Development of a Proximal Soil Sensing System for the Continuous Management of Acid Soil

Raphael A. Viscarra Rossel

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Australian Centre for Precision Agriculture
Department of Agricultural Chemistry and Soil Science
The University of Sydney
New South Wales
Australia

MMI

Certificate of originality

I hereby certify that the text of this thesis contains no material that has been accepted as part of the requirements for any degree or diploma in any university nor any material previously published or written unless the reference to this material is made.

Raphael A. Viscarra Rossel

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ABSTRACT

The notion that agriculturally productive land may be treated as a relatively homogeneous resource at the within-field scale is not sound. This assumption and the subsequent uniform application of planting material, chemicals and/or tillage effort may result in zones within a field being under- or over-treated. Arising from these are problems associated with the inefficient use of input resources, economically significant yield losses, excessive energy costs, gaseous or percolatory release of chemicals into the environment, unacceptable long-term retention of chemicals and a less-than-optimal growing environment. The environmental impact of crop production systems is substantial. In this millennium, three important issues for scientists and agrarian communities to address are the need to efficiently manage agricultural land for sustainable production, the maintenance of soil and water resources and the environmental quality of agricultural land.

Precision agriculture (PA) aims to identify soil and crop attribute variability, and manage it in an accurate and timely manner for near-optimal crop production. Unlike conventional agricultural management where an averaged whole-field analytical result is employed for decision-making, management in PA is based on site-specific soil and crop information. That is, resource application and agronomic practices are matched with variation in soil attributes and crop requirements across a field or management unit. Conceptually PA makes economic and environmental sense, optimising gross margins and minimising the environmental impact of crop production systems. Although the economic justification for PA can be readily calculated, concepts such as environmental containment and the safety of agrochemicals in soil are more difficult to estimate. However, it may be argued that if PA lessens the overall agrochemical load in agricultural and non-agricultural environments, then its value as a management system for agriculture increases substantially.

Management using PA requires detailed information of the spatial and temporal variation in crop yield components, weeds, soil-borne pests and attributes of physical, chemical and biological soil fertility. However, detailed descriptions of fine scale variation in soil properties have always been difficult and costly to perform. Sensing and scanning technologies need to be developed to more efficiently and economically obtain accurate information on the extent and variability of soil attributes that affect crop growth and yield. The primary aim of this work is to conduct research towards the development of an ‘on-the-go’ proximal soil pH and lime requirement sensing system for real-time continuous management of acid soil. It is divided into four sections.

Section one consists of two chapters; the first describes global and historical events that converged into the development of precision agriculture, while chapter two provides reviews of statistical and geostatistical techniques that are used for the quantification of soil spatial variability and of topics that are integral to the concept of precision agriculture. The review then focuses on technologies that are used for the complete enumeration of soil, namely remote and proximal sensing.

Section two comprises three chapters that deal with sampling and mapping methods. Chapter three provides a general description of the environment in the experimental field. It provides descriptions of the field site, topography, soil condition at the time of sampling, and the spatial variability of surface soil chemical properties. It also described the methods of sampling and laboratory analyses. Chapter four discusses some of

the implications of soil sampling on analytical results and presents a review that quantifies the accuracy, precision and cost of current laboratory techniques. The chapter also presents analytical results that show the loss of information in kriged maps of lime requirement resulting from decreases in sample size. The message of chapter four is that the evolution of precision agriculture calls for the development of 'on-the-go' proximal soil sensing systems to characterise soil spatial variability rapidly, economically, accurately and in a timely manner. Chapter five suggests that for sparsely sampled data the choice of spatial modelling and mapping techniques is important for reliable results and accurate representations of field soil variability. It assesses a number of geostatistical methodologies that may be used to model and map non-stationary soil data, in this instance soil pH and organic carbon. Intrinsic random functions of order k produced the most accurate and parsimonious predictions of all of the methods tested.

Section three consists of two chapters whose theme pertains to sustainable and efficient management of acid agricultural soil. Chapter six discusses soil acidity, its causes, consequences and current management practices. It also reports the global extent of soil acidity and that which occurs in Australia. The chapter closes by proposing a real-time continuous management system for the management of acid soil. Chapter seven reports results from experiments conducted towards the development of an 'on-the-go' proximal soil pH and lime requirement sensing system that may be used for the real-time continuous management of acid soil. Assessment of four potentiometric sensors showed that the pH Ion Sensitive Field Effect Transistor (ISFET) was most suitable for inclusion in the proposed sensing system. It is accurate and precise, drift and hysteresis are low, and most importantly it's response time is small. A design for the analytical system was presented based on flow injection analysis (FIA) and sequential injection analysis (SIA) concepts. Two different modes of operation were described. Kinetic experiments were conducted to characterise soil:0.01M $CaCl_2$ pH (pH_{CaCl2}) and soil:lime requirement buffer (pH_{buffer}) reactions. Modelling of the pH_{buffer} reactions described their sequential, biphasic nature. A statistical methodology was devised to predict pH_{buffer} measurements using only initial reaction measurements at 0.5s, 1s, 2s and 3s measurements. The accuracy of the technique was 0.1 pH_{buffer} units and the bias was low. Finally, the chapter describes a framework for the development of a prototype soil pH and lime requirement sensing system and the creative design of the system.

The final section relates to the management of acid soil by liming. Chapter eight describes the development of empirical deterministic models for rapid predictions of lime requirement. The response surface models are based on soil:lime incubations, pH_{buffer} measurements and the selection of target pH values. These models are more accurate and more practical than more conventional techniques, and may be more suitably incorporated into the spatial decision-support system of the proposed real-time continuous system for the management of acid soil. Chapter nine presents a glasshouse liming experiment that was used to authenticate the lime requirement model derived in the previous chapter. It also presents soil property interactions and soil-plant relationships in acid and ameliorated soil, to compare the effects of no lime applications, single-rate and variable-rate liming. Chapter X presents a methodology for modelling crop yields in the presence of uncertainty. The local uncertainty about soil properties and the uncertainty about model parameters were accounted for by using indicator kriging and Latin Hypercube Sampling for the propagation of uncertainties through two regression functions; a yield response function and one that equates resultant pH after the application of lime. Under the assumptions and constraints of the analysis, single-rate liming was found to be the best management option.

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Conceptual Basis of the Research and Aims

CONCEPTUAL BASIS OF THE RESEARCH AND AIMS

CONCEPTUAL BASIS

This work describes research towards the development of an ‘on-the-go’ proximal soil pH and lime requirement sensing system, and the methodology required to manage acid soil using a real-time continuous precision agriculture (PA) management system.

Soil acidity is quantified in terms of pH. Soil pH is a most informative soil property that is frequently measured because it is also a good indicator of soil quality. The management of acid soil is important in crop and pasture systems because its incidence is not only detrimental to plant growth and agricultural production, it also has socio-economic implications and may affect human health *e.g.* through the increased concentration of aluminium in water supplies. Soil acidity is a form of land degradation that affects approximately 33 Mha of agricultural land in Australia, and approximately 900 Mha worldwide. Its management is important.

LAND DEGRADATION IN AUSTRALIAN AGRICULTURE

Over the past two decades there has been increased awareness of environmental issues associated with conventional agriculture. The issues of greatest concern pertain to the environmental impact of agricultural systems and the degradation of agricultural land, particularly soil, water and vegetation resources. Such environmental degradation, and the reduced productivity from degraded land, is testimony to the inadequacy and inefficiency of conventional production systems that may have once been thought to be sustainable.

Land degradation may be defined as any natural or anthropogenic factor or combination of factors that disrupt the chemical, physical and biological balances of an agro-ecosystem, and which restrict its use and productive capacity. Soil degradation is a principal component of land degradation because it adversely changes the pedosphere. Soil degradation in Australian agriculture pertains to the deterioration of soil chemical, physical and biological properties. For example, soil chemical degradation resulting from the depletion of carbon and nitrogen sources in the soil, as well as the widespread soil acidification and salinisation that occurs in many productive regions of Australia. The deterioration of soil physical condition has caused reduced infiltration, higher incidence of compaction and/or the formation of a hard-setting layer throughout the cultivated horizons. A decline in structural stability has resulted in increased runoff and erodibility of Australian soil. Soil biological degradation has reduced the capability of the soil to cycle nutrients. The build-up of chemical residues in soil may be a consequence of the reduced biology that is required to decompose and cycle the increased amounts of residues generated by conventional agricultural management. Cultivation and fallow systems reduce faunal and microbial populations, indicating a decline in soil quality.

The notion that agriculturally productive land may be treated as a relatively homogeneous resource at the within-field scale is a common factor of these problems. This assumption and the subsequent uniform application of planting material, chemicals and/or tillage effort may result in zones within a field being under- or over-treated. Arising from these are problems associated with the inefficient use of input resources, economically significant yield losses, excessive chemical costs, gaseous or percolatory release of chemicals, unacceptable long-term retention of chemicals and a less than optimum growing environment. The environmental impact of crop production systems is substantial.

In this millennium, three important issues for scientists and agrarian communities to address are the need to efficiently manage agricultural land for sustainable production, the maintenance of soil and water resources and the environmental quality of agricultural land.

MANAGING ACID SOIL

Liming is the most rapid and effective method used to manage acid agricultural soil. Currently in Australia, agronomic management of acid soil by liming consists of low single-rate lime ($CaCO_3$) applications over an entire area of management – generally this area is contained within field boundaries regardless of size. Recommendations are based on either conjectural evidence, or only one and sometimes a few discrete observations that are averaged to derive the application rate.

Inevitably such single-rate applications of lime result in some areas of the field where the resource has been over-applied and other areas where under-applications have occurred. Intuitively the consequences of such actions are agronomically and economically unsound. Excessive applications of lime are uneconomical and may affect crop growth by inhibiting the availability of certain plant macro- and micronutrients. Conversely when lime is insufficiently applied amelioration is not accomplished and the availability of nutrients such as manganese and elements like aluminium may reach toxic levels, then affecting physiological processes in the growing crop.

The inadequacies of conventional whole-field management systems arise from the fact that soil is an inherently variable medium. Precision agriculture and site-specific liming are offered as more efficient alternatives to uniform agronomic methods of acid soil management, particularly now that much of the technology is readily available to producers.

PRECISION AGRICULTURE

Precision agriculture refers to the application of information technologies to agriculture. It is an agricultural management system that aims to identify soil and crop attribute variability, and manage it accordingly in an accurate and timely manner for near-optimal crop production. Unlike conventional agricultural management where an averaged whole-field analytical result is employed for decision-making, management in PA is based on site-specific soil and crop information. That is, resource application and agronomic practices are matched with variation in soil attributes and crop requirements across the field or management unit.

Conceptually PA makes economic and environmental sense, optimising gross margins and minimising the environmental impact of crop production systems. Although the economic justification for PA can be readily calculated, concepts such as environmental containment and the safety of agrochemicals in soil are more difficult to estimate. Nevertheless, it may be argued that if PA lessens the overall agrochemical load in agricultural and non-agricultural environments, then its value as a management system for agriculture increases substantially.

Presently, a PA management system requires collection and spatial referencing (using the Global Positioning System (GPS)) of environmental parameters such as soil and crop attribute information, databasing, spatial data analysis and mapping in a Geographical Information System (GIS), modelling and decision making in a spatial decision support system (SDSS), followed by the implementation of optimal and timely management (Figure 1). The implementation and outcome of management may then be recorded and used as input in a new cycle the following season.

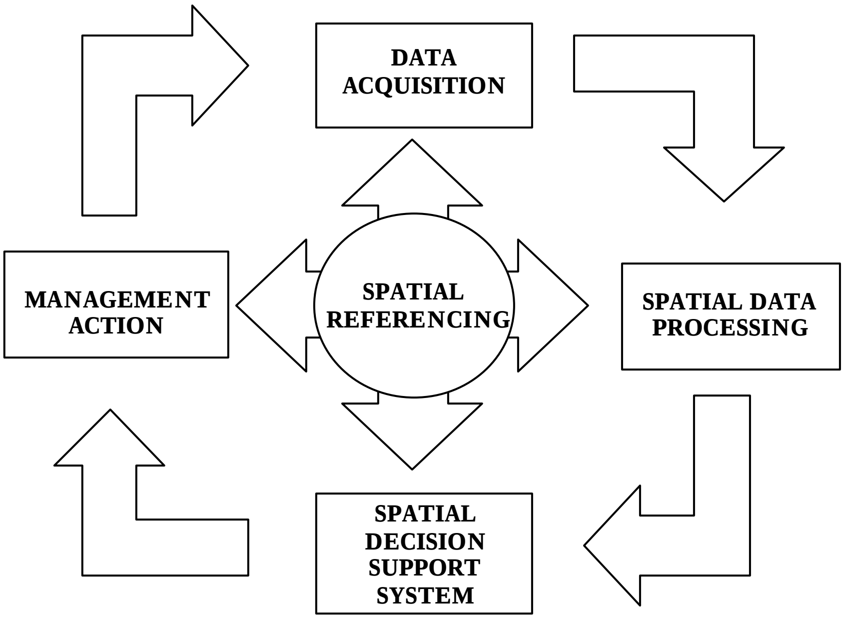

Figure 1 A continuous real-time precision agriculture (PA) management system

The PA management system (Figure 1) may be used to devise agronomically sensible management strategies which, depending on the degree of variability present in the field, crop response models, uncertainty models and economic models, etc. may be either uniform or differential. The ultimate objective of PA is to carry out all four phases in a single pass over the field 'on-the-go' and in real-time. This type of management system is referred to as continuous. However the four phases of the cycle are at different stages of development and real-time continuous operation is not yet possible. Thus the PA system must be applied and implemented using the GPS for spatial positioning during the data collection and management phases. Research is needed to device more efficient methods of data collection, and to develop SDSSs for continuous PA management.

Data Collection for Precision Agriculture

Data acquisition for PA involves more intensive sampling (*i.e.* at much higher resolutions) than that needed for conventional management. Routine soil maps, especially those at 1:100 000 readily available in Australia, are clearly inadequate for this purpose. Interim approaches between uniform and continuous site-specific management are currently being used.

A technique employed by users of PA combines grid or random sampling with digital elevation models and various other environmental data, and use geostatistics to interpolate. The production of accurate soil property maps then relies upon choosing a suitable grid resolution, quantitative soil analysis, and an appropriate spatial modelling and mapping technique. The size of the grid depends on the variable of concern and the trade-off between accuracy and cost. The production of accurate soil maps using an appropriate grid resolution is often laborious, time-consuming and much too costly for farmers to adopt. Conversely, if the resolution of the grid is too large, costs may be lowered but the loss of information results in inaccurate maps.

Zone or patch management techniques have been developed, whereby fields are stratified into smaller zones for sampling and management, based on the variability of exhaustive ancillary data sets such as yield, elevation, etc. Fuzzy clustering algorithms have also been used to divide fields into smaller management units.

Although these approaches may reduce the number of samples to collect, soil sampling and analysis is still much too laborious and expensive for the majority of Australian farmers since large areas are often involved. The development of ‘on-the-go’ proximal soil sensing systems that are timely, reduce the labour and lower the expense of soil sampling and analysis are imperative.

ADVANTAGES OF ‘ON-THE-GO’ PROXIMAL SENSING SYSTEMS

The implementation of PA at the farm or field level requires amongst other factors, the development of ‘on-the-go’ proximal sensing systems to collect the large amounts of soil information needed for management, with minimal labour, cost and effort. Research towards the development of ‘on-the-go’ proximal sensing systems to quantify soil variability and produce the information required for site-specific management in real-time is particularly important for the wide-scale adoption of PA.

The perceived advantages of such soil sensing systems are:

i. Elimination of costly and tedious sampling and analysis

ii. Efficient acquisition of fine spatial resolution continuous or continual data

iii. Real-time availability of results and the possibility for their integration with other field operations, *e.g.* variable-rate resource applications

iv. Minimal sample handling, *i.e.* no need for transport and storage

v. Elimination of laboratory induced variability

vi. Little expertise needed to operate the system after initial set-up.

AIMS OF THE RESEARCH

The conceptual basis of this work may be elucidated from the previous discussion. Its aims are as follows:

1. Describe the factors that converged in the development of precision agriculture
2. Provide a thorough literature review on topics that are relevant to the concept of precision agriculture and techniques used for the quantification of soil spatial variability, and the acquisition of soil data
3. Describe the geography, land use, vegetation and soil of the experimental site, with particular attention to the spatial variability of soil properties. Also describe the sampling strategy employed
4. Discuss the implications that precision agriculture has on current methods of soil sampling and analysis, and compare how sampling intensity affects map production
5. Compare various statistical and geostatistical methods for the analysis and mapping of non-stationary soil data
6. Review soil acidity and acidification and describe the components of a real-time continuous management system for acid soil
7. Conduct research towards the development of an ‘on-the-go’ proximal soil pH and lime requirement sensing system by:
    i. Evaluating the suitability of four potentiometric pH sensors for ‘on-the-go’ acquisition of soil pH and lime requirement information,

    ii. Investigating and assessing the electrochemical characteristics of a pH ion-sensitive field-effect transistor (ISFET) for its use as the sensor component in the proximal sensing system

    iii. Designing the analytical apparatus of the sensing system for ‘on-the-go’ field operation

    iv. Conducting kinetic experiments to describe the soil:0.01M $CaCl_2$ pH (pH_{CaCl_2}) and soil:lime-requirement buffer pH (pH_{buffer}) reactions, and devise a statistical methodology that may be used to predict equilibrium pH measurements at shorter time intervals than those suggested in the literature

v. Outlining the framework for the development of the sensing system

vi. Proposing the creative design of the ‘on-the-go’ proximal soil pH and lime requirement sensing system which includes the design for an ‘on-the-go’ soil sampling mechanism, and the data processing system to be used.

8. Derive a lime requirement calibration model using various soil types from southeastern New South Wales, that may be incorporated into the spatial decision support of a real-time continuous management system for acid soil. The model should be flexible and allow the use of data from the sensing system for real-time predictions of lime requirement
9. Conduct a glasshouse experiment to verify the use of the model derived in aim 8 and the rationale behind site-specific liming management
10. Assess the production and economic risks of liming using geostatistical uncertainty modelling

Each of the following ten chapters, in turn, addresses the aforementioned aims. Each chapter also encompasses topical conclusions. A general concluding statement with suggestions for future work is given at the end.

SECTION I

Chapter I

PRECISION AGRICULTURE: CONVERGENCE OF THREADS

1.1 INTRODUCTION

In the next five decades world population will increase dramatically, prompting a parallel need to increase global food supplies. Intensifying production is imperative to achieve this aim. However the physical and economic sustainability of current crop and livestock production systems worldwide is questionable. Land degradation is at the core of this uncertainty. In all of its forms, land degradation denies the efforts made to improve yields, and marginalises potentially productive arable land. Moreover, the availability and suitability of land where agriculture may be expanded is limited because of the continual decline in per capita arable land area and its uneven distribution.

Price regulation, subsidies and the protectionist policies of wealthier industrialised nations have become integral components of modern agricultural activity. Such actions exacerbate the uncertainty of agricultural production and add to the economic and environmental difficulties of producers in non-protectionist countries such as Australia. Obviously these problems are more intensive in industrially developing countries where demographic, economic and environmental problems are greatest.

If current trends continue, will humanity be able to produce enough food to adequately feed the future population? How will we all cope with and support this unprecedented growth? Are conventional methods of agricultural production compromising our planet’s resource base and environment? These are very pertinent questions whose answers are not straightforward due to the complex and dynamic nature of the subject. This chapter will not attempt to answer them but simply document how some of these issues, the increasing need for environmental awareness, the current global economy, together with advances in science, information and communication technologies, and increasing consumer demand for more stringent quality control and more vertically integrated operations, all converged to the development of the sustainable agricultural management system that is referred to as precision agriculture (PA).

Thus although this chapter may at first appear bleak, its theme is by no means pessimistic. It merely suggests that through scientific research in agriculture, and the consequent adoption of innovative, sustainable systems, it may be possible to avoid potential environmental and social disasters.

1.2 WORLD POPULATION AND FOOD SECURITY

As the world confronts increasing environmental, social and economic problems world population is often discussed. Population impacts nearly every aspect of our lives, from education, health and employment to the environment, methods of agricultural production, and scientific and technological developments.

Demographers project world population to grow from an approximate 6×10^{12} people in 2001 to 9.4×10^{12} people by 2050 and 10.4×10^{12} people by 2100 (United Nations, 1997). Population is predicted to stabilise at slightly under 11×10^{12} people by the year 2200 (United Nations, 1997). This medium fertility scenario estimates average population increases of 80 million per annum until 2015 and 50 million per annum by 2050 (Fischer & Heilig, 1998). The reasons for the extraordinary population increase, 80 % of which is expected in developing countries, are principally the great improvements in medical sciences, the age composition of the population and the lag-time needed for reductions in birth rates of the current population (Fischer & Heilig, 1998). Projections of low, medium and high fertility scenarios are shown in Figure 1.1.

The projections in Figure 1.1 account for the heterogeneous geographic nature of world population growth. The most substantial absolute and relative population increases are expected to occur in developing countries, particularly in Asia and Africa. Population in Europe is expected to remain constant while population in the remaining continents is expected to approximately double (Fischer & Heilig, 1998).

Malthusians[1.1] argue that we are about to arrive at a major checkpoint when the earth will reach and even exceed its carrying capacity due to constraints on land use and productivity. They point to the growing rate of extinction of species, global climatic change, more people living in poverty than ever before and the approximately 800 million famished and undernourished people, as indicators of their argument. However, by more objective analyses of the facts, the perception of the scientific community is that global and regional food security for the growing population is attainable but only with the adoption of sustainable technologies in agriculture and responsible environmental management.

[1.1] T.R. Malthus (1798) in his *Essay on the principle of population* suggested that population growth will always tend to surpass increases in food production.

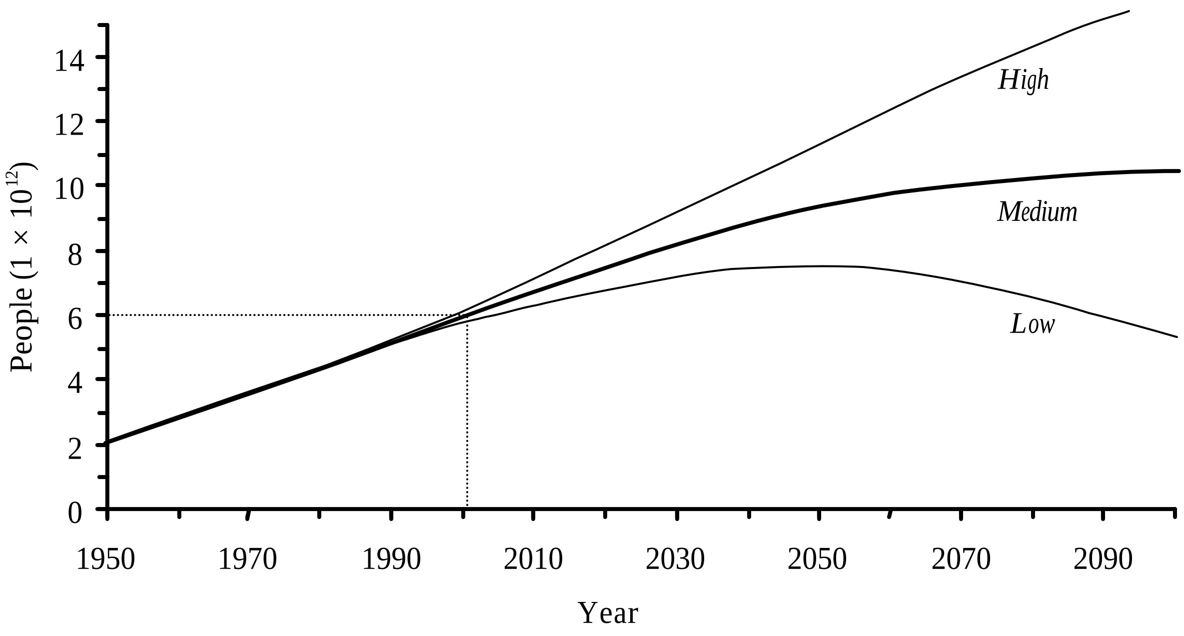

Figure 1.1 World population from 1950 to 2100. Projections for low, medium and high fertility scenarios, (United Nations, 1997).

Projections by the United Nations Food and Agricultural Organisation (FAO) and the International Food Policy Research Institute (IFPRI) suggest that agriculture worldwide can produce enough food to feed people in the year 2100. Although food security may be attainable, the greater problem is to ensure that all people are continuously and adequately fed. Periodic food shortages have occurred throughout the history of mankind. In this century, there have been a number of occasions, such as the food shortages that occurred in the post-war[1.2] years, the food shortages previous to the 'green revolution' and the widespread crop failures of the early nineteen-seventies in the United States of America (USA). Nevertheless, humanity has always progressed and devised more efficient ways of securing food and living requirements. Obviously with more people, we need to adopt more conscientious social policies, more innovative and economically and environmentally sustainable methods of production to support the needs and wants of the future population.

1.3 ARABLE LAND AREA

Coupled with the continuing increase in global population (Figure 1.1), there is a projected decline in the amount of available land suitable for cultivation. Lal & Pierce (1991) reported that the per capita area of arable land has been progressively declining

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[1.2] Refers to the periods following World War I (1914-1918) and World War II (1939-1945) from 0.45 ha in the early 1950s to an expected 0.15 ha in 2010 (United Nations, 1997). Trends show that it will continue to decline until the time world population stabilises in the year 2100 (von Uexküll & Mutert, 1995). Similarly the per capita area of grain harvested land has decreased from 0.23 ha in 1950 to 0.12 ha in 1990 and it is projected to be approximately 0.07 ha in 2030 (Brown, 1997).

Worldwide, the land area on which agriculture may be expanded is limited (von Uexküll & Mutert, 1995), particularly in Europe where a large proportion of land is already under cultivation (Table 1.1).

Table 1.1 Total Land Area and Arable Land Area by Continent (von Uexküll & Mutert, 1995)

Region	Total Land Area (Mha)	Cultivated Land Area		Potential Arable Land Area (Mha)
		(Mha)	(%)	
Africa	3 010	158	5.2	737
Asia	2 740	519	18.9	627
Australia and New Zealand	820	32	3.9	153
Europe	480	154	32.1	174
North America	2 110	239	11.3	465
South America	1 750	77	4.4	681
Former USSR	2 240	227	10.6	356
Total	13 150	1 406	10.6	3 190

Although there is considerable uncultivated arable land in North America, South America, Africa, Australia and New Zealand (Table 1.1), much of it may not sustain crop production because of climatic, edaphic and/or topographic factors. In developing regions, land resources could allow crop production on potentially arable land, however a large proportion of this land is unevenly distributed and only marginally suited to agricultural use due to severe soil, landform and climatic limitations (Fischer & Heilig, 1998). Furthermore potential regions for agricultural expansion may include areas of great natural biodiversity or fragile natural habitats, *e.g.* Amazonian regions of South America. This should deter governments from pursuing expansionist strategies that aim at converting such environments into land on which agriculture may be expanded.

Greater agricultural research and development efforts should be aimed at increasing productivity per hectare of land in a sustainable manner.

Meeting the food and fibre demands of the future population will need higher productivity levels for land now in production and the restoration of degraded land to reasonable levels of productivity. Increased food production must come primarily from productive areas through sustainable agricultural intensification so that the need for expansion into marginal and easily degraded non-agricultural land is alleviated.

1.4 DEVELOPING NATIONS

Discussing 'developing' countries as one of the 'threads' that converged towards the development of PA may at first appear misguided. However, the population and arable land area problems previously described are greatest in these nations. By the year 2010, land in developing countries will barely suffice to feed their expected populations if traditional methods of agricultural production continue to be used (FAO, 1998). Furthermore, the lack of income, infrastructure, information, agricultural inputs such as fertilisers, and trade policies that disadvantage such economies are reasons for the current and projected crisis in developing countries.

A great deal of political work is being done in the industrially developed world to promote the sustainable intensification of agricultural production systems (Alexandratos, 1995). It is important to transfer knowledge and technology in soil, water and nutrient management to developing nations, to encourage self-sufficiency and lessen dependence on imports and aid. Production increases in developing countries will only be achieved if the basic principles of crop production and sustainable management are understood (Greenland *et al.*, 1998). For example, fertiliser use in some of these regions must be increased to achieve higher yields, however it needs to be complemented with the knowledge of how to use fertiliser efficiently. This is not an easy feat and has to be done carefully according to the varying cultures, climates and economic conditions of the particular regions. The introduction of inappropriate technologies in fragile agroecosystems might have deleterious effects on the sustainability of food production (Quiroz *et al.*, 1995).

The transfer of technology and the implementation of PA in developing countries may seem inappropriate because of the economic cost associated with the technology. However, Bouma (1995) suggested that low-tech site-specific procedures in developing countries are just as feasible as the high-tech approaches in industrially developed countries. For example, quantifying the extent of soil variability is complex and very expensive, particularly for developing countries, but indigenous knowledge can be used to map soil according to micro-topographical, textural and fertility variation. Subsequently farmers may manually apply livestock manure or crop residues only to less fertile areas of a field. Low labour costs and relatively small field sizes may facilitate adoption of such management systems in developing countries. Quiroz *et al.* (1995) suggested that the introduction of PA to Andean eco-regions calls for the combination of scientific and indigenous knowledge. In this way PA may aid in substantially increasing crop production in the Andes with minimal environmental damage.

1.5 ENVIRONMENTAL AWARENESS

In recent decades, increased monoculture production of cash grain and fibre crops and greater reliance on chemical fertilisers and pesticides to maintain crop growth have resulted in large yields increases, greater availability of labour, greater export potential and large, profitable operations. However they have come with a cost to the environment and to society. Agricultural production uses large amounts of water, energy and chemicals, often with little regard to the long-term effects on the environment. The agricultural paradigm throughout most of the 20th Century was to produce more food or profit per unit area, without regard to the energy and material flows within agricultural production systems (Pierce & Lal, 1991).

Over the past two decades, awareness of environmental degradation caused by conventional agricultural management (simple homogeneous input and output systems) has increased as these practices have been found to neglect the long-term maintenance of our base resources. The issues of greatest concern include widespread soil degradation (*e.g.* Lal & Stewart, 1990), eutrophication of waterways by fertilisers (*e.g.* Koo & Williams, 1996) environmental contamination by pesticides and other agri-chemicals (*e.g.* Castelnuovo, 1995), and harmful atmospheric emissions (Lal *et al.* 1995). Although there isn’t firm evidence on the extent of some of these issues, intuitively their environmental costs are great but difficult to quantify, as are the enormous indirect costs implicit in the high-energy requirements of these practices.

The quality of many soils (soil quality is defined by Karlen *et al.*, 1997) all over the world has declined significantly since grasslands and forests were converted to arable agriculture and cultivation was initiated (Doran *et al.*, 1999). In the last decade, severe soil degradation has occurred over approximately 10 % of the earth’s arable land, mainly due to soil erosion, extensive cultivation, overgrazing, land clearing, salinisation, acidification and desertification (Oldeman, 1994). The most damaging forms of soil degradation in Australia were described in the previous section, Conceptual Basis of the Research and Aims.

Soil degradation has strong impacts on food and energy resources (Lal & Stewart, 1990), environmental quality and the greenhouse effect (Lal *et al.* 1995). It affects all aspects of human society through its adverse effects on environmental quality, agricultural productivity, human welfare and socio-economic stability (Lal, 1999). Figure 1.2 summarises these effects.

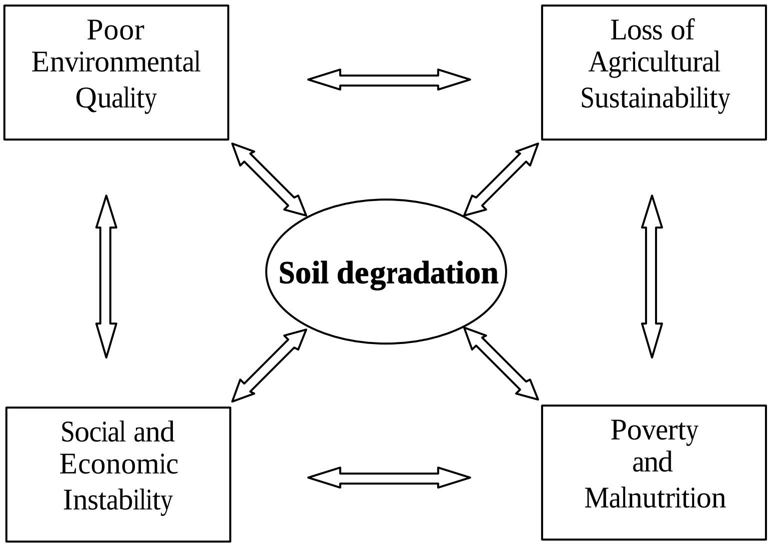

Figure 1.2 The cycle of soil degradation and its adverse effects on environmental quality, agricultural sustainability and the socio-economical aspects of human society. Adapted from Lal (1999)

As well as the aforementioned effects of soil degradation (shown in Figure 1.2), degradation has led to increased greenhouse effect, loss in biodiversity, lower returns per input of essential resources, reduced human health, uneven distribution of wealth, lowered standards of living and political instability (Lal, 1999).

1.6 WORLD ECONOMICS

Recent times have witnessed much of world agriculture in economic crisis. Some of the socio-economic ramifications of modern agriculture include the decreasing number of farmers, and the consequent deprivation of rural communities of their population and therefore their economic base (Alexandratos, 1995). Income generation is essential to achieve agricultural sustainability. Unstable agricultural prices, declining exports, widespread economic distress in rural and associated industries, and rising trade tension have resulted in many nations adopting policies which aim to protect their farmers. National protectionist policies, intended to isolate domestic producers from declining world markets by assisting to maintain farm incomes and stabilising market prices (Miner & Hathaway, 1988), are generating increasing instability in world agricultural trade and are continuing to create international conflict. The perpetrating governments of wealthier nations are responding to these problems with additional protectionist measures, whose consequences are now seen as major contributing factors to domestic and global economic unrest as well as over-production and the resulting international problem of falling agricultural commodity prices.

Internationally, protectionist trade policies (mostly non-tariff trade barriers) and export subsidies create confrontations within the trade system, such as the continuing subsidy war between the USA and the European Union (EU). These trade conflicts are in turn creating international crises in the World Trade Organisation (WTO) agreements, as governments are unable to resolve their differences through the application of existing trade rules. Governments face pressure from economically troubled rural communities to increase the level of support given, however this provokes conflict between primary agricultural producers and larger interest groups in society, including consumers and taxpayers. Governments in wealthier countries have responded with higher subsidies, often resulting in artificially sustained farm production and intensified export competition. Consequently, the economic difficulties of producers in non-subsidising countries such as Australia have deteriorated, further debilitating their economies.

The on going process of trade liberalization, now being taken a step further in the WTO negotiations for the Agreement on Agriculture (AoA), could make a significant contribution to global economic growth, however this is a slow and uncertain process. Furthermore, such negotiations have dramatically negative effects on small farmers in both industrially developed and developing countries. The AoA has the potential to severely undercut the remaining viability of small farm production, with potentially devastating consequences for rural economies and environments worldwide.

In Australia, a more efficient use of agricultural resources combined with economically and environmentally sustainable production systems that produce high quality products can provide the nation with a competitive advantage over competitors, leading to significant increases in economic growth. Obviously, this type of system is applicable to other international economies.

1.7 ADVANCES IN SCIENCE AND TECHNOLOGY IN AGRICULTURE

Historically, the betterment of human society has been associated with scientific and technological innovation. The earliest of these occurred with the development of tools that enabled hunters and gatherers to access a much wider range of foodstuffs and environments. This turning point in human history is often referred to as the tool making or cultural revolution. In time, further innovation resulted in the agricultural revolution, when hunters and gatherers became cultivators and herdsmen. As technology developed, the human population grew due to more stable food supplies and the relative security of a settled existence. The scientific or industrial revolution commenced three to four hundred years ago. Its main outcome was the improved standard of living of a growing population, which in part resulted from an increase in the efficiency of agricultural production. The mechanisation of agricultural practices may have contributed to such an increase in efficiency and the resulting increase in productivity of agricultural land and labor. This may be why agriculture has historically been associated with human prosperity.

These three most important demographic transitions in human history are depicted in Figure 1.3. The greatest advance in technology resulting from the industrial revolution was the development of steam power. Although the steam engine was not adapted for agricultural purposes, it later led to the mechanisation of agricultural practices. Farm machinery became larger and more powerful, making it possible to manage larger areas of land with less effort. It was then that agriculture in industrially developed nations began to operate under ‘economies of scale’. The size of farms increased as agricultural operations became faster and more efficient, with lower costs of production per unit of land, thus helping to supply adequate amounts of food and fibre for the growing population. However, mechanisation also led to increases in the size of the management unit and to the uniform management of increasingly larger areas of land. Such practices augmented to the problems associated with the misallocation of resources and related adverse environmental and socio-economic consequences (previously described).

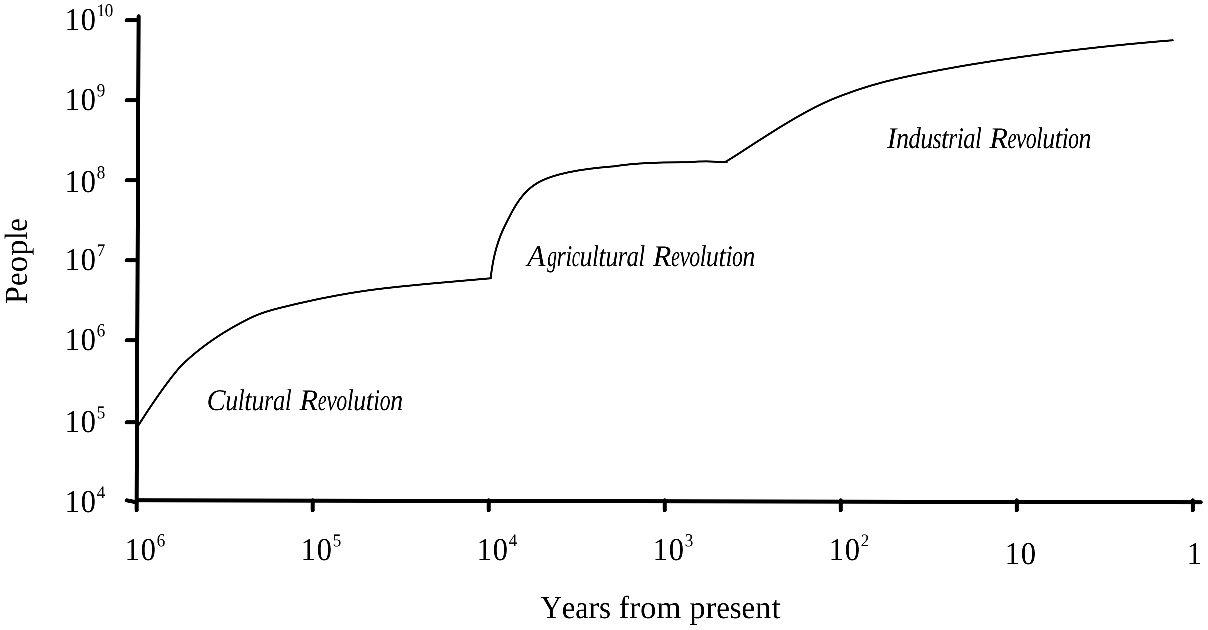

Figure 1.3 Logarithmic population curves through history, showing effects from the cultural, agricultural and scientific / industrial revolutions. Adapted from Welinder (1979)

Science has contributed greatly to agricultural productivity and growth, and has assumed a major role in more recent times. It has broadened our knowledge of the processes associated with and occurring in agricultural ecosystems, the effects that the environment has upon them, and the biological and chemical cycles within them. There have also been significant scientific breakthroughs in biotechnologies, plant breeding and genetics. Historically, scientific breakthroughs have occurred in response to specific issues, in particular regions (Campbell, 1979). Science has also provided answers to many agricultural problems. For example, in Australian agriculture the recognition of minor elemental deficiencies in particular soils, the use of legumes in crop rotations for the replenishment of soil nitrogen and the use of better yielding crop varieties, have resulted in a three-fold increase in wheat yields since the turn of last century (Burch *et al.*, 1987). Mechanisation has also played a part in such increased crop yields.

Two relatively recent scientific developments of worldwide significance that are particularly relevant to this work are discussed below.

1.7.1 THE GREEN REVOLUTION

The developments in plant breeding that occurred in the 1960s are commonly referred to as the ‘green revolution’. The green revolution was a package comprising material components of high-yielding varieties of primarily wheat and rice, but eventually maize and a range of other crops. It also bought about the use of larger amounts of irrigation, fertilisers and pesticides. On suitable land in suitable economic environments, use of green revolution technology resulted in large yield increases in many parts of the world. It certainly ensured that the food requirements of the growing population were met, and at an affordable price. Between the period 1960 to 1990 yields more than doubled, attesting to the achievements of the 'green revolution' (Figure 1.4).

The improved crop varieties relied heavily on the use of external inputs that were essential to provide good growing conditions for realising their genetic potential. Thus the green revolution resulted in significant increases in the use of irrigation and fertilisers required to maintain the high yielding crops. The genetically homogeneous monocultures also increased the potential for massive pest attacks, which in turn triggered large-scale applications of pesticides. Since then, such practices have no doubt contributed to the environmental contamination by agricultural chemicals and to land degradation problems.

Many agricultural scientists are hopeful that biotechnology can revitalise agriculture in the new millennium as the achievements of the green revolution slowly fade. As further applications of the green revolution are explored through biotechnologies, opportunities exists for breeding crop varieties that are tolerant to adverse soil and environmental conditions. For example, salt tolerant crop varieties and varieties that can withstand highly acidic soil, others that are drought resistant, or crops varieties that are resistant to certain diseases or pest attacks. However comparable yield increases to those achieved by the green revolution in the next few decades based on plant physiology and genetics alone are doubtful (Evans, 1998).

Recently, the use of genetically modified organisms (GMOs) in agriculture has been the source of many public debates. However discussion is needed on a more wholistic sense. Mostly, biotechnologies do not yet attempt to find ways to reduce the environmental impact of current crop production systems. These crops are usually input intensive and increase the use of agricultural chemicals in the production process. Consequently, they may also result in greater environmental contamination.

Innovations in genetic engineering are still largely at the laboratory stage and are subject to international debate concerning ethics, biological safety and intellectual property rights. Furthermore, it may take at least ten years for them to reach farmers' fields. Most genetic engineering in agriculture is conducted by large, horizontally integrated corporations that need to sell their products at premium prices to cover the cost of research. These companies have few competitors and are developing products for farmers or farming corporations who can afford to pay high prices for seed. The resulting products are of little value to farmers who cannot afford the technology.

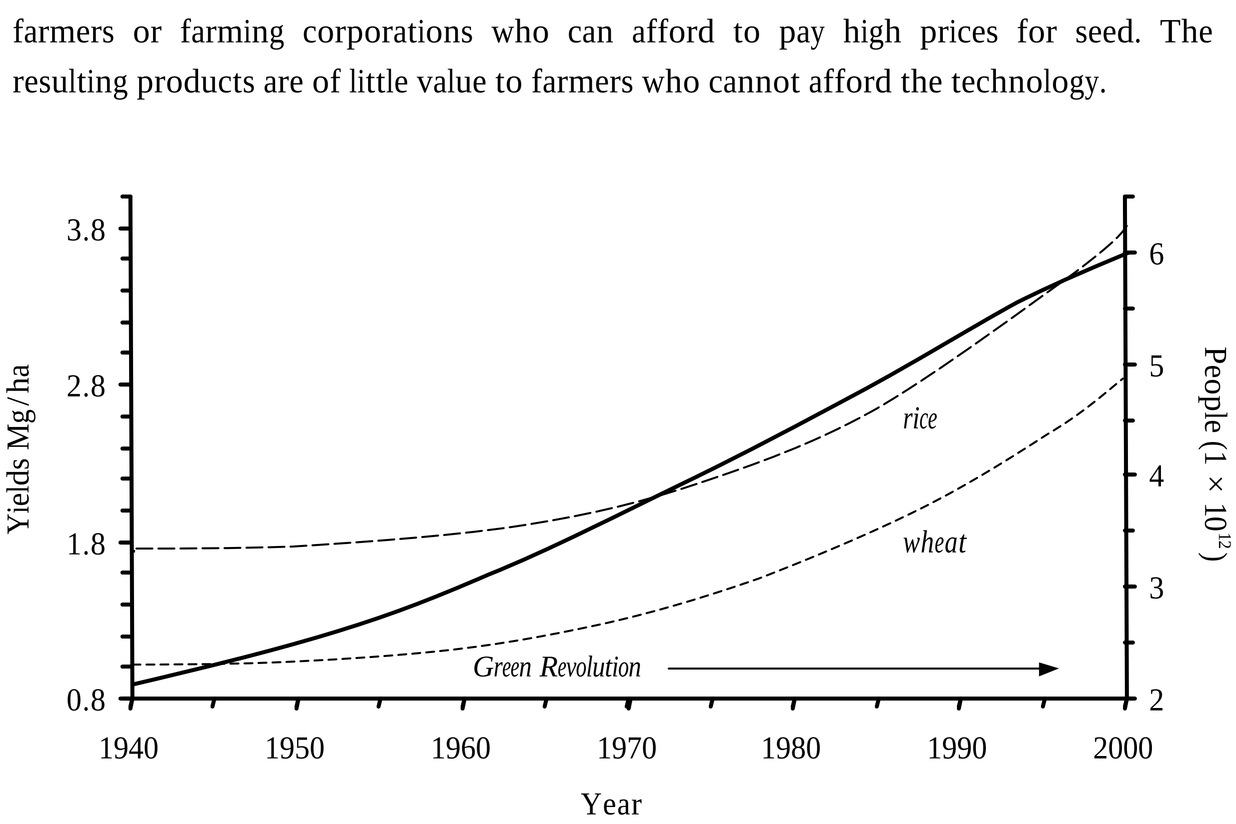

Figure 1.4 Trends in world population (solid line), world-average yields of wheat (dashed line) and rice (broken line). Adapted from Evans (1998).

1.7.2 DEVELOPMENTS IN STUDIES OF SOIL SPATIAL VARIABILITY

Jenny (1941) described the fundamental processes of soil formation. The state factor theory he developed suggested that soils and the ecosystems in which they occur can be related to climate (*cl*), organisms (*o*), relief (*r*), parent material (*p*), time (*t*) and unspecified factors (…) so that any given soil property (*s*) may be determined by a function of the state factors, *i.e.* $s = f(cl, o, r, p, t, ...)$. This deterministic model regards the spatial variation of soil as dependent on the complex combination of the soil forming processes (which are themselves influenced by the soil forming factors) and their balance in space and time (Jenny, 1941).

Given the complexity of soil, scientists have generally attempted to remove soil variability by defining homogeneous mapping units, which have insufficient detail to relate agronomic research results to soil types or specific soil properties. Resulting polygon maps or choropleths assumed that soil changes abruptly at soil boundaries, so that the homogeneous mapping units are made up of similar soil 'individuals' or pedons (Soil Survey Staff, 1975). As such, statistical analysis of soil spatial variability has been historically related to research and analysis of field plot data (Beckett & Webster, 1971) that lie within such mapping units. Experiments were designed to interpret the significance of agronomic treatment effects with little or no effort made to understand the results in terms of soil variability and condition (Wilding & Drees, 1983). Most of these studies relied upon analysis of variance (ANOVA) methods, where the variances associated with soil were diminished by randomisation, blocking and replication (*i.e.* the Fisherian approach to field experimental design and analysis (Fisher, 1925)). In this way scientists could increase the efficiency (*i.e.* achieve the same precision with less effort) of their experimental designs.

By the latter half of the 1960s, soil classification had reached the limits of its usefulness (Webster, 1994). Soil scientists needed to test the assumption that all soil mapped as a single unit or class had equal potential. Moreover they needed to know how variable soil was to decide on the number of samples necessary to characterise its properties correctly (Burrough, 1993). On occasions, ANOVA techniques were used to measure relationships between distance and variance (Beckett & Webster, 1971). However despite the variety of sampling plans used, these methods did not allow concise and complete descriptions of soil changes over distance (Campbell, 1978).

The advent of computers permitted more sophisticated methods for analysing soil spatial patterns (Webster, 1994). Methodologies for analysing spatial soil data evolved rapidly from using various kinds of regression, trend surface fitting (*e.g.* Walker *et al.*, 1968), and variance analysis, to multivariate methods of soil analysis (*e.g.* Norris, 1970), and perhaps most significantly, to using the theory of regionalised variables and its practice, geostatistics (*e.g.* Journel & Huijgbregts, 1978).

Geostatistics refers to statistics that pertain to the earth, in a geographical context, and denotes statistical methods that emphasise locations on a plane. The techniques of geostatistics in soil science are primarily used to predict the values of the property at unsampled locations and/or to estimate the average value of a soil property within some defined region. The method used for estimation is called kriging after its founder, D.G. Krige, who devised it for use in the mining industry to quantitatively describe and predict ore depositions (Journel & Huijgbregts, 1978).

In the mid- to late-1970s and early 1980s soil scientist realised the potential of geostatistical methods for soil variability studies (*e.g.* Beckett & Bie, 1976; Burgess & Webster, 1980a, b; McBratney & Webster, 1981). The last three decades have witnessed increased research in the use of geostatistics and great developments have occurred in the understanding of, and methodology used to quantitatively describe soil variability. Geostatistics is perhaps the biggest single advance in survey technology since the 1960s (Webster, 1998). The application of spatial variability studies and geostatistics, aided by developments in information and communication technologies, can now be used to manage agricultural land and make significant contributions towards the sustainable intensification of agricultural production.

1.8 INFORMATION AND COMMUNICATION TECHNOLOGY

Many of the developments in science, information and communication technologies were driven by war, thus the common phrase ‘war breeds innovation’. The competitive nature of the Cold War fuelled creativity among governments, scientists and inventors, resulting in some of the most significant developments in information and communication technologies in the last century. Since the end of the Cold War many of these technologies were made available to civilian users and industries other than the military (*e.g.* agriculture) to justify the enormous costs of development. The following provides a brief history of information and communications technologies and recounts only major developments that have had an impact on agriculture, enabling the development of PA.

1.8.1 COMPUTERS – HARDWARE AND SOFTWARE

Remarkable developments in computer technologies and computing sciences have been made since the emergence of the 'modern' electronic computer in the 1940s. In 1946 the Electronic Numerical Integrator and Computer, more commonly known by its acronym ENIAC was designed for the USA army during World War II to calculate cannon trajectories and other military computations. Throughout the 1950s and 1960s the scope and power of computers continued to expand into other areas of research. The most important milestone in computer history to this day occurred in the 1970s through the development of the silicon microchip. As a result, computers reduced in size dramatically, from being approximately the size of a large room in the 1960s to the size of a typewriter by the late 1970s, to the development of the first microcomputers in the early 1980s.

Presently, computers can be smaller than the palm of a human hand and their processors faster and more powerful than ever previously imagined. Developments in computer software have closely followed those in hardware, and together they have become indispensable for education and scientific research, as well as for most industries, businesses, and households. Computers in agriculture are now used for a wide range of tasks, ranging from scientific research to decision-making, automation of many farm operations, electronic mailing, marketing of produce, livestock identification, accounting, record keeping, etc.

One other important development in computing and communications technology has been the Internet. In 1968 the U.S. Department of Defence Advanced Research Projects Agency built a network of communications (ARPAnet), which was the predecessor of what we now know as the Internet (National Research Council, 1997). Now the Internet benefits the entire computing and communications community, including agriculture, and is bolstering the global economy like never before.

In agriculture, the Internet is beginning to be used to access marketing and weather information, to transfer research findings from the scientific community to producers, and to transfer and share information with the aim of making more informed management decision. The capability to integrate and support computer hardware and software in many rural communities in Australia is still low, but is rapidly increasing. Almost half (49 %) of 147 181 Australian farms with an estimated value of agricultural operations of A$5 000 or more owned or used a computer at March 1999, a 27 % increase over the number of farms using a computer at March 1998 (Australian Bureau of Statistics, 2000). Just under 18 % of farms were using the Internet at March 1999, a 65 % increase over the number a year before (Australian Bureau of Statistics, 2000).

1.8.2 SATELLITE SYSTEMS

In 1940 the U.S. National Defence Research Council developed LORAN, the first all-weather navigation system that combined radio signals and accurate time interval measurements. It was used in World War II to guide bombers to their targets and to improve the performance of long distance fighters. In 1957 the Soviet Union launched Sputnik, the world’s first artificial satellite. Fearing attack from afar and being distraught at being beaten by its Cold War rival, the USA launched itself into the ‘space race’ and established the National Aeronautics and Space Administration (NASA). In 1960 NASA successfully launched the first telecommunications satellite ECHO-1. It proved to be the promise and basis for satellite telecommunications.

In 1972 the first LANDSAT environmental monitoring satellite was launched, followed by a range of other similar purpose satellites (*e.g.* the SPOT system is a French earth observing satellite system). The purpose of these satellites is to provide repetitive acquisition of high-resolution multispectral data of the earth’s surface on a global basis.

Their remotely sensed images can be used to develop base maps for environmental impact studies, evaluating geological faults and structures, land planning, mapping soil, and to forecast crop yields.

Throughout the 1970s the USA government designed the NAVSTAR Global Positioning System (GPS) as a military navigation system, developed to provide 24-hour, all weather, real-time positioning worldwide (Clark, 1992). The former USSR responded with a system called the Global Navigation Satellite System (GLONASS). These positioning systems are now widely used in scientific research and in industries like agriculture and engineering. The GPS is the primary, most important enabling technology of PA.

1.8.3 GEOGRAPHICAL INFORMATION SYSTEMS (GIS)

An important development in software has been the development of the geographical information system (GIS). The development of GISs has paralleled the large improvements in computer performance, as well as the developments of the theories and analysis of spatial processes in various disciplines (including earth and soil sciences) and the greater social and environmental awareness.

Many of the innovations in the geographical application of information technology began in the late 1950s, when researchers began to envision the development of GIS. In 1959 a simple system called MIMO (Map In-Map Out) was developed for the application of computer technology to cartography (Coppock & Rhind, 1991). The principles of the MIMO system provided the origins for geo-referencing, data capture, data analysis and display, all of which are standard elements found in GIS software today. One of the earliest fully operational GISs was developed in the early 1960s in Canada (Coppock & Rhind, 1991). Its purpose was to analyse and store spatial data and produce statistics to develop land management plans for large areas of rural Canada. The maps classified land using various themes *e.g.* soil capability for agriculture, present land use, etc. (Johnston, 1983). In the 1970s, GIS research resulted in the development of various raster and vector systems and the 1980s brought about the creation of many companies working with GIS. Eventually, some of these companies developed commercial GIS packages. Since this time, various books on the principles of GIS for the earth sciences have also been published following a lot of educational and research interest (*e.g.* Burrough, 1986). In the 1990s major improvements have occurred in GIS software interfaces, making them ‘friendlier’ and available to a wider range of users.

Through the better use of information, GIS combined with developments in spatial data analysis (geostatistics), remote sensing and the GPS is enabling great improvements in the management of agricultural land and its base resources. The assembly of landscape, soil and crop attribute maps and maps of their spatial and temporal interrelationships, combined with appropriate agronomic experimentation, is proving to be vital for decision-making, sustainable land and agronomic management.

1.9 TOTAL QUALITY MANAGEMENT AND VERTICAL INTEGRATION

Total Quality Management (TQM) is a management system that focuses on people, process improvement, training, statistics and quality assurance (Rao *et al.* 1996). TQM may be traced back to post-World War II Japan, when quality control was introduced into Japanese manufacturing. Soon after, quality control progressed to TQM via the introduction of new statistical quality control measures (Blakemore, 1989). Since then Japanese manufacturing succeeded in producing high quality goods cheaply and has thus maintained a competitive advantage over its competitors.

The TQM approach is illustrated by the Deming or Shewart wheel (Blakemore, 1989), where major improvements in productivity occur as follows: (i) the need to change is recognised, (ii) a decision is made, (iii) the decision is acted upon and (iv) the action is sustained. During this process it is essential to plan, do, check, act, improve and standardise. This is the Japanese process called Kaizen (Rao *et al.* 1996). The continual improvement in productivity and quality is illustrated in Figure 1.5.

By continually rotating the wheel, improvements in productivity and quality are achieved by applying statistical quality control (Blakemore, 1989). Although TQM began in the manufacturing sector with the purpose of improving customer satisfaction and maintaining low production costs, it expanded into the service sector and more recently, into education and agriculture. Quality controls both revenue and cost, so it has the potential to improve the competitive advantage of agricultural industries (refer to Section 1.5).

Increasingly consumers are demanding more stringent quality control measures in agricultural production and processing. They are willing to pay more for high quality produce, grown with minimal chemical applications *e.g.* organically grown food. Consumer lobby groups are forcing producers to adopt systems whereby the integrity of their produce is guaranteed. One example of this occurs in the European beef industry whereby farmers are asked to keep records of breed type, diet, husbandry, etc. to create livestock ‘passports’ which accompany each animal through the processing chain to the consumer at point of sale. The consumer may access information via the Internet on the meat product right up to primary production. This system enables the industry to rapidly contain, at the farm or processing level, any chemical residue problems or food poisoning incidents that may occur, with little disruption to trade. Similarly in the wine industry, the labelling system provides the consumer with information on the region where the wine was made and in some instances the winery, winemaker, vineyard and grape variety grown.

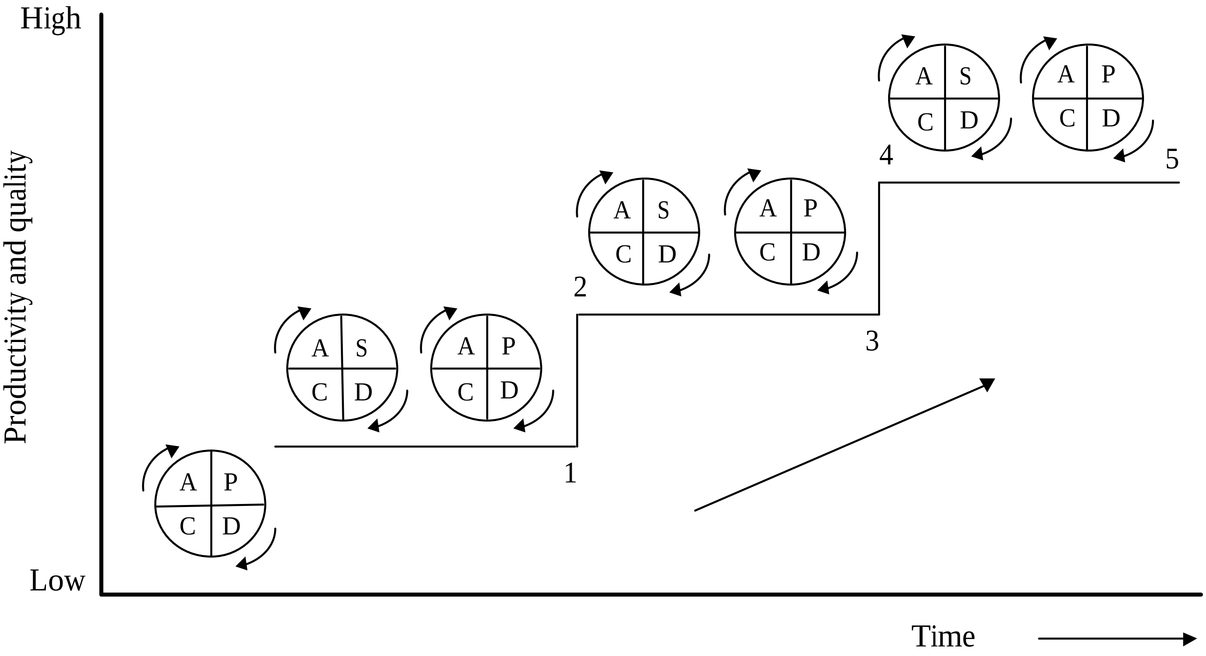

Figure 1.5 Continual improvements in productivity and quality applying the Demin or Shewart wheel to Kaizen, the continual desire to improve. To improve one must plan (P), do (D), check (C), act (A) and standardise (S). Progress between 1 – 2 and 3 – 4 represent major innovations, while progress between 2 – 3 and 4 – 5 represent improvements achieved through the application of statistical quality control. Adapted from Blakemore (1989)

In terms of continual improvements in productivity and quality (Figure 1.5), the agricultural objective is to continually improve the production process and product quality. This may be achieved by more efficiently using input resources, minimising product contamination and waste, and reducing the environmental impact of crop production systems.

Together with the increasing consumer demand for more stringent quality control in agriculture, economic, social and technological factors favour more vertically integrated agricultural operations (National Research Council, 1997). Vertical integration (VI) should not be confused with horizontal integration, or movements toward greater oligopoly or monopoly within an industry. Vertical integration occurs when a firm or a group of firms combines activities, unlike those it currently performs, and which are related to them in a sequence of marketing and production activities.

For example, subsistence agriculture is a fully integrated system. VI is nearly complete since most of the resources, production and decisions are made by the same individuals or cooperatives. However, the development of a market-oriented agriculture brought about specialisation and the disintegration of such systems. Using the wine industry as an example of VI in modern agriculture, different aspects of wine making, from the sourcing of the grape variety and production decisions to the wine making processes to marketing of the wine, are all integrated. In this instance integration provides consumers with a consistent, dependable product that is identified with a particular label. This control can only be achieved by outright ownership of the entire business or through tight producer marketing alliances. With a better understanding of the entire production process, the business is able to target particular markets with a suitable product, thus providing opportunity to value-add their product prior to sale.

Generally, TQM and VI in agriculture may be associated with positive results, including more efficient production, improved product quality, risk management, international competitiveness and food safety advantages. The future of agricultural production appears to encompass this type of stringent product control.

1.10 PRECISION AGRICULTURE

The convergence of all of the ‘threads’ outlined in this chapter, namely the growing population, issues of food security and arable land area, the increasing need for environmental awareness, the current global economy, developing countries, together with advances in science, information and communication technologies, and increasing consumer demand for more stringent quality control and more vertically integrated operations, resulted in the development PA.

In the literature, PA has been referred to as site-specific crop and soil management (Robert, 1989; Robert, *et al.*, 1991), farming by soil (Larson and Robert, 1991), variable-rate program (Mulla, 1993), computer-aided local resource management (Schnug *et al.*, 1993) and precision farming (Robert, 1994). Ultimately, all of these names refer wholly or in part to PA as defined in the Conceptual Basis of the Research and Aims.

In 1997 the USA Congress passed a bill on PA which formally defined it as ‘an integrated information- and production-based farming system that is designed to increase long-term site-specific and whole-farm production efficiencies, productivity, and profitability while minimising unintended impacts on wildlife and the environment by:

- combining agricultural sciences, agricultural inputs and practices, agronomic production databases, and precision agriculture technologies to efficiently manage agronomic systems;
- gathering on-farm information pertaining to the variation and interaction of site-specific spatial and temporal factors affecting crop production;
- integrating the information with appropriate data derived from remote sensing and other precision agriculture technologies in a timely manner in order to facilitate on-farm decision-making; and
- using the information to prescribe and deliver site-specific application of agricultural inputs and management practices in agricultural production systems.

One final point to mention is that the philosophy behind PA is synonymous to that of sustainable agriculture, which has also been widely defined (*e.g.* Brown *et al.*, 1987; Neher, 1992; Farshad & Zinck, 1993). Their philosophies include elements such as soil fertility and productivity, management strategies, human needs, economic viability, social acceptability, ecological soundness, timeliness and ethics. An advantage of PA is that its definition and practice both promote the use of innovative science and technology to manage agricultural land. As such PA has the potential to significantly contribute to the well being of humanity. Perhaps historians in the future will write about the 'Information and Communication Revolution' and the role of PA in helping to meet the food and fibre needs of the global population in an economically and environmentally sustainable manner.

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Chapter II

QUANTIFYING SOIL SPATIAL VARIABILITY AND THE PRACTICE OF PRECISION AGRICULTURE: A REVIEW OF THE LITERATURE

2.1 INTRODUCTION

Precision agriculture is an environmental management system for agriculture that aims to quantify the variations that occur in agricultural ecosystems, to provide accurate and precise information for its management (Chapter I). To achieve this, reliable information on the spatial (and temporal) variation of soil and crop parameters is essential. The methods used to collect information on soil and crop variability and the statistical techniques used to quantify the variation are particularly important.

This chapter presents a review of the literature describing classic statistical and geostatistical methods used to quantify soil spatial variability. Descriptions of each methodology are supported with corresponding literature reviews pertaining to the quantification of the spatial variability in soil pH. The chapter then focuses on precision agriculture and the research that has been conducted on each of the five components of the management system (Figure 1, Conceptual Basis of the Research and Aims). Emphasis is given to the methods used to collect data on the spatial variability of soil, particularly those that attempt a complete enumeration of field soil variables, namely remote and proximal sensing. The chapter closes with a review of developing options for the characterisation of fine-scale soil variability using proximal soil sensing systems, and emphasises that for further evolution and adoption of PA, their development is imperative.

2.2 QUANTIFYING SOIL VARIABILITY

No soil scientist is unaware that soil varies gradually, continually and sometimes abruptly through space and time. Most realise that a good quantitative understanding of soil variability is necessary for agronomic management and increasingly, they are aware of the existence of ‘tools’ that can deal with spatially variable data. Before starting the review and discussion on geostatistics, the basic tool for soil and crop variability studies, it may be useful to present a brief review of classical methods of statistical analysis as they are often used to describe the variability of soil and crop attributes.

2.2.1 CLASSIC STATISTICAL DESCRIPTIONS

Conventionally soil survey at the regional scale has been based on classed soil maps derived from measurements made at discrete points, where the soil within each class is assumed homogeneous and different from other classes. Similarly, conventional soil survey at the field and within-field scales consists of the collection of a few, discreet samples which are bulked and subsequently re-sampled for laboratory analysis. Agricultural management decisions are therewith based on mean-of-field results, which assume that the sampling unit mean is the expected value everywhere in the field. In this way, the probability distribution of the particular property and its value at any one place within the field or study area A, is thought to have been estimated, albeit with some error that is expressed by the within-unit variance. This is the basis of conventional agronomic management decisions using classical statistical methods. When only a small number of samples are collected this approach to prediction and quantification of the variability present within A is the only feasible option (Burgess & Webster, 1980a).

Mathematically, the expected value of a soil property s at any location within the field (x) is the sum of the general population mean m of the attribute for the whole field, and a normally distributed, spatially uncorrelated random component $e(x)$ that has a mean of zero, variance s^2 and standard deviation s , *i.e.:*

$$E[s(x)] = m + e(x) \tag{2.1}$$

The probability distribution of a soil population S, characterised by m and s^2, may be calculated from its sample population S' that is derived from a sample $(s_i, \ldots s_n)$. The parameters describing S' are the sample mean $\bar{s}$ and the sample variance v^2. The sample variance v^2 or its square root the standard deviation v describe the spread of the distribution around the mean, and may be defined by:

$$v^2 = \frac{1}{n}\sum_{i=1}^{n}(s_i - \bar{s})^2 \tag{2.2}$$

The sample variance is the average squared difference of the observed values from their mean. Both $\bar{s}$ and v^2 may be derived using least squares analysis and analysis of variance. Confidence limits can be determined from v^2. The smaller the v^2, the better the prediction. The standard deviation is often proportional to the sample mean, hence variability between sample populations may be compared using the standardised coefficient of variation (CV), which expressed as a percentage is defined as:

$$CV = \frac{v}{\bar{s}} \times 100 \qquad (2.3)$$

Therefore the CV describes the variability in the sampling population, present within the entire sampling region or field.

Classical Description of the Spatial Variability of Soil pH

Table 2.1 presents a literature review of the overall variability in soil pH characterised using classical statistical parameters, namely the mean, standard deviation and CV.

The median CV for soil pH in Table 2.2 is 5.7 %, and generally the standard deviation and CV increased with increasing sampling area. Similarly, Dampney *et al.* (1997) presented data showing that the mean CV of surface soil pH (0 - 15 cm) within 78 individual arable fields in England was 5.1 %. Field sizes in their study ranged from 4.5 to 51.8 ha and variation was greatest in larger fields. Thus Table 2.2 and the findings of Dampney *et al.* (1997) concur with the conclusions of Beckett & Webster (1971), *i.e.* that soil variation (as measured by the CV) increases with the size of the sample and the area sampled.

2.2.2 GEOSTATISTICS

Classical statistics assume that the variability around the mean is random and contains no reference to the geographical distribution of differences within the sampling units (Trangmar *et al.*, 1985). That is, the variable is a random variable (RV) with no spatial correlation. However research has shown that this is not the case, but rather that soil variables, such as soil pH, are continuous variables whose values at any location vary according to the direction and distance of separation from neighbouring samples *e.g.* Beckett & Webster (1971), Campbell (1978), Burgess & Webster (1980a), Yost et. al. (1982), Webster & McBratney (1981), Trangmar *et al.* (1985). Hence the notion of regionalisation of soil variables and the theory of regionalised variables.

The theory of ‘regionalised variables’, commonly referred to as geostatistics was first suggested by Matheron (1963), who defined it as: “…the application of the formalism of random functions to the reconnaissance and estimation of natural phenomena” (in Journel & Huijbregts, 1978). The practice originated in the mining industry where it was used to quantitatively describe and predict ore depositions (Chapter I). In the mid- to late-1970s and early 1980s soil scientists realised the potential of geostatistical methods for soil variability studies (Chapter I).

In soil science and PA, geostatistics is used to design optimal sampling schemes, and to quantify and predict the spatial distribution of variables at unsampled locations.

Regionalised Variables and Random Functions

In the context of this research, 'natural phenomena' refers to parameters of an agro-ecosystem *e.g.* crop and soil, which can be characterised by the spatial distribution of one or more RVs, *e.g.* soil pH, crop yield, etc. As these RVs are spatially distributed, they are referred to as regionalised variables (REV). Thus a regionalised soil variable REV $s(x)$ is considered a RV that takes different values s according to its location x within the field. REVs can be regarded as particular realisations of a set of RVs $\{S(x), x \in A)$. The REV is made up of a systematic or structured component that needs a certain functional representation, as well as a random component (Wilding & Drees, 1983). Accurate representation of soil spatial variability must account for both the structured and random components of the REV. The random function (RF) concept expresses both aspects of the REV.

A RF can be considered as a set of spatially dependant RVs $S(x)$, one for each location x in A, whose dependence on each other is specified by some probabilistic mechanism (Isaaks & Srivastava, 1989, pp. 218). The set of RVs for all locations within A is called a RF because it associates the RV S with any location x, thus expressing both random and spatially structured components of a REV. Just like the distribution of a RV $S(x)$ characterises the uncertainty about s at x, the RF $\{S(x), x \in A)$ characterises the joint spatial uncertainty over A.

Table 2.1 Classical statistical descriptions of the spatial variability of soil pH

Author	n	Units	Depth (cm)	Sampling	Mean	S.D.	Range	CV %
Peck & Melsted (1967)	256	H_2O			6.51	0.46	5.5 - 8	7.1
	256				6.21	0.44	5.5 - 8	7.1
Campbell (1978)	160	1:2 $CaCl_2$		1.6 ha	6.5	0.28		4.3
	160				6.5	0.17		2.6
Vander Zaag *et al.* (1984)	121	1:1 H_2O	0 – 15		5.71		5 – 6.7	
Tabor *et al.* (1985)	49		0 – 20	13 ha	7.33	0.18		2.4
Riha *et al.* (1986)	240	$CaCl_2$			2.76	0.13		2.5
	240				4	0.12		3
	240				2.83	0.12		2.1
Laslett *et al.* (1987)	121	$CaCl_2$		1 ha	4.49	0.21	4.02 – 5.04	4.7
	121	H_2O			5.26	0.21	4.8 – 5.82	4
Webster & McBratney (1987)	436	H_2O		77 ha	7.72	0.64		8.3
Miller *et al.* (1988)	99	1:1 H_2O		400 m	7.5	0.44	6.5 – 8.1	5.9
Samra et.al. (1990)	162	1:1 H_2O	0 – 30		7.64		7 – 8.3	
Boyer *et al.* (1991)	543	1:1 $CaCl_2$	0 – 10		4.5	0.3	2.8 – 6.1	7.6
Boekhold & Van der Zee (1992)	166	1:10 $CaCl_2$	25 – 30		5.87	0.32	5.17 – 6.74	5.5
Mulla (1993)	172		0 - 30	8 ha	6.09	0.66		10.8
Cambardella *et al.* (1994)	271		0 – 15	6.25 ha	6.25	0.78	5.06 – 8	12.5
Cattle *et al.* (1994)		1:5 H_2O			7.81[a]	0.51		6.5
					6.25[b]	0.51		8.1
Dobermann (1994)	117	1:2.5 H_2O	0 – 20		7.2	0.7	5.7 – 8.1	9.7
Dobermann *et al.* (1995)	105	1:1 KCl	0 – 15		2.61	0.12	2.33 – 4.01	2.3
Perez (1995)	28	2:1 H_2O			6.1	0.2	5.5 – 6.6	2.3
Pierce *et al.* (1995)	74		0 – 5	10 ha	6.5	0.9	5.2 – 8	1.4
	165		0 – 5	16 ha	6.6	0.9	5.2 – 7.8	1.4
	174		0 – 20	22 ha	6.7	0.4	5.7 – 7.7	6
Meredieu *et al.* (1996)	253	2.5:1 H_2O	0 – 20		6.5	0.39	6 – 7.3	6
Adderly *et al.* (1997)	480		0 – 10	30 ha	6.3	0.47	5.1 – 8.7	7.5
Median								5.7

[a] pH of cultivated soil; [b] pH of uncultivated Mallee soil

Stationarity

Stationarity is a decision implicit in all statistics. It allows the practitioner to define a data set or area over which the statistics calculated (*e.g.* averages, proportions, etc.) are assumed representative of the whole population and not only of particular individual locations. An important decision of many geostatistical studies is that of stationarity, *e.g.* inference using kriging algorithms (see below) require the user to make the assumption of whether or not the RF model is stationary. Therefore stationarity is a model decision, not an intrinsic property of the actual distribution of *s*-values and not a hypothesis that can be proven or refuted from the data (Journel, 1989). Webster (2000) stressed that the question and assumptions that pertain to the stationarity of soil can only refer to the statistical models of the soil and not to the soil itself. The reason for this being that we have ever only one realisation of the soil in a particular region, so assumptions of stationarity in the mean and variance are nonsensical (Webster, 2000).

A strictly stationary RF $S(x)$ has a distribution function (including all of its moments) that is always the same throughout A, *i.e.* its mathematical expectation or first-order moment throughout A is given by:

$$\begin{gathered} E\{S(x)\} = m(x) \\ E\{S(x+h) - S(x)\} = 0 \end{gathered} \tag{2.4}$$

where m is the mean, and h is the separation vector between sample locations, usually known as the lag. In contrast, RFs that are non-stationary have characteristics that change at any time and at any location. Intensively collected crop and soil information usually displays trends, which are often not detected by sparse sampling techniques.

In geostatistics, the interest is limited to the two first-order moments (second-order moments considered in geostatistics are the *a priori* variance, the covariance and the variogram) hence it suffices to assume their existence, and limit the stationarity assumptions to them (Journel & Huijbregts, 1978). A second-order stationary RF model has an expectation $E\{S(x)\}$ that does not depend on the support point x:

$$E\{S(x)\} = m, \quad \forall x \tag{2.5}$$

Furthermore, the covariance $C(h)$ of each pair of RVs $\{S(x+h), S(x)\}$ is the same throughout A and depends only on the lag h:

$$C(h) = E\{S(x+h)\cdot S(x)\} - m^2, \quad \forall x \tag{2.6}$$

The stationarity of $C(h)$ implies the stationarity of the sample variance v^2, semi-variogram $g(h)$ and correlogram $r(h)$ (Isaaks & Srivastava, 1989). Their relationship is discussed in a subsequent section of this chapter.

Second-order stationarity assumes the existence of a finite covariance and thus, a finite variance. As previously mentioned, this is not always the case with soil or crop data because there are many situations where neither an *a priori* variance nor a covariance exist but a semi-variogram may still be defined, other examples include spatially trended phenomena. In such instances, only the existence and stationarity of the variogram may be assumed and a more flexible form of stationarity called the intrinsic hypothesis adopted (Journel & Huijbregts, 1978, pp. 33-35).

Intrinsic Hypothesis

The intrinsic hypothesis describes a type of stationarity characteristics of the RF model. It is a shorter, more relaxed version of the second-order stationarity condition previously described. The intrinsic hypothesis also has an expectation $E\{S(x)\}$ that does not depend on the support point x (Equation 2.5). That is, the mean is the same at any two places separated by the lag h:

$$E[S(x+h) - S(x)] = 0 \tag{2.7}$$

and the variance of the increment $\{S(x+h) - S(x)\}$ for all vectors of h (depending on the length and orientation), is finite and does not depend on the location x in A:

$$\begin{aligned} \operatorname{var}\{S(x+h) - S(x)\} &= E\{[S(x+h) - S(x)]^2\} \\ &= 2g(h), \qquad \forall x \end{aligned} \tag{2.8}$$

where g is the semi-variance, and is the expectation of the sample variance v^2 for $\{S(x+h) - S(x)\}$. Thus from Equation 2.8, the intrinsic hypothesis is simply the second-order stationarity of the differences $\{S(x+h) - S(x)\}$. The conditions (Equations 2.7 and 2.8) constitute the intrinsic hypothesis of geostatistics, and when it conforms it contains all the information on the model of spatial variation for the soil attribute being studied. This hypothesis is widely applicable to soil (McBratney & Webster, 1986).

It is important to realise that second-order stationarity implies the intrinsic hypothesis, but that the opposite is not true since an intrinsic RF model need not be stationary of order two (Webster & Oliver, 1990; Trangmar et. al., 1985; Journel & Huijbregts, 1978). As a consequence, the intrinsic hypothesis renders the definition of the theoretical semi-variogram, which is discussed next.

Structural Analysis

In soil science, structural analysis refers to the characterisation of the spatial distribution of soil variables and their spatial dependence. The 'tools' used for structural analysis are the covariogram $C(h)$, the semi-variogram $g(h)$ and the correlogram $r(h)$. The correlogram describes the autocorrelation between values at a given separation distance h (Burgess & Webster, 1980). Following from the previous discussion on stationarity, v^2, $C(h)$, $g(h)$ and $r(h)$ of a second-order stationary RF are related by:

$$v^2 = \mathrm{var}\{S(x)\} = E\{[S(x)-m]^2\} \tag{2.9}$$

$$C(h) = E\{S(x+h)\cdot S(x)\} - m^2 \tag{2.10}$$

$$g(h) = v^2 - C(h) = \frac{1}{2}E\{[S(x+h)-S(x)]^2\} \tag{2.11}$$

$$r(h) = \frac{C(h)}{v^2} = 1 - \frac{g(h)}{v^2} \qquad \forall x \tag{2.12}$$

At zero lag (*i.e.* $h = 0$), $C(h)$ is equal to the sample variance v^2. As the lag h increases, $C(h)$ and $r(h)$ (the latter bounded by $-1 \leq r(h) \leq 1$) tend towards zero and the sill value of a bounded or transitive semi-variogram (described in a separate section below) tends towards the finite variance v^2. Therefore when variation is finite the assumption of second-order stationarity holds and the semi-variogram is complementary to a covariance function (Equations 2.10 and 2.11 above).

However when data do not display second-order stationarity, *i.e.* do not have finite variances between sample locations, $C(h)$ and $r(h)$ cannot be used as they are impossible to define (Isaaks & Srivastava, 1989). Thus the weaker assumptions of the intrinsic hypothesis should be adopted and the more robust semi-variogram used as the descriptor of spatial variability. In such instances the semi-variogram appears to increase without limit and is said to be unbounded because there is no finite or *a priori* variance.

Experimental Semi-Variograms

In an intrinsically stationary RF, the semi-variance at lag h is defined by the experimental semi-variogram, which is equal to half the expected square distance between sample values separated by a vector h (Equation 2.11). Hence it measures the average dissimilarity between data points separated by h. This implies that differences between sites are merely a function of their lag h and their direction, not their location x within A. The semi-variance may then be computed from the sample data using:

$$g(h)=\frac{1}{2N(h)}\sum_{i=1}^{N(h)}\left[s(x_i)-s(x_i+h)\right]^2 \tag{2.13}$$

where $N(h)$ is the number of sample pairs of observations separated by h apart, s is the value of the soil property described by its population S, and x is the spatial location of the particular point.

Theoretically sampling points that are closer together display smaller semi-variances than those points that are further apart. The semi-variogram for a given direction is illustrated as a graph of the semi-variance $g(h)$ against the lag distance h (Figure 2.1). This graph together with knowledge of the phenomenon studied can be used to enhance our understanding of the underlying mechanisms controlling the spatial variability patterns of the attribute in question (Oliver & Webster, 1986). The experimental semi-variogram may then be characterised by fitting a theoretical model to it. The most frequently used semi-variogram models in the agricultural and earth sciences are summarised in the following section.

Theoretical Semi-Variograms

As well as semi-variogram estimation, modelling of the semi-variogram is important for structural analysis, determination of sampling design and interpolation. The semi-variogram is modelled by fitting one of a number of (theoretical) functions to the experimental semi-variance values. The fitted functions are used to quantitatively describe the spatial variation of the particular soil property, and may thus be used to optimise sampling, to determine scale of spatial patterns and for prediction (Burrough, 1993).

The chosen function must obey certain mathematical constraints, described by McBratney & Webster (1986). Fundamentally, it must have an intercept on the ordinate, a section of constantly increasing semi-variance, and a sill. In two dimensions the theoretical function must also describe anisotropy (which is described below).

The intercept on the ordinate, *i.e.* the semi-variance at lag zero is defined by C_0 and is called the nugget variance (Figure 2.1). Although by definition the value of C_0 should be zero, the semi-variances tend towards positive values as the lag distance approaches zero. The value at which the semi-variance reaches a maximum is called the sill variance and is denoted by (C_0 + C), where C is the section of constantly increasing semi-variance due to the spatial dependence of the data (Figure 2.1). Roughly, the sill variance corresponds to the population variance s^{2}. The lag at which the semi-variogram reaches the sill variance is called the range and is commonly denoted by a (Figure 2.1). Beyond the range, the semi-variance has no relation to the lag and the data is not spatially dependent, *i.e.* it has no spatial structure.

However, not all models that satisfy these characteristics will serve. The fitted semi-variogram function must be an ‘authorised’ or ‘permissible’ function, or Conditional Negative Semi-Definite (CNSD). McBratney & Webster (1986) and Webster & Oliver (1990) provide good explanations of this constraint. Briefly, in a second-order stationary RF the covariance matrix must be either zero or positive, *i.e.* positive semi-definite. In situations where the variance appears to increase without limit and properties do not have definable covariances, provided that the intrinsic hypothesis holds, only the semi-variance of the property is considered. Therefore, with reference to the semi-variogram only, the function used to quantify the experimental semi-variogram must be CNSD. This condition is strict and only valid models must be used to characterise the semi-variogram. Two main families of functions describe simple forms of variograms: models that are bounded by a sill - called bounded or transitive models, and those that are not - referred to as unbounded modes.

Bounded (or Transitive) Models

These models are derived from the notion that the RF, of which the soil property measured is a realisation, depends on the amount of overlap of two blocks, *i.e.* a zone of transition (McBratney & Webster, 1986). Note that the sill value of transitive models is the *a priori* variance of the RF $S(x)$ which is second-order stationary with a definable covariance. The most commonly used transitive models in soil science are described in the following text.

The Spherical Model

The most common bounded semi-variogram model used in soil science is the spherical model (Figure 2.1). It was originally derived from the volume of intersection of two spheres (McBratney & Webster, 1986). Its formula is:

$$\begin{cases} g(h) = C_0 + C\left\{\dfrac{3h}{2a} - \dfrac{1}{2}\left(\dfrac{h}{a}\right)^3\right\} & \text{for } h \le a \\ g(h) = C_0 + C & \text{for } h > a \end{cases} \tag{2.14}$$

where a is the range of the model with a gradient $3C/2a$.

The Exponential Model

When the semi-variogram approaches the sill asymptotically, then it may well be represented by an exponential function. The exponential model (Figure 2.1) appeals to soil research because of its generality. Its formula is given by:

$$g(h) = C_0 + C\left\{1 - \exp\left(-\frac{3h}{a'}\right)\right\} \quad \text{for } 0 < h \tag{2.15}$$

where C is the asymptotic sill with no strict range. The effective range a' is analogous to the range of the spherical model as it also defines the spatial extent of the function. It is taken to be the lag where $g(a')$ is approximately equal to $(C_0 + 0.95C)$.

The Gaussian Model

The Gaussian model (Figure 2.1) has a sigmoidal shape. The model is rarely applied to soil data, but often found to characterise phenomena that is extremely continuous, *e.g.* topographical data. Its formula is given by:

$$g(h) = C_0 + C\left\{1 - \exp\left(-\frac{3h}{a'}\right)^2\right\} \tag{2.16}$$

As with the exponential case, C is the asymptotic sill and a' is the effective range defining the scale of spatial variation.

Unbounded Models

These models describe situations where soil appears to increase without limit as the lag distance increases (McBratney & Webster, 1986). Unlike the previous models, unbounded models are fitted to soil properties with an unlimited capacity for dispersion where neither their *a priori* variances nor their covariances can be defined (see above). In this sense then the RFs are only intrinsic and thus only the intrinsic hypothesis applies.

The Linear and Power Models

Equation 2.17 describes the family of semi-variograms that are called the power models.

$$g(h) = C_0 + wh^q \tag{2.17}$$

The reader is referred to McBratney & Webster (1986) for a more detailed description of the derivation of power models. Briefly, the parameter θ of equation 2.17 must take a value in between 0 and 2. When $\theta = 2$, the function is a parabola and differentiable, thus not no longer representing a random process. When $\theta = 0$, the function represents pure noise, which is impossible for a continuously varying process. The shapes of power models with $\theta = 0.5$, 1 and 1.5 are shown in Figure 2.1. When the $\theta = 1$, the function describes a linear semi-variogram (Figure 2.1). The linear model is the simplest in this group and it has been used to describe the spatial variability of soil properties (*e.g.* Burgess & Webster, 1980a; Gajem *et al.*, 1981; Tabor *et al.*, 1985).

Pure Nugget Variation

A pure 'nugget effect' occurs when $g(h)$ is positive and equal for all values of h, including $h = 0$. Using power model notation, pure nugget variation may be defined when $\theta = 0$. However what is required is a function that is positive for all values of h, but zero at $h = 0$. The Dirac function $d(h)$ accomplishes this, taking a value of 1 when $h = 0$, and zero otherwise (Webster & Oliver, 1990, p.232). The pure nugget semi-variogram is defined by:

$$g(h) = C_0\{1 - d(h)\} \tag{2.18}$$

The model is impossible for continuous variables such as soil. However it appears in soil data (*e.g.* Campbell, 1978) either because the shortest sampling interval is larger than the range of spatial dependence, or because there is large sampling and measurement errors or both. The pure nugget effect thus corresponds to a total absence of spatial correlation between variables *i.e.* it occurs when the variables are spatially independent. Therefore it characterises a very homogeneous soil and is associated with a strictly stationary RF (refer to 'Stationarity' section of this chapter). For example, if soil pH in an agricultural field is the variable of interest, it implies that no local differentiation in soil pH is possible and that the best estimator of soil pH in that field is the average pH.

Figure 2.1 shows the common forms of bounded and unbounded semi-variogram models that were described in the preceding text.

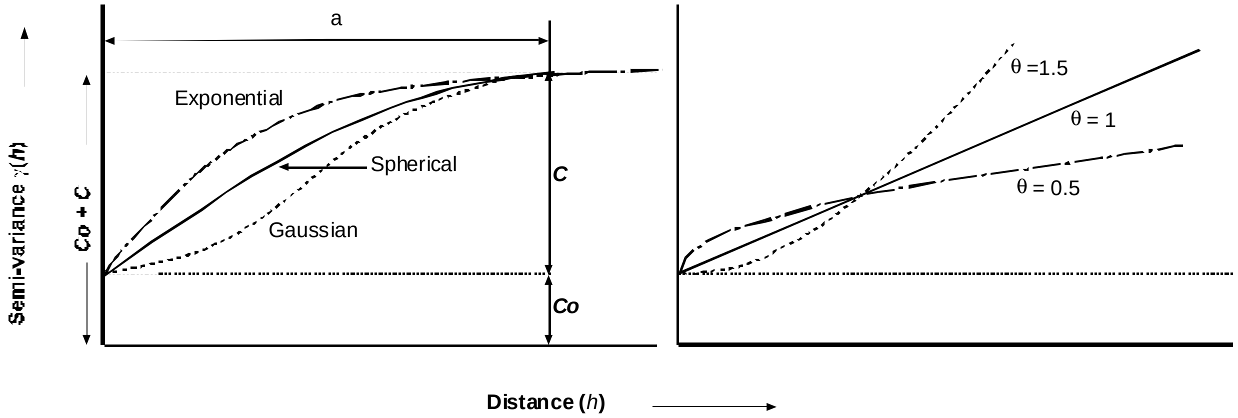

Figure 2.1 Bounded and unbounded semi-variogram models of soil properties

Other Models

Other less commonly employed models include the linear model with sill, the circular model, the pentaspherical model and anisotropic models. In some situations, the data call for a combination of two or more permissible models to fit the experimental semi-variogram. These are referred to as 'nested' models, *e.g.* a nugget and double spherical or exponential models. Webster (1985), McBratney & Webster (1986) and Webster & Oliver (1990) provide good descriptions of these other models that may be used to characterise soil spatial variability.

Anisotropy

The semi-variogram models previously described relate to isotropic models, where variation is assumed to be identical in all directions. However soil does not necessarily behave in an isotropic manner, rather it may be anisotropic. Anisotropy refers to soil that does not vary equally in all directions. In this case each direction will have its own semi-variogram model that differs from those in other directions. There are two general types of anisotropy that may be distinguished: geometric anisotropy and zonal anisotropy.

Geometric or 'affine' anisotropy occurs when the range changes with direction while the sill remains constant. This type of anisotropy may be accounted for by a linear transformation of the coordinates (Webster & Oliver, 1990, pp. 234-236). Burgess *et al.* (1981); McBratney & Webster, 1983; 1986) showed examples of geometric anisotropy is soil.

Zonal anisotropy occurs when the sill changes with direction while the range remains the same, *i.e.* the amount of variation changes according to direction. This type of anisotropy cannot simply be accounted for by a linear transformation of the coordinates (Journel & Huijbregts, 1978, pp. 181-183). Webster & Oliver (1990) indicated that this situation would certainly arise in studies of soil in three dimensions, where the vertical variation differs greatly from that in horizontal planes. Journel & Huijbregts (1978) further defined zonal anisotropy as a nested structure in which each component structure may have its own anisotropy.

Model Fitting and Selection

The common method of fitting a function to experimental semi-variance values is that of weighted least-squares. In theory the weights can be the inverse of the variance of the semi-variances estimates, however this variance is generally unknown (McBratney & Webster, 1986). Therefore the weights used for fitting are usually taken to be equal to the numbers of pairs of observations making up each estimate. The assumption in this case is that the weights are inversely related to the variance of the semi-variance estimates. McBratney & Webster (1986) provided a description and assessment of other methods used for fitting semi-variogram models.

Selecting the most representative semi-variogram model and its parameters can be difficult. The investigator's knowledge of the area and the phenomenon being studied should provide good qualitative information to aid with model selection. On occasions however, the investigator may have little pedogenetic grounds for choosing a particular model (McBratney & Webster, 1986). In such instances a more quantitative statistical method may be required that helps to achieve a balance between goodness of fit and parsimony in the model. McBratney & Webster (1986) suggested the use of the Akaike Information Criterion (AIC) (Akaike, 1973) to strike this balance. The AIC may be estimated by:

$$AIC = n \ln(RSS) + 2p \tag{2.19}$$

where n is the number of observations, p the number of estimated parameters and RSS the residual sum of squares. In a latter publication Webster & McBratney (1989) described the utility of the criterion in model selection. The model having the smallest AIC is the best fitting model.

The Spatial Variability of Soil pH

A literature review of the spatial variability in soil pH, described by semi-variograms is given in Table 2.2. The spatial variability of soil pH was reviewed because of its implications to the topic of this research. The spatial variability of other agriculturally relevant soil properties have been reviewed elsewhere (*e.g.* McBratney & Pringle, 1999).

For the most part, surface soil pH is characterised using the transitive spherical and exponential semi-variogram models (Table 2.2). Median values of the semi-variogram parameters (Table 2.2), suggest that soil pH is spatially correlated over a range of 121 m. The nugget ratio (*i.e.* $C_0/(C_0+C)$) of 14 % indicates that soil pH is strongly structured over the given range. In contrast, the relatively low overall variability measured by the median CV (Table 2.1) may be due to the indexing nature of the logarithmic pH scale. The implications and application of semi-variogram parameters for sampling and prediction are outlined in Chapter IV.

Table 2.2 Isotropic semi-variogram models and parameter values for soil pH

Author	Depth (cm)	Area (ha)	Interval (m)	Model	C_0	C	a (m)
Campbell (1978)		1.6	10	Nugget	0.04		
		1.6	10	Nugget	0.02		
Yost *et al.* (1982)	0 – 15		1000 to 2000	Exponential	0.1	0.43	3200
	30 – 45		1000 to 2000	Exponential	0.03	0.6	3400
Uehara *et al.* (1985)		0.0784			0	0.35	4
Tabor *et al.* (1985)	0 – 20	13		Linear	0.015	0.056	500
Riha *et al.* (1986)				Nugget			
Laslett *et al.* (1987)		1	10	Spherical	0.019	0.032	55
		1	10	Spherical	0.025	0.02	52.8
Trangmar *et al.* (1987)	0 – 20			Spherical	0.015	0.34	4100
Webster & McBratney (1987)		77	40	Spherical	0.021	0.33	185
Samra et.al. (1990)	0 – 30				0.06	0.64	117
Boyer *et al.* (1991)	0 - 10		1	Spherical	0.02	0.1	53
Mulla (1993)	0 – 30	8		Spherical	0.17	0.26	132
Cambardella *et al.* (1994)	0 - 15	6.25	2 to 25	Spherical	0.06	0.7	117
Pierce *et al.* (1995)	0 – 5	10	30 .5	Spherical	0.078	0.318	95
	0 – 5	16	30 .5	Spherical	0.127	0.474	354
	0 – 20	22	30 .5	Spherical	0.06	0.15	190
Kristensen *et al.* (1995)	0 – 25	10		Exponential	0	0.092	19
	0 – 25	10.9		Exponential	0	0.098	17
Birrell *et al.* (1996)	0 - 15	28		Spherical	0.055	0.11	125
Lark & Bolam (1997)	0 – 20	6.5		Spherical	0.04	0.04	35.7
Adderly *et al.* (1997)	0 - 10	30		Exponential	0.15	0.1	250
Median					0.035	0.21	121

Prediction using Kriging Algorithms

Kriging is a generic name adopted by geostatisticians for a family of generalised least-squares regression algorithms (Webster, 1996). There are a number of kriging algorithms that may be used depending on the stationarity condition, the probability distribution of the data or the application for which it is being considered. The simplest forms of kriging are ‘ordinary punctual (or point) kriging’ (Burgess & Webster, 1980a) and ‘ordinary block kriging’ (Burgess & Webster, 1980b). Punctual kriging pertains to estimates of point values, while block kriging involves estimating areas or ‘blocks’. Derivation of the ordinary kriging estimator requires the intrinsic stationarity assumptions previously described. Data that appear to possess trends (*i.e.* non-stationary data) can be interpolated using ‘universal kriging’ (Webster & Burgess, 1980). Soil data that exhibits lognormal or complex probability distributions where a linear estimator may not be adequate, can be interpolated using ‘lognormal kriging’ (Dowd, 1982) or ‘disjunctive kriging’ (Yates & Yates, 1988) algorithms. Journel & Huijbregts (1978) also provided brief explanations of the latter two methods. Wackernagel (1995) described yet another variant, ‘factorial kriging’, which aims at estimating and mapping the different sources of variation identified on the experimental semi-variogram. Journel (1983) described the technique of ‘indicator kriging’, which can be used to model the conditional cumulative distribution function non-parametrically. Goovaerts (1997) also provided a good description and discussion of indicator kriging. Finally, ‘co-kriging’ will allow the incorporation of secondary continuous information in the estimations (Journel & Huijbregts, 1978; McBratney & Webster, 1983).

Only ordinary kriging is described below, with reference to point and block kriging. Chapter V provides an outline of universal kriging and variants of the methodology, while Chapter X presents the key steps of indicator kriging and demonstrates an application.

Ordinary Kriging

Ordinary kriging is the principal method used for the prediction of regionalised soil variables at unsampled locations (Burgess & Webster, 1980a). Thus in PA, kriging is used to produce soil and crop property maps for site-specific management. It is a local estimation technique that provides the Best Linear Unbiased Estimator (BLUE) of the unknown variable being studied (Journel & Huijbregts, 1978). The technique is ‘linear’ because its estimates $s^*(x_0)$, are weighed linear combinations of the available data:

$$s^*(x_0) = \sum_{i=1}^{n} l_i s(x_i), \tag{2.20}$$

where n is the number of neighbouring samples, $s(x_i)$ represent the value of the soil property S at the ith sampling point and l_i are their respective weights. Kriging constraints these weights to sum to one:

$$\sum_{i=1}^{n} l_i = 1, \tag{2.21}$$

to ensure 'unbiased' estimation. Hence it tries to have the mean estimation error equal to zero:

$$E\left[s(x_0) - s^*(x_0)\right] = 0 \tag{2.22}$$

The estimation variance s^2_{est} at x_0 is given by:

$$s^2_{est} = 2\sum_{i=1}^{n} l_i g(x_0 - x_i) - \sum_{i=1}^{n}\sum_{j=1}^{n} l_i l_j g(x_i - x_j), \tag{2.23}$$

where $g(x_i - x_j)$ denote the semi-variance between the ith and jth sampling points. Recall that when the soil variable is isotropic the semi-variance depends on only the separating distance between data points, *i.e.* $g(x_i - x_j) = g(|x_i - x_j|)$.

Ordinary kriging is 'best' because it attempts to minimise the estimation variance, hence distinguishing it from other methods used for estimation (*e.g.* inverse distance methods). The minimisation of a function of n variables is generally accomplished by setting the n first partial derivatives to zero. The resultant equations and unknowns are then solved using methods for solving systems of simultaneous linear equations (Isaaks & Srivastava, 1989). However this procedure may not be correct for the minimisation of s^2_{est} since the solution is constrained such that the weights l_i, sum to 1. This problem of constrained optimisation requires the definition of the Lagrange parameter y, which is used to convert the constrained minimisation problem into an unconstrained one (Isaaks & Srivastava, 1989, pp. 284-285). Therefore the kriging variance s^2_{est} is minimised when:

$$\sum_{j=1}^{n} l_j g(x_i - x_j) + y = g(x_i - x_0) \qquad \text{for } i = 1,2,\ldots n. \tag{2.24}$$

where $g(x_i - x_0)$ is the semi-variance between x_i and x_0, as defined by the semi-variogram. Therefore the semi-variogram is essential for kriging.

The equations of the kriging system may be more efficiently solved using matrices. Equation 2.25 may then be written as:

$$\mathbf{A}\begin{bmatrix} l \\ y \end{bmatrix} = \mathbf{b}, \tag{2.25}$$

where **A** is calculated from the separation distance between each point using the semi-variogram model, vector **b** becomes an $n + 1$ by 1 matrix of the semi-variances between the sampling point and the point to be estimated, *i.e.*:

$$\mathbf{A}\begin{bmatrix} ?(\mathbf{x_1},\mathbf{x_1}) & ?(\mathbf{x_1},\mathbf{x_2}) & \cdots & ?(\mathbf{x_1},\mathbf{x_n}) & 1 \\ ?(\mathbf{x_2},\mathbf{x_1}) & ?(\mathbf{x_2},\mathbf{x_2}) & \cdots & ?(\mathbf{x_2},\mathbf{x_n}) & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ ?(\mathbf{x_n},\mathbf{x_1}) & ?(\mathbf{x_n},\mathbf{x_2}) & \cdots & ?(\mathbf{x_n},\mathbf{x_n}) & 1 \\ 1 & 1 & \cdots & 1 & 0 \end{bmatrix},$$

$$\begin{bmatrix} l \\ y \end{bmatrix} = \begin{bmatrix} l_1 \\ l_2 \\ \vdots \\ l_n \\ y \end{bmatrix}, \text{and } \mathbf{b} = \begin{bmatrix} ?(\mathbf{x_1},\mathbf{x_0}) \\ ?(\mathbf{x_2},\mathbf{x_0}) \\ \vdots \\ ?(\mathbf{x_n},\mathbf{x_0}) \\ 1 \end{bmatrix}.$$

Matrix **A** may then be inverted and multiplied by **b** for the determination of the kriging weights:

$$\begin{bmatrix} l \\ y \end{bmatrix} = \mathbf{A}^{-1}\mathbf{b} \tag{2.26}$$

Each weight is then multiplied by the sample data $s(x_i)$ and summed to obtain the estimate of the soil attribute at the particular point. Then the minimum estimation variance s^2_{est} is given by:

$$s^2_{est} = \mathbf{b}^{\mathbf{T}}\begin{bmatrix} l \\ y \end{bmatrix}, \tag{2.27}$$

where $\mathbf{b^T}$ is the transpose of vector **b**.

Kriging will therefore use the semi-variogram to estimate data at locations where there are no measurements, and under stringent hypothesis of normality and homoscedasticity, it provides an error variance that can be combined with the estimated value to derive confidence intervals (the uncertainty) at each location x_0 (Goovaerts, 1997). However, it is important to remember that the accuracy of the kriged estimates and the error variance from which the confidence intervals are derived will depend on how well the semi-variogram has been computed and modelled (Isaaks & Srivastava, 1989, pp. 504-506). Note also that with kriging, the sampling points closest to the unknown point being estimated contribute more weight than those further away. Burgess & Webster (1980a) indicated that for data on a regular grid only the nearest 16 to 25 points are sufficient for an accurate estimate.

Instead of single point estimates (x_0), it may be more useful to obtain average estimates for discrete areas or blocks (*B*) in a field *e.g.*, block estimates of soil properties over which resources may be applied using variable-rate technology, depending on soil variability. Block kriging provides a method for achieving this and, at the same time, evading some of the shortcomings of punctual kriging (see above). The technique estimates the average value for *B* with its centre at x_0. Although the user may define *B*, for PA commonly used block sizes range from 10 to 20 m. The kriging system is similar to the punctual system outlined above. However block kriging involves replacing the semi-variances between data points and the point to be estimated $g(x_i - x_0)$, by the average semi-variances between the data points and all points in the block *B*, $\bar{g}(x_i - B)$. The modifications to the kriging system are detailed in (Burgess & Webster, 1980b; Journel & Huijbregts, 1978).

The Nugget Effect and the Ordinary Kriging System

The nugget effect will also affect the estimates obtained from the ordinary kriging system (described above). A larger nugget will produce a more equal distribution of the ordinary kriging weights resulting in somewhat higher kriging estimates and a larger kriging variance (Isaaks & Srivastava, 1989, pp. 305-307). It will create discontinuities at the sampling points and smooth the kriging surface between them (e.g. Webster & McBratney, 1987). Higher nuggets will make estimation by ordinary kriging more like a simple averaging method, and if all the variance is nugget then the kriged surface will be flat between sampling points. The discontinuity problem does not arise with block kriging (e.g. Webster & McBratney, 1987) because the nugget variance is contained entirely in the within-block variance and does not contribute to the block-kriging variance (Webster & Oliver, 1990). Block estimates thus overcome the discontinuity problem and are more precise than punctual kriging estimates (see above).

The Smoothing Effect of Kriging

Kriging is a 'best' least-squares weighted linear estimator of a soil property at an unsampled location because it attempts to minimise the estimation variance. A shortcoming of the procedure is that estimated soil property values are generally much less variable than actual values. Typically estimation by kriging results in the overestimation of small, and the underestimation of large values. These artifacts produced by kriging are often referred to as the smoothing effect of kriging algorithms, and are a result of the fact that estimates are weighted linear combinations of several sample values (Isaaks & Srivastava, 1989, p. 420). Another drawback of estimation by kriging is that the smoothing effect is dependant on the configuration of local data (Goovaerts, 1998a). That is, smoothing is small close to data locations and increases as the site being estimated gets farther away from sampled locations. This uneven smoothing produces kriged maps that appear a lot more variable in densely sampled areas than in sparsely sampled ones (Goovaerts, 1997).

Stochastic Simulation

Another geostatistical technique for the aggregation of soil information, other than kriging, is geostatistical simulation (*e.g.* refer to Goovaerts, 1997; Deutsch & Journel, 1998). Unlike kriging whose design is to minimise the local estimation error variance, stochastic simulation aims to generate of a set of values that reproduces global statistics such as the sample histogram and the theoretical semi-variogram. Like kriging, stochastic simulation models honour data at their locations however, simulation produces less smooth maps reproducing areas of high and areas of low values as represented by the sample data. Nevertheless simulated values should be interpreted with care because the global constraints in simulation take precedence over the accuracy of the local predictions.

Therefore conditional simulations retain the statistics of the original data and the overall texture of the variation in the simulated values. It is for these reasons that simulated maps often appear more variegated and perhaps more realistic than kriged maps derived using the same sample information. Table 2.3 provides a comparison between the statistics of a sample data set (assumed to be reality), a kriging model and a simulated model.

The only statistic reproduced by the estimation model is the sample mean (Table 2.3). As previously mentioned, estimated values are less variable that those of the sample data due to the smoothing effect of kriging. The spatial variability of the estimation model is also generally lower than that of the spatially distributed attribute, the semi-variogram usually exhibits a lower nugget variance and an S-shaped curve characteristic of extreme continuity. All of the statistics of the simulated values are comparable to those of the sample data (Table 2.3).

Table 2.3 Comparison of a sample data set (considered as reality) to estimation and simulation models. Check symbols (✓) represent comparable statistics, while cross symbols (✗) represent statistics that are not comparable to their counterparts in the same row

Statistic	Reality	Estimation model	Simulated model
Random function	Spatially distributed sampled data set	Estimated values at unsampled locations	Simulated values at unsampled locations
Histogram	✓	✗	✓
Mean	✓	✓	✓
Variance	✓	✗	✓
Semi-variogram	✓	✗	✓

Simulation allows the derivation of many equiprobable realisations of the RF, each producing statistics comparable to the sample data (Goovaerts, 1999). However each realisation will be different form the others *i.e.*, conditional simulations (or stochastic models) are not unique. For example if maps of several realisations were produced and compared, differences between the maps in local areas would be evident. The question would then be which of the many equiprobable realisations does one select as the management map? To derive an optimal map one may average the large number of realisations together and use this E-type estimate (or expected estimate) as the management map. However the average of a large number of realisations is simply the kriged estimate. Therefore if the derivation of management maps is the only aim, then kriging is the simpler more effective option. On the other hand stochastic simulation may be preferred to kriging where the spatial variability of the field must be preserved (Goovaerts, 1999).

The more attractive advantage of stochastic simulation is its provision of a non-parametric measure of the spatial uncertainty from the differences between the many equiprobable realisations (Deutsch & Journel, 1998) (*c.f.* the more common Gaussian-type confidence intervals derived from kriging estimates and variances). For example, consider having 100 simulated realisations of the lime requirement of a field. Since each of these realisations is equiprobable, a histogram of all 100 simulated lime requirements may be constructed, it representing the probability distribution of lime requirements for the particular field. That is, the histogram provides a measure of the spatial uncertainty of lime requirements resulting from our imperfect knowledge of the spatial distribution of lime requirements in the field: segments of high lime requirement are deemed certain if seen on most of the realisations and *vice versa*. Each simulated map may also be used as input into models to investigate the local or regional impact of given scenarios (*e.g.* single-rate and variable-rate applications of lime) and the consequences of remediation (Goovaerts, 1998a). Such joint probabilities cannot be derived from conditional cumulative distribution functions (*ccdf's*) as each *ccdf* is specific to a single location and thus provides a measure of the local uncertainty (Goovaerts, 1999). Chapter X describes a method for modelling the local uncertainty about the value of a soil attribute s at location x.

Frogbrook (1999) compared the effect of sampling intensity on the reliability of soil potassium maps for variable-rate fertiliser application, produced by kriging and sequential-Gaussian simulation. She indicated that statistically, kriging produced more accurate values than simulation but that simulation did not smooth the data and hence preserved the spatial variability of potassium in the field. The comparisons by Frogbrook (1999) were made on single realisations and no useful conclusions were derived.

Techniques with Properties Intermediate to Kriging and Simulation

Olea & Pawlowsky (1996) developed a technique that compensates for the smoothing of kriging. Briefly, Olea & Pawlowsky's algorithm involved kriging the data and using cross-validation to run a regression of the estimation on true values. Inversion of the regression model removed the smoothing and produced the new estimator termed 'compensated kriging'. If some of the corrected values fell outside an admissible interval, the parameters of the linear regression model were modified using a trial-and-error procedure. The authors showed that the estimation surface generated by their technique had properties that were intermediate between those generated by ordinary kriging and stochastic simulations. That is, the histogram was well reproduced by the compensated kriging surface, which also approximated the semi-variogram, better than ordinary kriging but not as well as stochastic simulations. Olea & Pawlowsky (1996) concluded that compensated kriging was more accurate than stochastic simulations (*i.e.* smaller prediction error), but not as accurate as ordinary kriging. However the authors cautioned its use and suggested that better ways to model the smoothing and deeper knowledge of the technique are needed before it is used beyond the exploratory stage.

Goovaerts (1998b) suggested that a shortcoming of Olea & Pawlowsky's algorithm was the lack of control on the reproduction of spatial statistics such as the semi-variogram and on the preservation of desirable properties of kriging such as local accuracy. Goovaerts (1998b) presented an algorithm that combines the different local (estimation) and global (simulation) constraints into a single objective function, which is then used to post-process an estimated map using simulated annealing. The relative weights of the different constraints in the objective function allow the user to strike a balance between the smoothness of an estimated map and the variegation of simulated maps. Goovaerts (1998b) showed that the procedure produced maps that were more accurate than stochastic simulation but not as accurate as E-type estimation. The author concluded that by incorporating local estimation constraints in simulated annealing, the approach reduced the risk associated with the use of a single realisation for forecasting and planning.

2.4 PRECISION AGRICULTURE

Geostatistics is currently essential for the implementation of PA. It is used for spatial modelling and prediction of soil and crop properties at unsampled locations. Precision agriculture uses measured information on the spatial and temporal variability in soil, crop and environmental factors to site-specifically manage agricultural land within a management unit, for near optimal crop production (*e.g.* Larson & Robert, 1991; Robert *et al.*, 1995). It has been the subject of much research conducted worldwide *e.g.* Robert *et al.* (1993, 1994, 1995, 1996, 1998), Olesen (1995), Lake *et al.* (1997), Stafford (1997, 1999), and has encouraged the publication of the Journal of Precision Agriculture by Kluwer Academic Press. Many of the research papers published in such publications deal with the various phases, or components of the management system.

The four main phases of current PA management systems involve geo-referenced data acquisition, spatial data analysis, decision support and the implementation of optimal management, be it site-specific or uniform (Conceptual Basis of the Research and Aims). However, in real-time continuous operation where 'on-the-go' soil sensing systems are used to gather variability data only three phases are required, data acquisition, decision support and continuous implementation of management. In real-time operation, the use of a GPS for spatial referencing is not crucial however it may be important for record keeping and databasing.

Real-time continuous management systems integrating data acquisition, decision support and implementation in a single pass over the field are currently being researched and are under development but are not yet commercially available. Therefore for completeness, the four phases of a PA management system and the use of positioning technology for spatial referencing will form the basis of the subsequent review.

2.4.1 SPATIAL REFERENCING

Precision agriculture requires spatial referencing to establish ground position when conducting field-based operations, such as data collection and subsequent site-specific management. A robust and practical positioning system is therefore essential. Three types of positioning (or navigation) systems that may be used for spatial referencing include satellite based (Kruger *et al.*, 1994), local triangulation (Luellen, 1985), or dead reckoning (Sudduth *et al.*, 1994) systems.

Local triangulation systems rely on calculating a position relative to a configuration of ground based beacons. The first site-specific spreader units used a standard AgNav system with two sender units, one on each side of the field, and a receiver on a truck (Luellen, 1985). Triangulation between these three points gave the system constant information on the location of the spreader. Dead reckoning systems rely on the relative distance to the starting location for positioning, using direction, heading and the distance travelled as aids. However since only a relative position is obtained, errors tend to accumulate and position measurements are not repeatable unless permanent reference points are available on a field by field basis (Sudduth *et al.*, 1994). Due to the better accuracy, precision, and greater practicality and lower cost of satellite positioning, the use of both of these systems has been abandoned with preference to the latter. Satellite navigation systems are the important enabling technology of PA (Chapter I), and hence they will be briefly reviewed.

There are two major satellite navigation systems currently accessible to civilian users, the NAVSTAR GPS and GLONASS (Chapter I). The systems are very similar in design and operation, both consisting of a space segment that comprises of a constellation of dedicated satellites, a control segment that monitors, manoeuvrers and updates information to the satellite, and a user segment that determines ground positioning (Kruger *et al.*, 1994). The NAVSTAR GPS will be predominantly discussed in the following text, as it has been the more widely adopted system for civilian use. A reason for this may be that until recently, no commercial time receivers were available for GLONASS. However, there are a number of manufacturers currently developing receivers that will use both GPS and GLONASS signals. This may increase the incidence of sightings and potentially positional accuracy.

The fundamentals of GPS operation have been described in many other more specific publications, *e.g.* USA Government (1993), Kruger *et al.* (1994) Hofmann-Wellenhof *et al.* (1994). A number of publications also describe GPS operation with particular reference to PA, *e.g.* Auernhammer *et al.* (1994) described GPS operation for yield mapping, Larsen *et al.* (1994) described precision navigation for agricultural vehicles, while Lange (1996) and Tyler *et al.* (1997) provided more general reviews for general PA applications. The reader is directed to these texts for complete descriptions and explanations of GPS operation. Here it will suffice to briefly describe the most current developments and features that are relevant to PA.

The current GPS constellation consists of more than 24 satellites in six planes orbiting at an altitude of 20 000 km. The satellites are in 13 hour orbits and provide 24 hour coverage worldwide with four to ten satellites visible at any one point. To record a point position in four dimensions (*i.e.* x, y, z, and time), the user segment (or GPS receiver) must instantaneously resolve the position from four satellites. The receiver then converts x, y, z signals from three satellites into latitude, longitude, and elevation respectively, while the fourth satellite determines correction errors between the satellite and receiver timepiece (Kruger *et al.*, 1994). Hence the fourth satellite is used to synchronise the signals and improve the accuracy of the measured position.

Selective Availability (SA) refers to the technique that was intentionally used by the U.S. Department of Defense for the degradation of GPS signals. Selective availability was turned off a few minutes after 0400 hours UTC May 2, 2000 (midnight EDT May 1, 2000). Selective availability reduced the accuracy of stand-alone, single-receiver GPS measurements by altering (or dithering) the GPS satellite clock signals, and by modifying orbital elements of the broadcast navigation message (USA Government, 1993). The alterations were done in a coded manner, and could only be removed by authorised users. Selective availability caused horizontal positional errors on the order of ± 100 m (95 % confidence interval) (Figure 2.2a), and varied in a manner that prevented rapid averaging of positional data (Kruger *et al.*, 1994). The potential positional accuracy without SA has 95 % confidence intervals of 3 and 35 m (Figure 2.2b). The broad range in errors (3 m to 35 m) when SA is inactivated results from the variable nature of a number of other components that contribute to the overall error in the GPS signals. These errors include those caused by the signal travelling through the ionosphere and troposphere, orbital parameters, multi-path signal reception, GPS receiver noise, and geometric effects such as the Precision Dilution of Position (PDOP) (Kruger *et al.*, 1994).

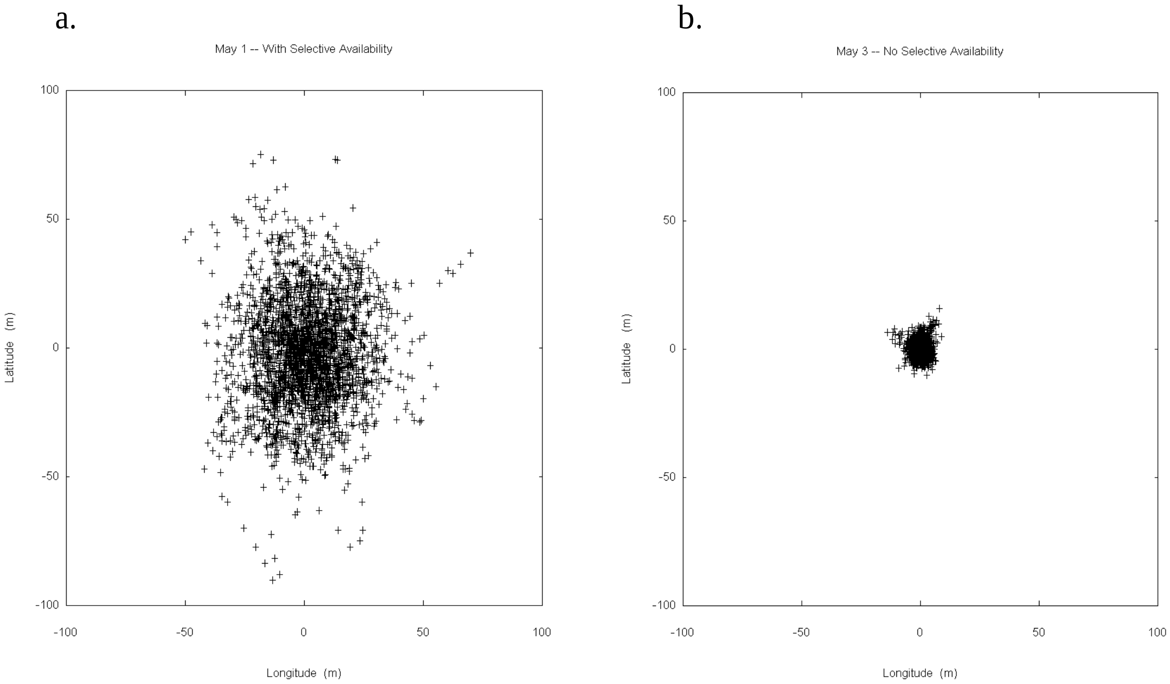

Figure 2.2 Positioning accuracy of the Global Positioning System (a.) with selective availability and (b.) without selective availability. Source: www.ngs.noaa.gov

Positional GPS errors can be reduced (whether SA is activated or not) to 1 to 3 m by using a differential GPS configuration, or DGPS. Differential GPS incorporates error corrections provided by a fixed GPS monitoring station with known surveyed position (Figure 2.3).

The monitoring station calculates the corrections by comparing its known location with that reported by the GPS satellites (Figure 2.3). The difference between the two represents a ‘differential correction’ that can be applied either in real-time using a radio-frequency communication link, or during post processing following sampling or surveying. Real-time DGPS results in more accurate positional calculations and the advantage of allowing the corrected information to be linked with other data such as soil property sensor signals, as the information is being collected ‘on-the-go’.

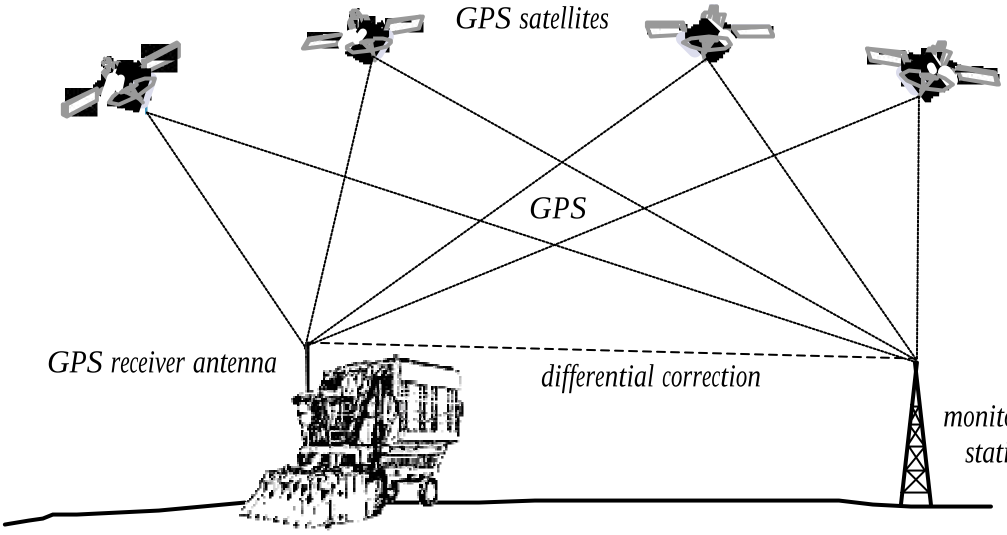

Figure 2.3 Operational configuration of a real-time Differential Global Positioning System (DGPS)

The discontinuation of SA will not eliminate the need for DGPS systems in PA since the level of accuracy required for site-specific management ranges between a few centimetres to a couple of metre depending on the operation being considered. For example Stafford (1996) suggested the following levels of accuracy: 30 m for variable fertiliser application, 10 m for yield mapping, 1 m for variable herbicide application, 10 cm for the avoidance of spray overlap and also row crop planting and 5 cm for seed bed structure. For soil sensing applications metre to sub-metre accuracy may be necessary. Although these figures are open to considerable debate they illustrate the wide range of positioning resolution that is required for site-specific management and the need for DGPS.

With the removal of SA, the largest source of error is distortion of the GPS signal as it travels through the ionosphere. Although an ionosphere correction model is broadcast over the navigation message, it is only partially successful in correcting the ionosphere sensed by a GPS receiver at any given location (Hofmann-Wellenhof *et al.*, 1994). Using DGPS with a single monitoring station may compensate for effects associated with ionospheric errors, however this ability may degrade with increasing distance from the monitoring station (Brown, 1989). Removal of the SA bias will not affect the accuracy of DGPS. However, DGPS corrections may not need to be broadcast as frequently any more. Hence, future commercial DGPS services may use less radio bandwidth and thus cost less to the end user.

Using a single fixed-base monitoring station (as previously described) assumes that all the positional errors apply equally to both the monitoring station and the mobile receiver unit. However as their separation distance increases (*e.g.* beyond 100 km), the receiver and monitoring station may be viewing different satellites and receiving the signals via different atmospheric travel paths, hence also experiencing different satellites errors (Brown, 1989; Clark, 1992). If this happens then the accuracy of the corrected position will decrease as the receiver unit gets farther away from the monitoring station.

Using two or more monitoring stations can reduce these errors (Brown, 1989). If a network of monitoring stations is used then the operational configuration is referred to as wide area differential GPS (WADGPS) (Mueller, 1994). In a WADGPS configuration, the fixed monitoring stations communicate with the GPS satellites and individual correction algorithms are calculated for each station. These are then transmitted to a master station that calculates a vector correction from all individual fixed stations and transmits the correction signal to a general geostationary communications satellite, which increases the broadcast range to receiver units being used in remote areas. Wide area DGPS can provide sub-metre accuracy that is spatially independent of the receiver unit location within the network.

There are numerous DGPS receivers commercially available with reported accuracy of ± 1 m, however this accuracy will depend on the specifications of the receiver unit and will be location and time dependant. Also, WADGPS corrections are available in Australia from a number of commercial organisations. For the majority of PA operations, these positioning configurations may be adequate. However, for operations requiring sub-centimetre accuracy such as accurate spray overlap control, vehicle guidance or digital terrain modelling, other more accurate modes of operation may be necessary. One recent innovation in positioning technology that provides real-time sub-centimetre positioning accuracy in three dimensions (*i.e.* x, y, z) is called real-time kinematic (RTK) GPS.

2.4.2 DATA ACQUISITION

A prerequisite of PA is the collection of spatial soil, crop and environmental data at finer spatial resolutions than that needed by conventional agronomic management systems. The collection of data at appropriate resolutions using conventional methods of sampling and laboratory analyses is inefficient because these techniques are time consuming, tedious and expensive. Presently, with the exception of crop yield data that may be collected continuously and in real-time using yield monitors, the acquisition of data for PA remains for the most part, reliant on discrete sampling and laboratory analysis (Sudduth *et al.*, 1997). However demand for data at similar resolutions to that acquired using yield monitors is encouraging worldwide research to devise field-based 'on-the-go' proximal soil property sensing systems that will automate the sampling and analyses procedures and produce fine-resolution results in real-time. Methods of soil data acquisition for PA, both discrete and complete enumeration techniques, will be reviewed in section 2.5. This section will review yield monitors only.

Yield Monitoring

Yield monitors are proximal-sensing systems for crop yield that consists of a DGPS, a crop flow sensor, a ground speed sensor and data acquisition equipment. Hence yield monitoring refers to the calibrated, continuous proximal sensing of crop yield using sensors that measure the mass flow, or volume of harvested crop per unit area, at each location within a field. The rate of produce flow into the harvester can be related to yield since the velocity swath width and position of the harvester is known. The first yield monitoring systems were commercially developed for grain crops, hence for the most part this review will refer to combinable grain yield monitoring. However fibre, fruit and tuber monitoring systems have similar operating principles and will not be excluded.

Depending on the design and operating principles, yield sensors may measure crop yield either directly or indirectly. Direct sensors include sensors that measure the actual mass or volume of harvested crop, while indirect sensors measure some parameter that can be functionally related to crop yield but require calibration to convert the measured parameter to yield (Pierce *et al.*, 1997). Indirect yield sensors measure grain mass flow either by gauging the force by which grain hits an impact-plate sensor, or by measuring the mass flow of grain using the attenuation of electromagnetic signals between a source and a detector. All yield sensors regardless of type are mounted on the harvester and measure the flow of clean produce at some point in the harvesting process. Borgelt (1993) described both types of sensors for combinable grain crops. Table 2.4 lists currently available yield monitoring systems for various crops. The yield monitoring systems in Table 2.4 are used together with DGPS to produce crop yield maps that provide estimates of the within-field spatial variability in crop yield. The production of crop yield variability maps is essential for the adoption and implementation of PA, and yield mapping is the most obvious first step towards its adoption.

Seasonal interactions between soil, crop and weather are usually large, therefore yield maps can show considerable temporal differences in grain yield (*e.g.* Stafford *et al.*, 1996) and grain quality (*e.g.* Stafford, 1999). Only when recorded over a number of seasons will yield maps aid with agronomic decision-making. Hence their spatial and temporal interpretation should follow a careful and informed analytical process (Sylvester-Bradley *et al.*, 1999).

Table 2.4 Yield monitoring systems and methods of operation for a variety of crops

	Yield monitoring technique		
Crop	Method	Sensor location	Examples in the literature
Grains (combinable)	Volume / light	Clean grain elevator	Hummel *et al.* (1995)
	Mass / force plate	Clean grain elevator	Vansichen & De Baerdemaeker (1991)
Cotton	Volume / light	Cotton shute	Wilkerson *et al.* (1994)
Sugarcane	Mass / grab loader		Saraiva *et al.* (1999)
Grapes			www.harvestmaster.com
Potatoes	Load cell	Conveyor	Rawlings *et al.* (1995)
Tomatoes & horticultural	Load cell	Conveyor	Pelletier & Upadhyaya (1999)
Peanuts	Load cell	Conveyor	Boydell *et al.* (1996)
Straw / forage	Mass / force plate	Delivery shute	Missotten *et al.* (1996)

Some yield monitoring systems (*e.g.* those for combinable grains), are prone to dynamic inaccuracies that should be corrected to avoid misinterpretations when yield maps are analysed. These inaccuracies result from the delay or lag that occurs between the point of harvest and the position of the flow sensor where the yield is actually measured. Birrel *et al.* (1996) measured the lag on grain combines to range between 8 s and 15 s. The mixing or convoluting of grain during the harvesting process is also an important factor (Whelan & McBratney, 1997). Both of these types of inaccuracies in the monitoring process need to be considered, and sensed yields de-convoluted if yield maps are to help resolve the site-specific causes of yield variation. Birrel *et al.* (1996) and Whelan & McBratney (1997) illustrated different approaches to model combine flow dynamics. The reader is directed to these texts for more detailed information. Ideally, yield-monitoring systems should accommodate non-intrusive sensing techniques that estimate yield mass flow without interfering with the dynamics of grain flow (Pierce *et al.*, 1997). The cotton yield sensors are of this type (Table 2.4).

Sensing grain quality (determined by grain moisture, protein and oil content) can significantly augment the value of yield monitoring because both grain moisture and protein content are spatially variable, both affect its price, and both can provide valuable information for the interpretation of yield maps (Reyns *et al.*, 1999). While studying the relationships between site-specific grain quality and yield, Reyns *et al.* (1999) indicated that the variation in grain moisture ranged between 9 and 16 % over a 10 ha field, while the range in protein content over the same field was 10 and 15 %. Information on site-specific grain quality may aid with the development of marketing plans through the detection of low grain quality areas of a field. Quantification of these grain quality parameters will also help understand the processes involved in crop nitrogen assimilation, and may help guide future site-specific nitrogen agronomy.

The combinable grain sensors described in Table 2.4 measure wet grain flow. The moisture content of grain affects both its volume and mass, hence it must also be measured in conjunction with grain flow for accurate yield monitoring. The most common approach to grain moisture sensing uses capacitance sensors (Pierce *et al.*, 1997), however alternatives include near infrared (NIR) and microwave techniques. A grain protein and oil content sensor prototype[2.1] that may be used during harvesting is now in a final testing phase and is due for release in the not-too-distant future. The sensor uses NIR reflectance at various wavelengths to measure protein and oil content.

2.4.3 SPATIAL DATA ANALYSIS AND PREDICTION

The next phase of current PA management systems involve spatial analysis of the collected data and the production of crop and soil resource variability maps. Following from the previous section 2.4.2, the collection of soil and environmental data at suitable resolutions is not yet possible and spatial data analysis and prediction techniques are needed to produce high-resolution maps from discretely sampled information. Spatial prediction may also be necessary for the processing of high-resolution data, such as that collected using proximal crop and soil sensing systems, as these data may be unevenly distributed in space.

Many spatial prediction methods are available for use in PA, some with more merit than others depending on the data and the minimum area of interest (MAI) (Whelan *et al.*,

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[2.1] Developed by Casa IH Advanced Farming Systems

1996). An assumption shared by all methods is that the variable in question varies more or less continuously in space. Laslett *et al.* (1987) grouped spatial prediction methods under three main headings: global or local, interpolating or non-interpolating, and smooth or non-smooth, predictors.

The distinction between global and local predictors lies in the amount and closeness of the data used for prediction *i.e.* global techniques use all the data for prediction at an unsampled locations while local predictors use only neighbouring data points. Local techniques are often based on partitioning the area containing the data sites into smaller units or neighbourhoods and fitting a function to each unit. Local methods that use a single function throughout may be preferred on large data sets since global techniques may be computationally expensive.

Interpolators require the prediction to exactly reproduce (or honour) data values at sites where data is available. However if large measurement errors exist (*i.e.* replicate values that differ) then the constraint may be somewhat relaxed because only one of the two measured replicates (or the mean) can honour the data. Kriging is usually thought to be an interpolator, although if a nugget effect exists the kriged surface will be discontinuous at the data sites. Laslett *et al.* (1987) indicated that definitions of interpolators should exclude such cases, otherwise the terms discontinuous or continuous appended to their description.

Smoothers are spatial predictors whose predicted surface and the first partial derivatives thereof are continuous. A non-smooth predictor is one for which the discontinuities of the predictor or its first partial derivatives are readily detected by the eye. Discontinuities of the second and higher derivatives are not usually apparent. Laslett *et al.* (1987) suggested that despite these definitions, the concept of smoothness of a spatial predictor is somewhat subjective.

Laslett *et al.* (1987) showed some of the prediction techniques that fall under the given groups and may be used to predict soil variables at unsampled locations. For example, global means and medians, local moving averages, inverse distance interpolation, Akima's interpolation, natural neighbour interpolation, trend surfaces, Laplacian smoothing splines, and various forms of kriging. Their study indicated that for soil data, all methods displayed some deficiencies, however they concluded that interpolators were generally very poor predictors, while of the non-interpolators, Laplacian smoothing splines and kriging performed best. In a subsequent study, Laslett & McBratney (1990) compared interpolators, Laplacian smoothing splines, intrinsic random functions, and universal kriging fitted by restricted maximum likelihood (REML). The authors indicated that the kriging technique fitted with the REML was consistently the best method.

Choosing an appropriate spatial prediction method will depend on both the sample size and the sampling intensity. Whelan *et al.* (1996) suggested that for PA the MAI (which may be an area ranging from approximately 10 m to 20 m for most cropping systems) must first be determined. The authors suggested that sampling intensity may be expressed by the number of observations per MAI, and sparse, moderate and intense categories defined as 0.0001 – 0.01, 0.01 – 1 and > 1 observations per MAI, respectively. Whelan *et al.* (1996) provided some provisional recommendations for spatial prediction methods that may be used in PA, with relation to sample size and intensity. These are given in Table 2.5.

Table 2.5 Provisional recommendations for spatial prediction methods to be used for precision agriculture with relation to sample size and intensity. Adapted from Whelan *et al.* (1996)

	Sampling intensity (no. of observations per minimum area of interest)		
	Sparse	Moderate	Intense
Sample size	0.0001 – 0.01	0.01 – 1	> 1
<10	NA	NA	NA
10–100	NA	?ID	?ID/NR
101-500	NA	GS	GS/NR
>501	NA/GS	LGS	LGS/NR

NA not applicable - don't do it
?ID inverse distance or some informal prediction method but there may be problems with the accuracy of the estimates
GS a geostatistical method such as ordinary kriging or universal kriging with a global variogram or Laplacian smoothing splines
LGS a local neighbourhood method kriging or Laplacian smoothing splines
NR spatial prediction will only be necessity if the sampling is uneven.

From Table 2.5, considering a moderate sampling intensity (0.01 – 1 samples per MAI), spatial prediction will not be useful where less than 10 samples are available. When 10 to 100 samples are available informal prediction methods like inverse distance (ID) interpolation may be used. Several authors (*e.g.* Laslett *et al.* (1987); Weisz *et al.* (1995); Gotway *et al.* (1996); Brus *et al.* (1996)) compared inverse-distance to kriging predictions and found the former to perform well for moderate sample sizes of no more than 100 observations. However these studies suggested kriging to be the 'safe' choice and criticised the inverse-distance methodology for its lack of provision of an error value for the estimate. Furthermore, Gotway *et al.* (1996) indicated that the inverse-distance methodology should not be applied blindly, as there is not one distance power that is optimal for all data. The authors recommended that for data sets with a high CV, the use of the distance power 1 will give most accurate results, but for data with relatively small CVs higher powers of distance may be more suitable.

When 100 to 500 samples are available geostatistical techniques (GS) such as kriging using neighbouring points and a global variogram will be suitable. For PA block kriging will be more suitable than point kriging since averaged prediction values over the block can be used to represent a management unit over which resources may be applied. In this sample size range, auxiliary information (*e.g.* proximally sensed soil data, or terrain attributes derived from digital elevation models (DEM), etc.) may be used to improve prediction through the use of geostatistical techniques such as co-kriging and regression kriging (Odeh *et al.*, 1995). For sample sizes greater than 500, such as data gathered using proximal crop and soil sensing systems, kriging with local variograms for each moving neighbourhood should be used. The local kriging procedure is described by Haas (1990).

Wollenhaupt *et al.* (1997) provided a review of prediction techniques for PA, including non-geostatistical methods such as moving averages, inverse distance, smoothing splines and trend surface analysis, and geostatistical methods such as point and block kriging. The authors indicated that the choice of spatial prediction method should depend on the data type, its statistics and configuration. Wollenhaupt *et al.* (1997) also suggested that both the sampling strategy and the prediction method should be considered.

Therefore, spatial prediction methods are used in PA to extend the information available from data sampled (or sensed) at sparse or unevenly distributed locations by estimating the values of variables at unsampled sites or areas, at an appropriate resolution. The chosen method should accurately represent the spatial variability of discretely sampled crop, soil and environmental variables while minimising the loss of useful information. In a real-time management system where ‘on-the-go’ soil sensing systems are used to gather high-resolution data, spatial data processing would be integrated into the DSS structure (Conceptual Basis of the Research and Aims). Here, other techniques that can characterise one-dimensional variability ‘on-the-go’ may be more applicable. For example, a Kalman Filtering algorithm (*e.g.* Brown & Hwang, 1992) may be integrated in the DSS of the real-time system to characterise the variability of transects traversed by the vehicle that also contains the sensing system and variable-rate applicator. In such instances a post-processed map of the variability would not be required.

2.4.4 DATA MANAGEMENT AND DECISION SUPPORT

Once soil, crop and environmental information has been collected and sparse or unevenly distributed data spatially processed to the required resolution, it needs to be stored, statistically analysed and interpreted before agronomic management decisions may be formulated. A spatial data management system such as a GIS used in conjunction with a spatial decision support system (SDSS) can be employed to meet these requirements. While a GIS may be used for storage, geographic manipulation (which may include spatial prediction), and display of the information, the SDSS may supply decision-makers with modelling capabilities, and choice for risk minimisation and tactical decision-making.

Geographic Information Systems for Precision Agriculture

Essentially a GIS is a database that can store, collate, manipulate and display geographical data of various origins (Burrough, 1986). It consists of three primary components: computer hardware, software, and an organisational context that includes skilled operators (Burrough, 1986). One of the main implementations of GIS in soil studies has been for agriculture, *e.g.* to identify suitable soils for agriculture (Burrough, 1986), to assist with rural planning and management (Fernandez *et al.* 1993), and more recently for PA (Casperan, 1995; Yule *et al.*, 1996; Swindell, 1997). The reader is referred to Burrough & McDonnell (1998) for a detailed description of GIS and its uses in land resource assessment.

Corner (1997) suggested that a GIS for PA should be customised specifically for PA applications, and that it should be capable of spatial prediction, modelling and databasing. For example, a farm GIS for PA may contain various geo-referenced layers for each field, *e.g.* proximal and remote sensing data, crop yield data and weather information for each season, as well as the farm's topography. The GIS may then be used to store, analyse, overlay and display the information. Bregt (1997) highlighted the need for the development of farm GIS for PA to also provide a platform for simple modelling, and in combination with a GPS to control the navigation of farm vehicles for the application of agricultural inputs.

Schröder *et al.* (1997) described LORIS (Local Resource Information System), a GIS specifically designed for PA. LORIS consists of several modules that enable the input of data from various sources, generation of raster files, databasing of rastered information, generation of maps and overlays, calculation of application maps by means of algorithms stored in a library and export of operation maps to memory cards. It is based on standard software (*i.e.* Excel®, Surfer®) implemented under a Windows® environment, and supports links to other programs developed in Access®. Schröder *et al.* (1997) suggested that LORIS has been used to derive fertiliser application maps and to perform variable-rate fertiliser spreading on 14 000 ha of farmland in Germany. The authors concluded that LORIS was proven to be particularly useful for PA applications

Spatial Decision Support Systems for Precision Agriculture

A SDSS for PA will help model the spatial data required for site-specific decision-making and may be used to formulate tactical management decisions that satisfy a predefined objective (*e.g.* maximum yield and quality, minimum cost, etc). Decision support systems (DSSs) in agriculture have been used to assist with agronomic and economic decision-making. However few DSSs have been employed in conventional management systems due to the limited amount of information required to derive single-rate (or uniform) management decisions. The use of DSSs in PA (*i.e.* SDSSs) is more relevant as PA uses greater amounts of information to manage within-field variability.

To determine the within-field multivariate causal relationships of yield variation in the system and devise spatially variable management decisions, the SDSS needs to integrate data from various sources and be based on the spatial and temporal interactions between soil, crop and environmental parameters. Subsequently this information can be used to determine whether the degree of observed variability warrants uniform, zone or continuous management, and the production and economic risks of each management plan. This SDSS phase of the PA management system is perhaps the most complex and diverse. These factors may be contributing to the slow development of SDSSs for PA.

Figure 2.4 illustrates a conceptual DSS based on that suggested by Petersen *et al.* (1993).

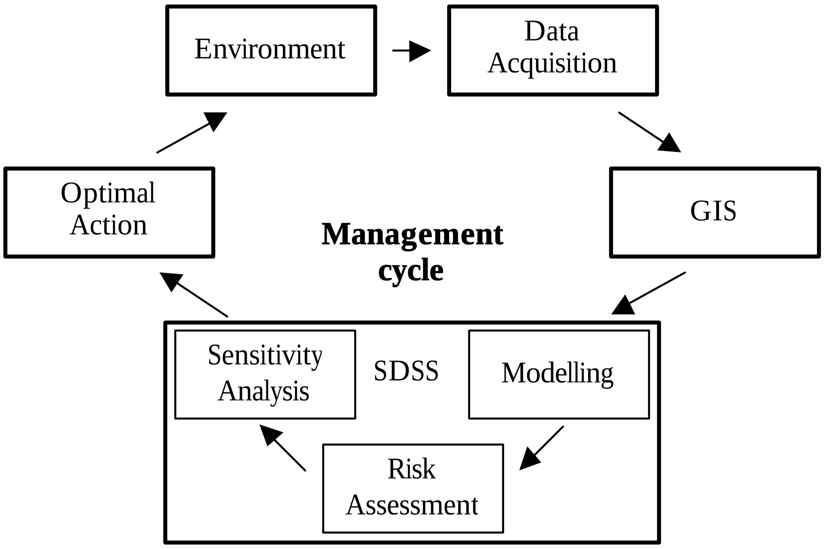

Figure 2.4 Conceptual diagram of a management cycle and decision support system (DSS). Modified from Petersen *et al.* (1993).

The diagram in Figure 2.4 is similar to the PA management system depicted in Figure 1 of the Conceptual Basis of the Research and Aims. The management cycle shown in Figure 2.4 illustrates the flow of geo-referenced information from the environment via data acquisition equipment (*e.g.* proximal sensors) to a GIS where the data may be stored, analysed, manipulated and mapped. The environmental data (soil, crop, weather, etc.) are then transmitted to the SDSS of the cycle where they may be modelled to predict the future likelihood of events from the information gathered, and ultimately derive management decisions. The ability of DSSs to estimate the consequence of decisions is of significant value in helping users compare the outcomes of different decisions (Audsley *et al.*, 1997). Risk assessment and sensitivity analyses may then be used to identify the differences and variations in the likely outcomes (*i.e.* their uncertainty), thus providing the user with a rational method for deciding on how management may be site-specifically applied over a field.

Risk assessment is based on repetition. In agriculture risk may be difficult to assess due to the expense and time required to conduct field experimentation. Gomez-Hernandez, 1996) indicated that this problem may be solved using RF models and geostatistical simulations. Some examples exist, *e.g.* Pachepsky & Acock (1997), Faechner *et al.* (2000). The latter study showed how the economic benefits of deep ripping (*i.e.* the expected increase in crop yield) can be assessed in the presence of sparse sampling. They used an economic model combined with geostatistical simulations to quantify the risk and the expected benefits of remediation.

The optimal management decision then results in an action to be executed within the environment, which is then monitored in a new cycle of information flow. Obviously, the quality of the decision will depend on the quality and suitability of the information used and the ability to analyse, interpret and conclude.

Soil and Crop Modelling

Our lack of understanding the reasons for yield variation makes up the principal 'information hole' in PA (Acock & Pachepsky, 1997). Only when we understand the reasons for that variability and consider all the limiting factors to crop growth will it be possible to derive decision and optimally manage yield variability. The only practical way to consider these factors is to model crop growth and attempt to simulate the principal mechanisms occurring in the soil-crop-environment system.

Bouma (1997) suggested the use of modelling techniques using calibrated and validated models to estimate crop growth, soil water regimes and solute fluxes. The author indicated that weather generators could be used to predict future weather conditions in the growing season and corresponding crop growth and nutrient leaching rates. Booltink *et al.* (1996) showed how simulation models combined with weather generators, fitted to long-term weather data could be used as a predictive tool to support farm management decisions. Therefore, predictive modelling (in both space and time) may be used to diagnose potential problems in the production system (*e.g.* nutritional, water storage, etc.), that may lead to reductions in crop growth and yield.

McBratney (1998) classed various types of quantitative models for resource assessment as empirical or mechanistic, and deterministic or stochastic. McBratney (1998) suggested that these types of models correspond to the Hoosbeek & Bryant (1992) hierarchical i-level framework, in terms of the scale and type of information required for modelling and management at the PA level. Adding to these, Bregt (1997) described static or dynamic models and qualitative or quantitative models. The author indicated that models constructed for real-world processes often contain combinations of some or all of the model types described above. Cook & Bramley (1998) provided a more arbitrary categorisation of some general types of models that may be used to predict crop yield response. The authors described intuitive, mechanistic, simulation and statistical models as well as expert systems and artificial intelligence. Cook & Bramley (1998) indicated that no one method would be suitable for all situations, however the authors suggested that with increasing availability and use of spatial and temporal data the more quantitative methods should perform better.

Early attempts to model crop growth involved empirical analyses of relationships (using regression and correlation methods) between crop yield and observational environmental data such as precipitation, temperature, cultural influences and soil treatments (Barnett *et al.*, 1997). However, empirical models are often criticised because of their empiricism, *i.e.* they are only useful within the range of data and environmental conditions from which they were developed. Once conditions change and the causal parameters of yield variation are not included in the model, empirical models will not perform well. Empirical models are also criticised on the grounds that they make no attempt to explain and represent the mechanisms of crop growth and yield variation (Acock & Pachepsky, 1997).

Some examples of empirical modelling include the work by Sudduth *et al.* (1996) who analysed the spatial relationships between crop yield and soil and site properties for fields and regions within fields using stepwise multiple linear regression, projection pursuit regression and neural networks. Using similar techniques Sudduth *et al.* (1997) looked at the relationship between crop yield and soil and topographic parameters. Shatar & McBratney (1999) expanded on the work of Sudduth *et al.* (1996) and examined the relationships between sorghum yield and various soil properties also using generalised additive models. Although these studies identified some specific factors that limited site-specific crop production, the challenge of identifying the causal factors of yield variation for site-specific management was made difficult by the fact that many other interrelated parameters and weather, pests and pathogens have major influences on production. Furthermore, such empirical models are less useful for understanding yield variability because they have no understanding of crop behaviour built into them (Acock & Pachepsky, 1997).

Barnett *et al.* (1997) attempted to overcome this problem by using a parsimonious hybrid modelling technique that incorporated agronomic and climatological data interpreted in terms of physiological knowledge of key influences on wheat development, *e.g.* rainfall from early reproductive stages to grain-filling. The authors reported reasonable yield predictions and suggested that these hybrids might be useful in refining wheat simulation models to improve their predictive capabilities.

The need for general models of crop behaviour, based on scientific understanding and physiological knowledge, stimulated the development of mechanistic crop models (Barnett *et al.*, 1997). Unlike empirical models, mechanistic crop models attempt to represent processes in the soil-crop-environment system, and at a plant and organ level (*e.g.* photosynthesis, transpiration, etc.) (Acock & Acock, 1991). Acock & Pachepsky (1997) indicated that the primary advantage of mechanistic crop models is that they can incorporate our collective knowledge of soil, crop and atmospheric processes. However, the authors also warned that the main weaknesses of mechanistic crop models result from the difficulties in representing our knowledge about plants in a computer, and perhaps more importantly, our still limited knowledge of plant behaviour. Over-parametrisation can be another problem of mechanistic crop models. Acock & Pachepsky (1997) warned that in using mechanistic models for PA, one must scientifically choose and adjust model parameters because a mechanistic model with a large number of parameters fitted to the data, quickly becomes an empirical model. Barnett *et al.* (1997) discussed and attempted to overcome this problem by developing the hybrid (empirical-mechanistic) model for determining wheat yields.

Mechanistic crop models have been used to derive fertiliser recommendations for conventional agronomic management (Cook & Bramley, 1998). Inevitably, attempts to site-specifically manage fertiliser applications have essentially been spatial variants of such models. A limitation of these variants is the lack of more information on the spatial distribution of soil and other environmental properties used to drive the models (Rawlings, 1996). These spatial data are needed not only to drive, but more importantly, validate the models.

The development of proximal soil sensing systems is imperative for the acquisition of greater amounts of spatial information. The ultimate aim is to develop a real-time PA system for continuous management (Conceptual Basis of the Research and Aims), where measurements, and yield predictions in the SDSS are made in real-time, followed by the implementation of informed management decisions.

2.4.5 IMPLEMENTATION OF MANAGEMENT

Precision agriculture in the form of site-specific soil and crop management requires farm equipment that can spatially vary resource application rates ‘on-the-go’, as the equipment moves through the field. The technology for the implementation of site-specific seeding, fertiliser application, liming, irrigation and pesticide applications is referred to as

Variable-Rate Technology (VRT), and was the first enabling technology of PA (National Research Council, 1997) .

Different VRT systems operate in either of two ways depending on the inputs to be applied and the source of information used to specify the spatially variable application rates. A review of application equipment and technology for site-specific management was given by Anderson & Humburg (1997). Briefly, commercial VRT systems may be either map-based or sensor-based. Map-based systems need a geo-referenced plan of the application rates for each management unit within a field, and a GPS to find and navigate these locations. Sensor-based systems do not need geo-referenced maps as applications are determined in real-time from information acquired using ‘on-the-go’ soil and crop sensing systems.

Presently, sensor-based systems are not as widely used as map-based VRT systems due to the unavailability of real-time, ‘on-the-go’ soil property sensing systems. Only a few of these sensing systems are commercially available (refer to section 2.6.2 and Table 2.11) and more testing for their use in a continuous management system is still required. The development of ‘on-the-go’ proximal sensing systems for the collection of information on the variability of agriculturally important soil properties is thus important. As previously mentioned, the aim of PA, a real-time, continuous management system for agriculture, is to collect site-specific spatial information, formulate a management decision and use VRT to act upon the decision, in a single pass over the field. Needless to say sensor-based systems are more efficient than map-based VRT. Chapter VI describes one a real-time continuous management system for acid soil.

2.5 DATA ACQUISITION FOR PRECISION AGRICULTURE

If our state of knowledge were perfect then perhaps all soil variation would be recognised as systematic (Wilding & Drees, 1983). Important to this statement is consideration of the methods of data acquisition and the sampling schemes used, because if the sampling resolution is too coarse then all variation may appear as random. In this latter case classical statistical analysis may be a feasible option for the characterisation of field soil variability. To accurately characterise soil spatial variability, we need to develop data acquisition methods that are more efficient than conventional, discreet sampling strategies. Bouma (1997) suggested that ‘…a major challenge for science is to present methods that can characterise variability in space and time in such a manner that farmers can use the information to improve their management’.

Presently, an important requirement for the implementation of PA is the derivation of a suitable sampling strategy, which combined with suitable spatial prediction methods may be used to obtain representations of the spatial variability of soil parameters. However sampling intensity is dictated by convenience and trade-off between resolution and cost. The development of more efficient methods of soil data acquisition (*e.g.* proximal soil sensing systems) is essential for the progression of PA into a fully operational, widely implemented management system. Proximal crop yield sensors have been developed and are widely used by farmers attempting to implement PA. What they are discovering is that although yield maps provide some idea on the patterns of yield variation, there is a great lack of spatial soil information and a ‘gap’ in the understanding of the causal factors of yield variation. Proximal soil sensing technologies that are able to collect spatial information at similar resolutions to proximal yield sensors need to be developed to close this information gap and fully implement PA to improve agronomic management.

The importance of sampling resolution and the differences between design-based and model-based strategies with respect to PA will be discussed in Chapter IV. What follows is a brief review of commonly used discrete sampling schemes.

2.5.1 DISCRETE SAMPLING

Conventionally, the characterisation of field soil for agronomic management has been based on sampling procedures that collect soil at discrete locations within a field. The most commonly used sampling techniques use either a random or systematic based approach. Currently sampling on a grid is thought to the best strategy for the production of accurate maps for site-specific management, however trade-off between sampling resolution, accuracy and cost has resulted in the development of sampling techniques designed specifically for PA. These aim to reduce the cost and effort of sampling while maintaining the accuracy necessary for map production. Still, there is a fundamental need for the development of more intensive methods of data acquisition.

A brief description of common sampling techniques is provided below. Automated discrete sampling devices will be discussed in a latter section of the chapter.

Simple Random Sampling

Simple random sampling requires samples to be collected in such a way that individual samples from the population have an equiprobable chance of being selected. Random number tables or computer aided random number generation may be used to determine sampling locations. Webster & Oliver (1990) indicate that uneven coverage and apparent clustering of sampling points makes this sampling technique inefficient and unsuitable for describing the spatial variability of soil, and hence PA.

Stratified Random Sampling

This method requires the total area of interest to be stratified before sampling points are chosen at random within each stratum. The strata should be chosen so that each cell differs with relation to the variable under study, otherwise there may not be much gain from stratification. Although this approached is deemed more efficient than simple random sampling, cover may be uneven and clustering of points may still occur. Webster & Oliver (1990) suggest that modest rather than dramatic gains in precision should be expected from stratification. A form of stratified sampling used in PA, termed ‘zone’, ‘patch’ or ‘direct’ sampling will be subsequently described under a separate heading.

Systematic Sampling

This sampling approach provides even coverage and potentially greater efficiency than the described random sampling methods (Webster & Oliver, 1990). In this method the points are located at regular intervals, hence the sampling is simple to implement. Webster & Oliver (1990) warn that if periodicities are present in the sampling population, and if these coincide with the period of the grid then substantial bias may be introduced to the sampled data. Webster & Oliver (1990) suggest that another disadvantage of systematic sampling is that on its own, the technique gives no entirely valid estimate of the sampling error since the sampling points are not randomised within the strata. Other systematic sampling patterns may include rectangular, triangular, or hexagonal configurations. Yfantis *et al.* (1987) examined the effects of various sampling configurations on the efficiency of kriging estimations.

At this point in time, grid sampling (with an appropriate sampling lag, determined by the semi-variogram) of agricultural fields combined with geostatistics, is thought to be the most accurate method for representing the status of field soil properties. However the costs incurred by intensive sampling and subsequent laboratory analysis are prohibitive for the majority of farmers, resulting in grid resolutions of 100 m or larger. Thus for properties that exhibiting ranges of spatial dependence smaller than 100 m, sampling at such a resolution may be less than optimal for spatial analysis (*e.g.* Birrel *et al.* (1996)). Subsequent sections in this chapter describe sampling strategies that have been developed for PA. These aim to maintain data accuracy and reduce the sampling cost and effort.

Stratified Systematic Unaligned Sampling

This method combines the advantages systematic sampling with randomisation. The approach involves stratifying the sampling area into coarse cells and superimposing a fine grid on each cell as a reference system. Commencing on a corner cell, a *x*-coordinate and a *y*-coordinate are randomly chosen within the reference grid. Moving onto the next cell the *x*-coordinate is retained but a new random value for the *y*-coordinate is chosen. The procedure is repeated as such for the remaining cells on that row. Then proceed with the columns starting from the same initial corner cell. Randomly select a new *x*-coordinate but hold the *y*-coordinate constant, repeating these steps for the remaining cells on that column. Sampling points are placed in the remaining cells so that the *x*-coordinate distances are the same along each row and the y-coordinate distances are the same along each column. In this way bias introduced by periodicities and trends may be avoided. Wollenhaupt *et al.* (1997) suggested that with the growing awareness of periodicities in soil test variables, this type of sampling may be desirable for site-specific management. As with systematic sampling, there is the inevitable tradeoff between appropriate grid resolution for accuracy and sampling cost.

Zone (Direct) Sampling

An alternative sampling scheme aimed to reduce the number of sampling sites and hence labour and costs has been proposed in the USA and Europe, the technique is termed zone or direct sampling. It is based on dividing fields into smaller units (or strata) based on fine spatial scale data such as yield, (acquired using yield monitors), proximal soil sensors (e.g. VERIS 3100), remote sensing and/or digital elevation models. Sampling is then performed within each zones depending on the variability present. Francis & Schepers (1997) suggested that selecting sampling areas on the basic concepts of soil colour, texture, slope, and past testing programs may be a good starting point. Franzen *et al.* (1998) used topography as the basis for stratification. Griffin (1999) used yield maps as a means of customising soil sampling regimes to increase nutrient map accuracy while minimising costs. Lark *et al.* (1999) used a similar approach, stratifying fields into regions using yield maps prior to sampling.

Purposive Sampling Schemes

A purposive sampling scheme termed the variance quad-tree (VQT) was proposed by McBratney *et al.* (1999). The approach is designed to sample sparsely in areas where variation is low and more intensively where variation is large. The VQT algorithm provides a means of partitioning the variance in continuous variables so that the resulting strata contain data of equal variability. The aim of the procedure is to maximise efficiency of the sampling scheme and minimise cost while ensuring that the variability within the sampling area is characterised effectively. McBratney *et al.* (1999) indicated that when data is available at the required resolution, the VQT sampling algorithm will provide a more efficient sampling method for covariates, than a regular grid. The technique is suitable for sampling schemes based on elevation data, remotely sensed imagery and proximally sensed attributes.

2.5.2 AUTOMATED MECHANISMS FOR DISCRETE SOIL SAMPLING AND ANALYSIS

McGrath & Skotnikov (1997) described the development and use of a discreet automated soil sampler used to collect, pack, position (using a GPS) and label soil samples. There is a plethora of similar soil sampling devices now commercially available, which aim to reduce the time and effort of soil sampling. A step up from these are sampling and analysis systems that transfer sample preparation and soil chemical analysis from the laboratory to the field or sample location. A sampling and analysis system for soil nitrate developed by Wild *et al.* (1997) is shown in Figure 2.5.

Figure 2.5 Field-based automated soil sampler and nitrate analysis system of Wild *et al.* (1997)

Lütticken (1999) described an automatic sampling system with a hydraulic auger that samples soil at predetermined, constant depths with an accuracy of one centimetre. The sampling depths range from 10 cm to 25 cm and samples may be collected in 4.5 seconds, from the time the auger is positioned on the soil surface, until it is retrieved. Before sampling, the farm and field data can be transmitted from the office to the computer of the sapling device via a digital telephone. Field boundaries and the size of the field may be determined using an on-board GPS, and a systematic grid with the desired cell size calculated before sampling. Lütticken (1999) indicated that soil sensors may be attached to the sampling vehicle for the simultaneous collection of more soil data.

These types of field-based sampling, and analysis system are significant steps towards the development of continual or continuous soil sensing systems, as they minimises handling, transport and labour costs. However they are still slow and inadequate for continuous management.

2.6 COMPLETE ENUMERATION

Techniques that attempt a complete enumeration of field soil variables are based on remote and proximal sensing (Viscarra Rossel & McBratney, 1998). Both remote and proximal sensing systems have the potential to supply useful soil information that may be used to formulate management decisions in a PA management system. Possibilities for the development and use of remote and proximal sensors exist in bands throughout the electromagnetic spectrum (Figure 2.6)

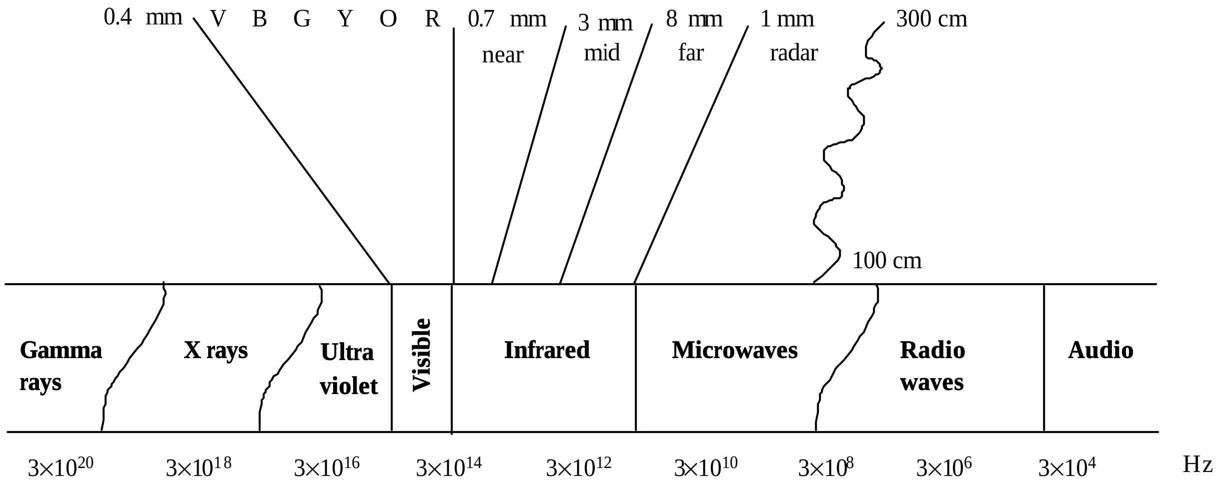

Figure 2.6 The electromagnetic spectrum. Adapted from Viscarra Rossel & McBratney (1998).

For example, in the high frequency end of the spectrum there is potential for the use of remote sensing radiometric methods (Billings, 1994) to map soil potassium. In the low frequency end of the spectrum, acoustic techniques may prove useful to proximally sense soil physical properties such as surface air porosity, air permeability and pore structure (Sabatier *et al.*, 1990). Possibilities for the development of soil sensing systems also exist in between these frequency ranges, in the visible, infrared, microwave and radio-wave portions of the electromagnetic spectrum. Worldwide research towards the development of such sensors and other electrochemical and mechanical sensors is currently ongoing.

2.6.1 REMOTE SENSING

A remote sensor is a device that collects data from a distance varying from a few metres to hundreds of kilometres (Mulders, 1987). Remote sensing or teledetection, in this context refer to techniques used for measuring the intensity of energy that is reflected from the Earth's surface. As such remote sensing may be used to collect information on the spatial and temporal variation of soil (*e.g.* Stoner & Baumgardner, 1981) and crop attributes (*e.g.* Taylor *et al.*, 1997). The sensed data may be kept in storable form as *e.g.*, photographs, in digital formats, etc., enabling simultaneously analysis of not only spatial but also temporal patterns.

Remote sensing techniques rely on the premise that different landscapes have characteristic reflectance spectra in various portions of the electromagnetic spectrum, *e.g.* Figure 2.7 shows characteristic spectra for soil, vegetation and water in the visible and short wave infrared (near infrared) portions of the spectrum.

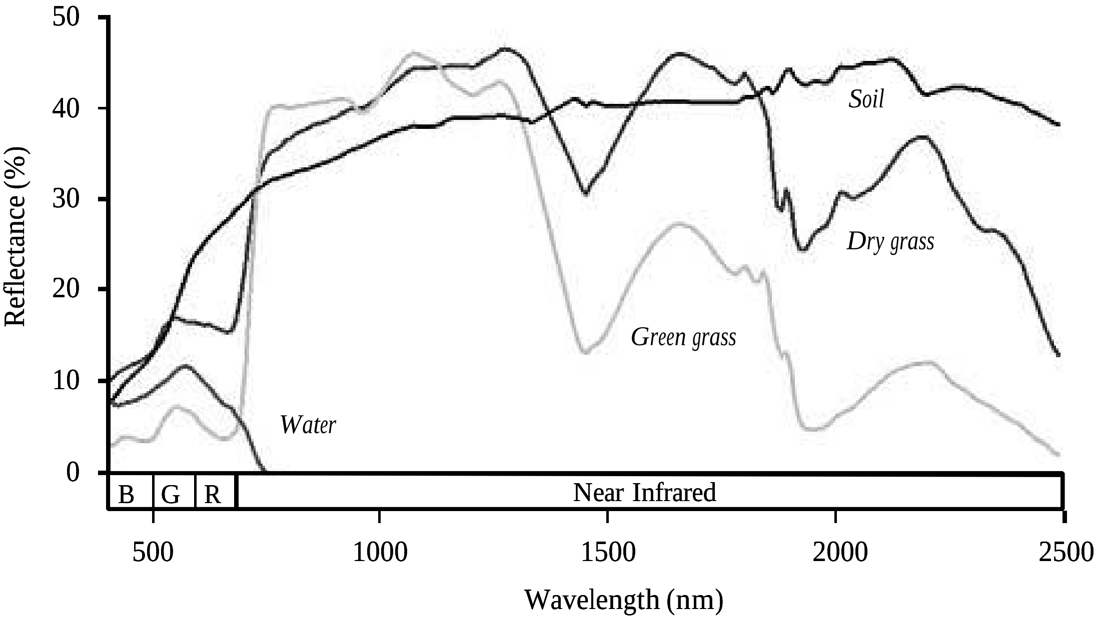

Figure 2.7 Reflectance spectra for soil, vegetation and water (adapted from Geoimage Pty Ltd)

Measurements in the visible part of the spectrum can be related to land-cover, while the infrared portion provides information on vegetation parameters such as the leaf-area-index (LAI). Soil measurements are usually based on bare soil surface condition rather than its association with crop type. A shortcoming of remotely sensed data for soil studies is that information may only be collected for the top few millimetres, which for most soil properties, is not representative of the soil profile. Nevertheless, remotely sensed images have been used to assess soil textural variability (*e.g.* Stoner & Baumgardner, 1981) and organic matter (OM) contents (*e.g.* Bhatti *et al.*, 1991). Furthermore remotely sensed reflectance data could be used in conjunction with meteorological, soils and other crop data to model crop growth, crop condition and yield (Moran *et al.*, 1997). Table 2.6 provides a summary of various forms of remote sensing and their use.

Table 2.6 Examples of remote sensing techniques and their use. Adapted from Corner (1997).

Technique	Platform	Example of its use
Visible and NIR	Aircraft, Satellite	OM, texture, soil water, LAI, biomass, crop stresses, crop damage
Thermal infrared	Aircraft, Satellite	Soil water, canopy temperature, crop moisture stress
Radar	Aircraft, Satellite	Soil water, surface roughness, LAI, biomass
Gamma ray emissions	Aircraft	Clay content, mineralogy

Although remote sensing is a potentially useful tool for agricultural management (Table 2.6), so far its use in PA has been limited because of problems associated with resolution. Resolution has four components, namely radiometric, spectral, spatial and temporal resolution (Corner, 1997). Radiometric resolution refers to the sensitivity of the sensing instrument and determines the subtlety of variation that it can detect. Spectral resolution describes the detail of the electromagnetic signal and determines the system’s ability to discriminate between objects with different spectra. It relates to the extent of the spectrum being sampled, the number of bands within that area and the width of those bands (Corner, 1997).

Spatial resolution refers to pixel size sensed in any one pass as well as to the size of features that can be discerned. The resolution of images captured from aircraft platforms is generally a function of the altitude from which they are taken. The unavailability of fine spatial resolution data is the most significant limiting factor for the use of remote sensing in PA. However, new companies that provide aircraft-based imagery at the resolution required for site-specific management are beginning to emerge. A number of companies also intend to make available fine-resolution satellite imagery. Temporal resolution refers to the timeliness with which data is available to the user. With satellite imagery temporal resolution is determined by the repeat cycle of subsequent passes of that satellite, however with aerial platform imagery data may be captured opportunistically.

For PA, remote sensing offers techniques that may be used to obtain complete representations of crop reaction to soil and environmental conditions, presenting managers with a potentially useful, cost-effective tool for site-specific decision-making. However much research in needed before the overall benefits of remote sensing are realised. The reader is referred to Moran *et al.* (1997) for a thorough review on the opportunities and limitations of remote sensing for PA. In this instance the uses of remote sensing in PA will be reviewed and categorised according to the platform from which the data is acquired (refer to Table 2.6).

Aircraft Imagery

Robert *et al.* (1991) used a crop free colour infrared aerial photograph at a scale of 1:6 000 together with a detailed county geo-referenced soil survey for variable application of anhydrous ammonia in a field of approximately 10.5 hectares. The author indicated that when relationships between photo tones and soil conditions are known, low altitude aerial photography could be used to refine delineations of soil survey maps for site-specific management.

Colour infrared, also called false colour infrared because the film does not show the same colours as are in nature, has also been used for the identification of management zones within which soil sampling may be directed (*e.g.* Frazier *et al.*, 1997). In an experiment conducted to contrast crop yield differences in uniformly managed versus specifically managed soil, Carr *et al.*, (1991) used colour infrared aerial photographs (and satellite images) to modify soil unit boundaries first delineated using a conventional soil survey.

Taylor *et al.* (1997) used high resolution Airborne Digital Photography (ADP) successfully, to map the within-field spatial distribution of crop parameters and yield potential for winter barley. Wood *et al.* (1998) extended the work by Taylor *et al.* (1997) by exploring possibilities of reducing field sampling to a practical level. They described the practicality of a methodology for field calibration of remotely sensed data as a source of information for the site-specific management of wheat and barley. The calibration was based on regressed values between field sampling and the Normalised Difference Vegetation Index (NDVI) derived from ADP. Tucker (1979) defined the index as:

$$NDVI = \frac{NIR - red}{NIR + red}$$

The NDVI ratio is related to plant photosynthetic activity and hence biomass production. The time integral of NDVI should represent total biomass, hence it may be related to potential yield (Plant & Munk, 1998).

Pettygrove *et al.* (1998) attempted to relate tomato yield with the vegetation index derived from colour infrared aerial photographs. Their results indicated that preceding harvest, NDVI was related to fruit yield and vine dry-weight. Wiegand *et al.* (1994) reported good correlations between NDVI and cotton yield. Plant *et al.* (1998) reported strong relationships between cotton yield and NDVI derived from colour infrared photographs. The authors suggested that remote sensing could detect differences in crop development due to soil textural differences within fields. Furthermore, they indicated that such information might be used to assist with irrigation management.

Multispectral imagery may also be used to study resource variability. Multispectral sensing may be useful for determining different terrain features (particularly in regions with large areas of bare soil) and to produce significantly different images for objects with slight spectral differences (Mulders, 1987). Soil has been shown to have spectral response in the visible and infrared (*e.g.* Dalal & Henry, 1996; Viscarra Rossel & McBratney, 1998). Yates *et al.* (1988) suggested that reflectance in the thermal infrared range provide an integrating indicator of underlying spatial variability in the status of available soil moisture for plant uptake. Therefore multispectral images of soil show potential for classification and detection of management zones.

Yates *et al.* (1988) suggested that reflectance in the thermal infrared range provide an integrating indicator of underlying spatial variability in the status of available soil moisture for plant uptake. Therefore multispectral images of soil show potential for classification and detection of management zones.

Soil properties have been shown to have spectral responses in the visible and infrared. Schuler *et al.* (1998) collected multispectral data (400-500 nm, 500-600 nm, 600-700 nm and 700-4500 nm) and evaluated it as a tool for the assessment of crop and soil variability as well as crop pest problems. They reported that visible patterns of the multispectral data were very similar to patterns of weed, disease and pest infestations evident in yield maps. Rew *et al.* (1999) obtained multispectral images (at 440 nm, 550 nm, 650 nm, and 770 nm) for detecting wild oats (*Avena* spp.) in a seedling triticale (X *Triticosecale*, Wittmack) crop. Rew *et al.* (1999) indicated that the technique has potential for weed detection and that it could also be used as part of a stratified sampling system.

Blackmer *et al.* (1996) identified wavelengths (radiation near 550 nm and 710 nm) for detecting N deficiency, as well as N stress in corn. The authors suggested that the data provided information for the development of a variable-rate application strategy. Bausch *et al.* (1997) assessed the N status of corn using a reflectance index that measured the ratio of NIR to green reflectance of a crop, compared to the expected ratio from a crop with no deficiency. The authors concluded that that the index provides a rapid index of N sufficiency.

Yang & Anderson (1996) determined management zones for sorghum using colour infrared aerial videography. Their results indicated that plant height, biomass and yield were significantly correlated with the red band, green band, and NDVI. Their results suggested the need to manage individual zones within a field differently.

Airborne gamma radiometry for mapping soil is based on the decay of unstable radioactive isotopes that occur naturally on the earth's crust. Decay may involve gamma ray emission, which can be recorded by a radiometric sensor. The aircraft mounted sensors have sodium iodide crystals which record emissions in four energy windows centred about the ^{40}K, ^{238}U and ^{232}Th isotopic emissions and one over the whole energy range (Billings, 1994). Mapping soil using radiometric techniques is based on sensing the relative differences in isotope concentrations between mapping areas, and not on the absolute concentrations of isotopes in the soil. Thus, areas are grouped into classes based on the intensity of the radiometric patterns sensed across the four channels recorded (Billings, 1994). Cook *et al.* (1996) applied ground and airborne gamma radiometry to identify the distribution of soil within a catchment in southwestern Australia. The authors concluded that radiometric data could provide valuable insight into the spatial distribution of soil-forming materials but little direct information of pedological variation. Cook *et al.* (1996) suggested that gamma radiometry is likely to be useful to soil survey only when considered jointly with other information such as terrain models or aerial photography.

Satellite Imagery

Remote sensing from satellites has been used for land resource assessment. More recently, the ease of availability of data from operational satellites such as LANDSAT, SPOT, ERS (Earth Resources Satellite), JERS (Japanese Earth Resources Satellite) and RADARSAT, has created the potential for these techniques to be used in PA.

The LANDSAT program, owned by the government of the United States of America, has operated continuously since it was launched on July 23, 1972. Thereafter, five more satellites have been successfully launched. The aim of LANDSAT was to provide repetitive acquisition of high-resolution multispectral data of the earth's surface on a global basis. The complete system consists of an observation platform in near-polar earth orbit and ground installations to receive, process and distribute the data provided by the sensors carried on board the satellite. The satellites operate from a repetitive, circular, sun-synchronous, near polar orbit, and on each dayside pass, scan a ground area extending 185 km^2 beneath the satellite (Mulders, 1987). Data from the satellites is collected in a continuous stream along a near vertical path as the satellites move from north to south (Mulders, 1987).

The first three satellites carried a Multispectral Scanner (MSS) as the main imaging instrument with a Return Beam Vidicon (RBV) as a subsidiary, while LANDSAT 4 and 5 included the Thematic Mapper (TM) sensor as well as the MSS. The MSS is an opto-mechanical scanning system that scans side to side during the passage of the satellite from north to south. Tables 2.7 shows the radiometric characteristics of the MSS sensor.

The TM sensor was first introduced in LANDSAT 4, and was designed to provide improved spectral and spatial resolution over the MSS scanner. The basic instrument was the same as the MSS, but had more sensitive detectors, better optics and lower orbit. These characteristics enabled the collection of data in seven bands, with improved ground resolution.

Table 2.7 Radiometric and spatial resolution characteristics of the Multispectral Scanner (MSS)

Band number*	Spectral range (nm)	Spatial resolution (m)	Relevant general application
1	500 – 600	80	Vegetation vigor, areas of shallow water
2	600 – 700	80	Vegetation types, chlorophyll absorption
3	700 – 800	80	Water bodies, biomass surveys
4	800 – 1100	80	Better penetration - water bodies, biomass

* The wavelength bands in the MSS sensor referred to as 1 to 4 in LANDSAT 4 & 5 were referred to as 4 to 7 in LANDSAT 1-2. LANDSAT 3 had an eighth band in the thermal infra-red region with a spatial resolution of 237 m.

LANDSAT 6 was launched in 1993 and contained the MSS and an Enhanced Thematic Mapper (ETM) sensor, however it was lost at launch. LANDSAT 7 was launched in April 1999 and it contained an Enhanced Thematic Mapper Plus (ETM+) sensor. The ETM+ sensor replicated the capabilities of the TM instruments in LANDSAT 4 and 5. However the primary new features of ETM+ were a panchromatic band with 15 m spatial resolution and a thermal infrared channel with 60 m spatial resolution. Table 2.8 shows the spectral regions, respective applications and resolution obtained by the TM ETM+ sensors. Currently, LANDSAT 5 and 7 are operational.

Table 2.8 Radiometric and spatial resolution characteristics of the LANDSAT 5 Thematic Mapper (TM) and LANDSAT 7 Enhanced Thematic Mapper Plus (ETM+) sensors

Band number	Spectral range (nm)	Spatial resolution (m)	Relevant general application
1	450 – 520	30	Differentiation of vegetation from soil
2	520 – 600	30	Vegetation vigor
3	630 – 690	30	Chlorophyll absorption
4	760 – 900	30	Water bodies and biomass surveys
5	1550 – 1750	30	Vegetation and soil moisture
6*	10400 – 12500	120 / 60	Soil moisture and plant heat stress
7	2080 – 2350	30	Hydrothermal mapping
8*	520 – 900	15	Large area mapping

* Band 6 of the EMT+ sensor in LANDSAT 7 had an improved spatial resolution of 60 m. The EMT+ sensor also had an extra panchromatic band with a spatial resolution of 15 m.

Neale (1991) indicated that commercial satellite sensors lack the spatial resolution for monitoring natural surfaces that are highly heterogeneous on a small scale. However the launch of satellites with greatly improved spatial resolutions are planned for the near future.

The SPOT system is a French earth observing satellite system. Each satellite carries two high-resolution visible (HRV) sensors with the capability of scanning in either multispectral or panchromatic mode. The SPOT satellites operate from a sun-synchronous, *quasi*-polar orbit at an altitude of 800 km. The swath width of each HRV sensor is 60 km, however when both sensors are scanning in a twin vertical viewing mode the ground area scanned is 117 km^2. Table 2.9 shows specifications of the systems.

SPOT 4 was launched in 1998, with a lifetime of more than five years. SPOT 5 will be due for launching in 2002. The instrument has a new imaging instrument – high resolution geometry (HGR). The system will have higher spatial resolution in panchromatic mode, namely 5 m and 2.5 m instead of 10 m, and 10 m instead of 20 m in multispectral mode. SPOT 5 will have the same band numbers as SPOT 4, however the panchromatic band will be the same as SPOT 1-2.

Table 2.9 Radiometric and spatial resolution characteristics of the SPOT sensors

System	Mode	Band number	Spectral range (nm)	Spatial resolution (m)
SPOT 1, 2, 3, 4*	Multispectral	1	500 – 590	20
	Multispectral	2	610 – 680	20
	Multispectral	3	790 – 890	20
	Panchromatic		510 – 730	10
SPOT 4*	Multispectral	4	1580 – 1750	20
	Panchromatic		610 – 680	10

* SPOT 4 contained the same multispectral bands as SPOT 1-3 and an additional fourth NIR band

Current uses of SPOT data include the preparation of base maps for environmental impact studies, evaluating geological faults and structures, forecasting crop yields, assessing natural disaster damage, and preparing thematic maps for urban and regional planning.

Research has tested the use of satellite imagery for mapping soil and crop condition using the LANDSAT and the SPOT programs. Currently, LANDSAT and SPOT imagery can be used at the regional and farm-scale to produce accurate DEMs, map soil and crop variability and predict final field-scale yield. However, so-far satellite based sensors have little potential for site-specific applications due to their coarse spatial (and temporal) resolution. Future launches of satellites such as SPOT 5 and greater availability of commercial satellite data with greater spatial resolution will satisfy the fine-resolution data requirements of PA. Table 2.10 lists some of the satellites that may become potentially useful for PA.

The biggest drawbacks with remote sensing systems such as those reviewed in Table 2.10, will be data management and the fact that for soil studies, the data is only representative of surface soil conditions. One other problem of their optical sensors is that their use is severely limited by weather conditions. Cloud cover poses the greatest restriction to the acquisition of data. Some of these limitations may be alleviated with the use of all-weather radar systems.

Table 2.10 Potentially useful satellite-based sensors for precision agriculture

Satellite and launch year	Spectral range	Spatial resolution
Resource 21 – 1999	Visible, NIR, SWIR	10 m
Orbital Sciences – 1997	Visible, NIR	2 m panchromatic 8 m multispectral
Space Imaging – 1997	Visible, NIR	1 m panchromatic 4 m multispectral
Earth Watch		
Early Bird – 1997	Visible, NIR	3 m panchromatic 15 m multispectral
Quick Bird – 1998	Visible, NIR	2 m panchromatic 4 m multispectral

Imaging radar (radio detection and ranging) measures the strength and roundtrip time of microwave signals emitted by a radar antenna and reflected off the earth's landscape. Alternately the radar antenna transmits and receives pulses at particular microwave wavelengths and polarizations. The wavelengths used range from 1 cm to 1 m, which corresponds to a frequency range of about 300 MHz to 30 GHz (Figure 2.7). For an imaging radar system, about 1500 high power pulses per second are transmitted toward the imaging area (Curlander & McDonough, 1991). Each pulse has a duration (or pulse width) of typically 10 - 50 μs. The pulse normally covers a small band of frequencies, centered on the frequency selected for the radar. Typical bandwidths for imaging radar are in the range 10 to 200 MHz.

At the Earth's surface, the energy in the radar pulse is scattered in all directions, and some is reflected back towards the antenna. This backscatter returns to the radar as a weaker radar echo and is received by the antenna. These echoes are converted to digital data and passed to a data recorder for later processing and display as an image (Curlander & McDonough, 1991). The Synthetic Aperture Radar (SAR) is a sensor used in airborne or spaceborne platforms to generate high resolution images of the earth surface using microwave energy (Curlander & McDonough, 1991). Some of the satellite systems include the Japanese JERS, the European ERS-1 and 2 and the Canadian RADARSAT, all of which carry an SAR sensor.

Apart from the mentioned problems of current remote sensing, there is also the fact that actual observations will always be needed to verify or ‘ground truth’ the images. It will always be better to have actual ground measurements, specially for properties that require ‘wet’ chemical analysis or for properties that have few spectral properties, *e.g.* soil pH and lime requirement. Therefore there is a fundamental need for research towards the development of proximal soil sensing systems.

2.6.2 PROXIMAL SOIL SENSING SYSTEMS

Viscarra Rossel & McBratney (1998) first suggested the term ‘proximal sensing’ to describe devices that are able to collect data from a distance that is in close proximity (~ 1 m or less) to the object of interest (*cf.* remote sensing). Proximal sensors are capable of gathering data intensively (*i.e.* at short lags) so that properties may be determined continually and almost continuously. The proximal distance from which measurements are taken may be defined by categorising the method of data collection as either non-invasive or invasive. Non-invasive proximal soil sensors provide estimates of soil condition at various depths from aboveground observations, usually at distances of less than 1 m above the soil surface. Invasive sensors disrupt the soil surface and penetrate the soil to either sense directly, or collect soil for external detection. Table 2.11 shows a categorical list of proximal sensing systems, some that are already available and most of which are currently under development.

Crop yield sensing systems were defined as proximal because the yield sensor built into the harvester records the magnitude of crop yield harvested while in close proximity to the produce. For PA, estimates of soil properties are needed at a resolution similar to that of proximally sensed crop data. Therefore proximal soil sensing techniques must be developed strategically to meet the demand for high-resolution soil data.

Recently a number of field-deployed proximal sensing systems for ‘on-the-go’ measurements have been developed and are commercially available. These include a soil OM sensor (Shonk *et al.*, 1991), a soil EC sensing system called the Soil Doctor® (Colburn Jr., 1998), a soil EC sensing systems called the VERIS 3100 (Lund *et al.*, 1999) and the Mobile Electromagnetic Induction Sensing System (MESS) for electrical conductivity measurements (Triantafilis & McBratney, 1998).

Soil Water

Paetzold *et al.* (1985) developed a tractor-mounted pulsed nuclear magnetic resonance (NMR) moisture sensor to collect data for the calibration of remotely sensed images. The unit constructed by Paetzold *et al.* (1985) consisted of a sensor with an electromagnet, a detection coil, and a tuning capacitor; and an electronics package made up of radio frequency, signal processing and power distribution subsystems. The unit was mounted on a tractor for ‘on-the-go’ sensing. Conventional NMR measurements of soil water rely on a strong, uniform and steady magnetic field being placed on the soil, to produce a ‘splitting’ of nuclear energy levels. The novel concept in the research conducted by Paetzold *et al.* (1985) was the use of two pole pieces at the bottom of the magnet to increase homogeneity of the static magnetic field in the measurement region. The authors used a magnetic gradient rather than a uniform magnetic field for this purpose, therefore making it also possible to make measurements in sample volumes of various dimensions and various distances from the instrument surface. Paetzold *et al.* (1985) described the two poles extended 10 cm into the soil, and allowed greater control of the magnetic gradient necessary for controlling measurement depth. The authors indicated that preliminary tests on clay and loamy sand correlated linearly with volumetric water contents at 30 mm and 51 mm depths. Paetzold *et al.* (1985) suggested that although more testing was required, the technique showed lots of potential for soil water sensing. A problem was the high power requirement of the sensor.

Table 2.11 Possible proximal soil sensing systems for various agronomically important properties

Soil property	Type of sensor/scanner	Mode of operation	Examples in the literature
Soil water	Nuclear Magnetic Resonance	Non-invasive	Paetzold *et al.* (1985)
	Near Infrared and fibre optics	N/A	Christensen & Hummel (1985)
	Microwave (incorporated into a tine)	Invasive	Whalley (1991)
	Capacitance	Invasive	Whalley *et al.* (1992)
	Capacitance multisensor	Invasive	Starr & Paltineanu (1998)
Soil water, clay content	Near Infrared	Invasive	Viscarra Rossel & McBratney (1998)
Soil water, pH, EC, OM, NO_3-N	Near Infrared / Visible	Invasive	Shibusawa *et al.* (1999)
Soil water, OC, total-N	Near Infrared	Non-invasive	Dalal & Henry (1986)
Clay, soil water, OM, CEC, CO_3	Near Infrared	Non-invasive	Ben-Dor & Banin (1995)
NO_3-Nitrogen	Ion Selective Electrode	Non-invasive	Adsett & Zoerb (1991)
	Ion Sensitive Field-Effect Transistor	Non-invasive	Birrell & Hummel (1997)
Mineral-Nitrogen	Near Infrared	Non-invasive	Ehsani *et al.* (1997)
Carbon and nitrogen	Near Infrared	Non-invasive	Morra *et al.* (1991)
OC, N, LR, pH, CEC, clay	Mid Infrared	Non-invasive	Janik *et al.* (1997)
Organic matter	Visible (660 nm)	Invasive	Shonk & Gaultney (1988, 1989)
	Near Infrared	Non-invasive	Sudduth *et al.*, (1989, 1990)
Organic matter and ground slope	Visible for OM, inclinometers for slope	Non-invasive	Yang *et al.* (1993)
pH	Flat surface Ion Selective Electrode	Invasive	Adamchuk *et al.* (1998)
pH and lime requirement	Ion Sensitive Field-Effect Transistor	Invasive	Viscarra Rossel & McBratney (1997)
Electrical conductivity / salinity	EM-38	Non-invasive	Lesch *et al.* (1992)
	EM-38 and EM-31	Non-invasive	Mankin *et al.* (1997); Triantafilis & McBratney (1998)
Electrical conductivity	Resistivity / Conductivity	Invasive	Lund *et al.* (1999)
Gaseous composition of soil air	Electronic polymer array-based odour sensing system	Non-Invasive	Persaud & Talou (1996)
Texture, compaction	Load cells	Invasive	Lui *et al.* (1996)
Structure	Microphones	Invasive	Sabatier *et al.* (1990)
Mechanical Impedance	Penetrometer	Invasive	Xiwen & Limin (1999)
	Penetrometer	Invasive	Sirjacobs & Destain (1999)
	Penetrometers	Invasive	Alihamsyah & Humphries (1991)

Note: EC = electrical conductivity; LR = lime requirement; OM = organic matter; OC = organic carbon; CEC = cation exchange capacity

Whalley (1991) described the development of a microwave soil moisture sensor for incorporation into a narrow cultivator tine. The sensor used microwave attenuation for measurements and consisted of a microwave source and detector connected by an electromagnetic transmission line. A commonly used transmission line called a ‘stripline’, consists of a low loss dielectric slab with a thin conducting strip on one side and a ground plane set at zero potential on the other. The dielectric component of the transmission line that separates the conducting elements must at least partly consist of the sample being tested, *i.e.* soil. When microwaves pass down the stripline the electric and magnetic vectors that result pass through the air space around the transmission line. When moist soil contacts the stripline the microwave energy is attenuated proportionally to the volumetric water content of the soil. However striplines are not suitable for placement in tines because they are not resistant to abrasive wear. Whalley (1991) described the development of a transmission line resistant to abrasive wear that may be incorporated into a narrow tine. The sensor was dynamically calibrated by measuring attenuation at 10.5 GHz, using a forward speed typical of those found during seed planting operations. The main limitation of the sensor was that it sampled relatively small volumes of soil, therefore being sensitive to soil structure, *i.e.* good calibrations were obtained in uniform soils but not in structured ones.

Whalley *et al.* (1992) described the development of a tractor-mounted capacitance sensor for ‘on-the-go’ soil water measurements. The sensor was shaped similar to a tine consisting of two capacitor electrodes separated by and insulator. The sensor described by Whalley *et al.* (1992) was basically a large parallel wire capacitor shaped like a tine so that it may be dragged through the soil. The capacitor electrodes were connected to an oscillator operating at approximately 150 Mhz. The signal was used to drive an LED that emitted into a fibre optic cable. The cable connected the oscillator with a frequency meter. The advantage of the capacitance technique is that it can overcome some of the problems associated with dynamic measurements of soil water. Namely, capacitance sensors have a large sampling volume compared to soil structural details; they can be built in a compact design and can be powered from a 12-volt tractor battery. However, the authors found that the sensor was not entirely independent of soil type. The effect of bulk density on the dielectric constant was to introduce a systematic bias to the measurements. Therefore the sensor was found to give calibrations that were affected by the soil’s bulk density.

Starr & Paltineanu (1998) assessed the capabilities of multisensor capacitance sensing systems to measure soil water content under long-term field-scale conditions. Their measurements involved real-time quantification of the spatial variability of soil water under plow-tillage and no-tillage corn. The authors reported that the capacitance probes proved to be highly sensitive and robust for field-scale, real-time soil water research.

Stafford (1988) also reviewed techniques available for measuring soil moisture content. The reader is referred to that publication for a more complete review of the techniques and methodologies used to sense soil water, as this has only considered the most promising methodologies which may be most suitable for ‘on-the-go’ sensing.

Soil Nitrate

Adsett & Zoerb (1991) developed a tractor-mounted, automated field monitoring station for soil nitrate. The sensing system consisted of a soil sampler, a nitrate extractor unit, a flow cell and controller and a nitrate ion-selective electrode. The unit operated at forward speeds of 3 km/h, sampled at 15 cm depth and operated in 30 s cycles. Although the nitrate ion-selective electrode was fast and accurate, the system had various limitations. The methodology employed for extraction was time consuming, particularly in varying soil types and conditions, were calibration was tedious. Adsett & Zoerb (1991) also reported that the nitrate extraction times for continual measurements were inconsistent. The authors modified a chain-slot cutter (similar to a chainsaw) for the sampling component and reported that it performed adequately, however Adsett & Zoerb (1991) noted that cleaning was a problem and its prolonged use in inherently abrasive soil was questioned. Their work showed that ion-selective electrode technology might be used in automated field monitoring systems for soil. The authors indicated that the system produced measurement accuracy for soil nitrate that was comparable to industry standards and colorimetric tests. This research demonstrated the possibilities of using common methods of soil analysis for ‘on-the-go’ measurements in the field. However as a final note Adsett & Zoerb (1991) suggested that more research and field-testing of the system is required because of the mentioned limitations.

Birrell & Hummel (1997) investigated the use of Ion Selective Field-Effect Transistors (ISFETs) and Flow Injection Analysis (FIA) systems for real-time soil nitrate sensing. ISFETs have some advantages over ion-selective electrodes. The authors researched the effects of various sample flow rates, sample injection and washout times on the capability of the ISFET / FIA system to predict nitrate concentrations. The authors reported that the system was capable of analysing samples within 1.25 s, making the system feasible for 'on-the-go’ soil nitrate sensing. However, Birrell & Hummel (1997) indicated that considerable improvements are needed in the automated extraction system before it may be used continuously. In their experiments, soil nitrate was extracted manually. Development of a rapid and robust automated soil sampler remains one of the major limitations in the development of such systems for ‘on-the-go’ sensing.

Ehsani *et al.* (1999) explored the possibility of rapidly sensing soil mineral nitrogen content using NIR reflectance in the 1800 to 2300 nm. Simulation studies determined the ability of Partial Least-Squares (PLS) and Principal Component Regression (PCR) techniques to relate NIR spectral data to soil nitrogen content in the presence of interfering effects and noise. Soil was tested in the laboratory and in the field, the latter producing a prediction standard error of around 8 ppm. Ehsani *et al.* (1999) indicated that both PLS and PCR were robust methods for soil nitrate predictions in the presence of interfering effects (*i.e.* unknown factors) provided the calibration set had similar effects, otherwise it failed. Therefore, NIR may be used to characterise soil nitrogen variation for site-specific nitrogen management provided the calibration is site-specific.

Soil Organic Matter

Shonk & Gaultney (1988) developed a prototype sensor to measure soil reflectance in real-time. The sensor used solid state light emitting diodes (LED) and a photodiode transducer to measure soil reflectance. The sensor was designed to measure soil colour changes within a field. Shonk & Gaultney (1989) described the sensor and its design. The sensor was mounted within a shank to protect it from rocks and other harsh debris, and also to facilitate soil penetration and take advantage of more uniform moisture conditions at 5 cm to 15 cm below the soil surface. The shank-mounted real-time soil OM sensor consisted of a compact transmitter and receiver modules that used light reflectance to measure soil OM (Figure 2.8). The sensor used single wavelength (660 nm) red light. The red LEDs and the sensor to measure soil reflectance (Figure 2.8b) were mounted on a tine that was attached to the front of an application vehicle (Figure 2.8a). The sensed data was transmitted to an on-board computer that calibrates chemical application rates. The authors produced soil OM maps for several fields, which were used to control the application of variable amounts of fertiliser and/or herbicides, using VRT.

Shonk *et al.* (1991) indicated that the sensor was useful in fine and medium textured soils with 1 % to 6 % OM, and that preliminary field tests at an operating speed of 6.5 km/hr produced accurate predictions (R^2 values ranging from 0.83 to 0.95). The limitations of the sensor were noted in soils with significant variations in texture and where OM was low (Shonk *et al.*, 1991). Shonk *et al.* (1991) suggested that the sensor might be calibrated in the field or using laboratory-derived calibration models. Re-calibration for each new soil type and moisture content level was required. The authors indicated that the soil OM sensor was licensed for commercial development by Tyler™.

a. b.

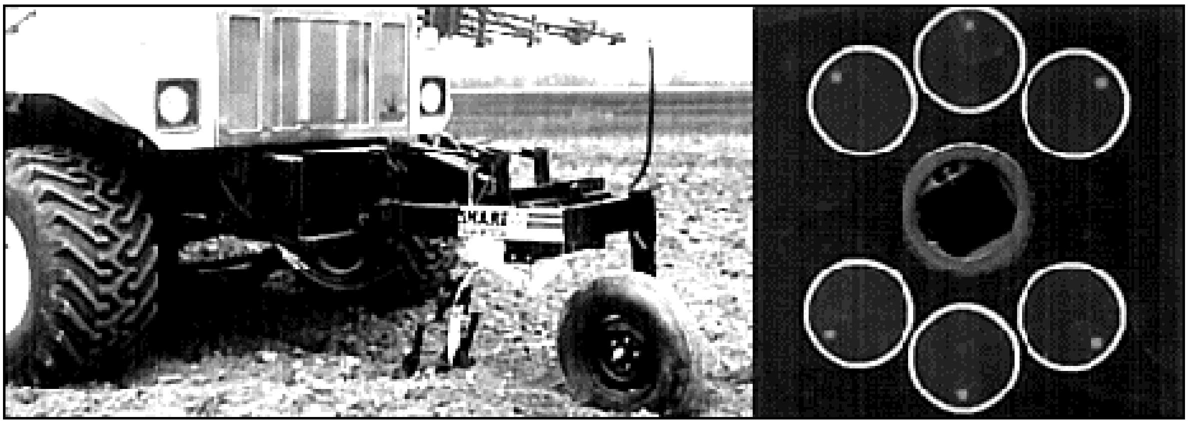

Figure 2.8 Tine-mounted soil organic matter sensor (a.) mounting system on a variable-rate herbicide applicator, and (b.) red-light (660 nm) emitters and sensor

McCauley *et al.* (1993) assessed the sensing system developed by Shonk & Gaultney (1988) and quantified the spatial variability of the sensed soil OM. The measurements from the sensor were reported to be more precise than those resulting from laboratory dichromate analysis. McCauley *et al.* (1993) also suggested that the high-frequency 'noise' of the signal from the sensing system, acquired in field tests, may actually represent the short-range variability of soil OM. This suggestion was based on the fact that under controlled tests, where the effects of ambient light and soil-to-sensor distance were blocked, similar fluctuations were observed. They obtained further support for this hypothesis by observing that the high-frequency variations were also evident in results obtained from consecutive dichromate oxidations (McCauley *et al.*, 1993). From these findings McCauley *et al.* (1993) derived an important conclusion: that although this level of variability will never be treated by site-specific management, understanding of the phenomena can aid in improving sensor design. That is, development should aim to produce sensing systems that measure this type of variability as closely as possible. This information may then aid with interpolation and map making for the application of input resources.

A portable NIR multiple wavelength soil OM sensor was developed by Sudduth *et al.* (1989). The sensor used a circular variable filter spinning at 5 Hz to provide sequential monochromatic, chopped light from a broadband source (Sudduth *et al.*, 1989). The monochromatic light was transmitted to the soil surface via a fibre optic bundle. This allowed for much of the sensor to be mounted remotely, away from the soil. The diffusively reflected light from the soil surface was detected by a lead sulphide photo detector (Sudduth *et al.*, 1989). The effective sensing range of the system was 1 630 nm – 2 650 nm. The sensor was both laboratory and field tested. Sudduth *et al.* (1989) indicated that the predictive capability of the system in the laboratory, using a range of soil types and moisture contents, was adequate and produced a standard error of prediction (SEP) of 23 % OM. Correlations of the spectral data with soil OM, and predictions of OM were accomplished using PLS regression. At that stage field testing was not successful.

Sudduth *et al.* (1990) evaluated the performance of the NIR-PLS OM sensing system using soils from a wide geographic range extending across north-central USA. They also attempted predictions of cation exchange capacity (CEC) and soil water using the NIR-PLS technique. Sudduth *et al.* (1990) concluded that predictions were less accurate as samples from an increasingly wider geographic range were considered. Good OM predictions, with a SEP of 28 % OM, were obtained using grouped data from the lower corn-belt. Sudduth & Hummel (1991) tested the sensor in the field and suggested that it was soil and moisture independent, thus more versatile than the single wavelength sensor. However the sensor is reported to be less robust than that previously described and shown in Figure 2.9.

Soil pH

Adamchuk *et al.* (1998) described the development of a prototype automated sampling system that allows ‘on-the-go’ measurements of soil pH. The system measures soil pH of naturally moist soil at field condition, no H^+ extracting solutions were used. It consists of a sampling shank that may be attached to an agricultural vehicle, a flat surface electrode, compressed air and rinsing-water circuits, a pH meter and a GPS. The authors reported that the flat surface electrode had a response time of between 3 and 6 seconds when tested in varying soil types, thus it was deemed suitable for ‘on-the-go’ operation. Adamchuk *et al.* (1998) designed the sampling shank so that it may be adjusted to sample at depths of approximately 10 cm to 20 cm. They described system operation as consisting of three steps: soil sampling, sample analysis and electrode rinsing. The duration of analysis ranging between five and six seconds. Obviously this is limited by the electrode’s response time.

Adamchuk *et al.* (1998) indicated that the accuracy of ‘on-the-go’ measurements was approximately 0.5 pH units. Thus the system does not provide similar accuracy to laboratory techniques. However the possibility for increased sample density may improve the quality of soil pH maps. The authors indicated that care needs to be taken when the sample is brought into contact with the sensor as its surface is made of glass. Therefore some modification of the sampling mechanism may be needed in the future. More testing of the system is required.

Adamchuk *et al.* (1998) proposed that the system may be used to map field lime requirement, using either multivariate techniques that depend on soil textural differences and their cation exchange capacity, or tables that combine soil pH and soil type. Chapter VIII describes the ineffectiveness and disadvantages of these methods for determining site-specific lime requirements.

Soil Electrical Conductivity

There are two main proximal methods that are used to measure the electrical conductivity through soil, an invasive, direct-contact electrode method and a non-invasive technique that uses electromagnetic induction for measurements (Table 2.11).

The VERIS 3100 (Lund *et al.* 1999) is the invasive soil sensing system, consisting of six coulter electrodes that are inserted into the soil to continuously measure the resistance to the flow of an electric current through soil (Figure 2.9). The equally spaced electrodes may be referred to as a Wenner array (Milsom, 1989).

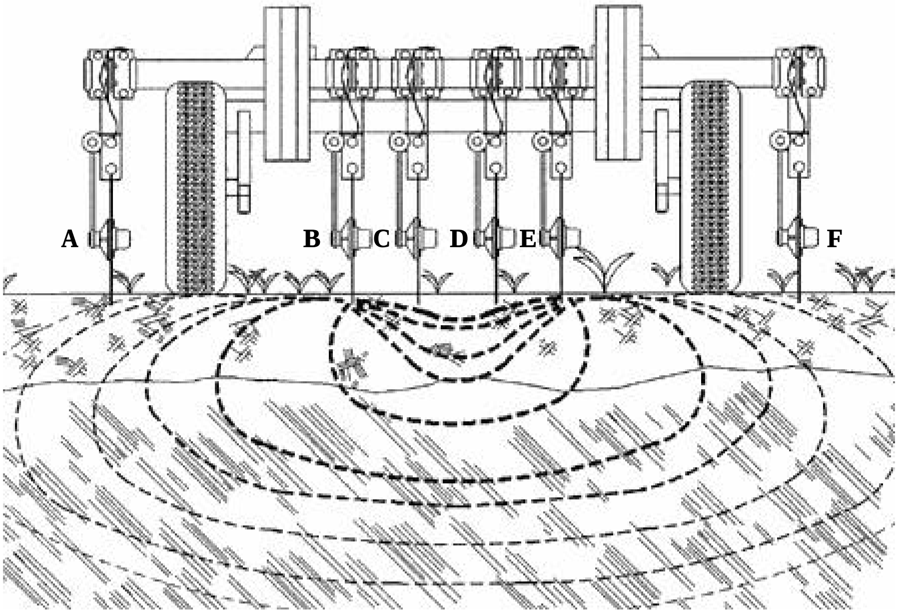

Figure 2.9 Operation of the VERIS 3100, an 'on-the-go' proximal soil (resistivity) electrical conductivity sensing system that uses two sensor arrays to measure conductivity at two depths, 0 – 30 cm and 0 – 90 cm. From Lund *et al.* (1999)

The system operates at two depths, 0 – 30 cm and 0 – 90 cm. The shallower measurements use the four inner coulters (labelled B, C, D and E in Figure 2.9) in the following manner: the outer (B and E) electrodes pass an alternating electrical current into the soil, while the inner electrode pair (C and D) measure the resistance of the soil to that electrical current. This is measure of resistance standardised over the distance separating the coulter electrodes is called the resistivity (see below). The deeper measurements use the four outer electrodes (A, B, E and F) and operate in a similar way: the outer (A and F) electrodes pass an alternating electrical current into the soil, while the inner electrode pair (B and E) measures the soil's resistivity to that current. Briefly, the relationship between resistance, resistivity and conductivity is given below. Electrical resistance (R) is given by:

$$R = \frac{V}{I}$$

where I is the flow of current between two electrodes and V is the voltage difference between them. Measuring R over a given length gives the resistivity (ξ):

$$x = 2p\mathrm{dR} = 2p\mathrm{d}\frac{V}{I}\,\mathrm{ohm}^{-1}\mathrm{m}^{-1}$$

where d is the given length. The electrical conductivity (EC) of the soil is inversely related to its resistivity:

$$\mathrm{EC} = \frac{1}{x} = \frac{I}{2p\mathrm{dV}}\,\mathrm{Sm}^{-1}$$

in units of siemens per metre (Sm^{-1}). Similar equations may be found in Malmstad & Enke (1963) and in Milsom (1989).

The VERIS 3100 coulter electrodes are inserted approximately six centimetres into the soil and the sensing system is towed through the field so that data acquisition occurs 'on-the-go'. The collected EC data is geo-referenced using a GPS. The EC values generated by the VERIS 3100 have been shown to vary according to the soil's electrolyte concentration and its connectivity (Lund *et al.*, 1999). These depend on the mainly the soil's water content and its texture, however effects due to temperature and soil bulk density may also be important. Chapter IV illustrates its use and provides some measured correlations of VERIS EC data to various soil properties.

Triantafilis & McBratney (1998) described the development of the MESS for electrical conductivity measurements. The sensing system consists of two electromagnetic induction (EM) instruments, the EM-31 and the EM-38 (Figure 2.10). The EM-31 measures EC to a depth of six metres while the EM-38 to two metres. The main advantages of this system is that it is non-invasive. As with the VERIS 3100, measurements will depend on the previously mentioned soil properties. However work is still needed to establish useful soil relationships.

Each EM instrument consists of a transmitter and a receiver. The transmitter irradiates a low frequency time-varying magnetic field that is propagated through conductive soil. This induces the formation of small Eddie currents, which in turn, induce a secondary magnetic field which is then detected by the receiver of the EM unit. The magnetic field may then be proportionally equated to the soil's electrical conductivity.

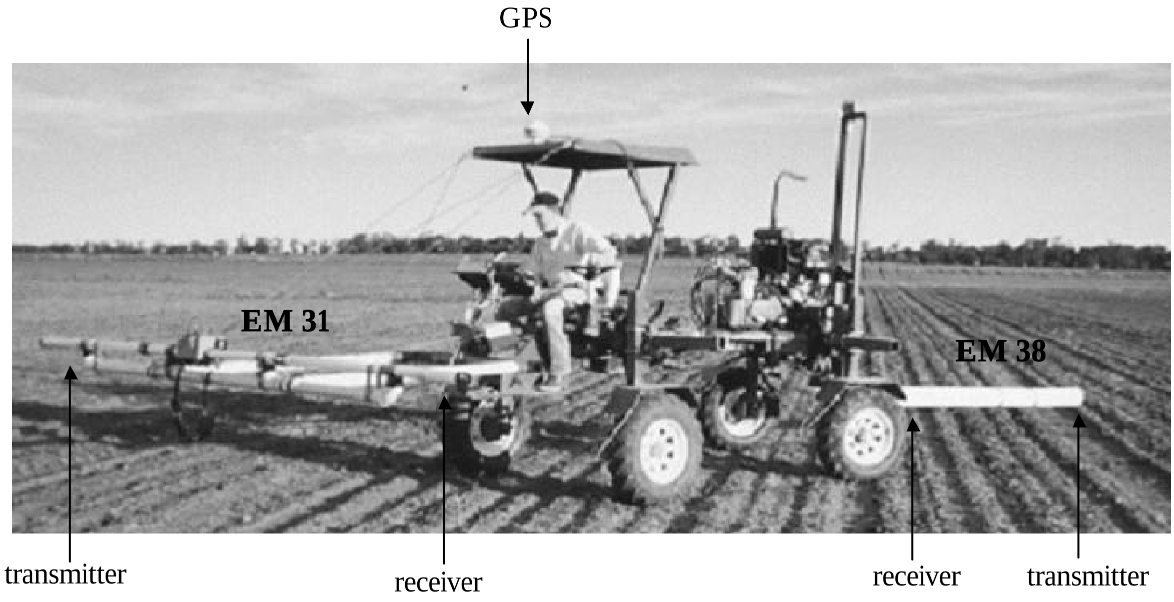

Figure 2.10 The Mobile Electromagnetic Induction Sensing System (MESS) for electrical conductivity measurements. The measurement depth of the EM-31 is six metres below the soil surface, while the measurement depth of the EM-38 is two metres.

Soil Physical Properties

Sabatier *et al.* (1990) showed that acoustic techniques (reflection and transmission in the audio-frequency range) may prove useful in determining soil physical properties such as surface air porosity, air permeability and pore structure. Their research consisted of measuring acoustic reflection and transmission in sandy, sandy loam and silty clay soil. The authors report that acoustically determined air porosity was within 10 % of the values that were determined gravimetrically. Sabatier *et al.* (1990) also reported that the technique showed the variation in soil condition with depth. The technique was able to detect permeable surface layers in clay (in a dry and loosely packed state), and the formation of a compaction pan.

Alihamsyah & Humphries (1991) developed techniques for ‘on-the-go’ soil mechanical impedance measurements, using horizontally operating penetrometers adapted to provide a continuous signal for the automatic control of soil implements. Cone and prismatic shape penetrometer tips were mounted on specially designed blades, which were coupled to load cells to provide the impedance signal. The sensor system was attached to a tractor and was tested at 2.2 and 6.4 km/h on sandy and loamy soil. Alihamsyah & Humphries (1991) concluded that the device was capable of measuring force continuously, and that both tips produced values that were related to standard vertical measurements. However, the authors indicated that the prismatic tip was less prone to damage.

Lui *et al.* (1996) emphasised the need for the development of sensing systems to rapidly quantify soil physical properties. Their research attempted the development of a soil texture/soil compaction sensor based on the draft requirement of an instrumented reference tillage tool. The chisel used to predict draft requirements comprised of two load cells to measure draft and one to measure vertical load. The sensor also consisted of a radar gun to measure ground speed, a displacement sensor, a dielectric moisture sensor to correct estimations, a linear potentiometer to measure depth, and a GPS. The device operated at a constant speed and a depth of approximately 30 cm. The authors concluded that adjustments are needed to the draft-moisture corrections in order to derive a texture compaction index. Most importantly, Lui *et al.* (1996) suggested that work is needed to verify results on various soil types.

Xiwen & Limin (1999) developed an automatic soil penetrometer for soil mechanical impedance measurements at different depths with a maximum of 40 cm. The device consisted of a stepping motor, transmission gears, a pulling and pressing sensor, a measuring staff and a cone body of stainless steel. The automatic soil penetrometer had three main functions, to penetrate the soil automatically with fixed speed, to return back automatically when it reaches the defined depth (max. 40 cm) and to stop and return back automatically when it meets obstacles such as stones. The system was attached onto a tractor for ‘on-the-go’ measurements. The authors indicated that measurements could be made every 30 m at various depths.

Different Soil Properties Using Various Techniques

The possibility exists for the use of a number of techniques that may, with more research, be adapted and used for continuous, proximal soil sensing.

Near Infrared Spectrophotometry

Dalal & Henry (1986) showed that it is possible to simultaneously measure total nitrogen (1 702 nm, 1 870 nm and 2 052 nm), soil moisture (1 926 nm, 1 954 nm and 2 150 nm) and organic carbon (1 744 nm, 1 870 nm and 2 050 nm) using non-destructive NIR reflectance spectrophotometry. However the authors indicated that at lower concentrations of total nitrogen predictions were poor. Furthermore Dalal & Henry (1986) suggested that the technique does not render itself to predictions across a wide range of soil colours.

Morra *et al.* (1991) used NIR to measure total carbon (1 766 nm, 2 206 nm, 2 226 nm, 2 246 nm and 2 346 nm) and nitrogen (1 246 nm, 1 646 nm, 1 726 nm, 1 826 nm and 2 366 nm) concentrations on a range of soil types. The authors concluded that the method can be used to predict carbon and nitrogen concentrations of soil size fractions.

Ben-Dor & Banin (1995) used NIR for the simultaneous prediction of clay (1 472 nm, 1 870 nm, 1 905 nm, 2 097 nm, 2 186 nm and 2 333 nm), moisture (2120 nm and 2362 nm), cation exchange capacity (CEC) (1 064 nm, 1 322 nm, 1 412 nm, 1 431 nm, 2 016 nm, 2 097 nm, and 2 333 nm), carbonate content (1483 nm and 1647 nm) and OM content (1 043 nm, 1 412 nm, 1 585 nm, 1 941 nm, 2 017 nm and 2 388 nm). Ben-Dor & Banin (1995) suggested that the methodology is rapid and likely to be useful for a relatively homogeneous soil population. However the authors recommended further experimentation with the methodology for its use in soil science.

Mid Infrared Spectrophotometry

Janik *et al.* (1997) proposed the use of mid infrared (MIR) diffuse reflectance soil analysis as a surrogate for conventional extractive or digestive laboratory techniques. They suggested that MIR is faster, cheaper and that it allows the acquisition of more intensive data sets. The soil chemical properties which the authors predicted using MIR spectrometry include soil water, particle size, organic carbon and nitrogen, pH, lime requirement, soil carbonates, and various elements. Janik *et al.* (1997) concluded that mid infrared spectrometry combined with PLS prediction provides quantitative and qualitative results which are comparable in accuracy with many of the conventional laboratory techniques. Furthermore, that MIR is particularly useful for studies where low cost, minimal preparation and fast acquisition of results is needed. However, infrared spectroscopy is unlikely to replace soil chemical extractions for properties dependent on soil solution chemistry, such as N, P, K and for properties that are in low concentrations such as nitrate-nitrogen. So far, soil analysis using mid infrared spectroscopy has not been widely reported and more research still needed to verify its accuracy and utility.

Other Possible Techniques

A non-invasive, polymer array-based odour sensing system currently used for truffle detection/harvesting (Persaud & Talou, 1996), could perhaps be modified and used 'on-the-go' for determining the gaseous composition of soil air. The sensor system contains twenty sensors used for continuous odour measurement, measuring odour intensity. Such techniques need to be tested for their ability to provide agronomically significant information.

Finally it may be relevant to mention some of the capabilities of NASA's Mars Microrover – 'Sojourner' (Figure 2.11). Sojourner was sent to the planet Mars to perform a number of scientific and technological experiments. An Alpha, Proton X-ray Spectrometer (APXS) was attached to the Sojourner to determine the elemental composition and mineralogy of rocks and soil on and around the landing site. The rover is also capable of performing basic soil mechanics experiments, measuring torque, topsoil compactness and density.

Although Sojourner cannot collect soil samples, future rovers in the year 2003 will have the mechanism to do so. Similar autonomous or semi-autonomous vehicles with soil property sensing systems and scanners attached may be possible for 'on-the-go' collection of various soil data.

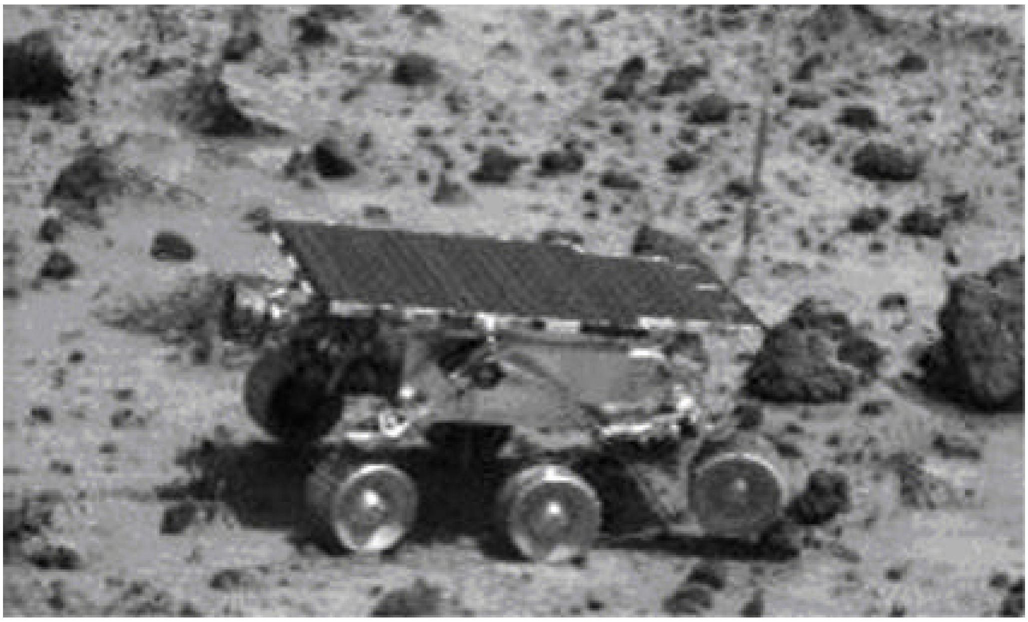

Figure 2.11 Photograph of NASA's Micro-rover 'Sojourner' operating on a Martian landscape. Sojourner is capable of determining the elemental composition and mineralogy of rocks.

2.7 CONCLUDING REMARKS

The review presented both classic statistical and geostatistical methods used to quantify the spatial variation in soil and crop parameters. Descriptions of each methodology were supported with corresponding literature reviews pertaining to the quantification of the spatial variability in soil pH. Under conventional agricultural management systems the spatial variation of agronomically important properties is often considered to be problematic. Geostatistics can be used to quantitatively describe the spatial variability of such properties. Precision agriculture uses this quantitative spatial information to accurately and precisely manage agricultural land.

Each of the five components of a precision agricultural management system were reviewed. Emphasis was given to data collection and acquisition methods for precision agriculture, and particularly to techniques that attempt a complete enumeration of soil, namely remote and proximal sensing. Finally, some of the developing options for the characterisation of fine-scale soil variability using proximal soil sensing systems were described. Precision agriculture uses spatial (and temporal) information to site-specifically manage agricultural land, according to its variability. The development of 'on-the-go' proximal soil sensing systems is imperative for the acquisition of soil variability information at the spatial resolution needed for site-specific management.

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SECTION II

Chapter III

DESCRIPTION OF THE EXPERIMENTAL FIELD: SOIL SAMPLING, ANALYSIS AND THE SPATIAL VARIABILITY OF SURFACE SOIL CHEMICAL PROPERTIES

3.1 FIELD SITE DESCRIPTION

The field site for the conduct of this project is situated in a commercially operating farm at Kelso, in central-west NSW, Australia (Figure 3.1). Its geographical reference is -33° 24’ 04” S and 149° 38’ 51” E, with a maximum elevation of 741 m above sea level.

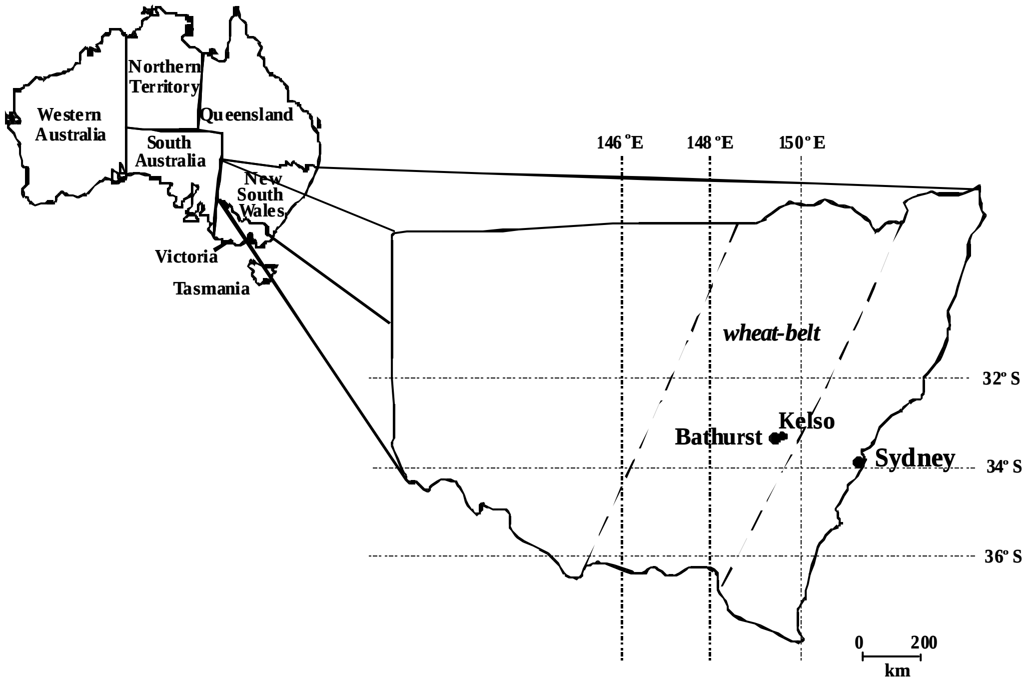

Figure 3.1 The experimental site located at Kelso in the eastern portion of the NSW wheat-belt

The district has an average annual rainfall of 630 mm, the incidence of rain intensifying from October through to February. Average daily maximum and minimum temperatures range from 11°C (July) to 27.7°C (January) and from 0.6°C to 13.3°C, respectively. The median yearly period between first and last frost is approximately 250 days. The long-term monthly climatic averages are shown in Figure 3.2.

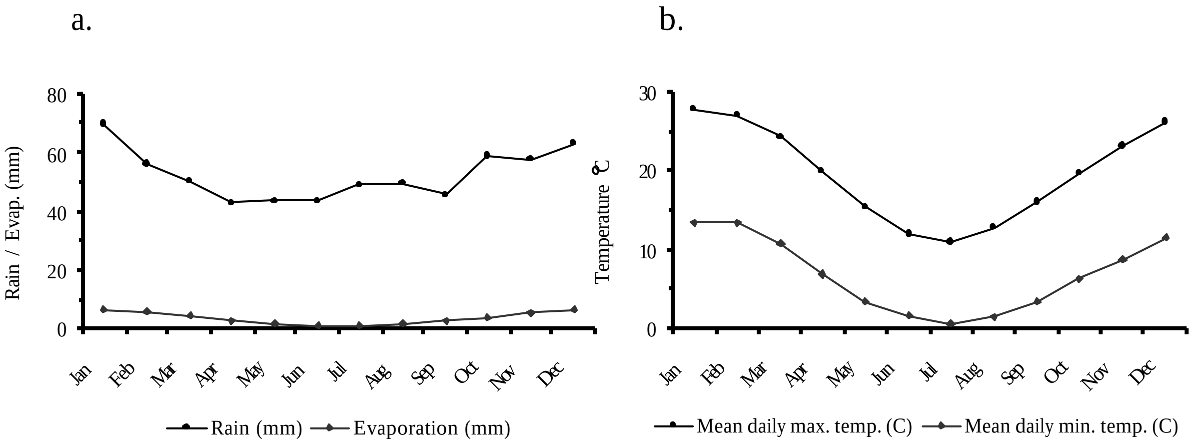

Figure 3.2 Monthly climatic averages for the Kelso / Bathurst area showing (a.) average rainfall and evaporation, and (b.) average maximum and minimum temperatures (Bureau of Meteorology, 1999)

Natural vegetation in the area is now sparse but consists of medium-low eucalyptus forests with a distinctively open appearance. Amongst other, some of the common species found include red ironbark (*Eucalyptus sideroxylon*), box (*Eucalyptus microcarpa*), and scribbly gum (*Eucalyptus racemosa*). The understorey is made up of low shrubs and grasses.

Kelso is situated in the Lachlan Fold Belt whose surface geology comprises Cambrian to early Carboniferous complexes. The rock types within stratigraphic units consist of granite, grandiorite, monzonite and admellite. Hence generally the resultant soil types are medium to coarse textured neutral to acid sands.

Land use in the region consists of cropping and grazing on native and improved pastures. Farms are generally medium in size ranging from approximately 200 to 5 000 ha. The predominant forms of agriculture consist of wheat (*Triticum aestivum*) and sheep production. The most common oilseed grown in the area is canola (*Brassica napus*), which is produced on a significance scale as an alternative to wheat. Canola provides a rotation crop in the cereal production system, and is used as a disease-break crop and as a means to significantly improve soil physical condition. The area sown to canola each year varies markedly from year to year due to climatic and market conditions, pests and disease, and the outlook for wheat.

The experimental site had not been cropped since 1994, prior to which it had been on a two year grain crop, three year pasture cycle. At the time of sampling the field was under constant fallow, acting as pasture for sheep.

3.1.1 THE LANDSCAPE AND SOIL OF THE EXPERIMENTAL FIELD

The experimental field has an undulating topography with a relief of 12 m and a maximum slope of 8.5 % (Figure 3.3).

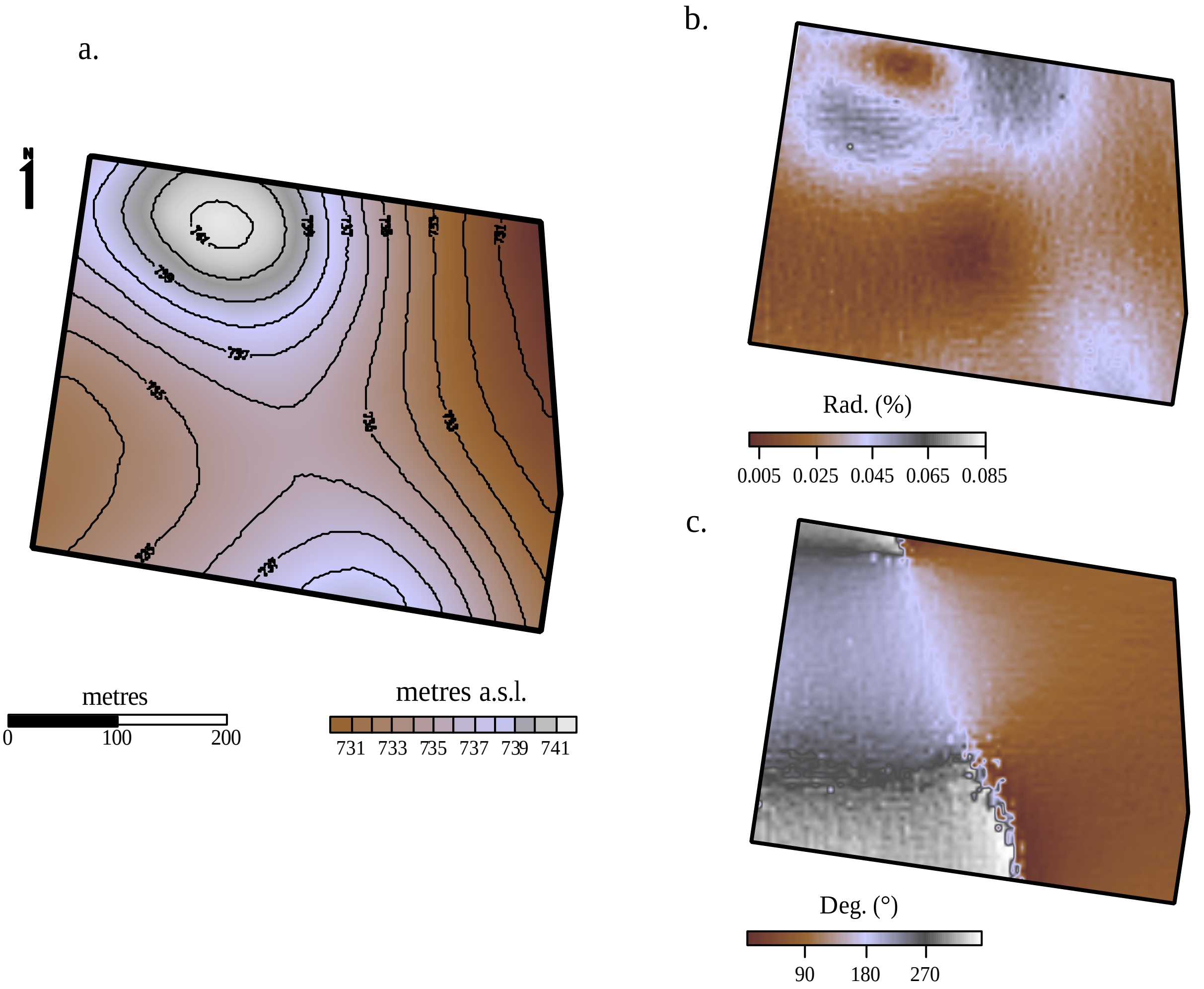

Figure 3.3 Topography of experimental field site, (a.) elevation in metres above sea level (a.s.l.), (b.) slope in radians (equivalent to percent) and (c.) aspect in degrees

Both aspect and slope were calculated using algorithms described in Burrough and McDonnell (1998). The undulating topography of the region resulted in the formation of two very general profile types occurring in what may be seen as a short toposequence in the experimental field. The profile description of the soil on the upper slope is shown in Table 3.1.

Table 3.1 Profile description: upper slope: Red Chromosol (Isbell, 1996)

Horizon	Depth (mm)	Description
A_{11}	0 – 200	7.5YR $^5/_4$, LSCL, pH 4.55, diffuse boundary to:
A_{12}	200 – 300	5YR $^4/_4$, SCL, pH 4.51, sharp boundary to:
B	300 – 800+	2.5YR $^4/_6$ (red), MC to HC, pH 5.50

Texture classes: Light Sandy Clay Loam (LSCL); Sandy Clay Loam (SCL); Medium Clay (MC); Heavy Clay (HC)

The soil on the upper slope (Figure 3.3) has a duplex profile with a sharp textural difference between the A_{12} and B-horizons (Table 3.1). The A_{11} horizon had a crumbly consistency with moderate force required to disrupt the soil. Soil pH was lowest in the A_{12} horizon and highest in the haematite-rich B-horizon.

The profile description for the soil on the lower slope of the field (Figure 3.3) is shown in Table 3.2.

Table 3.2 Profile description: lower slope: Brown Kurosol (Isbell, 1996)

Horizon	Depth (mm)	Description
A1	0 – 200	7.5 YR $^5/_2$, LSCL, weak crumb, pH 4.52, diffuse boundary to:
A2	200 – 400	10 YR $^6/_2$, SCL, pH 4.08, sharp boundary to:
B	400 – 800+	10 YR $^4/_2$, 2.5 Y $^5/_1$ mottles HC, pH 5.02

Texture classes: Light Sandy Clay Loam (LSCL); Sandy Clay Loam (SCL); Heavy clay (HC)

The profile described in Table 3.2 is also duplex. The main differences from the previous (Table 3.1) were the presence of an A_2 horizon, the mottled B-horizon and lower pH values throughout the profile. These characteristics are typical of soil lower in the toposequence, with levelling slopes (Figure 3.3b). The A_2 horizon and the mottled B-horizon indicate periodic saturation of the profile. The low pH values of the upper horizons indicated the presence of toxic concentrations of aluminium and manganese.

The imposition of traditional soil ‘types’ and taxonomic classification on the description of the soil of the experimental field is given solely for completeness. The concept of soil ‘type’ is unimportant to this work. Instead the focus is the development of quantitative techniques for the collection of useful data for continuous site-specific soil management using precision agriculture technology.

3.2 DISCREET SAMPLING STRATEGY

During a reconnaissance survey, a diagonal transect sample was used to collect soil along the toposequence present in the experimental field, to derive some of the exploratory statistics, including variograms for determination of an appropriate sampling strategy (and spatial inference). Thirty-two replicated samples (64 samples in total) at 20 m intervals were collected for this purpose. The samples were dried, ground, sieved and analysed in the laboratory for pH_{CaCl_2}, and lime requirement using the SMP buffer procedure (Shoemaker *et al.*, 1961). The analytical methods are described in section 3.3 below. The sampling points and resulting pH and lime-requirement transects are shown in Figure 3.4.

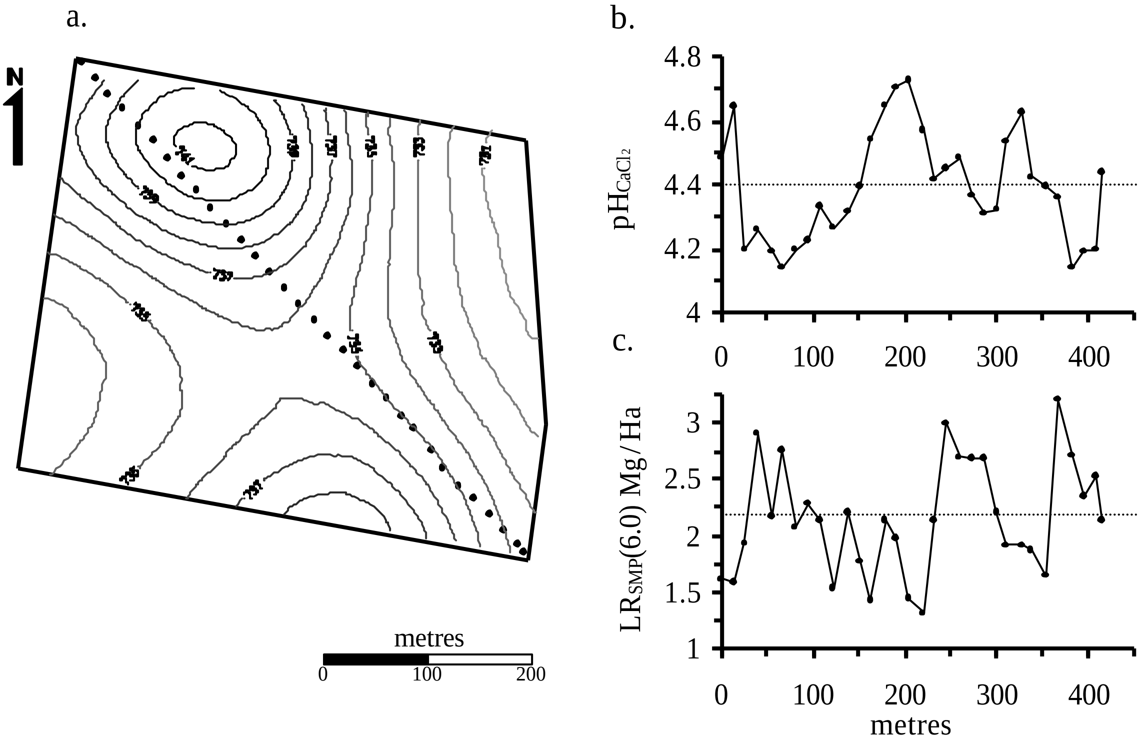

Figure 3.4 (a.) Points where samples where collected during the reconnaissance stage, (b.) corresponding pH_{CaCl_2} and (c.) lime requirement to a target pH of 6.0 (LR(6.0)) transects

Figure 3.4b shows a general trend in pH_{CaCl_2} along the transect starting at approximately 50 m, pH_{CaCl_2} increasing from approximately 4.2 to 4.7 at a distance of 200 m. the average soil pH_{CaCl_2} was 4.4 (dashed line on Figure 3.4b), ranging from 4.10 to 4.75. The lime requirement to a target pH of 6.0 (LR(6.0)) transect (Figures 3.4c) displays greater short range variability than pH_{CaCl_2}, with an average lime requirement value of 2.2 Mg/ha, and a range of 1.3 to 3.2 Mg/ha. This figure also provides and indication of the economic risk attached to averaged, single-rate lime applications in the field. (These risks are described and quantified in Chapters IX and X).

To produce reliable predictions and accurate management maps, the chosen sampling strategy should relate to the scale of spatial variation that the user wishes to resolve. The sampling strategy may otherwise be too intensive resulting in greater cost and effort than necessary, or if the sampling is too sparse (greater than the range of spatial variation), it may not provide spatially correlated data that is useful for spatial inference and map production. The experimental semi-variograms with fitted spherical models (Chapter II) are shown in Figure 3.5 below. Although only 64 points were used to calculate the variograms, the fitted models appear to conform to the experimental values; hence it is assumed that the variogram estimations were robust.

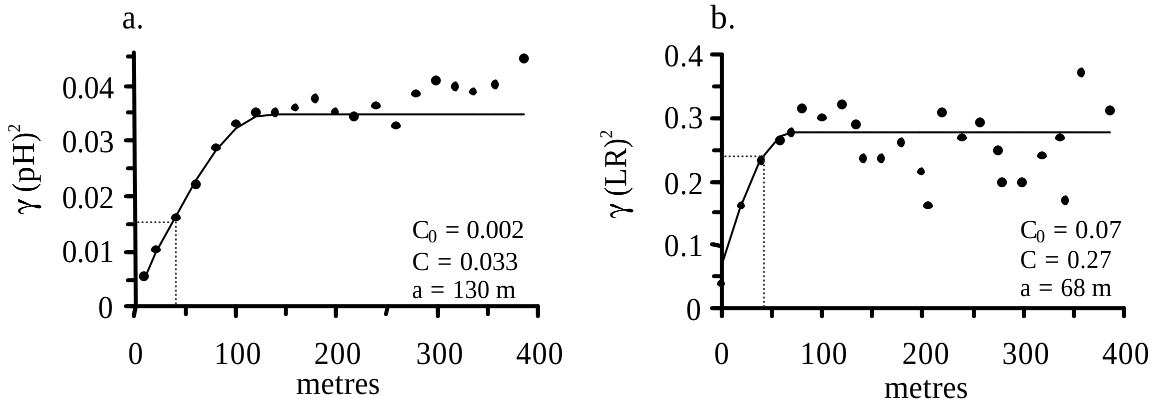

Figure 3.5 (a.) pH_{CaCl_2} and (b.) lime requirement (LR) semi-variograms and model parameters

From Figure 3.5a, the expected kriging variance for pH_{CaCl_2} must lie between 0.002 the nugget value and 0.033 the sill, which is equivalent to a range in standard errors of 0.04 to 0.18 pH_{CaCl_2} units. Setting a maximum permissible error of 0.1 pH_{CaCl_2} units and considering the pH_{CaCl_2} range along the transect (Figure 3.4b), resulted in an equivalent variance of 0.016, and an optimal sampling interval of approximately 40 m. The pH_{CaCl_2} transect (Figure 3.4b) and corresponding variogram (Figure 3.5a) hinted at the presence of trend in the pH data.

The equivalent ranges in standard errors for LR(6.0) were 0.26 to 0.53 Mg/ha. A maximum permissible error of slightly under 0.5 Mg/ha, results in an equivalent variance is 0.24 Mg/ha, and an optimal sampling interval of approximately 40 m. Note that the chosen 40 m grid interval spacing is well within the range of spatial dependence for both variograms in Figure 3.5. The sampling layout sample collection and bulking strategy for the experimental field is shown in Figure 3.6 below.

Two separate bulked samples (replicates) were collected at a depth of 0.25 m for analysis at each of the 122 grid nodes (Figure 3.6a) resulting in a total of 244 samples. The bulking strategy at each node consisted of combining five soil cores 1 m apart into one bulked sample (Figure 3.6b). The analytical results are shown in the proceeding section of this chapter.

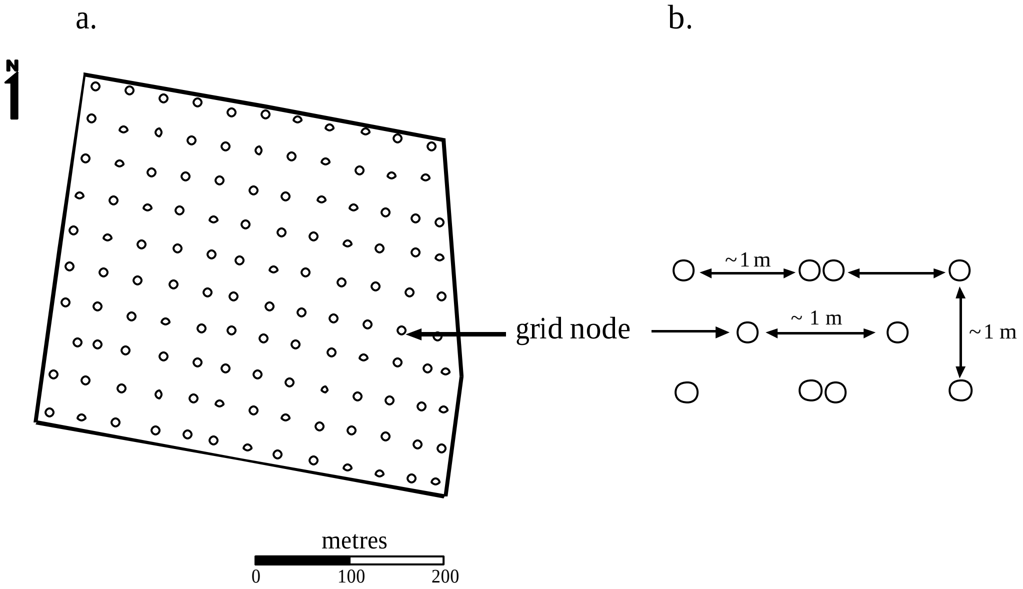

Figure 3.6 (a.) 40 m grid soil sampling layout and (b.) bulking strategy at each grid node. Total of 122 samples in duplicate (*i.e.* 244 samples in total).

3.3 SOIL ANALYSIS

After collection the soil was oven dried, ground and sieved to a size fraction < 2 mm, and sub-sampled for analyses. Soil pH was measured in a 1:5 soil solution ratio in both 0.01M $CaCl_2$ and H_2O (White, 1969). Although measurements in a solution of 0.01M $CaCl_2$ are preferred by many authors (Adams, 1984; McLean & Brown, 1984) pH measurements in water were made since it is probably the more common method of analysis in laboratories. Lime requirement was determined using the SMP buffer procedure (Shoemaker *et al.*, 1961), The Mehlich buffer method (Mehlich, 1976), the Woodruff buffer (Woodruff, 1948) and the New-Woodruff buffer method (Brown & Cisco, 1984). Organic matter was determined using the dichromate oxidation method of Walkley & Black (1934). Cation exchange capacity (CEC) was measured using the

$(AgTU)^+$ method and exchangeable aluminium by the 1M KCl method, both described in Rayment & Higginson (1992). Nitrate nitrogen, available phosphorus (Colwell) and exchangeable potassium were measured colorimetrically using procedures described in Rayment & Higginson (1992).

Clay content was determined using the hydrometer method described by Gee & Bauder (1986). Water content and field soil bulk density were determined using the methods described by Klute (1986).

3.4 SURFACE SOIL PROPERTY STATUS

As previously mentioned, soil analytical results provide information about the rhizosphere and its ability to support plant growth. The soil from the experimental field was analysed for a multitude of agronomically relevant chemical and physical attributes, whose results served as indicators of soil condition and were used in the analytical portions of subsequent chapters. The soil property distributions and characteristics are described in the following sections.

3.4.1 SOIL CHEMICAL PROPERTIES

Table 3.3 provides a summary of the distributions of soil chemical attributes relevant to the work presented here. The soil from the experimental field ranged from acidic to very acidic, was low in organic carbon, nutrients and CEC, had toxic levels of aluminium for plant growth and required relatively large amounts of lime (Table 3.3). Chapters VIII and IX deal with amelioration of this acid-induced infertile soil.

Table 3.3 Surface soil chemical properties and recommended ranges for optimal plant growth

Chemical properties	Mean	S.D.	Median	CV	Range	Recommended
pH_{CaCl_2}	4.37	0.25	4.34	5.83	3.90 - 5.38	*6 - 7*
pH_{H_2O}	5.29	0.27	5.25	5.01	4.78 - 6.30	
Buffer-pH_{SMP}	6.55	0.13	6.56	1.92	6.13 - 6.81	
LR_{SMP}(6.5) Mg/ha	3.36	1.33	3.22	39.45	0.59 – 7.75	
Buffer-$pH_{Mehlich}$	5.85	0.1	5.86	1.75	5.52 - 6.08	
$LR_{Mehlich}$(6.5) Mg/ha	6.39	1.33	6.34	20.83	3.13 – 10.99	
Buffer-$pH_{Woodruff}$	6.61	0.07	6.61	1.12	6.37 - 6.76	
$LR_{Woodruff}$(6.5) Mg/ha	7.14	1.58	7.13	22.07	3.76 – 12.07	
OC dag kg^{-1}	1.32	0.28	1.3	21.54	0.78 - 1.98	*> 3*
NO_3-N^* mg kg^{-1}	3.25	3.56	1.9	109.42	0.9 - 15	*> 30*
P_{Col}^* mg kg^{-1}	14.94	4.79	15	32.03	6 - 29	*17 – 25*
K^* mmol(+) kg^{-1}	5.44	2.45	5	45.09	1.5 - 13	*3 - 20*
Ca^* mmol(+) kg^{-1}	23.92	8.17	22	34.15	11 - 46	*> 50*
Al^* mmol(+) kg^{-1}	1.78	1.31	1.3	73.92	0.2 - 7.7	*< 2*
Al^* %	5.32	4.59	3.68	86.28	0.48 - 23.33	*< 5*
CEC^* mmol(+) kg^{-1}	38.8	11.46	36	29.57	22 - 72	*120 - 400*
E.C.* mS m^{-1}	4.29	1.19	4	27.67	2 - 7	*0 - 30*

Note: where properties are marked with * $n = 51$, otherwise $n = 244$

3.4.2 SOIL PHYSICAL PROPERTIES

Table 3.4 provides a summary of the distributions of soil physical attributes in the experimental field.

Table 3.4 Surface soil physical properties

Physical properties	Mean	S.D.	Median	Range
Clay dag kg^{-1}	14.1	2.9	14.0	8.0 – 24.0
Sand dag kg^{-1}	70.6	5.1	69.7	58.0 – 84.0
Bulk density* g cm^{-3}	1.67	0.11	1.70	1.60 - 1.85
Water Content* g g^{-1}	0.15	0.02	0.16	0.12 - 0.18
$Solid_V{}^*$ % (m^3m^3 × 100)	63.3	4.1	62.4	58.4 - 69.7
$\theta_V{}^*$ % (m^3m^3 × 100)	25.9	3.2	26.8	20.4 - 29.5
$Air_V{}^*$ % (m^3m^3 × 100)	10.8	6.5	11.8	1.9 – 20.0
Porosity*	36.7	4.1	37.6	30.3 – 41.6

Note: where properties are marked with * $n = 10$ otherwise $n = 122$

The soil texture class of the field ranges from a loam to a silty-loam to a sandy-clay-loam. At the time of sampling, and under those moisture conditions, the average volume fraction of air was only slightly higher than the 10 % critical value required for unimpeded plant growth (Table 3.4). Although the average bulk density was moderate, it was at the critical value for unimpeded plant emergence for the corresponding texture classes and water contents of the field (Table 3.4). Bulk density values were used for lime requirement calculations to a depth of 20 cm of soil (Chapter VIII), and in the liming of pots in the glasshouse experiment (Chapter IX).

3.5 SPATIAL VARIABILITY OF FIELD SOIL CHEMICAL PROPERTIES

Soil scientists study soil by sampling, usually by random or grid sampling (refer to Chapter II) and the prediction of values at unsampled locations is dependent on the degree of spatial dependence (as determined by the semi-variogram) that exists amongst samples. In general, the larger the sampling area, the higher the attribute variance and hence the greater the dissimilarity between samples.

Table 3.5 shows the variogram models and parameters for the various soil chemical properties from the experimental field.

Table 3.5 Description of the spatial variability of soil chemical properties in the experimental field

Property	Model	C_0	C_1	C_0/C_0+C_1	a	ω
$pHCaCl_2$ (units)^2	Exponential	0.02	0.13	0.15	677	
	Linear	0.026				0.00013
OC (dag/kg)^2	Exponential	0.031	0.18	0.15	862	
	Linear	0.0238				0.0002
CEC (mmol(+)/kg)^2	Spherical	37.5	116.6	0.24	267	
Ca (mmol(+)/kg)^2	Exponential	15.2	66.6	0.19	127	
Al (mmol(+)/kg)^2	Spherical	0.2	1.4	0.13	279	
NO_3^- (mg/kg)	Spherical	10	3.38	0.75	86	
P (mg/kg)^2	Spherical	6.1	18.3	0.25	171	
K (mmol(+) kg^{-1})^2	Spherical	0	7.65		273	
		C_0	C_1	a_1	C_2	a_2
LR(6.5) (Mg/ha)^2	Double exponential	0.15	1.02	27	120	10000

The semi-variogram models and parameters for the various soil chemical attributes listed in Table 3.5, describe their spatial variability in the experimental field and will be used in proceeding chapters for interpolation and map production.

The proportion of the nugget variance to the sill variance (C_0/C_0+C_1) illustrates the short-range variability of the soil as well as the inaccuracies of the sampling and analysis methods (Chapter II). For lime requirement, a double exponential semi-variogram model (Equation 4.2, Chapter IV) was fitted to the experimental data and the ratio C_0/C_0+C_1 was 0.13. The only property with an extremely large proportion of nugget variance was nitrate, indicating the inappropriateness of the sampling strategy and analytical methodology (Table 3.5). The ranges of spatial dependence for the attributes shown in Table 3.5 varied from 86 m for nitrate to 279 m for aluminium.

The semi-variograms for pH_{CaCl_2} and OC (Table 3.5) indicate the presence of spatial drift in the data. The ranges of the transitive semi-variograms far exceed field boundaries. So unbounded linear models were also fitted. The spatial modelling and mapping of these trended data is dealt with in Chapter V.

3.6 CONCLUDING REMARKS

This chapter provides a general description of the environment and the farming systems in the region surrounding the farm and field of experimentation. In more detail, it provides the reader with quantitative descriptions of the field site, soil condition at the time of sampling, and the spatial variability of surface soil chemical properties that are relevant to the management of acid soil. It also describes the methods of sampling and laboratory analyses. The descriptive statistics of the data provide the basis for the work being presented.

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Chapter IV

PRECISION AGRICULTURE AND ITS IMPLICATIONS FOR SOIL SAMPLING AND ANALYSIS

ABSTRACT

Soil is variable. Traditionally, descriptions of this variability have involved discrete soil sampling and subsequent laboratory analysis. Now that greater quantities of soil data are needed for the formulation of site-specific management decisions using precision agriculture techniques, conventional methods of sampling and analysis are proving to be slow, tedious and costly. Methods that reduce the time, cost and labour, and also improve the accuracy of current techniques are needed. For this purpose it is imperative that soil analytical chemistry becomes field-based and that 'on-the-go' proximal soil property sensing and scanning systems be developed. This chapter discusses the implications that precision agriculture has for current methods of sampling and analysis. The variability of a number of agriculturally important soil chemical properties was investigated and the 'nugget' variance discussed in terms of its importance in determining the proportion of not only short-range spatial variation, but also sampling and measurement error, and its implications for the development of proximal sensing systems. Comments are made on the accuracy of current laboratory methods. Analytical variances are compared with world-average and estimated nugget variances for the experimental field. The comparison shows that analytical precision needs to be maintained or improved when developing proximal sensing systems or adapting analytical methods for use in precision agriculture. Cost comparisons shows that soil chemical analytical costs are much too large for economic use in precision agriculture, costs in Australia being higher than in the USA. The negative effect of decreasing sampling resolution on the production of variable-rate lime application maps is illustrated. The advantages of using an 'on-the-go' proximal soil electrical conductivity sensing system are demonstrated. The conclusion this chapter draws is that, for large-scale implementation of precision agriculture, the development of field-deployed, 'on-the-go' proximal soil sensing systems and scanners is tremendously important. These sensing systems or scanners should aim to overcome current problems of high cost, labour, time and to some extent, imprecision of soil sampling and analysis to more efficiently and accurately represent the spatial variability of the measured properties.

4.1 INTRODUCTION

Soil may be regarded as a non-renewable resource that is highly variable and extremely complex, particularly from a chemical standpoint. It is imperative that we get the best possible understanding of the nature, properties and interactions of our soil, if we are to make the most efficient use of it for food and fibre production and simultaneously preserve it for future generations (Chapter I). Soil sampling and analysis have traditionally been the tools used to gain this understanding, where the resultant information is used as a reliable description of the area of interest. Although these traditional methods of soil sampling and analysis have aided our comprehension of soil, there are improvements that need to be made, particularly now that a larger amount of accurate and precise soil information is required for managerial decision-making (Chapter II).

Precision agriculture (*e.g.* Lake *et al.*, 1997, Chapter II) demands accurate, rapid and economical methods to obtain information on the fine-scale spatial variability of soil (Conceptual Basis of the Research and Aims; Chapter II). However sampling and laboratory testing is slow, tedious and much too costly because vast quantities of data are essential for the formulation of site-specific management decisions. These procedures may also be inaccurate and produce imprecise results, especially if the methods are not quantitative, or if conducted incorrectly. Precision agriculture needs not only that conventional methods of soil sampling and analysis be improved or replaced by techniques that reduce the time, cost and labour required, but also improve the accuracy and maintain, or better still improve the precision of results. For example, McCauley *et al.* (1993) indicated that a visible-wavelength ‘on-the-go’ soil OM sensing system produced better results than laboratory dichromate analysis (Chapter II). They proposed that the finding was to be expected because dichromate oxidation is the least quantitative technique used to determine soil OM.

One of the imperatives of PA is for soil analytical chemistry to become field-based (McBratney *et al.*, 1996). This is a view shared by many researchers working on the development of field-based proximal sensing and scanning systems for various chemical soil properties. The latter portion of Chapter II reviewed emerging proximal soil sensing systems for PA. Sudduth *et al.* (1997) also looked at the necessity for sensors in PA and inferred that there is a tremendous need for the development of automated sensing technologies. However, the state of development of soil sensors or sensing systems for agriculturally relevant soil properties varies considerably, and while some of these are well on their way to commercialisation, much research and development effort is still required. In the mean time, interim solutions to the sampling problem need to be addressed to overcome the shortcomings of current discrete sampling methods.

This chapter contains six sections. The first discusses the implications of soil sampling on analytical results; the second proposes routine soil chemical analysis for PA; the third compares the accuracy and precision of current laboratory methods; the fourth compares the cost of analysis in Australia and in the USA. The fifth section compares the effect of sampling size on map production and the sixth section describes the use of the VERIS 3100 ‘on-the-go’ proximal soil sensing system.

4.2 IMPLICATIONS OF SOIL SAMPLING ON ANALYTICAL RESULTS

In deciding upon a sampling strategy it is important to keep in mind that the accuracy of analytical results is ultimately determined by the accuracy of the sampling procedure and the way in which samples are handled after collection. There are differing opinions amongst soil scientists on what the best sampling method is, to obtain an adequate description of the field soil properties and their spatial interactions. Brus & de Gruijter (1997) produced a comprehensive discussion paper that described and compared the performance of ‘design-based’ and ‘model-based’ sampling strategies. These strategies may be defined by their source of randomness (Brus & de Gruijter, 1997). Briefly, in a design-based strategy that uses classical sampling designs and inference, the sample locations x_i are selected using a random selection procedure, while the value of s at any given location and time is regarded as fixed. In a model-based strategy the sample locations are assumed to be fixed and the value of the soil property s at each location random, thus forming a random variable $s(x_i)$. The observed value at x_i is regarded as a realisation of the random variable.

Since the late 1970s and coinciding with the adoption of geostatistics by soil scientists, there has been much research in trying to describe and quantify the spatial variability of soil (Campbell, 1978; Burgess & Webster, 1980; Burgess *et al.*, 1981; Yost *et al.*, 1982; Trangmar et. al., 1985; Webster & McBratney, 1987; Webster & Oliver, 1990; Goovaerts & Chiang, 1993). Mostly, the procedures involve first determining the experimental variogram and then observing the implications it has for sampling and estimation. The advantages of using geostatistics for planning soil sampling designs were described by Burgess *et al.* (1981); McBratney & Webster (1983) and Webster & Burgess (1984). Webster & Oliver (1990) showed how to apply classical statistical theory to obtain a ‘good sample’ from an area, and detailed various commonly used sampling designs. A number of these, their advantages and disadvantages from a PA point of view are reviewed in Chapter II.

Lark (1997) suggested that in some instances the cost and effort of sampling and analyses needed to estimate the semi-variogram before deciding on a sampling design, has prevented the adoption of geostatistics by soil scientists. This also applies to PA. Webster & Oliver (1990) proposed that robust semi-variogram estimation require at least 100 data points. Webster & Oliver (1992) stated that a semi-variogram computed from 152 points would generally be satisfactory, while one from 225 data will be reliable. Gascuel-Odoux & Boivin (1994) found similar results and suggested that the consistency of both experimental and theoretical semi-variograms increases with sample size. In their case 150 data points found this consistency. The implication is that the number of samples needed to estimate the variogram in advance of full-scale sampling might be a serious obstacle to adoption for farming enterprises.

If cost and effort are a prohibitive for reconnaissance sampling, it may be useful to use median semi-variogram parameters from databases (*e.g.* for soil pH, shown in Table 2.2 of Chapter II) to determine optimal sampling designs, and resolution. McBratney & Pringle (1999) proposed another alternative and suggested the use of average and proportional semi-variograms to overcome the cost and effort of reconnaissance sampling. They calculated the average and proportional semi-variograms (proportional where appropriate) from semi-variograms gathered from the literature. Pettitt & McBratney (1993) proposed the use of stratified random transect sampling in different directions to overcome cost and effort of sampling. The technique has properties that are intermediate between design-based and model-based strategies.

Presently in PA, systematic (*e.g.* square grid) sampling of agricultural fields combined with geostatistics (the model-based approach) is thought to be the best method to derive accurate representations of field soil. Hence most accurate for deriving variable-rate input application maps. However, as previously mentioned, a major obstacle is the cost and effort associated with sampling and analysis.

Although model-based sampling has often been suggested as the more appropriate sampling method, Brus & de Gruijter (1997) showed that the design-based approach is also a valid methodology for spatial sampling and estimation. They showed that soil scientists have generally dismissed the approach since the introduction and application of geostatistics in soil science (see previous paragraph). Brus & de Gruijter wrote that the design-based strategy is dismissed by soil scientists based on the false assumption of independence (they point to particular examples in the literature, including the work by McBratney & Webster (1983)), and that hence model-based strategies were thought to be optimal. The authors indicated that in design-based sampling independence is determined by the sampling design, and hence has a different meaning to that in the model-based approach. In the model-based sampling independence is determined by the postulated model for the process studied (Brus & de Gruijter, 1997). Brus & de Gruijter (1997) provided a decision tree to help choose between design-based and model-based sampling strategies. The tree asks the practitioner to consider aspects such as the type of request, the importance of objectivity in the estimates, the need for separate estimates of the estimation variance for all points or subregions, the interest in valid and accurate estimates of the estimation or prediction variance, the quality of the model, the strength of autocorrelation between points and the sample size. Their paper does not suggest that one technique is better than the other, certainly there are different circumstances where each of the techniques is applicable, instead it provides some quantitative indicators of the efficiencies of both. The authors concluded that the use of design-based strategies should be given more attention.

4.2.1 AN INTERIM APPROACH TO SAMPLING FOR PRECISION AGRICULTURE

Design-based and/or model-based sampling are both inefficient in PA because of the high cost incurred by sampling and analysis. In the absence of more cost-effective and efficient methods to collect soil information, an interim approach between uniform within field management and continuous site-specific management has been developed in the USA and Europe. It is thought to encompass an alternative (biased) sampling scheme that aim to reduce the number of sampling sites and associated costs and labour (Figure 4.1).

This approach which may be termed ‘zone’ or ‘patch’ management is based on dividing fields into smaller zones based on fine spatial scale data such as yield (acquired using yield monitors), proximal soil sensors (e.g. VERIS 3100), surface reflectance, remote sensing and digital elevation models. Sampling is performed within the zones and is followed by the delineation of management units. This technique has been euphemistically called ‘smart farming’. Chapter II reviewed this and other sampling techniques for PA.

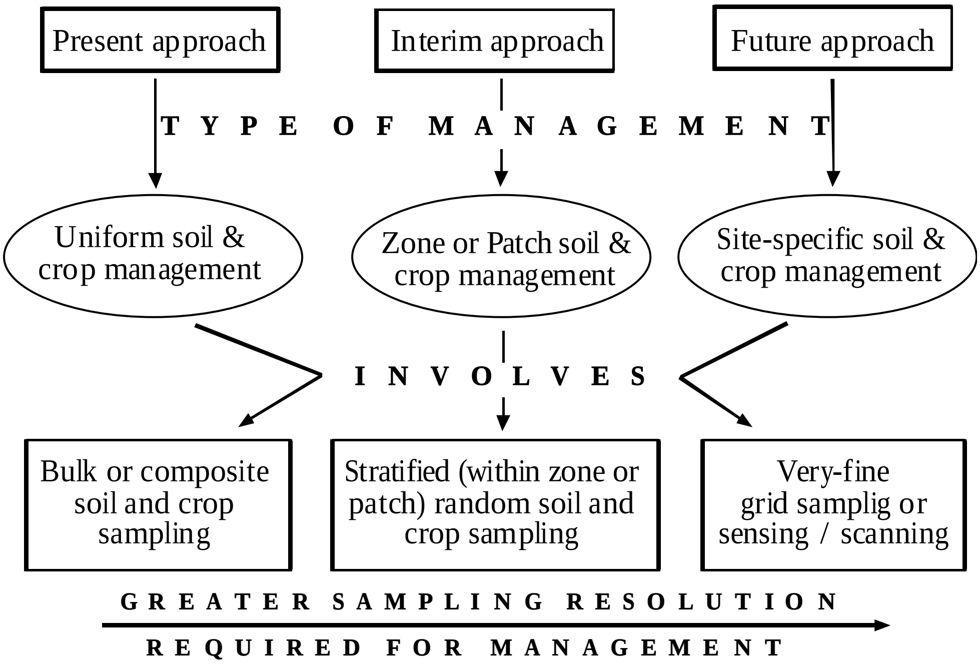

Figure 4.1 Management systems and required sampling schemes: Uniform, selective and continuous soil and crop management.

4.2.2 SAMPLE COLLECTION AND HANDLING

Consideration of sample size and method of sample collection is also necessary for accurate representation of field soil. McBratney & Webster (1983) demonstrated a method for determining the number of observations required for accurate representation of the sampling unit, taking into account the spatial dependence of soil properties. Sampling and bulking strategies were discussed by Webster & Burgess (1984). A method to determine the number of cores required for bulked sampling of soil by first estimating the variogram is suggested by Oliver *et al*., (1997).

Sample handling after collection is also important, especially for properties such as nitrogen or ammonium nitrate, for in these cases samples should be cooled as quickly as possible after collection to prevent further microbial activity. Failure to do so results in inaccurate analytical results as microbial activity may produce changes in the concentrations of these nutrients.

Sample preparation also requires proficient handling because before analysis the soil sample has to be dried, ground and sieved, before a sub-sample is taken for analysis. These stages provide further opportunities for laboratory-induced variability, which may result in unreliable analytical data.

Correct, unbiased soil sampling is hence essential for reliable laboratory analysis since analytical results are expected to be representative of the field soil status (Melsted & Peck, 1973). Therefore the sampling strategy needs to be designed in such a way that laboratory analysis of the collected soil samples may accurately reflect the true ambient and nutritional spatial variability within the field.

4.3 ROUTINE SOIL CHEMICAL TESTS FOR PRECISION AGRICULTURE

Through the analysis of a soil's chemical properties, we are able to draw some conclusion on that soil's environment and the availability of nutrients required for the growing crop to be able to realise its full potential. The soil chemical properties of most interest in PA include pH; mineral nutrients - particularly the macronutrients nitrogen (N), phosphorus (P) and potassium (K); organic matter (OM), and cation exchange capacity (CEC). These properties should be part of routine chemical analysis for PA, while properties such as soil electrical conductivity (EC), and lime requirement (LR) should be measured as required.

4.3.1 SOIL PH

Soil pH is an important property that measures the intensity of the soil's acidity or alkalinity, and as such is one of the most indicative measurements of the soil's chemical properties and condition. The pH of a soil is highly related to the solubility and therefore availability for plant uptake of various compounds, the relative bonding of ions to exchange sites, and the activities of various micro-organisms. Of particular interest to agriculture are the pH dependent symbiotic interactions of *Rhizobia* and host legumes. Therefore soil pH is indicative of the soil's condition and is also the causative factor of many reactions occurring in soil. With the advent of the glass electrode and much improved electronics, pH has become one of the most rapid, simple and therefore widely employed soil analytical procedures (White, 1969). McLean (1982) describes the various methods used to determine soil pH.

4.3.2 ORGANIC MATTER

Organic matter (OM) is a complex soil property important for crop production. Its abundance will have implicating effects on various processes occurring in the cropping system, including nutrient availability. For example it may directly influence the amount of fertiliser and herbicide that should be applied for a crop to succeed. Therefore the amount of organic matter in soil is routinely described when conducting chemical analysis, however its quantification is often difficult and subject to error. Nelson & Sommers (1982) describe the various techniques available for determining the organic matter content of soil.

4.3.3 MINERAL NUTRIENTS - PARTICULARLY N, P, K

Soil mineral nutrients, particularly N, P, and K are important factors affecting crop growth. If ignored when making management decisions, deficient amounts of these will result in much reduced crop growth, yield and quality while all other input costs will nevertheless still be incurred (Carter, 1992). Accurate diagnosis and subsequent amendment of mineral deficiencies in soil is vital to the production of quality crops. Inaccurate diagnosis will result in the placement of incorrect amounts of fertiliser, leading to not only economic loss but also in some cases, environmental pollution. Common analytical procedures for determining total soil nitrogen are outlined by Bremner & Mulvaney (1982); organic nitrogen by Stevenson (1982); and inorganic nitrogen by Keeney & Nelson (1982). Keeney & Nelson (1982) also discuss the use of ammonium and nitrate specific ion electrodes for determining the inorganic nitrogen content of soil. Methods for determining total soil phosphorus, organic phosphorus, fractionation of soil phosphorus and some indices of phosphorus availability are reported in Olsen & Sommers (1982). Some of the procedures used to estimate potassium fertiliser needs are outlined in Knudsen *et al.* (1982).

4.3.4 CATION EXCHANGE CAPACITY

The cation exchange capacity (CEC) of a soil is a measure of the quantity of readily exchangeable cations neutralising negative charge in the soil. Thus it provides information on the ability of the soil to retain ions, of particularly interest are those which are plant nutrients. The various methods used to determine the CEC are outlined in Rhoades (1982); and exchangeable cations in Thomas (1982). Sources of error in conventional CEC determinations are described in Rhoades (1982).

4.4 ACCURACY AND PRECISION OF LABORATORY METHODS

Schnug (1997) gave a definition of accuracy and precision for analytical quality. The accuracy and precision of analytical results are directly related to the sampling, handling and analytical procedure of the system. The accuracy of the analytical results is considered as the proximity to the true value. It relies on the choice of certified, referenced analytical method and valid calibration of the measurement instrument

(Houba *et al*., 1996a, b). The precision of the analytical results describes the error or reproducibility of results. Analytical precision may be improved by proficient laboratory discipline and in-house control mechanisms (Schnug, 1997). Inaccuracy (measured by the root mean square error) may be defined as containing both bias (measured by the mean error square) and imprecision terms:

$$inaccuracy^2 = bias^2 + imprecision^2 \tag{4.1}$$

This equation is similar to the one given by Kempthorne & Allmaras (1965).

Hence the accuracy of analytical results also encompasses the precision and bias of analyses. As such, PA should perhaps be better named ‘Accurate Agriculture’? Table 4.1 shows the imprecision of analytical results as measured by the variance of repeated analyses for various soil chemical properties in a number of studies.

Table 4.1 Published analytical variances for soil chemical analyses

Property	pH		C (dag/kg)	N (mg/kg)		P (mg/kg)		K (mg/kg)
	v^2		v^2	v^2		v^2		v^2
Loveday (1974)			0.002				1.2	
Tchuenteu & Ngakanou (1994)	0.006	0.009	0.009				5.492	
Quaggio *et al.* (1994)		0.017					11.56	
		0.01					4.41	
		0.005					2.496	
Miller *et al.* (1996)	0.04	0.053	0.044	1.96	6.25	4.41	9	1445
	0.036	0.053	0.044	0.25	2.25	8.41	9	1369
	0.044	0.053	0.044	1.96	6.25	4.41	9	1444
Wolf *et al.* (1996)		0.028						948.64
Mean variance (v^2)	0.0295		0.0287	3.153		6.308		1301.66

4.4.1 SPATIAL VARIABILITY OF FIELD SOIL CHEMICAL PROPERTIES

The soil chemical properties whose spatial variability is of particular relevance to agricultural management are pH, organic matter, nutrients (N, P, K), CEC (and constituent cations), and in certain instances electrical conductivity and lime requirement. When required, knowledge of how these properties vary in an agricultural field aids with the formulation of management maps for site-specific resource application or remediation. Moreover, their spatial variability is relevant because of the direct or indirect effects they have on crop yield.

Spatial variability of soil chemical properties occurs in both horizontal and vertical directions, and may be initially explained by the various processes and reactions that occur during the formation of soil. The main factors interacting and causing this variability are parent material, climate, time, topography and soil organisms (Jenny, 1941; Chapter I). Although one of the aims of cultivation is to make soil less variable, (*e.g.* Cattle *et al.* (1994) demonstrated that cultivated soil was more homogeneous than that which is in its natural state), further variability may be introduced by agricultural practices. For example, variability resulting from nutrient uptake, leaching, and management practices that change the chemical balance of the soil such as fertiliser and lime applications. Bouma & Finke (1993) noted that uneven fertiliser spreading can further increase the spatial variability of soil nutrients. In the case of soil organic matter, Jenkinson (1988) suggested that it may vary according to the spatial variation of the factors that affect its accumulation and decay, namely pH, soil water, oxygen availability, soil texture and management.

McBratney & Pringle (1999) summarised published research describing and comparing the magnitude of variability in soil properties relevant to PA. The soil chemical properties described in the study include pH, organic carbon, nitrate-nitrogen, phosphorus, potassium and organic carbon. The spatial variability of soil organic matter has also been reviewed and summarised by McCauley *et al.* (1993).

4.4.2 SHORT-RANGE OR 'NUGGET' VARIATION

Semi-variograms in soil science describe the spatial variability of soil properties as a function of distance. Plotting the average semi-variance against the lag distance separating pairs of observations derives a semi-variogram. The review in Chapter II provided the mathematical derivation of the semi-variance $g(h)$, and the various models that may be fitted to the experimental data to describe the semi-variogram. The parameters of interest in a semi-variogram were shown in Figure 2.1 of Chapter II. The following will elucidate the implications of the nugget variance C_0 on sampling and analysis.

Initially the terms 'nugget variance' and 'nugget effect' were interchangeably used to refer to the spatial variability of gold bearing deposits (Journel & Huijbregts, 1978). However they have now been generalised and are commonly used in the geostatistical vocabulary to represents the unexplained, random variance often caused by very short-range spatial variation (much shorter than the sampling interval) and sampling and measurement errors (Chapter II). Thus, the presence of nugget variation implies that the shortest sampling interval is larger than the range of spatial dependence, or that there is sampling and measurement errors, or both. The nugget effect is of particular interest to the topic of this research.

Pitard (1994) described the nugget phenomenon with reference to ore exploration, nevertheless it may apply to soil science. Pitard (1994) noted that the 'nugget effect' is the result of at least seven types of variability. The first type of variability is that of the true in-situ, fine-resolution random variability. The second through to fifth types describe variability components that may arise during all sampling and sub-sampling stages such as fragmentation, segregation, selectivity and poor sample recovery. The sixth type describes the variability component that may arise from sample or sub-sample handling and preparation after collection such as contamination, loss, alteration of chemical properties and human error. The final type of variability is described as that introduced by the analytical technique. Pitard (1994) added that precision problems or error in analytical techniques would with no doubt inflate the nugget variance. A proportion of the nugget variance is therefore partly due to sampling and measurement error, and Burrough (1993) suggested that as such, the nugget variance sets a lower limit to the precision of the sampling and analytical technique employed. Therefore, the prevention of sampling biases and analytical imprecision are important in soil science and PA.

Having discussed the nugget variance and the factors that contribute to it, some of its implications for analytical precision will now be educed. The analytical variance can only be smaller than or equal to the nugget variance ($\nu^2 \leq C_0$), since analytical error is an integral component of the nugget variance. If the analytical variance is equal to the nugget variance ($\nu^2 = C_0$), then it must be the only factor contributing to the nugget effect. Therefore in this case, the precision of the analytical method employed needs to be improved to allow detection of the other contributors to the nugget variance and the spatial relationships. On the other hand, if the analytical variance is smaller than the nugget variance (v^2 < C_0), then other factors such as those previously suggested, must also be contributing to the nugget effect. If the analytical error variance is much smaller that the nugget variance (v^2 << C_0), then more samples should be collected since insufficient sampling and sampling error may be largely contributing to the nugget variance. Table 4.2 shows a comparison of nugget and analytical variances for some important soil chemical properties.

Table 4.2 Comparative summary of variogram models (after McBratney & Pringle, 1999), nugget variances and analytical variances for a number of soil chemical properties

Property	pH	C^E (dag/kg)^2	NO_3-N^E (mg/kg)^2	P^E (mg/kg)^2	K^E (mg/kg)^2
Best model^A	1	3	2	3	4
Mean	4.567	0.983		7.1 - 15.3	254
Nugget variance (C_0)					
World-average^B	0.0358	0.0126	1.71	3.364	2490
Estimated^C	0.0117	0.005		4.917	11466
Analytical variance (v^2)					
Published^D analytical	0.0295	0.0287	3.153	6.308	1301
Estimated analytical	0.0067	0.0067		5.208	10956

Note: C_0 denotes the nugget variance

[A] proportional variogram models: 1 = average spherical; 2 = constant nugget, proportional spherical; 3 = proportional nugget, proportional spherical; 4 = proportional nugget, proportional exponential as in McBratney & Pringle (1999)

[B] estimated from equations given by McBratney & Pringle (1999)

[C] estimated nugget variance from the experimental field at Kelso, NSW, Australia.

[D] averaged analytical variance from a number of studies as shown in Table 4.1

[E] properties whose variances depend on the mean value as given.

The ensuing implication of Table 4.2 is that if soil analytical techniques are to be improved and adapted, or fully developed for PA, for most of the soil chemical properties listed, they should yield no less precise results than they do now. That is, the precision obtained by current analytical methods should be maintained or improved. For example by comparing 'published analytical v^2' with 'world-average C_0' in Table 4.2: for soil pH and potassium, current analytical methods appear to be sufficiently precise, while for organic carbon, nitrate and phosphorus, improvements in the precision of current analytical techniques should be considered when developing more efficient analytical methods, or proximal sensing systems for use in PA. McCauley *et al.* (1993) suggested that determinations of soil organic matter by laboratory dichromate oxidations were imprecise. They also suggested that the development of soil sensing systems should aim to measure short-range variability as closely as possible as the information may aid with interpolation and map making for the application of input resources. The work by McCauley *et al.* (1993) is reviewed in Chapter II.

The relative similarity of the ‘estimated C_0’ and ‘estimated analytical v^2’ for organic carbon and phosphorus in Table 4.2, indicates that for these properties the analytical variance makes up the nugget variance almost entirely. However it is important for the reader to note that the figures on Table 4.2 are only considered to be indicative estimates.

4.5 CURRENT COST OF ANALYTICAL TECHNIQUES

Fine-scale characterisation of the degree and extent of spatial (and temporal) soil variability is needed for accurate agricultural management. Whelan *et al.* (1996) suggested that for PA, management units of 10 m or less may be required. McBratney & Pringle (1999) calculated the expected kriging confidence limits that may result from various combinations of sample spacings and site-specific management block sizes, for different soil properties. Similarly, Table 4.3 shows the sample spacing required to achieve certain confidence if implementing site-specific management on 10 m and 100 m blocks. Table 4.3 also shows the corresponding number of samples and the analytical costs (for the soil properties shown in Tables 4.1 and 4.2), in Australia and the USA.

Presently, the implementation of PA in broadacre cropping systems is uneconomical because the cost of soil (sampling and) chemical analysis is very high (Table 4.3). For example from Table 4.3, if a wheat farmer in the wheat-belt of NSW, Australia, wants to apply lime differentially across a 50 ha field by managing 10 m × 10 m blocks, he would need to sample on a 30 m grid to obtain a resolution of ±0.25 pH units. The number of samples required subject to these specifications would be 555. Analytical costs for that field, not including sampling, sample preparation and handling/delivery costs, would be A$ 10 212 (a reasonable approximation). Obviously these would be much larger if sampling and other costs were included. The implication emphasised in Table 4.3 is that unless methods that reduce the costs of sampling and analyses are devised, PA will not develop from its present embryonic stage into an economically and environmentally sustainable management system.

Table 4.3 Examples of sample spacing, and analytical cost in Australia and the United States (in A$) to perform kriging to a sufficient accuracy

		Required sample spacing (m), number of samples and analytical cost (A$) for a 1 ha field if wanting to manage 10 m or 100 m blocks							
Property	95% C.I.	10 m blocks	No. samples	Cost A$[a]	Cost USA$[b]	100 m blocks	No. samples	Cost A$	Cost USA$
pH	±0.25	30	11.1	204	56	100	1	18	5
C[c] (dag/kg)	µ ± 10%	22	20.7	460	151	78	1.6	36	12
N[c] (mg/kg)	µ ± 10%	<10	>100	>2,290	>950	40	6.2	185	59
P[c] (mg/kg)	µ ± 10%	<10	>100	>2,250	>670	34	8.7	196	58
K[c] (mg/kg)	µ ± 10%	18	30.9	599	207	68	1.4	27	9

Note: sampling costs, sample preparation and delivery are added costs not taken into account.

[a] Average and range of analytical costs in Australia (per sample); pH $18.4 ($8 - $35); C $22.2 ($10 - $23); NO_3-N $29.9 ($12 - $44); P $22.5 ($10 - $35); K $19.4 ($8.7 - $35)

[b] Approximate analytical costs in the USA (per sample): pH $5; C $7.3; NO_3-N $9.5 , P & K $6.7ea.

[c] Sample spacings shown depend on the mean value and hence will change with the mean (as in McBratney & Pringle, 1999).

Precision agriculture requires vast amounts of information on the soil properties which are relevant to crop growth. Evidently, collection of large amounts of representative data through sampling and analysis is difficult and uneconomical. How can we increase efficiency and reduce costs? The suggestion made in this work and certainly by various researchers worldwide is that the development of methods for the complete enumeration of crop and soil properties by remote and particularly proximal sensing systems is essential.

4.6 EFFECT OF SAMPLING INTENSITY ON MAP PRODUCTION

As previously discussed, sampled information and spatial prediction methods are used to predict values at unsampled locations. The maps produced are presumed to be reliable descriptions of the spatial variation in the area of interest. Although the maps may appear plausible, their quality and reliability will depend on the sampling, analysis, spatial modelling and prediction technique used. Indeed, it is the combination of sampling design and prediction method used that determines the accuracy and other properties of the estimates (Brus & de Gruijter, 1997). Comparisons of various interpolation methods for the estimation of soil properties at unsampled locations are given by Laslett *et al.* (1987), and for PA by Whelan *et al.* (1996). Chapter V deals with a comparison of some techniques used for the modelling and mapping of sparsely sampled soil properties that exhibit spatial drift. This section is constrained to only dealing with sampling intensity. All spatial prediction is conducted using geostatistical techniques.

Some attention has been given to the effects of sampling intensity on the reliability of predictions for map production in PA for example, Birrel *et al.* (1996), Mohamed *et al.* (1996), and more recently Frogbrook (1999). The latter author demonstrated the effect of sampling intensity on the reliability of kriged and simulated (refer to Chapter III for descriptions of kriging and geostatistical simulation) phosphorus maps.

A 100 m (and 100 yard) grid spacing is said to be the commercially standard sampling intensity for agricultural crop management in the US (Birrel *et al.*, 1996) and Europe. Griffin (1999) indicated that in the UK, variable rate application of fertiliser and lime has been based on soil maps produced from 100 m interval grid samples. This procedure was criticised by many researchers including Birrel *et al.* (1996), Whelan *et al.* (1996), Griffin (1999) and Frogbrook (1999) because 100 m spacing may be far too sparse to derive a variogram, model the variation and produce accurate interpolated resource application maps.

4.6.1 SAMPLING INTENSITY AND LIME REQUIREMENT

The effect of sampling intensity on the reliability of lime requirement (to a target pH of 6.5) (LR(6.5)) predictions is demonstrated using two data subsets of the original 244 sample data set (Chapter III). The first subset presents an 80 m square grid with 32 replicated observations and the second a 120 m square grid with 18 replicated observations (Figures 4.2d and 4.2f respectively). The 120 m subset corresponds to roughly 1 sample per hectare.

Experimental semi-variograms were computed for each data set and the fitted model parameters used in ordinary point kriging to interpolate the lime requirements on to a 5 m grid. In this instance, point kriging was used rather than block kriging to enable statistical comparisons of the effects of grid spacing on the accuracy of predictions. Normally PA requires the use of block kriging as it is more sensible to manage areas of land rather than points. The semi-variogram fitted to the 40 m grid data was a double exponential model given by:

$$g(h) = C_0 + C_1 \times (1 - \exp^{-\frac{h}{a_1}}) + C_2 \times (1 - \exp^{-\frac{h}{a_2}}) \tag{4.2}$$

where $\gamma(h)$ is the semi-variance of points separated by distance h; h is the distance between points; C_0 is the semi-variance at $h = 0$; C_1 is the magnitude of the first auto-correlation in the data ($C(a_1) - C_0$); C_2 is the magnitude of the second auto-correlation in the data ($C(a_2) - C(a_1)$); a_1 is the distance at which the first auto-correlation structure ends; and a_2 is the distance at which semi-variance becomes independent of distance (*i.e.* the distance where the second auto-correlation structure ends).

The 80 m and 120 m grid data were fitted with exponential semi-variograms. Their form is given in Equation 2.15 of Chapter II. The semi-variograms are shown in Figures 4.2a, 4.2c and 4.2e respectively. The grid sample spacing and resultant maps are shown in Figures 4.2b, 4.2d and 4.2f.

The map on Figure 4.2b illustrates the localised feature of point kriging. A block kriged map would appear somewhat smoother. The semi-variogram in Figure 4.2a and the 40 m grid map in Figure 4.2b are thought to be the more accurate representations of the field’s lime requirement variation. The sub-sample maps will be compared to this data. The 80 m grid data subset (Figures 4.2c), shows a less structured semi-variogram with no points at short lag distances. The resulting map on Figure 4.2d illustrates the degradation of the local variation, resulting in a much smoother map with clearly overestimated lime requirements on the western portion of the field. This loss of information effect due to increasing grid resolution is further exemplified by the semi-variogram and interpolated map of the 120 m sample grid (Figure 4.2e and 4.2f). The experimental semi-variogram shows no structure and provides no semi-variance information at short lags (Figure 4.2e), thereby producing an uncertain estimate of the nugget variance. The interpolated map on Figure 4.2f looks like a smooth trend surface with no local variability. Lime requirement values were overestimated on the western and central portions of the field, and underestimated in southern parts of the field.

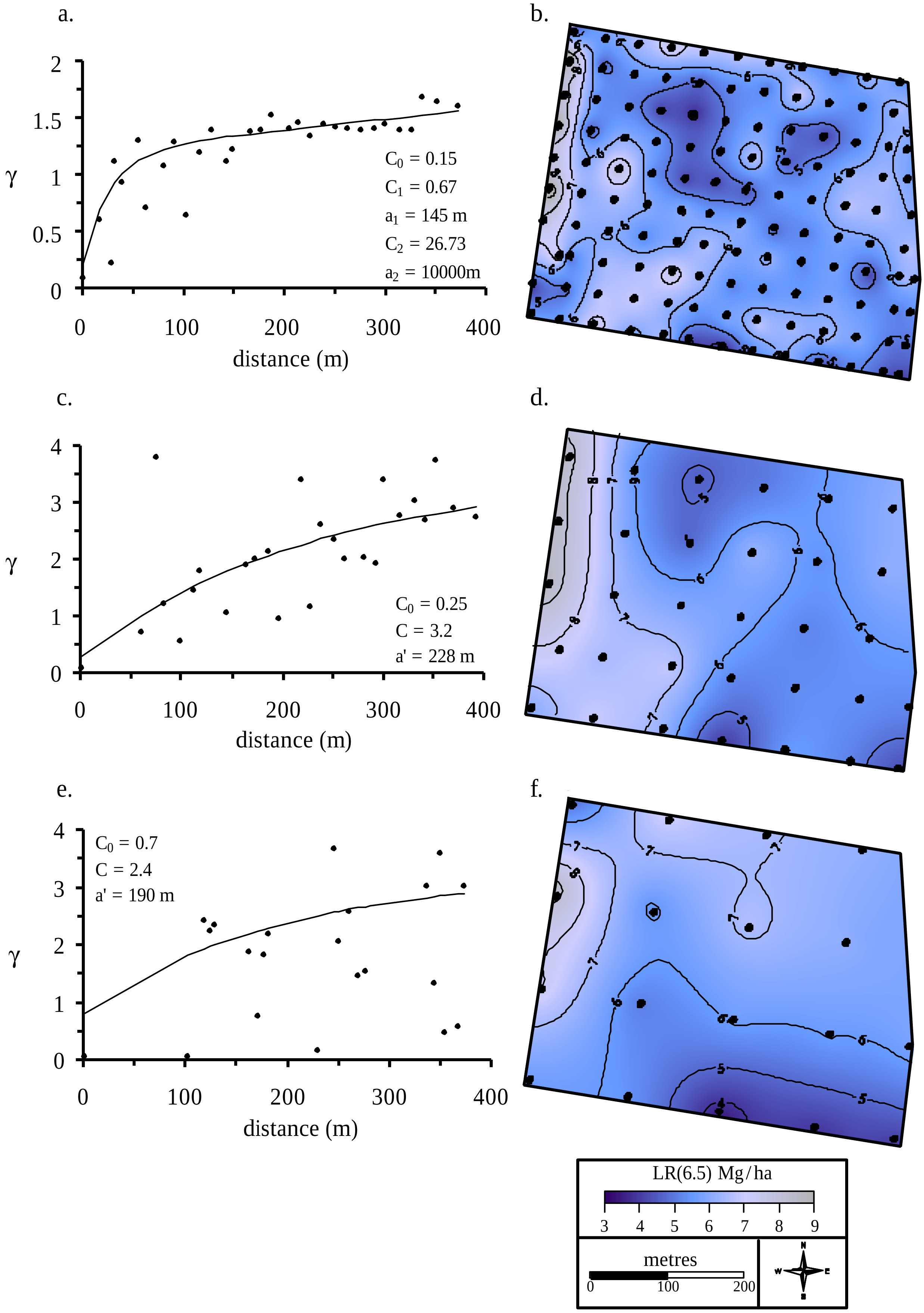

Figure 4.2 Experimental variograms with fitted exponential models for (a.) LR(6.5) 40 m grid, (c.) 80 m grid, and (e.) 120 m grid. Point kriged maps shown in (b.) 40 m grid, (d.) 80 m grid, and (f.) 120 m grid.

Figures 4.3a and 4.3b illustrate the loss of information and the inaccuracy of predictions resulting from sparser grid sample spacing.

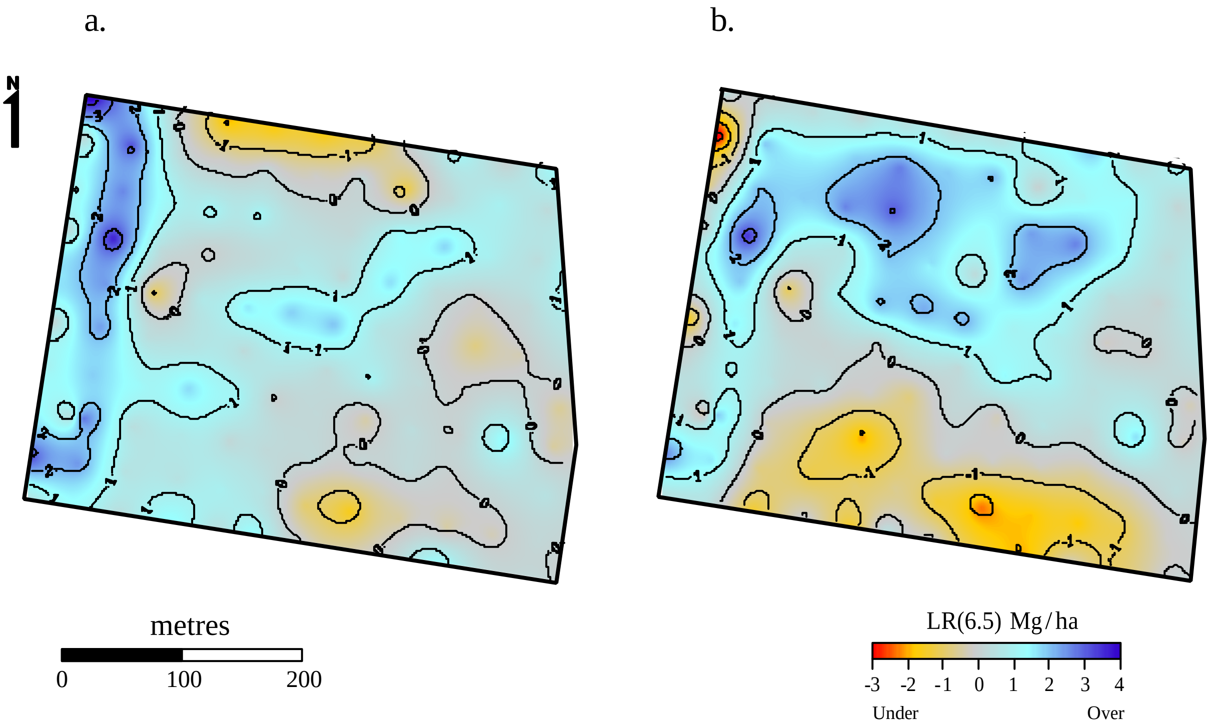

Figure 4.3 Difference maps between point kriged estimates of the different grid sample sizes (a.) 80 m – 40 m and (b.) 120 m – 40 m

The difference maps on Figure 4.3 provide a visual representation of the loss of information and increasing inaccuracy in the variable-rate lime application maps, as the sample size decreases and grid spacing increases. Like the point kriged maps from which they were derived, the maps on Figure 4.3 are unbiased.

If accurate estimates and maps are required for resource application and management decisions, then initially, the sample size should be related to the scale of variation and the sampling design must be sound. As previously suggested, the development of ‘on-the-go’ sensing systems for a variety of soil properties will facilitate the collection of more data at finer spatial resolutions. These data may then be used to accurately represent field soil variability, from which unbiased, sound management decisions may be derived. An example of data acquired using a commercially available soil electrical conductivity sensing system is given below.

4.7 INTENSIVELY COLLECTED SOIL DATA USING THE VERIS 3100

A description of the VERIS 3100 and its operation is given in Chapter II. The VERIS sensing system was used to characterise the soils' electrical conductivity (EC) in the experimental field. A classed map of the raw surface soil data (0 – 30 cm) is shown in Figure 4.4.

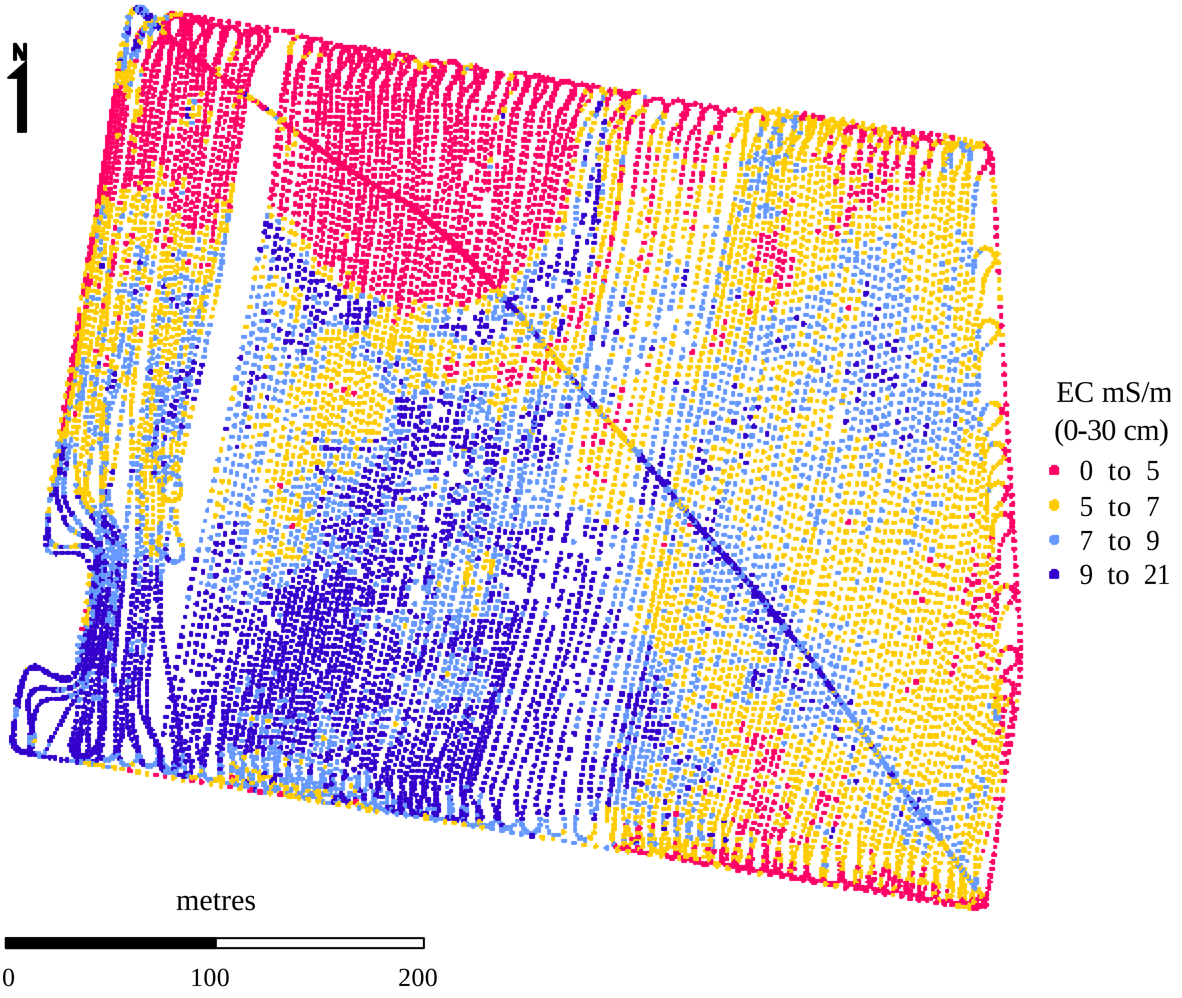

Figure 4.4 Sensed soil electrical conductivity measurements 0 – 30 cm. VERIS 3100 raw data, classed into distribution quartiles

Figure 4.4 illustrates the effectiveness of soil data collection using 'on-the-go' proximal soil sensing systems. A total of 15 300 data points were collected in six hours! The VERIS sensing system was towed behind a four-wheel drive vehicle at 15 km per hour, except along the SE to NW diagonal transect when the vehicle was driven at a maximum speed of 10 km per hour resulting in data acquisition at much shorter intervals.

In PA, when sample size and intensity are large (*e.g.* with intensively collected yield or soil data), local ordinary kriging (Haas, 1990) should be used for spatial prediction (Whelan *et al.*, 1996). Thus the raw VERIS 3100 data (Figure 4.4) was interpolated using ordinary block kriging (Chapter II) with local exponential variograms, using VESPER (Variogram Estimation and Spatial Prediction with ERror) (Minasny *et al.*, 1999). Local kriging uses points within a local neighbourhood for the calculation of the variogram and kriging matrices (Haas, 1990). The technique is particularly useful in the presence of non-stationary covariance structures where the stationarity restrictions imposed by global variogram fitting may not apply (refer to Chapter II and Chapter V). Figure 4.5 shows the interpolated map of the surface (0 – 30 cm) soil EC.

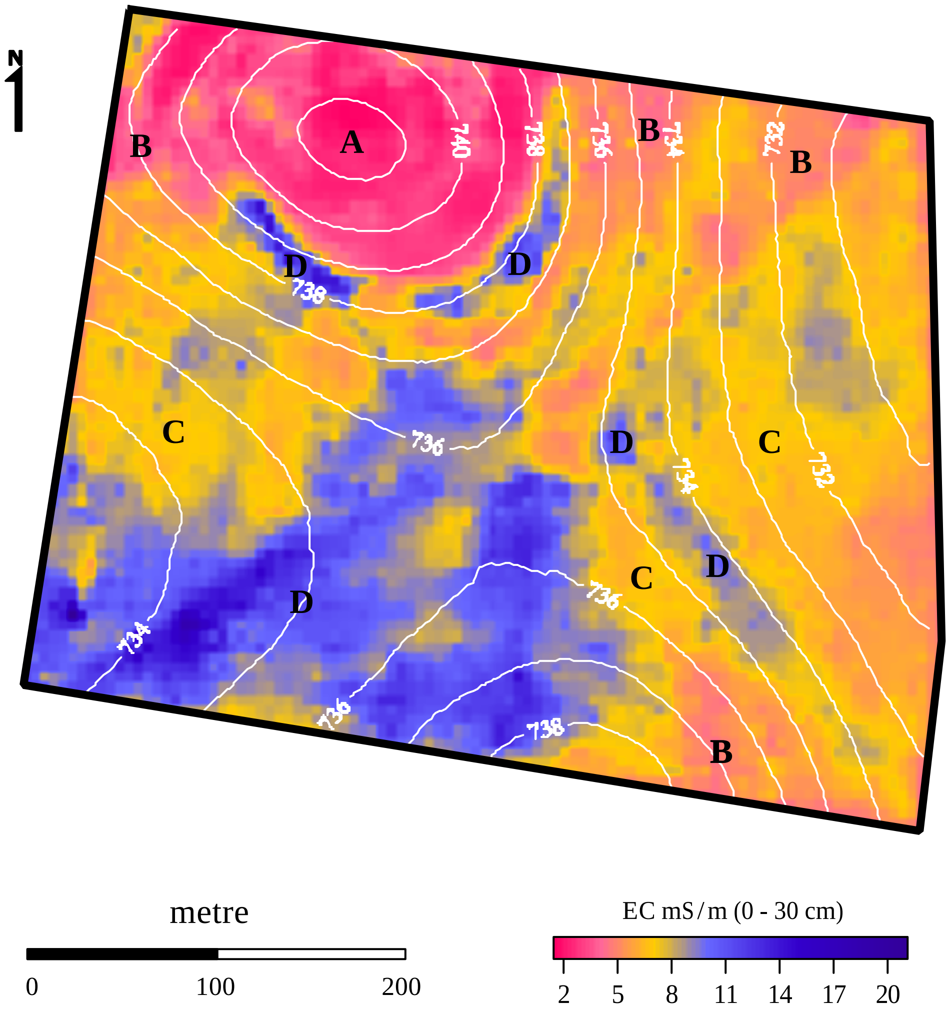

Figure 4.5 Block kriged map of VERIS 3100, surface soil (0 – 30 cm) electrical conductivity data, and elevation contours. Similar regions of conductivity are respectively labelled A, B, C and D

The interpolated map in Figure 4.5 has a narrower range of values than the actual classed map (Figure 4.4). This smoothing effect is typical of kriging algorithms (Chapter II).

The correlation of elevation with EC was poor ($\rho = 0.25$). Nevertheless, elevation contours were draped over the VERIS EC map to help with interpretation of some of the distinct EC patterns of the field. Four main regions may be distinguished from the map on Figure 4.5. These are labelled A, B, C and D and (roughly) correspond to the data quartiles. On the upper slope of the field (region A, Figure 4.5), EC is extremely low and is indicative of a highly leached, coarse textured soil. On the central portion of the field (regions C, Figure 4.5) and where constant decreases in elevation occur (regions B), the higher EC values may associated with the transitional movement of water and leachate down slope and with the accumulation of residual base cations. The highest EC values occur in south-central and south-western areas (regions D), where there is a ‘dip’ in the field between the 734 m and 738 m contours (Figure 4.5). Coincidentally, these regions of high EC correspond to regions in the field with the highest clay contents (18 % and 24 %), and highest water contents (25 to 29 % at the time of sensing) (refer to Table 3.4 of Chapter III for descriptions of the field soil physical properties). Both the higher clay and water content of the soil are conducive to a higher soil electrical conductivity (Lund *et al.*, 1999). The higher EC in these regions may also be due to the accumulation of base cations transported by the leachate from the more elevated parts of the field. Another feature that is apparent on the EC map is the cross pattern over the entire field (Figure 4.5). It corresponds to the pattern in which the previous wheat crop was harvested, and may represent compacted soil due to vehicle traffic. Also, further field investigations are needed to ascertain the reasons for the high conductivity values closely following the 738 m contour (regions labelled D, Figure 4.5) on the northern portion of the field.

As described in the previous chapter, the VERIS sensing system measures soil electrical conductivity at two depths, namely 0 – 30 cm and 0 – 90 cm. From these two measurements one may derive estimates for the 30 – 90 cm depth using:

$$30 - 90\,\mathrm{cm} = 1.5 \times (0 - 90\,\mathrm{cm}) - 0.5 \times (0 - 30\,\mathrm{cm}) \tag{4.3}$$

Raw data and interpolated maps of the 30 – 90 cm layer are shown in Figures 4.6 and 4.7 respectively.

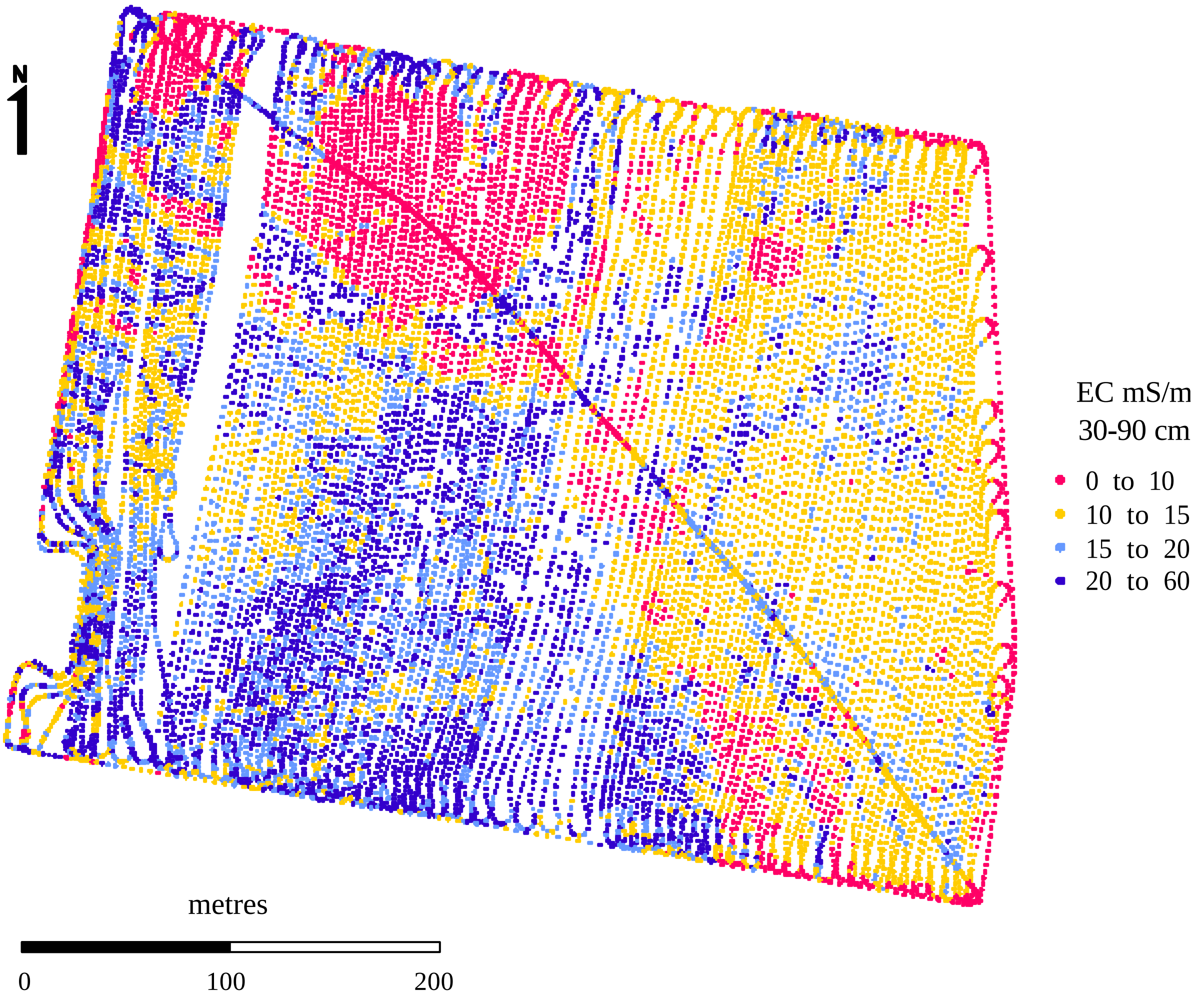

Figure 4.6 Sensed soil electrical conductivity measurements 30 – 90 cm. VERIS 3100 raw data, classed into distribution quartiles

The 30 – 90 cm soil conductivity is higher and more homogeneous than the EC of the surface soil (compare Figure 4.4 with Figure 4.6). This is to be expected because of the more stable and similar soil environment at depth, and the greater amount of conductive material present (*e.g.* clay, soil water) (Tables 3.1 and 3.2 Chapter III). The smoother, interpolated map is shown in Figure 4.7.

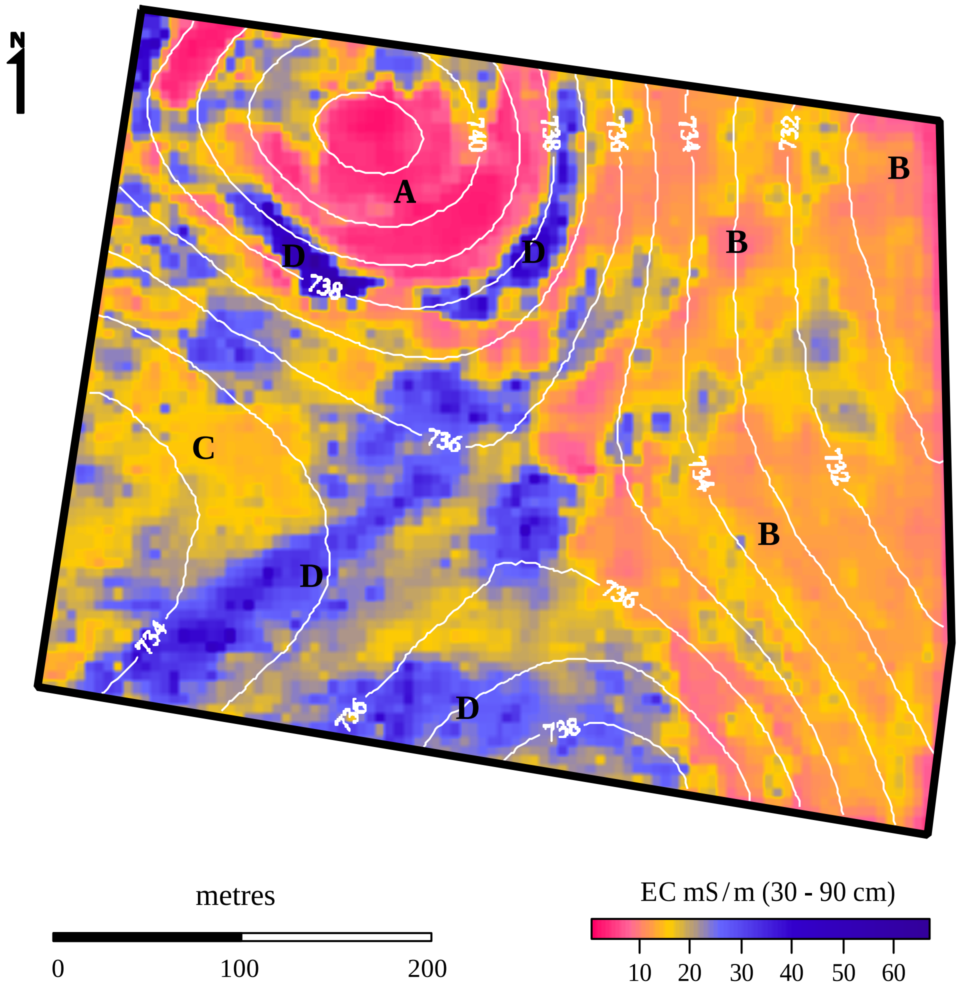

Figure 4.7 Block kriged map of VERIS 3100 30 – 90 cm electrical conductivity data, and elevation contours. As with the map on Figure 4.5, similar regions of conductivity are respectively labelled A, B, C and D

The subsurface soil (Figure 4.7) has higher EC than the surface soil (Figure 4.5), but similar features are apparent. Highly leached, low conductivity soil in the higher slopes (region A), and higher conductivity soil in the southern portion of the field (region D). The EC of the eastern half of the field is more homogeneous than the surface soil (compare Figure 4.5 and 4.7).

4.7.1 Correlations of VERIS EC Measurements with Soil Properties

Soil conductivity measurements result from the fact that soil materials are conductive, *i.e.* soil is able to transmit an electrical charge. For example, clays are highly conductive, silts have medium conductivity and sands have low conductivity. Soil electrical conductivity measurements have been used to identify variations in texture and other related soil properties such as soil water, OM, CEC, etc. (Lund *et al.*, 1999). Therefore measurements

may be used to delineate similar and contrasting regions of a field for example, to device sampling schemes (section 4.2; Chapter II). Table 4.4 shows correlations between surface soil chemical and physical properties of the experimental field and VERIS 0 – 30 cm EC measurements

Table 4.4 Linear correlations between VERIS EC measurements and soil properties

Soil property	pH$_{CaCl_2}$	pH$_{H_2O}$	OC dag/kg	Clay dag/kg	Sand dag/kg
E.C.$_{VERIS\ 0\text{-}30}$ mS/m	0.35	0.32	0.36	0.72	-0.65

Soil property	pH$_{Mehlich}$	LR(6.5)	CEC mmol(+)/kg	Al mmol(+)/kg	Ca mmol(+)/kg
E.C.$_{VERIS\ 0\text{-}30}$ mS/m	-0.13	0.12	0.62	-0.31	0.58

Soil property	NO_3-N mg/kg	P mg/kg	K mmol(+)/kg	E.C.$_{1:5}$ mS/m
E.C.$_{VERIS\ 0\text{-}30}$ mS/m	0.25	-0.07	0.44	0.29

VERIS conductivity measurements were highly correlated to clay content (and negatively correlated with sand content) (Table 4.4), thus as reported by Lund *et al.* (1999), the VERIS sensing system may be used to identify variations in soil texture. As expected the CEC of the soil (and its exchangeable cations Ca, K and Al) showed good correlations to VERIS measurements (Table 4.4). Reasonably good correlations were also established between VERIS measurements and soil pH in both 0.01 M $CaCl_2$ and H_2O, however none were nearly as high as 0.78, reported by Lund *et al.* (1998). VERIS EC was poorly correlated to Mehlich lime-requirement buffer (pH$_{buffer}$) values and lime requirements to a target pH of 6.5. Surprisingly, soil 1:5 electrical conductivity measurements were poorly correlated to VERIS conductivity measurements. Lund *et al.* (1999) reported some preliminary good correlations between VERIS measurements and crop yield. The reason for such promising correlations may be the highly influential effects of soil water and texture on crop yield.

VERIS measurements can be used to identify soil variability in a field (*i.e.* similar and contrasting regions) and then used to design direct sampling schemes and subsequently management units for the implementation of zone management (section 4.2; and Chapter II). Like with elevation data (*e.g.* Moore *et al.*, 1993), VERIS data may be used as exhaustive ancillary data for the prediction of other important soil attributes (*e.g.* Bishop & McBratney, 1999).

4.8 CONCLUDING REMARKS

Traditional crop management systems do not require large amounts of information for the formulation of management decisions. Precision agriculture does. Current techniques that are used to obtain and analyse samples at such intensities are clearly inadequate. They have not previously needed to cope with such demand. This chapter suggests that for PA we need to develop analytical techniques that are rapid, less labour intensive, economical and no less accurate than the current methods to efficiently characterise field soil variability. Current sampling and analysis techniques are time consuming, costly, labour intensive, and in some instances inaccurate and imprecise. While sensing systems are being developed to overcome these problems, the solution to the sampling and analysis dilemma is being addressed. In doing so, it should be clear that the sampling procedure and the way in which samples are handled after collection ultimately determine the accuracy of analytical results. Soil properties like pH, OM, N, P, K and CEC should form the basis for routine soil chemical analysis in PA.

A cost comparison indicated that for routinely measured soil chemical properties, Australian soil analytical costs are much higher than those in the USA, although costs of analysis in the USA were high. Therefore current analytical costs for economically efficient production using precision agriculture techniques are unrealistic. Sampling, preparation and handling costs were not taken into account. Obviously if these were accounted costs would be much higher.

The effect of sampling intensity on lime-requirement map production was investigated. As the sample size decreased and grid spacing increased, information was lost, modelling of the experimental variogram was difficult and uncertain, and consequently the accuracy of the variable-rate lime application maps decreased. To produce accurate resource application maps the initial sampling design must be sound and the sample size should be related to the scale of variation. Other factors such as data analysis and spatial modelling techniques were not considered but their effect on map production is acknowledged. The development of ‘on-the-go’ proximal soil sensing systems for a variety of properties will facilitate the collection of more data at finer spatial resolutions.

The VERIS 3100 mobile sensing system was used to characterise the soil electrical conductivity in the experimental field. Its use demonstrated the advantages of using an 'on-the-go' proximal sensing device as 15 300 data points were collected in six hours. Briefly, geostatistical manipulation of intensively collected data was described. Correlations between VERIS EC measurements and various other soil properties were drawn. Highest correlations were found between EC and clay content, sand content, CEC and constituent cations, while moderate correlations with pH and OC. EC was poorly correlated to lime requirement.

The development of 'on-the-go' proximal soil sensing systems and scanners with no less, or improved accuracy is hence essential for the adoption and implementation of precision agriculture. Their development is also important for the evolution of precision agriculture into a real-time continuous management system.

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Chapter V

SPATIAL MODELLING AND MAPPING METHODS FOR SPARSELY SAMPLED SOIL THAT EXHIBITS SPATIAL DRIFT

ABSTRACT

Accurate representations of the spatial variability in field soil properties are needed for accurate resource assessment and site-specific soil and crop management. The previous chapter looked at the implications that precision agriculture has for current methods of sampling and analysis, and the effect of sampling intensity on the production of variable-rate maps. As well as correct, unbiased soil sampling and laboratory analysis, the choice of spatial modelling and mapping technique is important for reliable results and accurate representations of field soil variability. There are various good examples in the literature that compare spatial modelling and mapping techniques for resource assessment and precision agriculture. This chapter constrains itself to comparing some of the methods that are used for modelling and mapping sparsely sampled soil that exhibits spatial drift. The data used in the comparison was soil pH and organic matter from the experimental field at Kelso, NSW. The methods compared include generalised additive models, trend surface polynomial regressions, local trend surface regressions, a combination of regression methods with kriging of the regression residuals, global ordinary kriging, local ordinary kriging, and intrinsic random functions of order k. The data was split into a prediction and a validation set, from which the models were assessed. The root-mean-square-error was used to quantify the accuracy of the predictions and the Akaike Information Criterion compared their performance in terms of goodness of fit and model parsimony. Results show that the intrinsic random functions of order k technique were superior to all other methods tested. Local ordinary kriging, containing relatively few points in the neighbourhoods, dealt with the non-stationarity of the data better than ordinary kriging. Kriging performed better than regression residual-kriging and regression-based methods were the least accurate. The most unexpected result was the poor performance of regression residual kriging.

5.1 INTRODUCTION

An accurate representation of soil spatial variability is needed for resource assessment and site-specific management. The previous chapter looked at the implications that precision agriculture has for current methods of sampling and analysis, and the effect of sampling intensity on the production of variable-rate maps. As well as correct, unbiased soil sampling and laboratory analyses, the choice of spatial modelling and mapping technique is important for reliable results and accurate representations of field soil variability. There are various good examples in the literature that compare spatial modelling and mapping techniques that may be used for these purposes (*e.g.* Laslett *et al.*, 1987; Gotway *et al.*, 1996; Wollenhaupt *et al.* 1997). The reader is referred to these for an assessment of the comparisons and results of such work. This chapter constrains itself to comparing some of the methods that are used for modelling and mapping soil that exhibits spatial drift.

On occasions, properties of sparsely sampled soil have a tendency to change continuously over the landscape. In the geostatistical literature, this tendency or trend is commonly referred to as spatial drift (*e.g.* Journel & Huijbregts, 1978). Geostatistically, the occurrence of spatial drift implies that the mathematical expectation of the Random Function (RF) model $S(x)$, *i.e.* $E\{S(x)\}$ is non-stationary within A (Chapter II). Some common examples of data that display spatial drift characteristics include soil properties that are related to landform attributes such as elevation, as well as high-density soil and crop data sets, like those that are collected using 'on-the-go' proximal crop and soil sensing systems (Chapters II and IV).

Recall from Chapter II that the questions and assumptions that pertain to stationarity, refer to the statistical models of the soil and not to the soil itself. Kriging algorithms in their simplest form may be distinguished according to the model considered for the trend (Chapter II). Inference requires the user to make a decision on whether or not the RF model is stationary. A stationary RF model suggests that its characteristics are translation invariant within the study area, while a non-stationary RF model has characteristics that change with location (and with time) (Wackernagel, 1995; Chapter II). For example, estimation by ordinary kriging (OK) needs a stationary RF model because the trend component is limited to a single constant (mean) term within a given neighbourhood (Chapter II). Conversely, universal kriging (UK) models the trend using a non-stationary RF model that takes different values in space. Like all kriging algorithms, UK provides minimum error-variance estimates.

Webster & Burgess (1980) provided a review of UK and its applications in soil science. They suggested that UK is not widely applicable in soil survey except when measurements are made on contiguous volumes of soil. Here, it will suffice to briefly outline the UK methodology to understand the work being presented. With UK, the non-stationary RF model $S(x)$ can be expressed as the sum of a deterministic trend $m(x)$, and a stochastic residual term $R(x)$ such that:

$$S(x) = m(x) + R(x) \tag{5.1}$$

where $m(x)$ may be viewed as the 'large-scale' non-stationary regular and continuous variation component of the model. The trend $m(x)$ is modelled as a weighted sum of known functions $f_l(x)$ (usually low-order polynomials), and unknown coefficients b_l, $l = 0,1,\ldots,n$, such that:

$$m(x) = \sum_{l=0}^{n} b_l \, f_l(x) \tag{5.2}$$

By convention if $n = 0$, the function $f_0(x) = 1$ for all x, *i.e.* $f_0(x)$ is constant, and is the case for simple kriging. In the case of UK, $n > 0$ and the trend component is a function of x, taking different values as x changes within local neighbourhoods (Journel & Huijbregts, 1978). $R(x)$ in Equation 5.1 represents the 'small-scale' component of the variability, representing the fluctuations of $S(x)$ around its mean value. Statistically, $R(x)$ is represented as a zero-mean (*i.e.* $E\{R(x)\}=0$), second-order stationary process characterised by its covariance or variogram function (Journel & Huijbregts, 1978). Assuming such conditions, it can be deduced that $E\{S(x)\}=m(x)$.

Theoretically the UK model is written in terms of the semi-variogram of residuals g_R, in practice however, g_R is unknown (Webster & Burgess, 1980). This is one of the problems of UK that Armstrong (1984) alluded to, the other is the difficulty in estimating both $m(x)$ and g_R simultaneously. g_R cannot be determined from measured values of $S(x)$ without knowing the drift $m(x)$, and $m(x)$ cannot be determined without knowing g_R. To estimate one of the components, it is necessary to assume that the other is known. This induces a bias in the estimates. As a result, UK has been the subject of much criticism, *e.g.* Armstrong (1984), Neuman & Jacobson (1984) and Journel & Rossi (1989).

The bias described in the previous paragraph may be overcome using a technique called restricted maximum likelihood (REML) (Kitanidis, 1983). Laslett & McBratney (1990) assessed the technique and concluded that its advantage compared to maximum likelihood methods is the consequent reduction in prediction error. Stepwise iterative general least-squares procedures for simultaneous estimations of the global drift and the residual semi-variogram (*e.g.* Neuman & Jacobson, 1984) can also be used to minimise the bias. In situations where high-density data is available (such as that collected from proximal crop and soil sensing systems) it may also be possible to reduce the size of the neighbourhoods to allow for *quasi*-stationary modelling, without adjusting the model to account for the trend. This latter method is the basis for local kriging (*e.g.* Chapter IV).

Estimation with local search neighbourhoods has also been proposed as the simpler, preferred model than those that account for trend (*e.g.* Journel & Rossi, 1989). All of these techniques that improve on the UK methodology have been developed, generally eliminating the need for UK.

The modelling techniques compared in this work include three forms of regression in which the Cartesian coordinates are used to predict the target soil property, global and local ordinary kriging, regression residual-kriging and the generalised covariance technique called intrinsic random function of order k.

5.1.1 REVIEW OF PREDICTION METHODS USED IN THIS WORK

Generalised Additive Models

Generalised additive models (GAM)s allow the detection of non-linearities in the data by incorporating them into the model and optimising the fit iteratively. The predictors in the equation are modeled non-parametrically using a scatterplot smoother used to identify the non-linearities in the data. Hastie & Tibshirani (1990) described the process. The additive predictor may be described by:

$$Y(x) = a + \sum_{i=1}^{j} f_i(x_i) \tag{5.3}$$

where each x_i, $i = 1,2,...,j$ are predictor variables described by their non-linear functions f_i. Several smooth terms are iteratively fitted to the f_i functions in the GAM using the scatterplot smoothers. In turn these may be used to introduce the non-linearity of the predictor variables by adding a limited range of transformed predictant variables to the model, *e.g.* quadratic and cubic terms. Venables & Ripley (1994) described an alternative approach that involves splitting the range of the predictant variable and fitting a piecewise constant function such as a polynomial, or optionally a spline function. Hastie & Tibshirani (1990) suggested that the small drawback of the non-parametric techniques is that to be successful, the underlying function needs to be reasonably smooth.

Trend Surface Regression Models

Trend surface (TS) analysis was one of the earliest and most widely used methods of global spatial prediction. TS polynomial models constitute a type of polynomial least-squares regression where the geographic coordinates of the dependant variable replace the predictor terms in the equation. The surface is approximated by a polynomial expansion of the geographic coordinates. The coefficients of the polynomial function may be determined using the least-squares estimation procedure, ensuring that the sum of the squared deviations from the predicted trend surface is minimum (Venables & Ripley, 1994). The TS of degree *r* may be expressed as a linear combination of polynomials in the spatial coordinates (*x*,*y*) by:

$$Y(x, y) = \sum_{0 \le k+l \le r} b_{kl} x^k y^l \tag{5.4}$$

The unknown coefficients are found by solving a set of simultaneous linear equations that include the sums of powers and cross products of the predictor parameters. The number of coefficients in the TS regression may be determined by (r + 1)(r + 2) (Venables & Ripley, 1994).

There are a number of problems encountered when fitting trend surfaces to data, the most obvious of these is the great simplicity in form compared to natural surfaces. Polynomial TSs tend to accelerate towards extreme values in areas where there are no data points such as towards the edges of the data sets (commonly referred to as 'edge-effects'), making TSs particularly prone to the generation of exaggerated estimates.

Local Trend Surface Polynomial Regression Models

The difficulties and disadvantages of fitting polynomials as global TSs may be overcome by using local trend surface (LTS) regression models. As the name suggests LTS regressions fit a local trend surface to data. This is achieved by fitting either a linear or quadratic polynomial surface to each predicted point by weighted least-squares (Venables & Ripley, 1994). The weights ensure that local data points are more influential. Therefore there needs to be a neighborhood containing the predictant in which the regression surface is approximated by a function from a specific parametric class such as polynomials of degree 1 or 2 (Cleveland *et al.*, 1992). The methods of fitting consist of smoothing the response as a function of the geographic predictors, and may be classed as non-parametric regression procedures (Cleveland *et al.*, 1992). Venables & Ripley (1994) suggested that the degree of smoothing is arbitrary and often selected to suit mapping aesthetics.

Ordinary Kriging and Local Ordinary Kriging

Ordinary kriging (OK) is used for the estimation of a continuous variable at unsampled locations using a linear combination of neighbouring observations. OK accounts for local fluctuations of the mean by limiting the domain of stationarity of the mean to a local neighborhood centered on the location x_0 being estimated. Like all other kriging algorithms, OK provides an optimal estimate in that it is unbiased and has a minimum error variance. Chapter II provides a description of the OK technique.

Ordinary kriging using a local variograms is termed local ordinary kriging (LOK). LOK is particularly useful in the presence of a non-stationary covariance structure, such as that found in intensively collected proximally sensed data, as it aims to overcome the stationarity restrictions imposed by global variogram fitting. For example, Whelan *et al.* (1996) suggested its use for spatial predictions in precision agriculture where both sample size and intensity are large, *e.g.* yield data collected with an ‘on-the-go’ yield monitor; soil EC data collected using the VERIS 3100 (refer to Chapter IV).

Local ordinary kriging requires the calculation of the semi-variogram parameters for observations in a predetermined neighbourhood (*c.f.* LTS technique), thus limiting the intrinsic hypothesis (Chapter II) to only those distances within the neighbourhood. In essence this corresponds to a *quasi*-intrinsic hypothesis, which is a compromise between the scale of homogeneity of the data, and its abundance (Journel & Huijbregts, 1978). Within the moving neighbourhoods, the expectation of the covariance can be considered as stationary if there is sufficient data to make statistical inference possible. Defining the size of the neighborhood that will influence the model is left to the operator’s judgement. Webster & Oliver (1992) suggested that semi-variogram fitting should be conditioned on the inclusion of 100 or more observations to ensure a reasonably robust estimation (Chapter IV). Once the local semi-variogram has been estimated OK is performed using the points in the neighbourhood.

Intrinsic Random Function of Order k

Estimation by kriging using the variogram assumes the preservation of the intrinsic hypothesis of geostatistics (*i.e.* constant mean and finite variance depending on the length and the orientation of a given vector, but not on its position in the neighbourhood (Chapter II)). When spatial drift occurs and these stationarity conditions are not met, the use of OK for estimation is inadequate. This is the reason for which UK was proposed.

Journel & Huijbregts (1978) and Journel & Rossi (1989) provided more thorough descriptions of UK than that given in the introduction of this chapter, and Armstrong (1984) alluded to the problems that led to it being considered an 'old-fashioned' technique. As such, UK methodology is commonly replaced in favour of other techniques, one of which is the theory of intrinsic random functions of order k (IRF-k). Like UK, IRF-k is a technique that aims to characterise the drift by a linear combination of stationary deterministic functions (Wackernagel, 1995). However, the theory employs the generalised covariance function rather than the semi-variogram as the tool for structural analysis and hence in the computation of the kriging matrices. Using the non-stationary RF model or IRF-k $S(x)$, the value of the soil attribute s at any location x_i, $i = 1,2,\ldots,n$ in a two-dimensional space, may be determined by:

$$S(x) = m_k(x) + R_k(x) \tag{5.9}$$

where $m_k(x)$ is the the drift represented as a k^{th} order polynomial, and $R_k(x)$ is the residual term that accounts for the erratic fluctuations around the drift. $R_k(x)$ has a generalised covariance $K(h)$ associated with it (Wackernagel, 1995). The drift component may be characterised as a global polynomial of order k over a given neighbourhood, in the following manner:

$$m_k(x) = \sum_{l=0}^{n} b_l f_l(x) \tag{5.10}$$

where b_l, $l = 0,1,\ldots,n$ are unknown coefficients, and $f_l(x)$ are linear combinations of functions (generally monomials) of the Cartesian coordinates x, y. The drift then depends on the order of k, the number of monomials n, and the $n + 1$ number of basis functions as follows:

constant drift: $k = 0$, $n = 0$, $m(x) = b_0$

linear drift: $k = 1$, $n = 2$, $m(\mathrm{x}) = b_0 + b_1 x + b_2 y$

quadratic drift: $k = 2$, $n = 5$, $m(\mathrm{x}) = b_0 + b_1 x + b_2 y + b_3 x^2 + b_4 y^2 + b_5 xy$

Note that in the case of a constant drift, the process is basically intrinsically stationary.

The system of equations is basically similar to those arising in UK. The difference being that rather than working with the explicit forms of the drift function, IRF-k attempts to determine the covariance of the residuals by filtering out a polynomial drift. The filtering is accomplished by considering not only zero-order ($k = 0$) increments of $S(x)$ as in simple and ordinary kriging, but also higher order increments (*i.e.* $k = 1$ or $k = 2$). Generally, the increment of order k filters the polynomial drift of similar order.

McBratney *et al.* (1991) also provided a thorough explanation of the technique together with examples of its use in soil science.

Regression Residual-Kriging Methods

As the name suggests, regression residual-kriging (RRK) combines regression of the attribute *s* as a function of its Cartesian coordinates for simultaneous estimation of the global drift, and the residual semi-variogram. The technique is closely based on the universal kriging methodology previously outlined, where the drift term represents the regular and continuous variation of $S(x)$ at the scale of observation, and the residual term accounts for the erratic fluctuations around the drift. Its advantage is that it allows for the subjectively choice of the trend model, unlike universal kriging or generalised covariance techniques (IRF-k) that make no attempt to define the global nature of the drift.

Like with UK, its disadvantage is the introduction of bias in the estimated residuals when they have been previously calculated as the difference between the original data and the drift estimated by regression. The RRK technique relies on estimating the drift $m(x)$ of the attribute *s* using regression analysis so that $m(x) = \hat{Y}(x)$, then estimating the residuals by:

$$\hat{R}(x) = S(x) - \hat{Y}(x) \tag{5.13}$$

Assuming that the regression residuals $\hat{R}(x)$ and the regressed values $\hat{Y}(x)$ are uncorrelated, estimates are obtained by solving a modified OK system written for the residuals. OK of the residuals is accomplished by:

$$R^*(x) = \sum_{i=1}^{n} l_i \hat{R}(x_i) \tag{5.14}$$

where l_i are kriging weights, and $\hat{R}(x_i)$ are the residual components corresponding to n measurement points of $S(x_i)$, $i = 1,2,\ldots,n$ in the domain. Estimates of *s* at unsampled locations are acquired by summing the kriged regression residuals $R^*(x)$ and the regressed drift estimates according to:

$$S^*(x) = \hat{Y}(x) + R^*(x) \tag{5.15}$$

where $R^*(x)$ represent the kriging estimates of the regression residuals, $\hat{R}(x)$.

Neuman & Jacobson (1984) also describe a similar approach by considering groundwater levels in an aquifer. Odeh *et al.* (1994, 1995) described similar procedures for the prediction of soil properties from landform attributes.

5.2 METHODS

5.2.1 STUDY SITE AND EXPERIMENTAL DESIGN

The study area is the 17 hectare agricultural field described in Chapter III. The field was sampled on a regular 40 m grid resulting in 122 grid nodes. At each grid node two samples one metre apart where collected. The sampling and bulking strategy is given in Chapter III. Of these 244 samples, six outliers were removed before the analysis, hence *l* = 238 (Figure 5.1b).

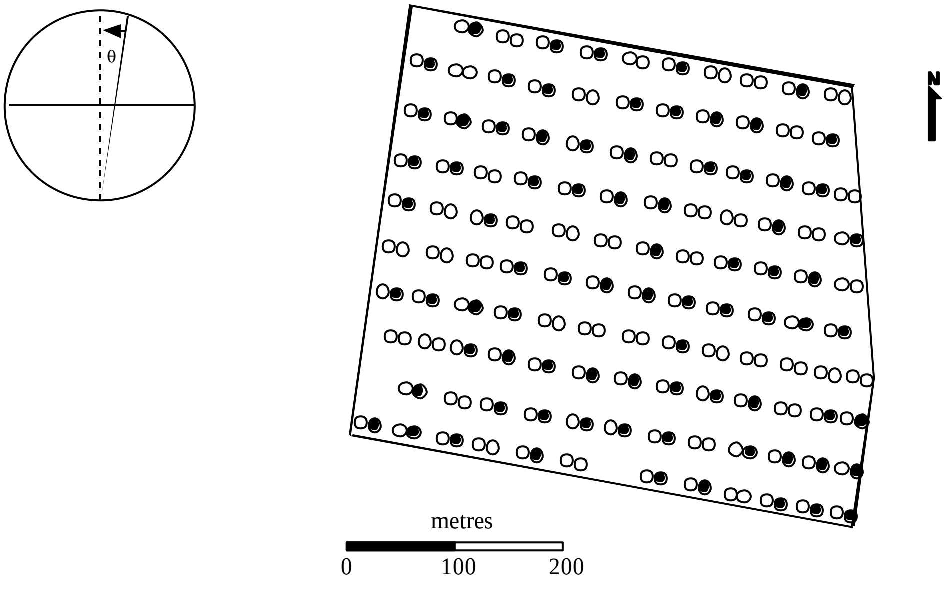

a. b.

Figure 5.1 (a.) Angle of coordinate rotation (q = -8.5°), and (b.) field layout showing two sampling points 1 m apart at each of the 119 nodes. Prediction sites (*n* = 158) are represented by (?) and validation sites (*m* = 80) are represented by (?).

Figure 5.1a shows the angle of coordinate rotation used to rotate the sampling points perpendicular to the plane before spatial analyses were conducted. Methods of chemical analysis for soil pH and organic carbon are described in Chapter III.

5.2.2 Exploratory Data Analysis

The frequency distributions of the pH and OC data sets were derived. Classed plots were produced to show the general trends of the raw data in the field. The averages of the data for each row (in the north-south direction), and column (in the east-west direction) of the grid were calculated and plotted to more clearly show the spatial trends in the data. To detect anisotropies in the soil pH and OC data, semi-variograms for the four principal directions were computed, *i.e.* north to south, north-east to south-west, east to west, and south-east to north-west.

5.2.3 Comparison of the Methods Tested by Cross Validation

The cross-validations procedure whereby a validation data set is re-estimated from a non-overlapping prediction data set, both collected within A, was used to compare the prediction methods tested. Two-thirds of the samples ($n = 158$) were used for prediction and the remaining one-third of samples ($m = 80$) for validation (Figure 5.1b).

5.2.4 Modelling of the Spatial Trend

The modelling techniques compared may be grouped as stand-alone regression-based techniques and regression residual-kriging, global and local ordinary kriging, and IRF – kriging. The forms of the methods used are shown in Table 5.1.

Table 5.1 Models compared. Generalised additive model (GAM); quadratic trend surface (TS 2); linear & quadratic local trend surfaces (LTS 1 and 2); global ordinary kriging (GOK) with spherical (Sph.), exponential (Exp.), Gaussian (Gauss.), linear (Lin.) and power function (Pow. Fn.) semi-variograms; local ordinary kriging (LOK) with both spherical and exponential semi-variograms; and intrinsic random function of orders 1 and 2 (IRF- 1 and 2).

Regression and RRK	Kriging		IRF-k
	Global	Local	
GAM: $Y(x) = s(e) + s(n) + s(e\times n) + s(e^2) + s(n^2)$ TS 2: $Y(x) = e + n + (e\times n) + e^2 + n^2$ LTS 1: $Y(x) = e + n + (e\times n)$ LTS 2: $Y(x) = e + n +(e\times n) + e^2 + n^2$	GOK – Spher. GOK – Exp. GOK – Gauss. GOK – Lin. GOK – Pow. Fn.	LOK – Spher. LOK – Exp.	IRF – 1 IRF – 2

Note: Using the regressions models, the Cartesian coordinates easting (e) and northing (n) were used to predict the target soil property. The s in the GAM represents the smoothing term (Venables & Ripley, 1994).

To test the predictions of GOK with trended data, isotropic variation of pH and OC was assumed and a number of transitive and unbounded, authorised variogram models, *i.e.* models which are conditional negative semi-definite (CNSD) (Chapter II), were fitted to the prediction data sets (Table 5.1).

The variogram model parameters were then used for GOK estimations. The minimim number of data used for GOK interpolation was set at 100 points. The number of data points used for LOK was 25.

5.2.5 INDICES USED TO DETERMINE THE ACCURACY OF PREDICTIONS

The accuracy of prediction of the spatial modelling techniques tested (Table 5.1), involved the computation of three indices, namely the root-mean-square-error of prediction (RMSE), the residual sum of squares (RSS) and the Akaike Information Criterion (*AIC*). The RMSE is a measure of the accuracy of predictions (accuracy encompassing both bias and precision, refer to Chapter IV). The RMSE is calculated by:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{m}\left[s^{*}(x_i) - s(x_i)\right]^2} \tag{5.16}$$

where: $s^{*}(x_i)$ is the predicted value, and $s(x_i)$ is the observed value at location x_i. The more accurate the prediction, the smaller the RMSE.

The AIC is used to ascertain the method that most satisfactorily compromises between goodness of fit and parsimony (Chapter II). The index is used to determine the procedure that most optimally strikes a balance between the residual sum of squares (RSS) and the number of parameters (*p*) used in the prediction. The equation for the calculation of the AIC is given by Equation 2.19 in Chapter II. There most efficient model is one for which the AIC is smallest. The residual sum of squares (RSS) may be calculated by:

$$RSS = \sum_{i=1}^{m}\left[\left(s^{*}(x_i) - s(x_i)\right)^2\right] \tag{5.17}$$

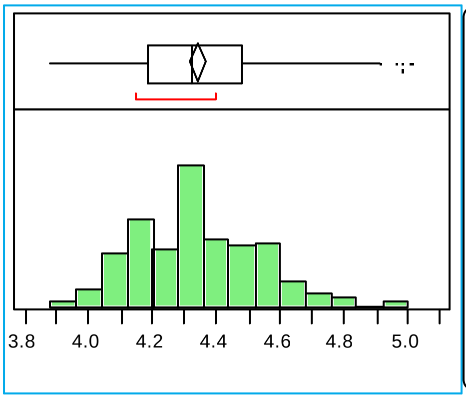
The RSS was used in calculations of the AIC. The latter was also used to assess the goodness of fit and parsimony of the fitted semi-variogram models used for GOK.

5.3 RESULTS AND DISCUSSION

5.3.1 EXPLORATORY DATA ANALYSIS

Histograms and summary statistics for soil pH and OC are given in Figure 5.2. From Figure 5.2, both sets of data are slightly skewed, with median values that are slightly smaller than their respective means. The pH variability in the field, as measured by the coefficient of variation (CV), was low at 5 %. Organic carbon is more variable in the experimental field, with a CV value of 21 %. Both of these CVs are consistent with what is reported in the literature for the respective properties (Chapter II).

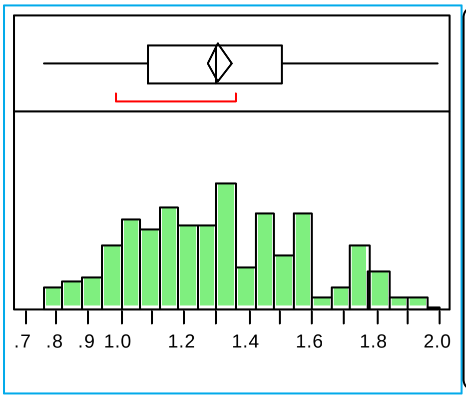
a.



Quantiles		
maximum	100.0%	5.02
	99.5%	5.01
	97.5%	4.91
	90.0%	4.62
quartile	75.0%	4.48
median	50.0%	4.33
quartile	25.0%	4.19
	10.0%	4.09
	2.5%	3.99
	0.5%	3.88
minimum	0.0%	3.88

Moments	
Mean	4.35
Std Dev	0.22
Std Error Mean	0.01
Upper 95% Mean	4.38
Lower 95% Mean	4.32
N	238.00
Sum Weights	238.00
Sum	1035.13
Variance	0.05
Skewness	0.56
Kurtosis	0.39
CV	5.02

b.



Quantiles		
maximum	100.0%	1.99
	99.5%	1.99
	97.5%	1.89
	90.0%	1.75
quartile	75.0%	1.51
median	50.0%	1.30
quartile	25.0%	1.09
	10.0%	0.98
	2.5%	0.82
	0.5%	0.77
minimum	0.0%	0.76

Moments	
Mean	1.32
Std Dev	0.28
Std Error Mean	0.02
Upper 95% Mean	1.35
Lower 95% Mean	1.28
N	238.00
Sum Weights	238.00
Sum	313.00
Variance	0.08
Skewness	0.30
Kurtosis	-0.61
CV	21.19

Figure 5.2 Histograms and summary statistics of soil (a.) pH$_{CaCl_2}$ and (b.) organic carbon (OC) in the experimental field (*l* = 238)

Primary observations of the raw geo-referenced pH and OC sampled data revealed general spatial trends. Classed maps of data values are shown in Figure 5.3.

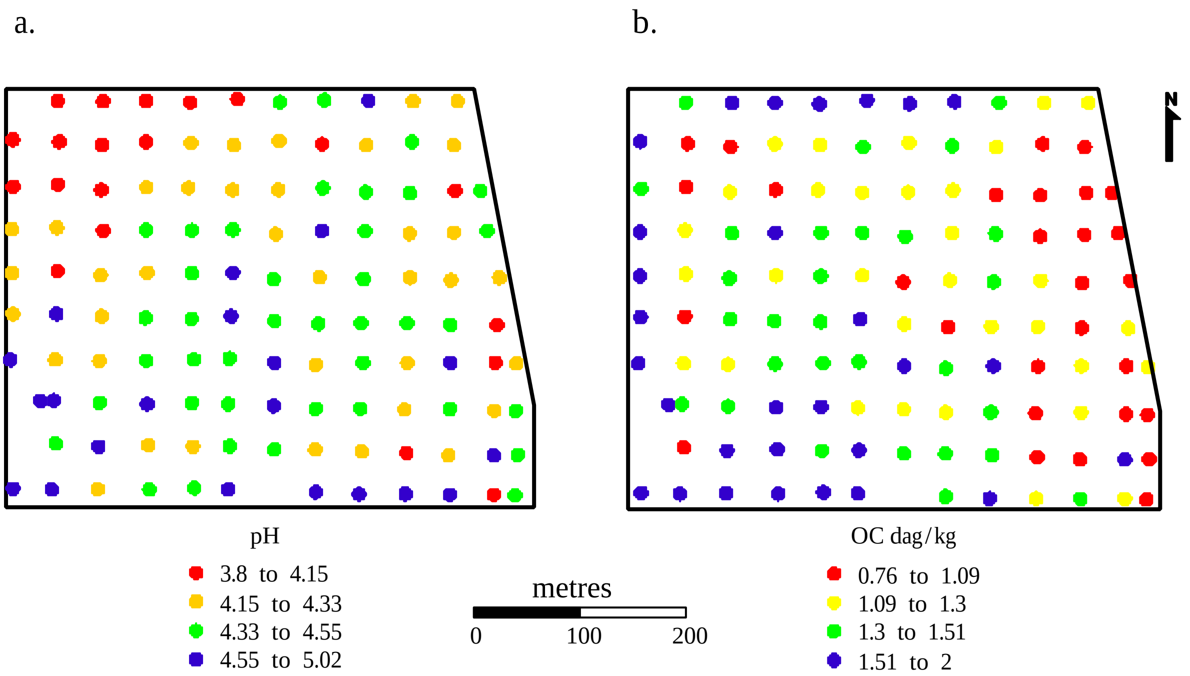


Figure 5.3 Classed maps of soil (a.) pH$_{CaCl_2}$ and (b.) organic carbon (OC) in the field

Figure 5.3a shows smaller pH values in the northern parts of the field, pH generally increasing in the southern direction. Figure 5.3b portrays the occurrence of lower OC values in the eastern parts of the field. The OC data appears more variable than the pH data (Figure 5.2). The spatial trends in both pH and OC data are better illustrated in Figure 5.4, where column and row data averages were calculated and plotted.

There is a distinctive pH trend in the north-south direction, average pH values increasing from approximately 4.1 to 4.7 (Figure 5.4a). The local trends in the pH data (Figure 5.4b) may be attributed to the topography of the field (Chapter III). The lowest average pH values occur at around 90 m east, corresponding to the most elevated section of the field where the soil is mostly leached. Figure 5.4c & d show the averaged north to south and west to east OC data respectively. The clearly distinguishable trend in OC occurs across the field in the west-east direction, OC values increasing from approximately 0.8 dag/kg to 1.7 dag/kg.

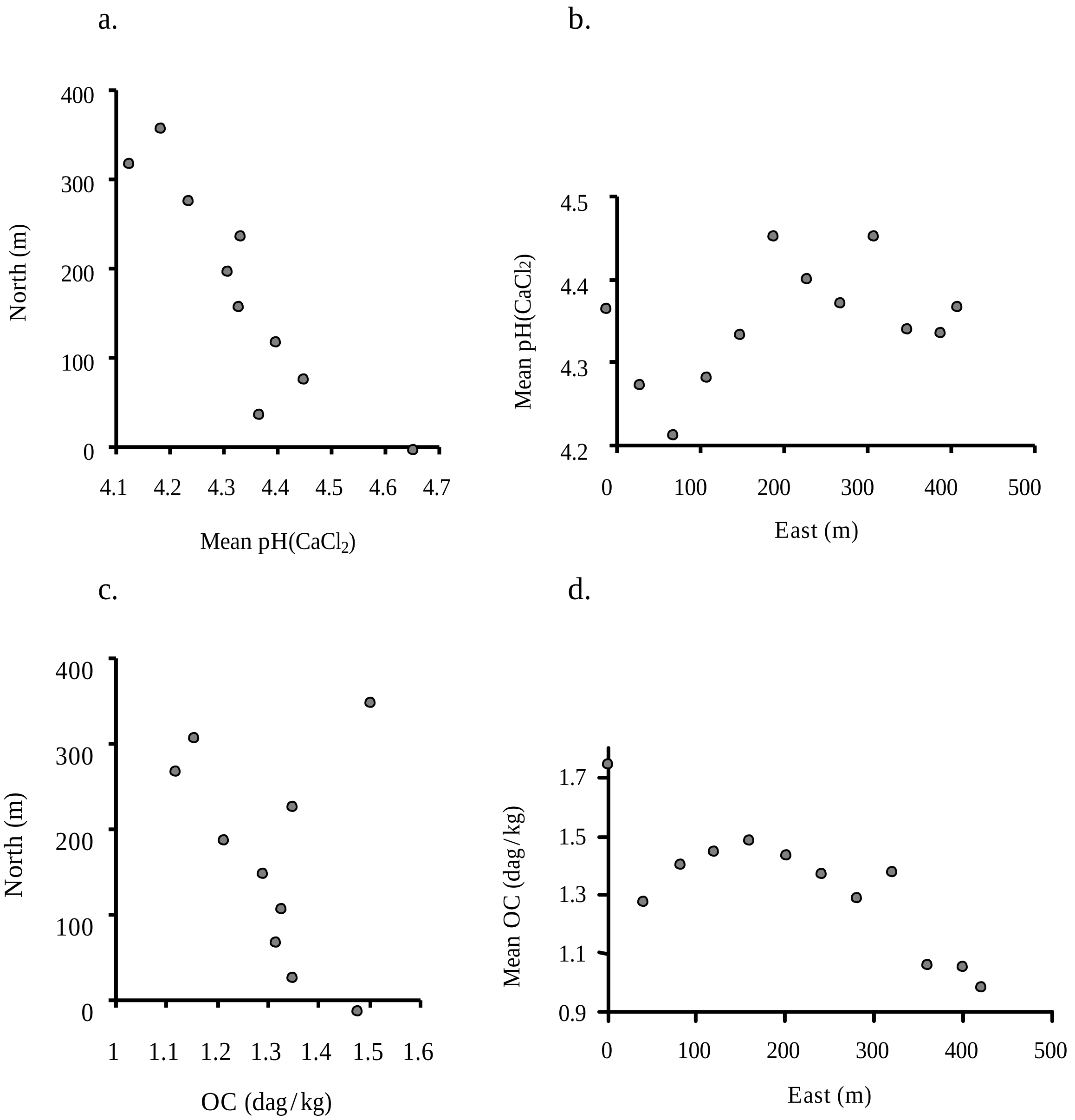


Figure 5.4 Averaged soil pH and organic carbon (OC) data in the northern (a. & c.) and eastern (b. & d) directions respectively.

5.3.2 STRUCTURAL ANALYSIS

The spatial autocorrelations of both the pH and OC data change with direction (Figures 5.5a & 5.5b). The processes involved are not solely a function of distance but also direction, *i.e.* are anisotropic. The directional variograms possess particularly small nuggets that may be easily extrapolated to the origin. These features together with the apparent concavity of the curves reflect the almost continuous variation of the data in specific directions.

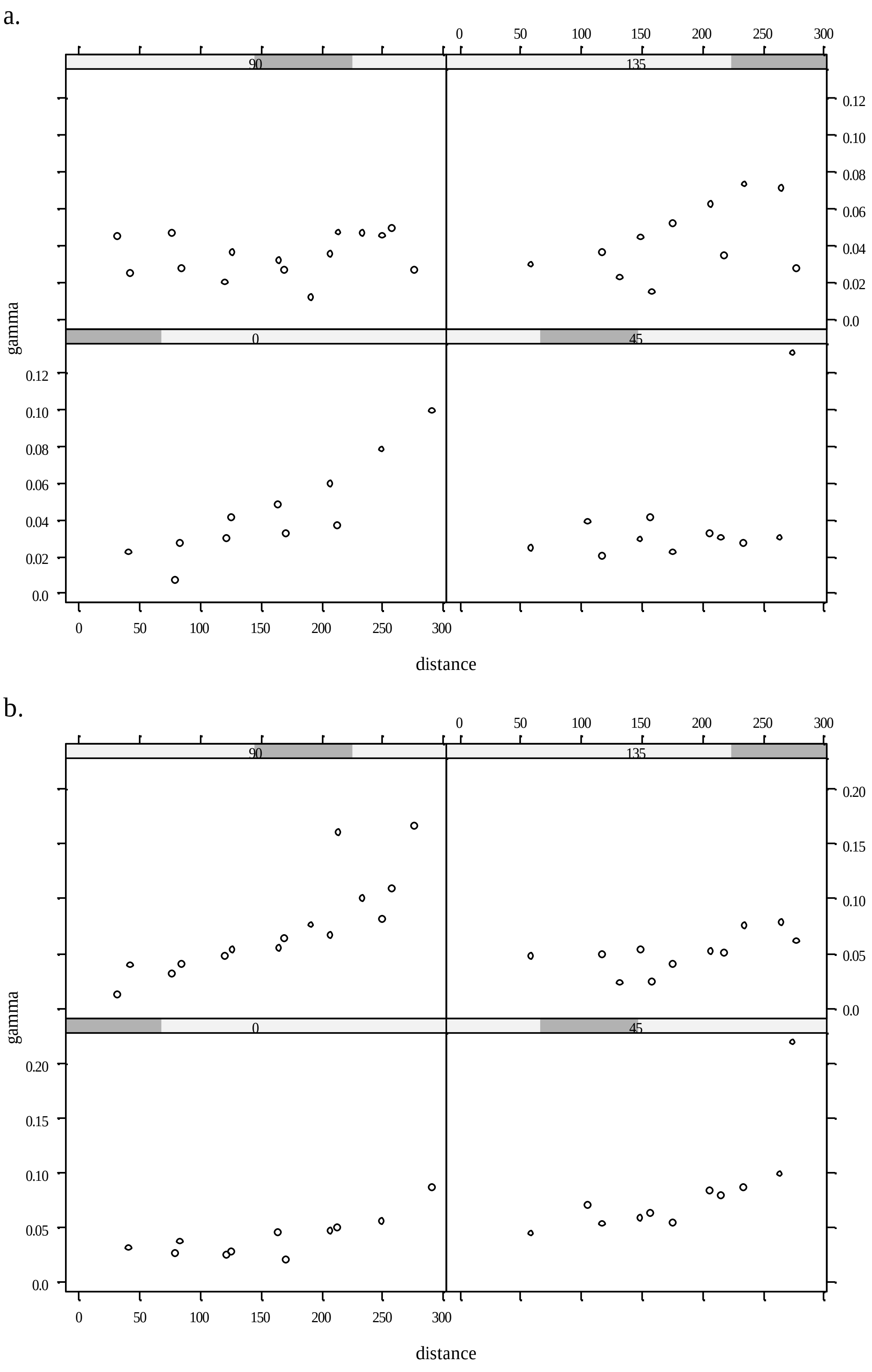


Figure 5.5 Directional semi-variograms for the four principal directions for (a.) pH and (b.) OC

The directional pH semi-variograms appear somewhat similar in the 45° and 90° directions while semi-variograms for the 0° and 135° directions appear anisotropic (Figure 5.5a). The 0° directional pH semi-variogram may present a case for zonal anisotropy. The variogram exhibits greater semi-variances than the other directional semi-variograms and has no apparent bounds. This observation is also consistent with the detected north-south trend in the pH data that was identified through exploratory data analysis in the preceding section. The OC directional semi-variograms (Figure 5.5b) appear similar in the 45° and 90° directions, and similar in the 0° and 135° directions. In the east to west and northeast to southwest directions, the semi-variograms increase continuously with no bounds. This concurs with previous observations of non-stationarity of the OC data in this direction (Figure 5.4d). The directionally dependent semi-variograms depict the non-stationarity of the data in the north-south (for pH) and east-west (for OC) directions (Figure 5.5).

The isotropic experimental semi-variograms for pH and OC were computed and are shown in Figure 5.6.

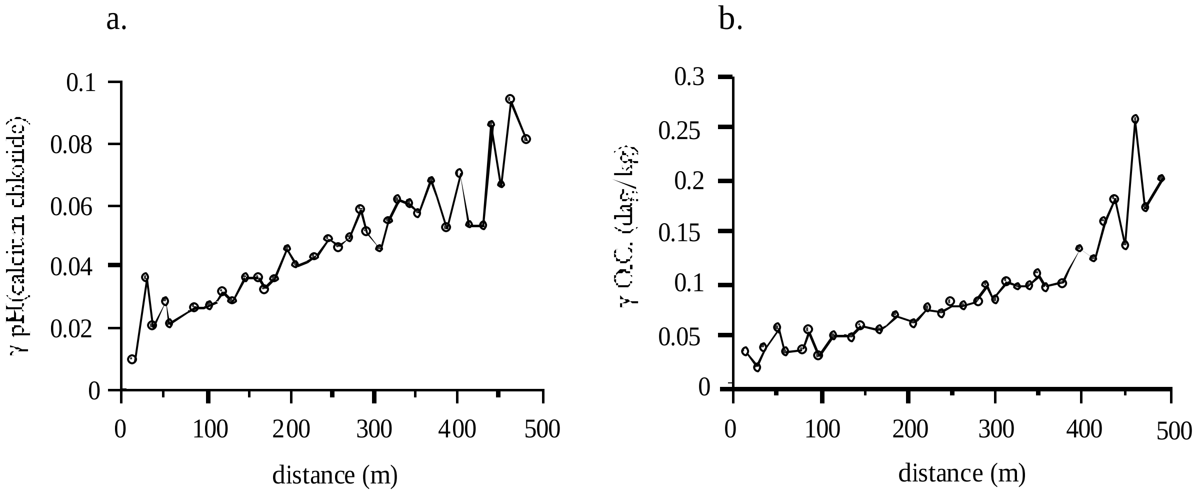


Figure 5.6 Isotropic experimental semi-variograms for soil (a.) pH and (b.) OC.

Both the pH and OC data show similar characteristics, that of increasing semi-variance with no sill (Figure 5.6a & 5.6b respectively). Demonstrated by the slight concavity of the variogram, the OC data appears more strongly trended than the pH data (Figure 5.6b). Subsequent results describe various methods for dealing with the drift detected in the soil pH and OC data.

5.3.3 MODELLING OF THE SPATIAL TREND

The validation and prediction data sets are shown in Figure 5.1b. Statistical summaries of the pH and OC prediction and validation data sets are given in Table 5.2.

Table 5.2 Summary statistics for prediction and validation data sets

Summary	Prediction set (*n* = 158)		Validation set (*m* = 80)	
Statistics	pH	OC dag/kg	pH	OC dag/kg
Mean	4.36	1.32	4.33	1.30
Median	4.33	1.30	4.34	1.30
Variance	0.052	0.075	0.038	0.084
Minimum	3.88	0.76	3.88	0.80
Maximum	5.02	1.99	4.91	1.96
CV	5.25	20.77	4.52	22.14

Both prediction and validation data sets (Table 5.2) appear alike and hence are suitable for the comparative research presented here. The data sets for cross-validation are fairly normally distributed and exhibit similar ranges (Table 5.2). The mean values of each set differ slightly, supporting the preliminary observations of non-stationarity of the data. Larger discrepancies of the variances in the two data sets provide further evidence.

The types of models fitted to the soil pH and OC data are given in Table 5.1. For GOK, the parameters of the transitive and unbounded variograms models that best fitted the experimental variogram data are shown in Table 5.3.

Table 5.3 Transitive and unbounded semi-variogram models and parameters fitted to the pH and OC data.

	Transitive					Unbounded				
	model	C_0	C	a (m)	AIC	model	C_0	ω	Exp.	AIC
Soil pH	Sph.	0.022	0.0527	491	278	Lin.	0.026	0.000126		194
	Exp.	0.02	0.115	677	200	Pow. Fn.	0.022	0.000134	0.97	199
	Gauss.	0.03	0.0491	325	268					
OC dag/kg	Sph.	0.033	0.0953	457	315	Lin.	0.0238	0.0002		176
	Exp.	0.031	0.178	862	231	Pow. Fn.	0.036	0.0004	1.41	205
	Gauss.	0.04	0.1427	397	297					

Linear models fitted both the pH and OC variogram data best, producing smaller AIC (Table 5.3). Exponential models for both data sets produced ranges that extend far beyond field boundaries, reiterating previous observations of non-stationarity in the data. Spherical and Gaussian models were not appropriate, as shown by their high AIC values (Table 5.3), and the shape of the experimental semi-variograms in Figure 5.6. Although power function models appear suitable (relatively low AIC values, Table 5.3), they were unstable and are generally not recommended for use with soil data. Nevertheless as previously described, all of these models were used for GOK in the comparative study (Table 5.1).

Where the assumptions of model stationarity do not apply because of the presence of drift, as is the case with the pH and OC data, it may be more appropriate to first model the trend and use the semi-variograms of the residuals g_R to perform the structural analysis and kriging. This is the basis for the UK methodology and its derivates (refer to section 5.1 above). For the regression residual-kriging methods (see above), the semi-variograms of the regression residuals are shown in Figure 5.7 and the parameters given in Table 5.4.

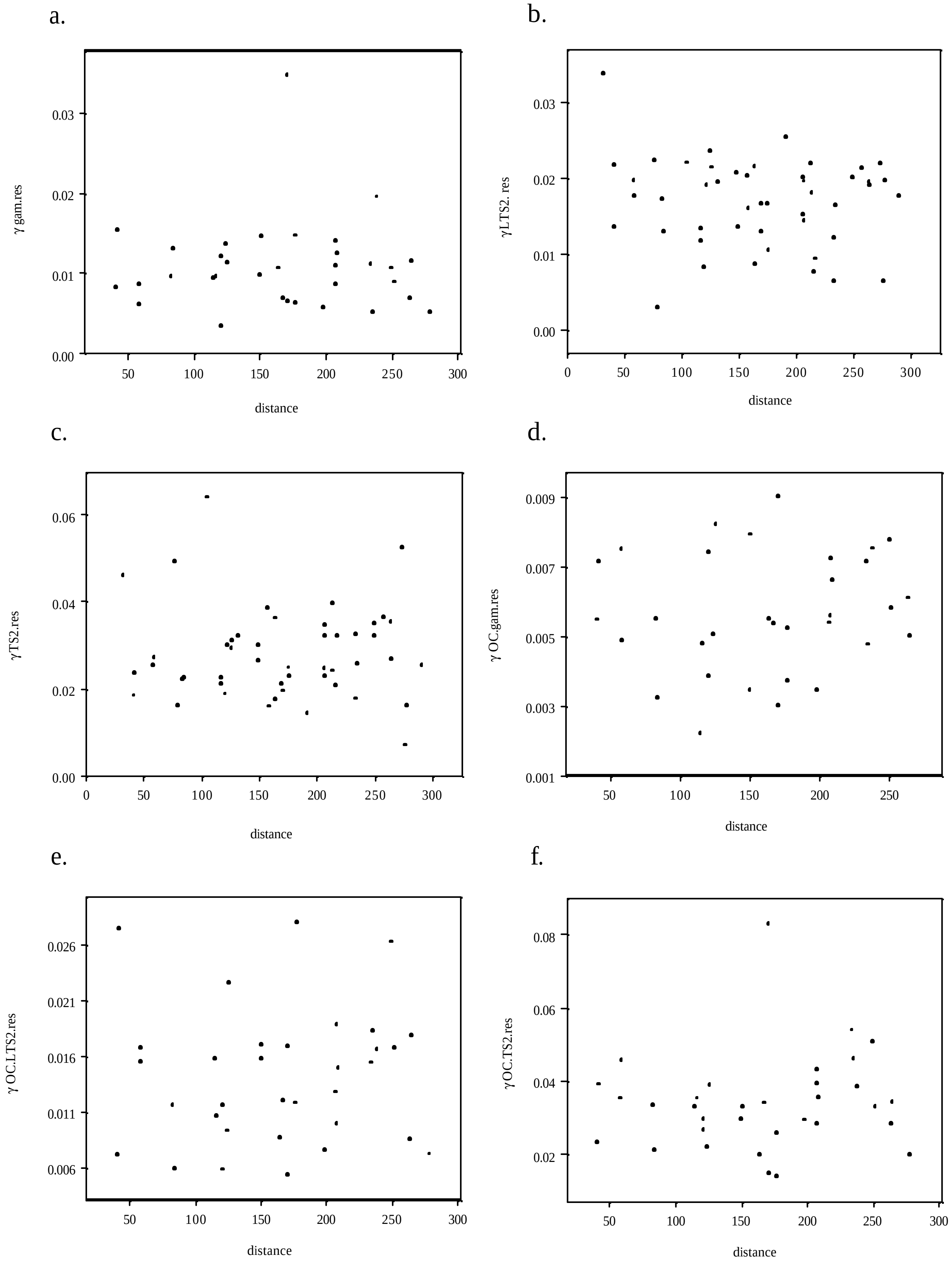


Figure 5.7 Semi-variograms of the residuals from the pH (a.) GAM, (b.) LTS 2, (c.) TS 2, and the organic carbon (OC) residuals for the (d.) GAM, (e.) LTS 2, (f.) TS 2 fitted models

Table 5.4 Spherical (Sph.) semi-variogram (Var.) parameters used for kriging of the residuals resulting from the generalised additive models (GAM), quadratic trend surface (TS 2), local linear trend surface (LTS 1), and local quadratic trend surface (LTS2) regression models, for both soil pH and organic carbon (OC)

Soil property / model	C_0	C	a (m)
Soil pH			
GAM RRK Sph. Var	0.011		
TS 2 RRK Sph. Var	0.026	0.004	425
LTS 1 RRK Sph. Var.	0.022	0.0002	457
LTS 2 RRK Sph. Var.	0.018		
Soil OC (dag/kg)			
GAM RRK Sph. Var	0.0054	0.0002	280
TS 2 RRK Sph. Var	0.03	0.003	307
LTS 1 RRK Sph. Var.	0.021	0.0007	336
LTS 2 RRK Sph. Var.	0.014	0.0003	299

The semi-variograms of the residuals lacked structure (Figure 5.7 and Table 5.4). The reason for this may be that the regression models used accounted for not only the trend in the data, but also for most (and in some instances, all) of the structure. In some instances where automatic fitting showed pure nugget effects, but some structure was evident in the data, spherical models were fitted manually to the residuals data. The semi-variogram parameters shown in Table 5.4 were used for GOK of the residuals.

5.3.4 COMPARISON OF PREDICTION METHODS

A statistical comparison of the predictions methods tested, for the soil pH data are shown in Table 5.5.

Table 5.5 Comparison of spatial prediction methods for soil pH. (Abbreviations of the models compared are the same as in Table 5.1)

Model	No. of parameters	R^2	RSS	RMSE	AIC
IRF – 1	3	0.97	0.11	0.037	-172
IRF – 2	6	0.74	0.94	0.109	7
GOK – Spher. Var.	3	0.75	0.82	0.101	-10
GOK – Exp. Var.	3	0.76	0.78	0.099	-14
GOK – Gauss. Var.	3	0.55	1.48	0.136	37
GOK – Pow. Fn. Var.	3	0.73	0.89	0.106	-3
GOK – Lin. Var.	2	0.73	0.89	0.106	-5
GAM	49	0.66	1.13	0.119	107
TS 2	6	0.48	1.68	0.145	54
LTS 1	8	0.59	1.34	0.129	39
LTS 2	16	0.65	1.21	0.123	46
GAM RRK – Sph. Var.	52	0.64	1.19	0.122	117
TS 2 RRK – Sph. Var.	9	0.42	1.94	0.156	71
LTS 1 RRK – Sph. Var.	11	0.56	1.45	0.135	52
LTS 2 RRK – Sph. Var.	19	0.65	1.27	0.126	56
LOK – Spher. Var	80	0.92	0.27	0.093	55
LOK – Exp. Var.	80	0.82	0.56	0.104	113

From Table 5.5, the GAM was the most accurate predictor of the regression-based methods. However, the large number of parameters used in the additive, fits made GAM the least parsimonious of the group. Regression residual-kriging techniques did not significantly improve the predictions of the stand-alone regression methods (Table 5.5), although in other experimental studies (*e.g.* Neuman & Jacobson, 1984; Odeh *et al.*, 1994 and 1995), the technique performed well. In this work, the poor performance of regression residual-kriging was due to the lack of spatial structure in the semi-variograms of the resiuals. These were either all nugget effects or possessed negligible structure

(Figure 5.7 and Table 5.4). LOK predictions with a spherical semi-variogram were accurate (Table 5.5), eventhough only relatively few data points were used in the local neighbourhoods. However the total number of semi-variogram parameters used was high, thus LOK rendered a higher AIC than most of the other methods (Table 5.5). An unbounded linear variogram model best fitted the pH data (Table 5.3), however GOK with an exponential semi-variogram produced the best predictions of the group (Table 5.5). IRF – 1 produced the best predictions of soil pH. To illustrate the performance of the various procedures, maps of predicted soil pH were produced using the best method from each group (Tables 5.5). These maps are shown in Figures 5.8.

Descriptive statistics of the predicted soil pH data (Figure 5.8), are given in Table 5.6.

Table 5.6 Statistics of soil pH predictions derived from the best predictors from each of the groups tested. For the sample data *n* = 238, for the predicted data *n* = 7 137

Method	Mean	S.D.	Min.	Med.	Max	CV
Sample data	*4.35*	*0.22*	*3.88*	*4.33*	*5.02*	*0.05*
IRF – 1	4.34	0.19	3.80	4.34	5.16	0.04
LOK – Sph. Var.	4.35	0.16	3.89	4.37	4.91	0.03
GOK – Exp. Var.	4.35	0.15	3.99	4.37	4.75	0.03
GAM	4.34	0.14	4.00	4.35	4.88	0.03

The IRF – 1 technique produced a variable map (Figure 5.8d), and statistics that most closely resembled the sample data (Table 5.6). LOK produced more accurate predictions (RMSE = 0.093, Table 5.5) than GOK and the GAM, respectively. In this order, the prediction of soil pH became less variable, as shown by the standard deviation and coefficients of variation of predictions (Table 5.6). In the same order (*i.e.* IRF – 1, LOK, GOK, GAM), the ranges of the predicted data became narrower and the maps smoother, the IRF – 1 technique produced the most variagated map (Table 5.6 and Figure 5.8, respectively).

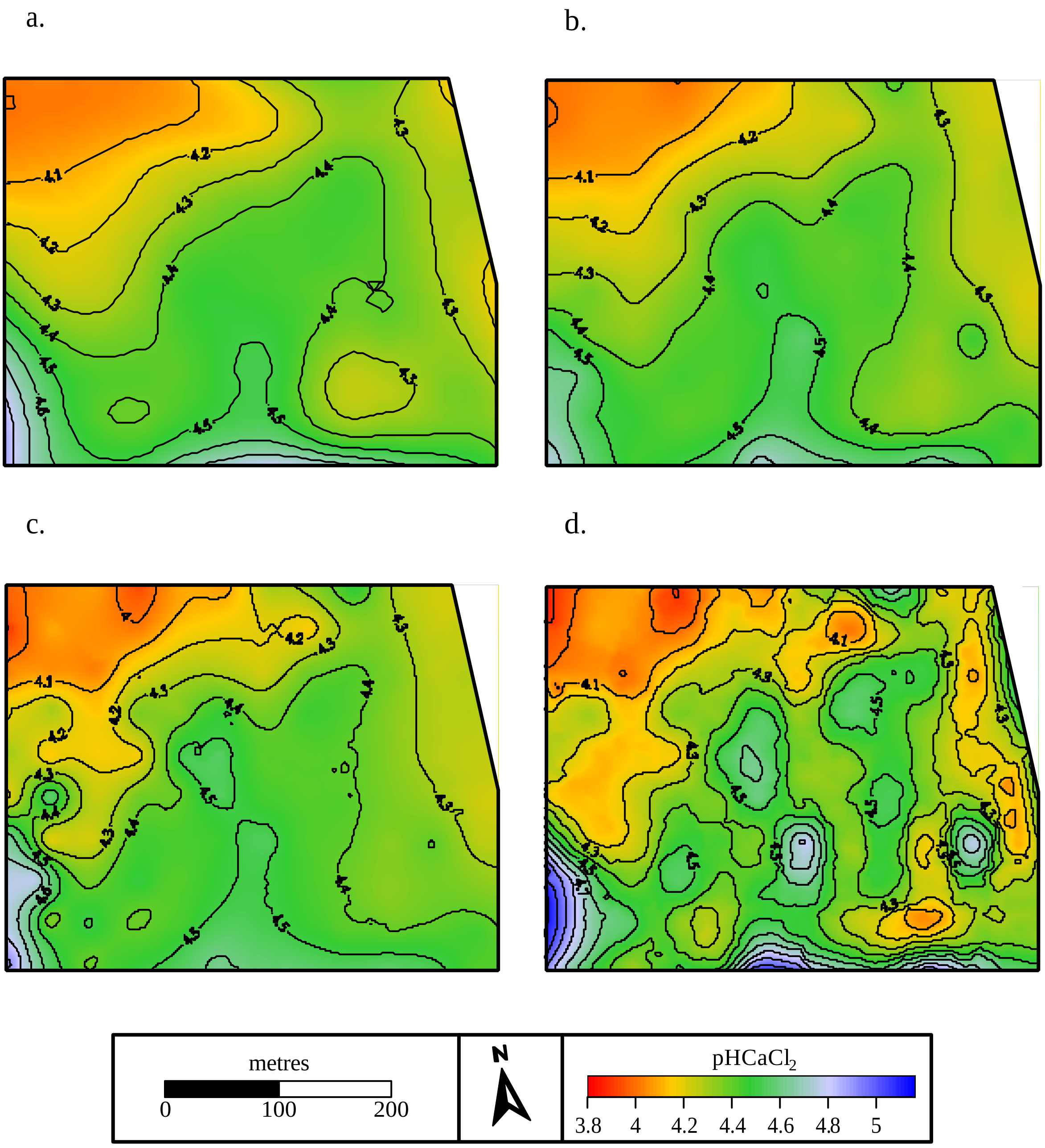


Figure 5.8 Maps of soil pH: (a.) generalised additive model (GAM), (b.) global ordinary kriging (GOK) using an exponential semi-variogram, (c.) local ordinary kriging (LOK) with a spherical variogram, and (d.) intrinsic random function of order 1 (IRF – 1). The latter method produced the most accurate predictions (Table 5.5)

The comparison of methods used to predict soil OC are shown in Table 5.7.

Table 5.7 Comparison of spatial prediction methods for soil organic carbon (OC). (Abbreviations of the models compared are the same as in Table 5.1)

Model	No. of parameters	R^2	RSS	RMSE	AIC
IRF – 1	3	0.96	0.26	0.058	-100
IRF – 2	6	0.96	0.29	0.061	-86
GOK – Spher. Var.	3	0.75	1.92	0.155	58
GOK – Exp. Var.	3	0.76	1.85	0.152	55
GOK – Gauss. Var.	3	0.52	3.25	0.202	100
GOK – Pow. Fn. Var	3	0.63	2.64	0.182	84
GOK – Lin. Var.	2	0.79	1.67	0.144	45
GAM	48.6	0.61	2.64	0.182	175
TS 2	6	0.51	3.28	0.203	107
LTS 1	8	0.57	2.91	0.191	102
LTS 2	15.5	0.67	2.25	0.168	96
GAM RRK – Sph. Var.	51.6	0.61	2.64	0.182	181
TS 2 RRK – Sph. Var.	9	0.46	3.64	0.213	121
LTS 1 RRK – Sph. Var.	11	0.56	2.99	0.193	110
LTS 2 RRK – Sph. Var.	18.6	0.67	2.34	0.171	105
LOK – Spher. Var	80	0.89	0.81	0.12	143
LOK – Exp. Var.	80	0.83	1.34	0.134	183

From Table 5.7, the LTS 2 was the most accurate and parsimonious predictor of the regression-type techniques. As for the soil pH data, regression residual-kriging techniques did not improve the accuracy of predictions (Table 5.7). Similarly, LOK predictions with a spherical semi-variogram were accurate, however the large total number of semi-variogram parameters used rendered LOK less suitable than most of the other methods (Table 5.5). The linear semi-variogram model best fitted the OC data (Table 5.3), and in this instance, it also produced the best GOK predictions of the group (Table 5.7). IRF – 1 produced the overall best predictions of soil OC. To illustrate the performance of the various procedures, maps of predicted soil OC were produced using the best method from each group (Tables 5.7). These maps are shown in Figures 5.9.

Descriptive statistics of the predicted soil OC data (Figure 5.9), are given in Table 5.8.

Table 5.8 Statistics of soil organic carbon predictions derived from the best predictors from each of the groups tested. For the sample data *n* = 238, for the predicted data *n* = 7137

Method	Mean	S.D.	Min.	Med.	Max.	CV
Sample data	*1.32*	0.28	*0.76*	*1.30*	*1.99*	*0.21*
IRF – 1	1.30	0.23	0.77	1.30	1.97	0.18
LOK – Sph. Var.	1.31	0.19	0.82	1.33	1.74	0.15
GOK – Lin. Var.	1.31	0.18	0.97	1.32	1.71	0.14
LTS 2	1.30	0.17	0.95	1.29	1.89	0.13

The IRF – 1 technique produced the best map (Figure 5.9d), and statistics that most closely resembled the sample data (Table 5.8). LOK produced more accurate predictions (RMSE = 0.12, Table 5.7) than GOK and the LTS 2, respectively. In this order, the prediction of soil OC became less variable, the ranges of the predicted data became narrower (Table 5.6), and the maps smoother (Figure 5.9). IRF – 1 produced the most variagated map (Figure 5.8).

5.4 CONCLUDING REMARKS

For both the soil pH and organic carbon data, intrinsic random functions of order k produced the most accurate and parsimonious predictions of all of the methods tested. Of the remaining methods local ordinary kriging was most accurate, even though a minimal number of points in each neighbourhood was used for predictions. However, in terms of the Akaike Information Criterion, local kriging performed badly as it was the least parsimonious. Global ordinary kriging performed better than the regression and regression residual-kriging methods.

These results were for the most part anticipated since the method that rendered best results was originally developed to ‘filter out’ the drift component of the random function and to overcome the problems associated with universal kriging.

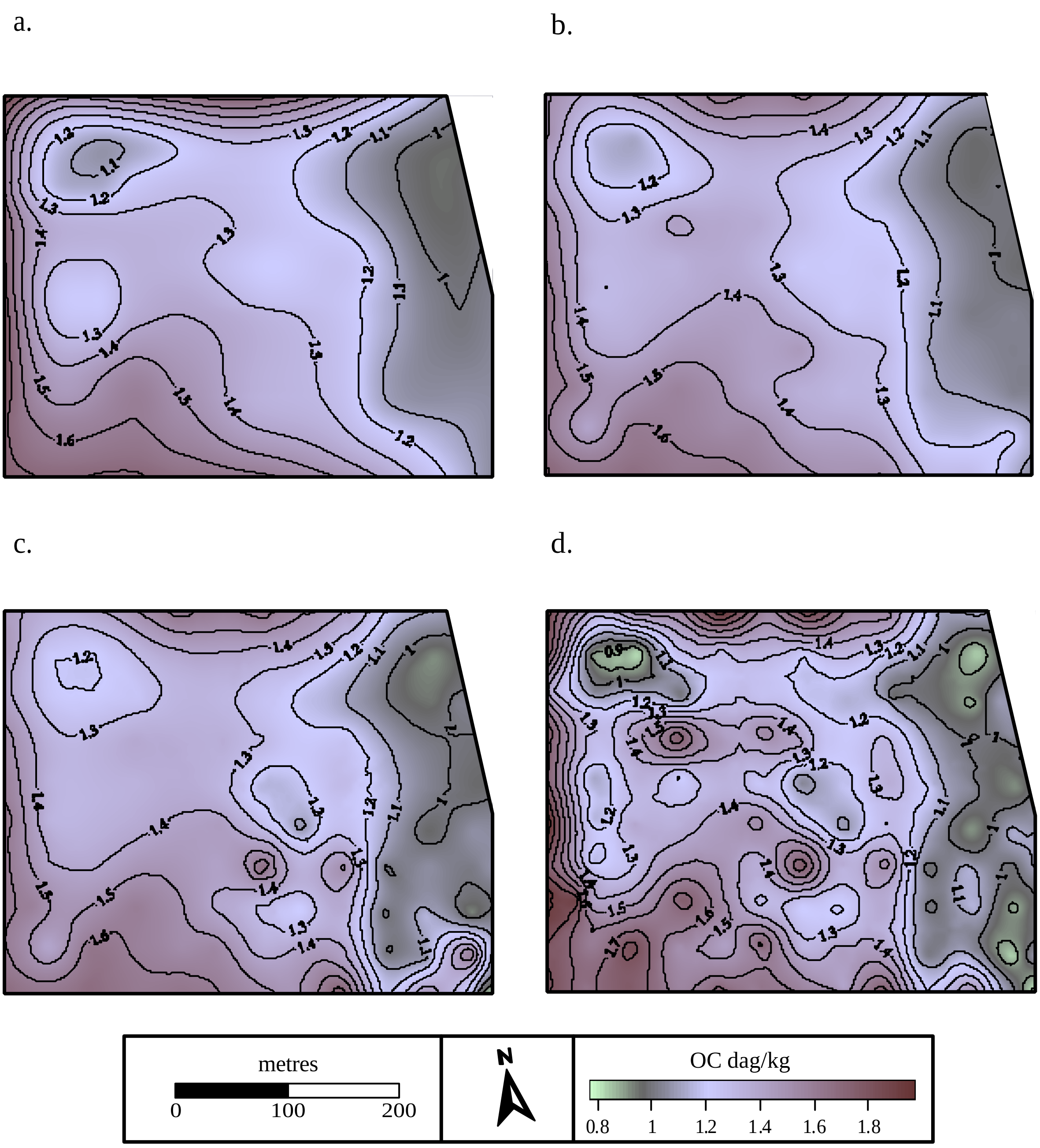


Figure 5.9 Maps of soil organic carbon (dag / kg) showing the general trend in prediction accuracy of the methods tested: (a.) quadratic local trend surface (LTS 2), (b.) global ordinary kriging (GOK) using a linear semi-variogram, (c.) local ordinary kriging (LOK) with a spherical variogram, and (d.) intrinsic random function of order 1 (IRF – 1). The latter method produced the most accurate predictions (Table 5.7)

Unexpectedly however, regression residual-kriging that aims to first define the global nature of the drift using a subjective trend model, performed poorly. The method was expected to produce similar results to, or better than, the intrinsic random function method, as it has done in other experimental studies. One reason for its poor performance was the little or no remaining semi-variogram structure in the regression

residuals. These results implied the presence of only deterministic trends in the pH and OC fields that could be easily modelled by trend surface regression analysis. Obviously this was not the case. The bias introduced in modelling the trend component of the random function needs further investigation. These non-conforming results may be due to the use of only a single validation, where the particular data subsets may not necessarily represent the actual pH and OC drifts in the experimental field. An improved validation method suggested by Goovaerts (1999, pers. comm.) is to conduct the analysis for a number of randomly selected jackknifes and compute statistics from them.

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SECTION III

Chapter VI

SOIL ACIDITY AND ACIDIFICATION: A PROSPECTIVE MANAGEMENT SYSTEM FOR ACID SOIL

6.1 INTRODUCTION

The topics of soil acidity and soil acidification are fundamentally important to the long-term stability of agricultural production systems in many regions of the world. A soil is said to be acidic when its pH is below 7. Soil acidification is a process that occurs over time, starting with the colonisation of rock surfaces by algae and thallophytic plants such as lichens. The acids produced, mainly from biochemical cycles (such as the carbon and nitrogen cycles), are involved in the dissolution of parent material during the process of soil formation (Jenny, 1941). Hence soil acidity is a variable process that depends on the type of parent material, local climate, organisms present and the length of time it has weathered (not as a consequence of weathering (Ulrich, 1991)). Soil may then be naturally acidic, neutral or alkaline.

Under natural conditions soil acidifies gradually with time, albeit aided by natural disturbances such as drought, atmospheric pollutant depositions (Brunet *et al.*, 1996), etc. However while many soils may be naturally acidic, the rates of acidification are augmented by anthropogenic practices that disturb the natural balance of the rhizosphere. For example, Lewis *et al.* (1987) indicated that in South Australia, after 30 years of sown pasture pH had decreased by as much as one unit. Conyers *et al.* (1996) showed that dryland agricultural practices in southeastern Australia acidified the 0 – 20 cm soil layer by approximately 0.5 pH units in 12 years. Slattery *et al.* (1998) indicated that in 15 years of continuous cropping (lupins-wheat rotation) soil pH of the top 0 – 20 cm layer had decreased by as much as 1.5 pH units.

In an agricultural ecosystem, most of the augmented acidification occurs because of imbalances between the inputs (*e.g.* chemical applications) and outputs (*e.g.* leaching and removal of produce) of the system. For example the ‘green revolution’ encouraged the use of immoderate amounts of nitrogenous fertilisers and irrigation water (Chapter I). Their antagonistic effects on production and the environment were particularly noticeable once the initial yield benefits started to fade. One of the discernible after-effects that remains is soil acidification and its adverse effects on crop yields and overall soil quality. The detrimental effects on soil quality refer to the inability of acid soil to support agricultural productivity. This is mainly due to the increased solubility of phytotoxic elements such as aluminium and manganese (when absorbed in high concentrations). Acid soil is also more prone to other forms of land degradation such as nutrient depletion and erosion. Consequences on human health include the entry of soluble toxic elements into water tables, rivers, storage dams and hence into consumable produce. For example a significant concern is the increased concentrations of aluminium in water supply dams and its possible links to Alzheimers's disease. Therefore the acidification of agricultural land is considered a form of land degradation that has adverse effects on not only production but also soil quality.

The present chapter will define soil acidity and acidification, summarise the causes and consequences of soil acidification as well as existing and potential management opportunities that may be employed to retard, arrest or even reverse acidification in agricultural ecosystems. To provide some reference to the extent of the problem and the need for a sustainable management system, discussion will continue with a review of the extent and degree of global soil acidification as well as that which occurs in Australia. Consequently, a real-time continuous management system for acid soil is proposed.

6.2 SOIL ACIDITY

Soil acidity (or alkalinity) is measured in terms of pH which is the logarithm of the reciprocal of the hydrogen ion activity in solution, *i.e.* $pH = -\log[H^+]$. The pH scale ranges from 0 to 14 and pH may be measured using a variety of colorimetric and potentiometric techniques, all of which measure the intensity of the acid (*i.e.* the concentration of H^+ in the soil solution), or base present in solution. Soil pH is a most informative and easily measured soil property and hence it is perhaps the most widely measured soil attribute. Soil pH is a good indicator of soil quality. Soil pH varies both in time and in space. Chapter II presents a literature review of the reported spatial variability of soil pH.

Schofield & Taylor (1955) and White (1969) both described and reviewed the measurement of soil pH. Ahern *et al.* (1995) derived relationships between pH measurements in water (pH_{H_2O}) and in a 0.01M $CaCl_2$ solution (pH_{CaCl_2}). Measurements in 0.01M $CaCl_2$ are generally preferred as the method minimises the effect of salts on pH, also reducing errors due to junction potentials and suspension effects (Peech *et al.*, 1953). Measurements of pH_{CaCl_2} are usually 0.5 to 1 pH unit lower than those made in pH_{H_2O}.

By definition, when soil pH falls below 7, it is deemed to be acidic, but many farm and soil managers do not usually consider a soil acidic until pH_{CaCl_2} falls below 5.5 when the soil is already moderately acidic. The reason for this may be that at pH values above 5.5, the solubility of phytotoxic elements such as aluminium is low. The term ‘acid soil’ is also sometimes used to refer to infertile soil or soil that is likely to become infertile if the pH drops further. A reason for the use of the terms is that acid soil frequently exhibits infertility problems. Acid soil inhibits the availability of certain nutrient (*e.g.* calcium, molybdenum), aggravates leaching of macronutrients (*e.g.* calcium, magnesium) below the root zone and encourages the accumulation of increasing concentrations of toxic elements (*e.g* aluminium) all adversely affecting biological processes and hence crop productivity. However care needs to be taken when using the term ‘acid soil’ to refer to soil infertility because some naturally acid soils support productive farming systems, *e.g.* soils in the high-rainfall Central Tableland areas of NSW and southeastern Victoria (see below).

6.2.1 SOIL ACIDIFICATION

Soil acidification is the process whereby acids (*e.g.* nitric, carbonic and organic) added to the soil dissolve the basic soil-buffering compounds (Helyar, 1976). Soil processes involve reactions that produce acids and reactions that neutralise the acids produced, for example in a natural ‘untouched’ ecosystems acids produced are very nearly in equilibrium with neutralising processes (Ulrich 1991). In such instances, soil acidification occurs over many thousands of years since the rates of acidification are slow. In contrast, the acid-base imbalance in agricultural soil is far greater due to increased rates of acid addition and base removal from the system, causing accelerated rates of acidification. That is, agricultural soil acidifies over shorter periods of time (*e.g.* Slattery, *et al.*, 1998; Lewis *et al.*, 1987, Williams, 1980). Coventry *et al.* (1996) conducted a ling-term rotation trial in southeastern Australia and evaluated the effects of some rotations, stubble handling and tillage practices on the relative rates of soil profile acidification over a 12 year period. All of the treatments in their experiments acidified the soil over the time period of the study, at a rate equivalent to the loss of 46 to 95 kg $CaCO_3$/ha/yr. The acidification of the topsoil layers is shown in Figure 6.1.

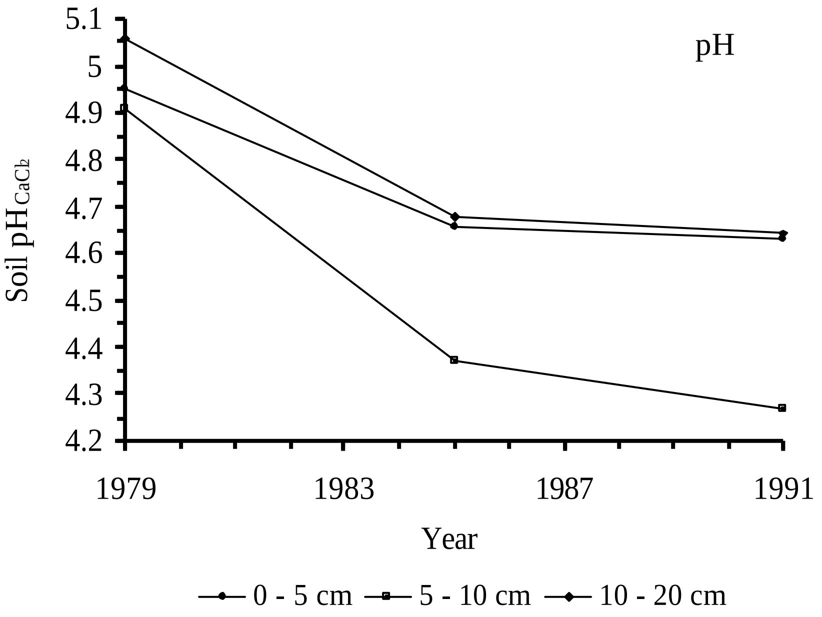

Figure 6.1 Change in the pH profile of the surface 20 cm of soil over 12 years as a result of dryland agricultural management practices. (adapted from Coventry *et al.* (1996))

The processes responsible for soil acidification have been comprehensively reviewed elsewhere (*e.g.* Kennedy, 1992; van Breemen, 1991; Helyar & Porter, 1989; Adams, 1984). Most research reporting on the rates of soil acidification are based on temporal changes in pH (some examples were given above). However changes in soil pH are not particularly useful in explaining the rates or significance of soil acidification. van Breemen (1991) used capacity (*e.g.* the amount of acid or base added) rather than intensity factors (*e.g.* pH) in titration curves for the characterisation of soil acidification. The reason for this is that soil pH cannot be predicted in a simple manner from the amount or acid or base added due to strong soil buffering in certain pH ranges. Particularly at pH values greater than 7 and lower than 4 (Figure 8.6, Chapter VIII). van Breemen (1991) discussed the nature and importance of acidification due to acid additions, biogeochemical cycles and nutrient assimilation, defining the acidification processes in terms of changes in capacity factors. Hence the effects of increased inputs of acid on soil acidity are determined by the soil's buffering capacity and the kinetic effects following the additions of the acid. Obviously, additions of base (*e.g.* $CaCO_3$) to ameliorate the net inputs of acid are also affected by both of these factors. Amelioration by liming is required to balance the net acid additions and to maintain soil pH at a desirable level for plant growth. Liming is discussed in detail in Chapter VIII.

Helyar & Porter (1989) discussed the processes and rates of soil acidification in agriculture in terms of biogeochemical cycles (mainly carbon, nitrogen), and suggested the concept of an ecosystem H^+ pool from which inputs and outputs of H^+ to and from the H^+ pool occur. The acids causing the acidification of agricultural soils are derived mainly from the carbon and nitrogen cycles. Organic acids are produced in plants from the assimilation of sugars by photosynthesis from carbon dioxide and water, while nitric acid is produced during the conversion of nitrogen into proteins. Both these processes involving the cycling of carbon and nitrogen are neutral (Helyar, 1976). Soil acidifies only when the inputs and outputs of the system occur in different proportions, inducing an acid reaction. Helyar & Porter (1989) defined the acidifying effect of the nutrient cycles important in agricultural ecosystems using the following equation:

$$\begin{aligned}\text{Acid addition (mol./ha/unit time)} &= (C_{cycle} + N_{cycle} + A_{alkali} + A_{acids}) \\ &= (OA_{ac} + OA_{ex} - OA_{ad} + HCO^-_{3\,ac} + HCO^-_{3\,ex} - HCO^-_{3\,ad}) \\ &\quad + (NH^+_{4\,ad} - NO^-_{3\,ad} - NH^+_{4\,ac} + NO^-_{3\,ac} + NO^-_{3\,ex} - NH^+_{4\,ex}) \\ &\quad + (-L_{ad}) \\ &\quad + (H^+_{ad}) - (H^+_{ex})\end{aligned} \tag{6.1}$$

where OA represent organic anions, A represent additions, L represent liming materials such as $CaCO_3$, *ac*, *ex* and *ad* represent material accumulated in, exported from, or added to the ecosystem. Helyar & Porter (1989) indicated that nutrient cycles involving sulfur, iron, aluminium and manganese where not included because they are of minor importance in soil acidification. However these cycles are recognised as being significant causes of seasonal pH fluctuations in periodically saturated soil. Aluminium and manganese are also understood to influence the management of acid soil because when they are present in high concentrations (as Al^{3+} and Mn^{2+}) in the soil solution they are phytotoxic.

6.3 PRIMARY CAUSES OF AGRICULTURAL SOIL ACIDIFICATION

In this instance a more applied discussion of the main causes of soil acidification in agricultural ecosystems will be given. The main causes and relative proportions in agriculture (given by Helyar & Porter, (1989)) being the leaching of excess nitrate below the root zone (40 – 51 %), accumulation of organic matter (34 – 43 %), product removal (12 – 15 %), and other sources including the misuse of nitrogenous fertilisers (< 4 %).

6.3.1 LEACHING OF NITRATE-NITROGEN

In soil, nitrate is a very soluble ion and following rainfall or irrigation, excess amounts of nitrate not consumed by the plant are easily leached below the root zone into the ground water, or lost in run off. When soil nitrate is lost through leaching, the soil is left more acidic (Equation 6.1), and soil acidification becomes of particular agronomic and environmental concern. The effect of nitrate leaching is to replace cations such as calcium, magnesium and potassium with protons. Therefore the nitrogen cycle contributes towards acidification proportionally to the amount of nitrogen lost via leaching, run-off (and product removal, refer to section 6.3.3). This form of acidification is the major contributor to the acidification of arable soils (Williams, 1980).

Some evidence that leaching is involved in the process of acidification is given by Helyar *et al.* (1990). These authors suggested that good correlations between rainfall and the distribution of acid soil in Australia partly reflect the role of leaching in the transport of organic anions and nitrate from the soil. Similarly, Ahern *et al.* (1993) showed that soil acidity in Queensland was extensive in high rainfall areas. Helyar *et al.* (1990) indicated that the correlations are accentuated where the seasonality of rainfall is extreme, for example in winter-rainfall climates of southern Australia where plant growth is slow and annual precipitation exceeds 500 mm. These authors also suggested that in areas of moderate rainfall, where active plant growth is possible at any time of year, reduced nitrate leaching occurs and the rate of acidification is lower.

6.3.2 ACCUMULATION OF ORGANIC MATTER

Drastic changes in the levels of organic matter in soil are unlikely in stable ecosystems (Kennedy, 1992). However in agriculture, changes in organic matter due to the implementation of ley farming systems have had an effect on the degree of soil acidification. In Australian agriculture the regular use of fertiliser and improved pastures, particularly the dinitrogen fixing legumes like subterranean clover resulted in the increased accumulation of organic matter. Williams & Donald (1957) indicated that increased soil acidification in pastures was partly due to the accumulation of organic matter. Helyar & Porter (1989) presented examples suggesting that as soil organic matter levels increased, soils acidified. Williams (1980) also indicated that the rate of acidification is likely to be greatest in light textured and poorly structured soils of increasing organic matter content. Although raising the organic matter content of soil has beneficial structural effects, the accumulation of acids resulting from the carbon cycle can be a significant cause of soil acidification (Equation 6.1).

Increased organic matter levels in soil suggest that more nitrate-nitrogen can be produced through mineralisation. Therefore in addition to acidification from accumulation of organic matter, the potential for further acidification from leaching and run-off is increased. This implies that the need to more actively reduce loss of nitrate becomes increasingly important as soil organic matter levels increase.

6.3.3 REMOVAL OF AGRICULTURAL PRODUCE

The objective of agricultural systems is the production of consumable and saleable products. Their removal off the land is an inevitable consequence. From the time when agrarian societies developed, the purpose of agricultural production systems has remained similar, although methods of production have changed and the magnitude of production is obviously greater. Soil acidification due to the removal of large amounts of agricultural product off the land, occurs because both plant and animal produce are slightly alkaline. Their removal has a net acidifying effect on the soil.

Ridley *et al.* (1990) used Equation 6.1 to compare the sum of carbon and nitrogen cycle acid addition components with the total calculated acid addition of a pasture production system. The authors assessed the importance of these cycles in the acidification of soil. Ridley et al (1990) indicated that carbon and nitrogen cycle acidification in an annual pasture production system accounted for 65 and 35 %, respectively, of the net acid addition on a fertilised field. The greater contribution of the carbon cycle may be attributed to higher stocking rates and greater product removal (hay, wool and meat) from the system.

Nutritional uptake by plants consumes a large proportion of basic cations (such as Ca^{2+}, Mg^{2+} and K^{+}) over anions (White, 1997). When these cations are present in excess amounts in plant and animal tissue, they are balanced by organic anions, which when exported in the form of saleable and waste products off the land (Equation 6.1), result in excess H^{+} in the soil. Slattery *et al.* (1991) calculated the ash alkalinity of several farm products to determine their potential contribution to soil acidification processes and hence the lime-required to counteract the removal of alkali from the system. A summary of their results is given in Table 6.1. The alkali removed by pastures like lupins is greater than for cereals such as wheat, barley and triticale (Table 6.1). Therefore pasture legumes have a greater potential for acidifying soil based on product removal, and hence require the greatest amount of lime to replace lost alkali from the soil. The data on Table 6.1 implies that (in both cropping and pasture enterprises) management strategies that include lime replacement for exported farm produce should be considered to minimise soil acidification (Slattery *et al.*, 1991).

Table 6.1 Equivalent amounts of lime ($CaCO_3$) required to replace the alkali removed in farm produce of north-eastern Victoria, Australia. Adapted from Slattery *et al.* (1991).

Plant Product	Yield Mg/ha	$CaCO_3$ kg/ha/yr
Lucerne hay	3 – 7	540 – 1260
Mixed grass hay	3 – 7	270 – 630
Lupin	0.6 – 1.3	12 – 26
Barley	1.2 – 2.3	10 – 18
Triticale	1 – 2.8	7 – 20
Wheat	1.2 – 2.1	11 - 19

6.3.4 INEFFICIENT USE OF FERTILISERS

Nitrate-nitrogen (NO_3^-) is the main form of nitrogen consumed by plants from the soil, and is used for growth and development. Nitrate is supplied to the soil either from fertilisers (*e.g.* nitrate, ammonia, urea, or organic materials) or through atmospheric nitrogen fixation by legumes. Nitrate fertilisers do not have an acidifying effect, but nitrification of ammonia and urea, or nitrification of mineralised organic matter are both processes that generate acidity (Kennedy, 1992; Ulrich, 1991). Usually the acid produced is neutralised by alkaline plant discharges during plant uptake of the nitrate formed. However if nitrate is supplied in greater amounts than that demanded by plants, for example when excessive ‘blanket’ rates of fertiliser (particularly ammonia and urea) are applied then higher rates of soil acidification can occur in areas of the field where over-applications have occurred.

Inadequate use of fertilisers can lead to accumulations of excess nitrate in the soil solution hence leaching of nitrate together with metal cations may occur, and consequently soil acidifies (refer to section 6.3.1). Different forms of nitrogenous fertilisers have different effects on soil pH. Hence the amount of acidification that results from their use depends on the type of fertiliser used and how it is managed. The potentially acidifying reactions all occur due to nitrification. For example, nitrification of ammonia fertilisers produces protons and as such is always acidifying (nitrifying equations are given in Kennedy (1992)).

Malhi *et al.* (1995) indicated that with increasing application rates of nitrogenous fertiliser, pH values of the topsoil layer were markedly reduced, inducing increased concentrations of aluminium, iron and manganese. Manoharan *et al.* (1995) showed that the use of diammonium phosphate was a significant factor in the acidification of soil. The various nitrifying reactions of ammonia fertilisers are given in Kennedy (1992 pp. 120-121). Table 6.2 shows the acidifying effect of various forms of nitrogenous fertilisers and expresses the acid addition in terms of the amount of lime needed to neutralise the effect of adding 1 kg of applied nitrogen to the soil. Two extreme situations are shown in Table 6.2.

Table 6.2 Rates of soil acidification expected from various forms of nitrogenous fertilisers. Adapted from Cregan & Helyar (1986).

Source of nitrogen	$CaCO_3$ (kg $CaCO_3$/kg applied N) required to balance acidification	
	0 % nitrate leached	100 % nitrate leached
High acidification – *e.g.* ammonium sulfate, monoammonium phosphate	3.7	7.1
Medium acidification – *e.g.* diammonium phosphate	1.8	5.3
Low acidification – *e.g.* urea, ammonium nitrate, anhydrous ammonia, biologically fixed (legume) N	0	3.6
Alkalisation – *e.g.* sodium and calcium nitrate	-3.6*	0

Note: * equivalent to applying 3.6 kg $CaCO_3$/kg applied N.

The second column of Table 6.2 presents a case where the crop takes up all of the nitrogen applied, while the third column presents one where all of the nitrogen is lost by leaching. Realistically, acid addition from fertiliser use is likely to be somewhere in between these two extremes depending on the efficacy of fertiliser management. It may be speculated that site-specific fertiliser usage (refer to section 6.5.1) will on average result in much lower nitrate leaching than single-rate ‘blanket’ applications. Also, ammonium fertilisers may never realise their full acidifying potential because ammonia (NH_3) can be lost by volatilisation from soil at higher pH values, or because of denitrification (Kennedy, 1992). However, acid addition through inefficient fertiliser use is an important source of acidification in some agricultural systems, requiring lime applications to neutralise it (Equation 6.1).

6.4 PRINCIPAL CONSEQUENCES OF SOIL ACIDIFICATION

Soil acidity adversely affects soil quality. It is detrimental to plant growth and hence agricultural production, it degrades productive and potentially productive land, it has socioeconomic implications and may affect human health. The following subsections briefly describe the consequences of soil acidification in agriculture as biological, chemical and physical.

6.4.1 SOIL BIOLOGICAL CONSEQUENCES

The most important biological consequence of soil acidification is the decline in agricultural productivity, therefore crop production on soils that are very acidic is not sustainable. Furthermore the choice of crops that can be grown on this land is restricted to acid-tolerant species. One of the reasons for the loss in yield is the disruption to soil biological processes caused by low pH levels. The most widely reported effects of acid soil on agriculturally important organisms are summarised below.

Different microbial groups have different pH optima; hence their biodiversity in acid soil differs from neutral or alkaline soil. Most microorganisms have a well-defined pH optimum for growth and a range in which growth is possible (Lynch, 1995). For example, generally fungi have pH optima below those of bacteria. Typically, soil bacteria are sensitive to low pH values, and grow poorly in acidic soil (Robson & Abbott, 1989). For example, when leguminous crops are grown, nodulating bacteria (*Rhizobia*) fail to establish their associations when soils are acidic. Also, ammonifying and nitrifying bacteria, *Nitrosomonas* and *Nitrobacter*, are both affected by acidic soil. Robson & Abbot (1989) indicated that a drop in soil pH from 6.5 to pH 4 almost completely suppressed nitrification.

Together with decreases in pH, the concentration of soluble elements like aluminium and manganese may increase and reach levels that are toxic to soil microorganisms (Glenn & Dilworth, 1991). Coventry & Evans (1989) indicated that aluminium was particularly toxic to *Rhizobia*. Robson & Abbot (1989) showed the adverse effects of high concentrations of soluble aluminium and manganese on nitrifying bacteria.

Soil faunal communities (*e.g.* invertebrates and arthropods) are sensitive to pH and hence acid soil. Lavelle *et al.* (1995) suggested that soil fauna are generally unable to adapt to acid soil conditions. They indicated that the population of large invertebrates (*e.g.* earthworms and termites) was lower in acid soil. Their abundance has clear implications on other soil properties like organic matter content and soil structure.

6.4.2 SOIL CHEMICAL CONSEQUENCES

Some of the agriculturally important chemical consequences of soil acidification include the increased solubility of phytotoxic elements, reduced cation exchange capacity and plant nutrient deficiencies. All of these have adverse effects on plant growth and crop production.

Elemental Toxicities

The solubility of aluminium and manganese (the latter being an essential plant nutrient – see below) in soil increases as soil pH decreases. When in high concentrations, both of these elements can be phytotoxic and can reduce agricultural productivity. Under acidic conditions, their increasing concentrations in the soil solution are of particular concern. Iron toxicity may also be important, but only in chemically reduced soil.

Various studies have suggested that the phytotoxic forms of aluminium are the free ion and labile monomeric forms Al^{3+} and $AlOH_2^+$, $Al(OH)_2^+$ respectively (*e.g.* Ritchie, 1989; Noble *et al.* 1988; Helyar & Conyers, 1987; Pavan & Bingham, 1982). The concentration of each of these increases logarithmically as pH decreases and at pH_{CaCl_2} levels below 4.5, equivalent to 5 % aluminium saturation, crop growth is inhibited (Hazelton & Murphy, 1992; Juo, 1977). Chapter IX explores these relationships further. Helyar & Conyers (1987) indicated that as pH decreases, the rates of increase of $AlOH_2^+$ and $Al(OH)_2^+$ are two-thirds and one-third respectively that of Al^{3+} and that their activity is lower at potentially toxic levels. Therefore in most of the literature, Al^{3+} is reported as the culpable species considered as causing toxicity in plants. The principal effect of aluminium toxicity is disruption of the structure and function of root systems. The damage has obvious implications on crop growth and yield (*e.g.* Parker, 1995; Noble *et al.*, 1988).

The Mn^{2+} ion is the form of manganese absorbed by plant roots that is essential for growth. However, when absorbed in excessive amounts it is phytotoxic, as it disrupts photosynthesis and certain enzyme action (Sumner *et al.*, 1991; Fox *et al.*, 1991).

Nutritional Deficiencies

Nutrient deficiencies in acid agricultural soils are widespread (Evans, 1991). Either increased adsorption or nutrient losses via leaching may cause soil infertility. For example, soil acidity may cause increased phosphorus adsorption, or it may reduce the soil's capacity to retain basic cations essential for plant nutrition. Consequently cations in the soil solution may be leached out below the root zone together with negatively charged ions such as nitrate. The nutrients of particular concern include phosphorus, calcium, magnesium, potassium and molybdenum.

Some ambiguity exists over the effects of soil acidity on phosphorus availability (Sumner *et al.*, 1991). Generally, acid soil provokes an increase in the adsorption capacity of soil for phosphorus, causing a decrease in its availability as soil pH drops. Therefore in acid soils with pH_{CaCl_2} values smaller than 5.5, phosphate availability and uptake by plants may be reduced (Sumner *et al.*, 1991; Edwards, 1991). Conversely raising soil pH above neutral values will also result in a decrease in phosphorus in solution, due to the formation of insoluble calcium phosphates. The ambiguity pertains to findings that suggest that soil solution phosphorus can also decrease with increases in pH, even under acidic conditions (*e.g.* Munns & Fox, 1976). Several studies cited by Sumner *et al.* (1991) suggested that this transient behaviour may be due to sorption of added phosphorus on newly precipitated hydroxy-Al surfaces.

Calcium is a dominant exchangeable basic nutrient cation in most agricultural soil (Dolling & Ritchie, 1985). The main equilibria determining the solubility of Ca in soil involves $CaCO_3$ (calcite, or more commonly referred to as lime), soil-Ca and simple cation exchange (Sumner *et al.*, 1991), such that:

$$\mathrm{CaCO_{3(S)}} + 2\mathrm{H}^{+} \Leftrightarrow \mathrm{Ca}^{2+} + \mathrm{H_2O} + \mathrm{CO_2} \tag{6.2}$$

Equation 6.2 suggests that when the soil condition is acidic, $CaCO_3$ dissolves to produce Ca^{2+}, which is held on cation exchange sites and in the soil solution. In very acidic soil all of the $CaCO_3$ is dissolved and calcium exists mainly in its soluble form as Ca^{2+} which can be easily leached below the root zone, causing nutritional deficiencies. Calcium deficiency may also be induced by high levels of soluble aluminium, which antagonises calcium uptake by plants (Huang *et al.*, 1995).

The behaviour of magnesium in soil is similar to that of calcium. However its solubility in acid soil is determined by magnesium silicates such as vermiculite, and dolomitic limestone (a mixture of $CaCO_3$ and $MgCO_3$) (Sumner *et al.*, 1991). Magnesium competes poorly with calcium and aluminium for colloidal exchange sites (Sumner *et al.*, 1991). When large quantities of calcium are added to the soil or when the soil is acidic, magnesium may be displaced from exchange sites resulting in an increased concentration of Mg^{2+} in solution. As a consequence Mg^{2+} can be lost from the soil by leaching. Hence as pH drops less magnesium is found in exchangeable form and more is present in solution as Mg^{2+}, which can be lost by leaching. Also, as pH increases above neutral levels, due to applications of $CaCO_3$, Ca^{2+} may displace Mg^{2+} into solution causing it to leach from the rhizosphere.

Soil acidity reduces the cation exchange capacity of variable-charge soils, and hence their ability to retain potassium (Sumner *et al.*, 1991). This results in greater quantities of potassium being present as K^+ in the soil solution, which is then prone to leaching. Therefore the lower the pH of a soil, the less likely potassium is retained on exchange sites. Calcium and magnesium can create imbalances with respect to potassium, leading to problems of availability and uptake.

Molybdenum is a trace element needed by plants for the assimilation of nitrate into proteins, and also for nitrogen fixation by legumes. Molybdenum deficiency may then result in the disruption of symbiotic associations of nitrogen-fixing bacteria in legumes. Decreases in soil pH may cause Molybdenum deficiency in plants, as it is highly insoluble in acid soil. Molybdenum availability is often assured by simply liming acid soil (Cregan *et al.*, 1989).

6.4.3 SOIL PHYSICAL CONSEQUENCES

The effects of soil acidification on soil physical properties relate mainly to soil structure and aggregation. von Uexküll & Mutert (1995) indicated that the productivity of many acid soils around the world are affected by soil physical factors that include low water holding capacity, susceptibility to crusting, erosion and compaction. The literature on this subject is not very extensive, however there is evidence indicating that liming has beneficial effects on not only soil pH but also soil structure (*e.g.* Norton & Zhang, 1998). Chan & Heenan (1998) reported increases in macro- and micro-aggregate stability of cultivated soils after liming. The authors indicated that three-years after liming the improvements in structural stability extended to 7.5 cm depth. These benefits result from the elevated ionic strength in solution and the domination of Ca^{2+} on the exchange sites. Both these factors affect clay flocculation or dispersion, which influence the soil's physical properties.

6.5 MANAGEMENT OF ACID SOIL

Helyar (1991) outlined the fundamental basis of soil acidification and discussed techniques currently used for acid soil management. The management of acid soils should build on knowledge of the acidification process, its causes and consequences, and should not ignore the fact that all of these processes vary in time and space. Taking these into account, there are a number of ways in which acid soils may be managed for near-optimal agricultural productivity. In this instance only the most practical and efficient methods will be discussed and some recommendations made on how they may be incorporated into a site-specific management system for acid soil.

6.5.1 SITE-SPECIFIC SOIL MANAGEMENT

Increasing rates of soil acidification and the threat of extensive soil acidity in agricultural soil is a significant problem curtailing production, and may become increasingly more so if effective management strategies for amelioration are not implemented. Conventional acid soil management involves the use of tolerant plant species, rotations, or low single-rate applications of lime over an entire area of management (or management unit) – generally this area is contained within field boundaries regardless of size. Recommendations are then based on either conjectural evidence, or only one and sometimes a few discreet observations that are averaged to derive the application rate. The final application rate is then the averaged value plus 10 or 20 % to cover variability. These types of management are deemed inefficient since for example, reliance on crop choice alone will not correct acidity, and single-rate applications of lime do not optimise the efficiency of resource use.

In the early 1980s growing awareness of the environmental and economic problems associated with resource misallocation in agriculture, and the need for soil conservation led to the development of PA (Chapter I). Site-specific management is the fundamental principle behind the agronomic concept that is collectively referred to as PA. Currently, PA is made up of five key components, namely spatial referencing, data acquisition, spatial data processing, decision support and timely implementation of management. Once geo-referenced data is collected, each of the other components is conducted separately at different times. The reason for this is that real-time continuous management systems have not yet been developed (section 6.7). Chapter II reviewed the current state of each of the five components of a PA management system.

Site-specific management is based on more accurately matching resource application and agronomic practices with soil and crop requirements as these properties vary in the management unit. More accurate application of input resources may avoid the adverse economic and environmental consequences of conventional management practices, such yield losses due to sub-optimal resource applications, excessive chemical costs, gaseous and percolatory release of chemicals, and a less than optimal growing environment (McBratney *et al.* 1996). For the management of acid soil, single-rate applications of lime and fertilisers over the entire management unit will inevitably result in some areas where the resource has been over-applied and other areas where under-applications have occurred. Intuitively the consequences of such actions are agronomically and economically unsound. For example, excessive applications of lime are uneconomical and may affect crop growth by inhibiting the availability of certain plant nutrients, *e.g.* phosphorus (section 6.4.2). Excessive application of nitrogenous fertilisers may result in nitrate leaching, further acidifying the soil (section 6.3.1) and increasing the environmental impact of production. Conversely when lime is insufficiently applied, amelioration of the acidity is not accomplished and the availability of nutrients such as manganese and elements like aluminium may reach toxic levels, then affecting physiological processes in the growing crop and ultimately their yield (section 6.4.2).

Site-specific management provides agricultural managers and decision-makers with a practical tool that may be used to manage soil and crop variability in each management unit. By doing so, the environmental impact of crop production systems may be minimised and production efficiency and profitability maximised. These are the economic and ecological basis of PA.

6.5.2 LIMING

Economic loss (from yield reductions) and the producer's narrower choice of enterprise (*i.e.* there will be an opportunity cost) are direct consequences that soil acidity has on production. The most rapid and effective method to ameliorate soil acidity is to incorporate lime ($CaCO_3$) or less commonly dolomite (a mixture of $CaCO_3$ and $MgCO_3$) into the top 200 mm of soil, where the greater density of crop roots occur. The application of lime to soil has a number of functions depending on the reasons for liming. The most common reason is the amelioration of acid soil, be it to reclaim inherently acidic land or to amend acid soils resulting from agricultural production. Banding or pelleting lime onto the seed at sowing is also a common practice used to aid with the establishment of temperate pasture legumes (Evans, 1991), however once the plants have established, supplementary liming is rarely practiced. Lime can also be applied as a preventative treatment for soil infertility, and to supply calcium and magnesium to deficient soils. Liming raises the pH of acid soil, thus the action of nitrogen fixing bacteria becomes uninhibited and nitrogen fixation increases. McLean & Brown (1984) suggested that nitrogen mineralisation from plant residues and organic matter increases when lime is applied to acid soil.

Although lime is primarily applied to raise soil pH and amend toxicities associated with acid soil, liming has also been used to improve soil structure. Calcium in the soil solution displaces excess sodium and magnesium, promoting flocculation and therefore aggregation and soil structural stability. For example, liming materials are effective in reducing aggregate breakdown by raindrop impact, surface sealing and crusting, surface runoff and surface water erosion (Norton & Zhang, 1998). During *et al.* (1984a, b) suggested that limed soils have greater water holding capacity, and attributed the growth response of pasture to this factor. These authors also measured improvements in the stability of limed soil aggregates and speculated that liming improved infiltration during heavy rain.

The overall reactions of lime in acid soil include $CaCO_3$ and Al^{3+} hydrolysis, ion exchange reactions, free H^+ neutralisation and ionisation of hydrogen from the functional groups of OM, layer silicates and sesquioxides (Norton & Zhang, 1998). Breaking down Equation 6.2, the hydrolysis of carbonate can be coupled as follows:

$$CaCO_3 + H_2O \rightarrow Ca^{2+} + HCO_3^- + OH^- \qquad (6.3)$$

The latter half of Equation 6.3, $HCO_3^- + OH^-$ is neutralised to form $CO_2 + H_2O$, as shown by Equation 6.2. The neutralisation of soil solution H^+ will encourage the sequential hydrolysis of Al^{3+} along with its hydroxyl compounds so that (from Sparks, 1995):

$$2Al^{3+} + 3CaCO_3 + 3H_2O \Leftrightarrow 3Ca^{2+} + 2Al(OH)_3 + 3CO_2 \qquad (6.4)$$

Obviously if dolomite is used, the final product will be exchangeable Mg^{2+} as well as Ca^{2+}. Liming shifts the equilibrium to the right-hand-side of Equation 6.4, reducing the solubility, concentration and hence phytotoxicity of Al^{3+}. As previously mentioned, liming can also affect soil physical properties. After the reaction of lime with the acid soil, Ca^{2+} will predominate on exchange sites and when these are saturated, excess calcium in the soil will raise the soil solution's ionic strength and keep clay particles flocculated.

A soil's lime requirement may be defined as the amount of lime needed to neutralise the exchangeable acidity of the top 200 mm of soil (Chapter VIII). The most accurate methods to predict the lime requirements of acid soil are the lime-requirement buffer procedures (Chapter VIII).

6.5.3 ACID-TOLERANT PLANT SPECIES

Aniol (1991) reviewed the genetics of acid-tolerant wheat plants. Plant species and cultivars that are genetically tolerant to acid soil conditions (hydrogen, aluminium and manganese toxicities as well as calcium deficiency) are commonly used to maintain farm productivity on these soils. Their use on farms is a low cost management option that may easily adopted by managers, however tolerant plant species will not amend acid soil or lower the rate of acidification. Moreover, the use of acid-tolerant plants could result in movement of the excess acid down the profile and lower soil pH at depth, where amelioration is much more difficult (Evans, 1991).

Nevertheless, acid-tolerant plant species have a role in the management of acid soils. For example, tolerant plants may be site-specifically introduced into areas of the field where liming is deemed uneconomical, or where the soil is acidic below the depth that can be ameliorated by lime, even if excess amounts are applied. In many productive farming systems in Australia, where it not for the use of tolerant species productivity would have been noticeably diminished (Evans, 1991). However, there is a risk that reliance on crop choice alone and not liming to correct acidity may ultimately result in productivity losses as the soils continue to acidify (Scott & Fisher, 1989). Concomitantly the number of crop species and varieties that can be grown becomes increasingly more limited.

6.5.4 EFFICIENT USE OF WATER AND FERTILISERS

The aim of a long-term acid soil management system is to retard, arrest and even reverse the acidification of agricultural soil. For the system to succeed an integrated approach to management is required. Thus, together with a spatially variable liming strategy and the use of acid-tolerant plants when and where required, more efficient applications of irrigation water (the cause of alkali losses by leaching) and fertilisers (a source of acid) are necessary. Sections 6.3.1 and 6.3.4 respectively, discussed both of these causes of soil acidification. Site-specific management through variable-rate resource application may provide the opportunity to improve the efficiency of water and fertiliser usage.

6.5.5 SUPPLEMENTARY MANAGEMENT PRACTICES

Other types of management that may be integrated in the management program include suitable crop rotations and enterprise diversification, to optimise both biological and economic objectives.

6.6 THE EXTENT OF SOIL ACIDITY

Estimates of the intensity and extent of acid soil globally and that which occurs in Australia are given in the following sections. These estimates are provided for the reader to speculate on the ensuing consequences of agricultural soil acidification if suitable management is not implemented.

6.6.1 GLOBAL DISTRIBUTION OF ACID SOILS

According to FAO (1998) estimates, approximately 3 940 Mha (equivalent to 30 %) of the global ice-free land area is made up of acid soils. Figure 6.2 shows the global distribution of acid soils irrespective of land use, with pH_{H_2O} values smaller than 5.5 (approximately equivalent to $pH_{CaCl_2} < 4.5$).

The regional distribution of acid soils by land use is given in Table 6.3. The highest regional share of acid arable soils occur in Asia, Latin America and Europe, while the highest share of acid soils under pastures occur in Latin America, Africa and Asia respectively (Table 6.3).

Approximately 11 % of the global land area (1 406 Mha) is currently being cultivated (Chapter I), of which 15 % is acidic with pH_{H_2O} values smaller than 5.5 (Table 6.3). von Uexküll & Mutert (1995) suggested that low or minimum input systems are not sustainable on acid soils, but with adequate inputs and good management, acid soils can be highly productive. In industrially developed countries with modern agricultural techniques, most acid soil can be made productive by site-specific liming to target pH_{CaCl_2} values between 6 to 7, and by variable-rate fertiliser applications to increase soil fertility. In ‘developing’ nations, site-specific management of acid soil may also be possible using local resources and low-tech procedures (Chapter I).

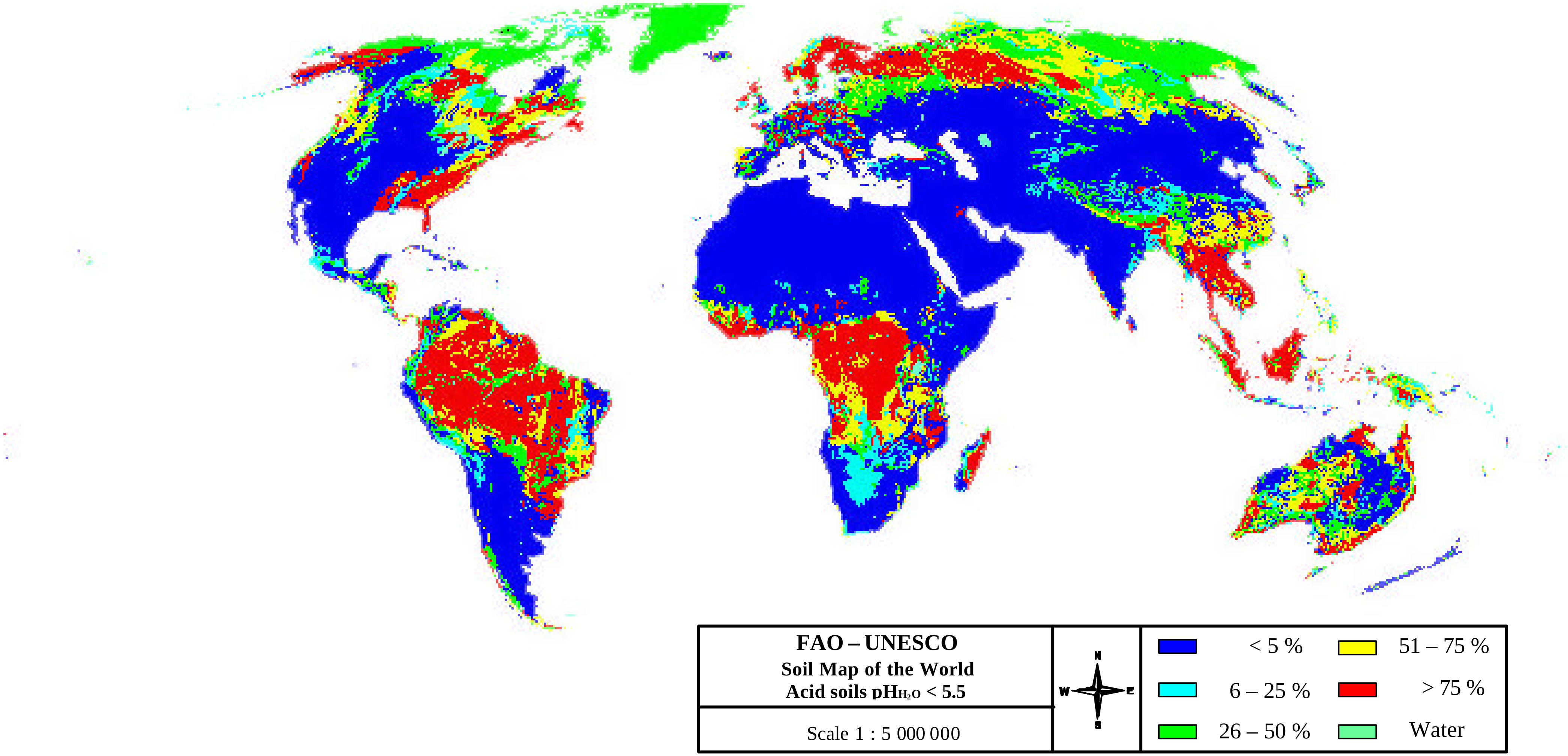

Figure 6.2 World distribution of acid soils with pH_{H_2O} values smaller than 5.5. Adapted from FAO (1998). The map was derived from 400 soil profiles and provides only estimates

The largest obstacle to increasing productivity in acid agricultural soils in ‘developing’ countries is poverty. Consequently, deforestation continues as farmers exploit the residual fertility of cleared land for a few seasons, then abandon it and move on. Approximately 24 % of land on earth (3 190 Mha) is considered to be potentially arable land that could possibly be used for farming in the future (Chapter I). However 78 % (2 500 Mha) of this potentially arable land is composed of acid soils, most of which occur in the tropics (von Uexküll & Mutert, 1995). Technology transfer is an important part of the global effort to increase yields in these acid soils so producers may afford to purchase the inputs necessary to sustain long-term soil fertility (Chapter I).

Table 6.3 World acid soils by land use (Mha) by main region. Source of data from which calculations were made: von Uexküll & Mutert (1995)

Region	Arable	Forests	Pastures	Other	Total
Asia	90	725	117	112	1044
Latin America	55	590	230	80	955
North America	8	490	49	115	662
Africa	11	450	195	3	659
Europe*	40	311	28	12	391
Oceania**	8	55	80	96	239
World (Mha)	212	2621	699	408	3940
World Total*** %	15.1	65.1	20.5	9.7	30

* Including European part of FSU.

** Includes Australia and New Zealand

*** Calculations based on: Total arable land area = 1 406; Total forests = 4 028; Total pastures = 3 402; Total other = 4 205; Total global land area = 13 150 Mha

6.6.2 DISTRIBUTION OF ACID SOIL IN AUSTRALIA

Agriculture is the most extensive form of land use in Australia, comprising of 463.8 Mha or approximately 60 % of the total land area, which is roughly 769.2 Mha (ABS, 1998). Livestock grazing accounts for the largest area of agricultural land use, and 44.3 Mha or 9.4 % of agricultural land is used for crop and pasture production. (ABS, 1998).

Cregan *et al.* (1989) estimated that the area of strongly acidic soils in Australia with pH_{CaCl_2} values below 5.0 was in excess of 15 Mha, much of which is the very productive agricultural land in southeastern Australia. The authors suggested that only a few objective estimates of the extent and severity of the problem are available on a State or even regional basis. Ridley *et al.* (1990) indicated that soil acidity limits crop and pasture production over at least 14 Mha in southern Australia (Table 6.4). The authors wrote that some of these soils are naturally acidic while others have experienced rapid acidification due to inadequate methods of agricultural production. Ridley *et al.* (1990) also suggested that areas of greatest concern occur in southeastern Australia. Evans (1991) estimated that the total area of acid agricultural soils with pH_{CaCl_2} values below 4.8 in Australia was 24.1 Mha. The author suggested that areas of greatest concern occur in the highly productive agricultural regions of the wheat-belt as well as on the high rainfall coastal areas of New South Wales (NSW) and Victoria (Table 6.4). Evans (1991) indicated that in some of these areas accelerated acidification occurs because liming is not part of the management strategy.

Commissioned by the Land and Water Resources Research and Development Corporation (LWRRDC), AACM International Pty Ltd (1995) reviewed the extent of soil acidification in Australia. They suggested that approximately 35 Mha of agricultural soil is highly acidic with pH_{CaCl_2} values smaller than 4.8. The data provided by the AACM International Pty Ltd (1995) review indicated that the magnitude of the problem is greatest in NSW than elsewhere (Table 6.4), however that Queensland soils had greater potential for acidification as the state has 32 Mha of moderately to slightly acidic soil. Table 6.4 shows the data quoted in the above studies.

Ahern *et al.* (1994) described the acid surface soil distribution and extent in Queensland, and reported similar results. They suggested that two-thirds of the total area are mapped as having acidic surface soils, one-third with strongly acidic ($pH_{CaCl_2} < 4.7$) and approximately one-third or 38 Mha with moderately acidic soils (pH_{CaCl_2} 4.7 – 5.2). However Ahern *et al.* (1994) did not indicate what proportion of this land is used for agriculture.

The studies shown in Table 6.4 do not provide information on the sampling design or intensity used to derive the estimates. It is assumed that these estimates were made from data based on soil and land use factors, existing low-resolution soil maps and only a relatively few actual soil pH measurements. Hence the accuracy of the estimates is limited since the surveys aim to cover a large area of land that may exhibit a lot of variability. A spatially oriented sampling design would be required to derive accurate estimates of the regional and state-wide extent of soil acidity in Australia.

Table 6.4 Extent of acid agricultural soils in Australia (Mha) with pH_{CaCl_2} values smaller than 4.8

State of Australia	AACM (1995)	Evans (1991)	Ridley *et al.* (1990)
New South Wales	13.5	9.5	7
Victoria	3	4.8	5
Queensland	8.4	2	
Western Australia	4.7	4	1.5
South Australia	2.8	2.8	0.4
Tasmania	1	1	
Total	33.4	24.1	13.9

A further limitation of these estimates is the temporal factor. For example since these studies were made, soil survey work conducted by CSIRO indicate that the total area of acidic agricultural soils in South Australia has reached 3.85 Mha (CSIRO, 1999). Therefore the data shown in Table 6.4 provide only rough approximations of the extent and distribution of acid agricultural soils in Australia.

Agricultural lime use in Australia is low by world standards, but its use is increasing. Lime use estimates in Australia of less than 200 000 Mg/yr were made by Cregan *et al.* (1989). The authors provided a comparison of lime use with New Zealand and the USA, and quote figures of 1.5×10^6 Mg/yr and 30×10^6 Mg/yr respectively. However such international comparisons are not useful indicators of whether or not liming should be expanded. A more useful test would be to assess if lime usage is at a sufficient level to neutralise the excess acids produced (Equation 6.1), which would otherwise further soil degradation and limit the choice of crops that a producer can grow. Evans (1991) collected data from around Australia and suggested that lime use could exceed 500 000 Mg/yr. Figure 6.4 (below) shows estimates for regional lime use in NSW.

Some of the reasons for this historical abstinence in the use of lime in potentially acid and acid soil are the high costs associated with liming (Conyers *et al.*, 1996), prevailing commodity prices and misinformation on the benefits of liming. Transporting lime from the quarry to the farm often involves large distances resulting in costly transport and hence lime applications compared to the value of the lime itself. Evans (1991) suggested that many producers believe that investments in lime are wasted where acid-induced infertility has not been adequately diagnosed and where acid-tolerant species are grown. Most of these affected farms have probably never had any lime applied. Obviously their situation could have been avoided by strategic lime applications. With the recognition of the problems in plant production associated with accelerated rates of soil acidification, the use of lime is increasing. Cregan *et al.* (1989) provide an extensive review of plant responses to liming in Australia.

Distribution of acid soil in New South Wales

Helyar *et al.* (1990) provided estimates of the extent and distribution of soil acidity in NSW. The authors measured surface soil (0 – 10 or 0 – 15 cm) pH_{CaCl_2} values and mapped them according to land capability categories and existing soil resource maps. Mean pH_{CaCl_2} values were written onto an overlay of the soil map (scale 1:2 000 000). Hence the accuracy of these estimates is also limited by sub-optimal sampling and mapping techniques, as previously described.

A map of the distribution of acid soils and soils at risk of becoming strongly acidic in NSW is shown in Figure 6.3. Soil pH patterns reflect differences in climate, higher rainfall areas to the east are more acidic (Figure 6.3). The Coastal sands along the north coast and soils high in silica, some developed on sandstone parent materials in the southeastern portion of the State are good examples of soils with pH_{CaCl_2} values smaller than 4.25. Many of the soils with pH_{CaCl_2} values between 4.25 and 4.5 also occur in coastal regions but also extend further inland with more prominence in southern rather than northern regions. Some of these regions extend into areas of the wheat-belt where crop production is the main agricultural industry (Figure 6.3). For example, the experimental field on which the work presented here was conducted, in Kelso (Figure 6.3), occurs where soil pH_{CaCl_2} values between lie between 4.25 and 4.5 (Chapter III).

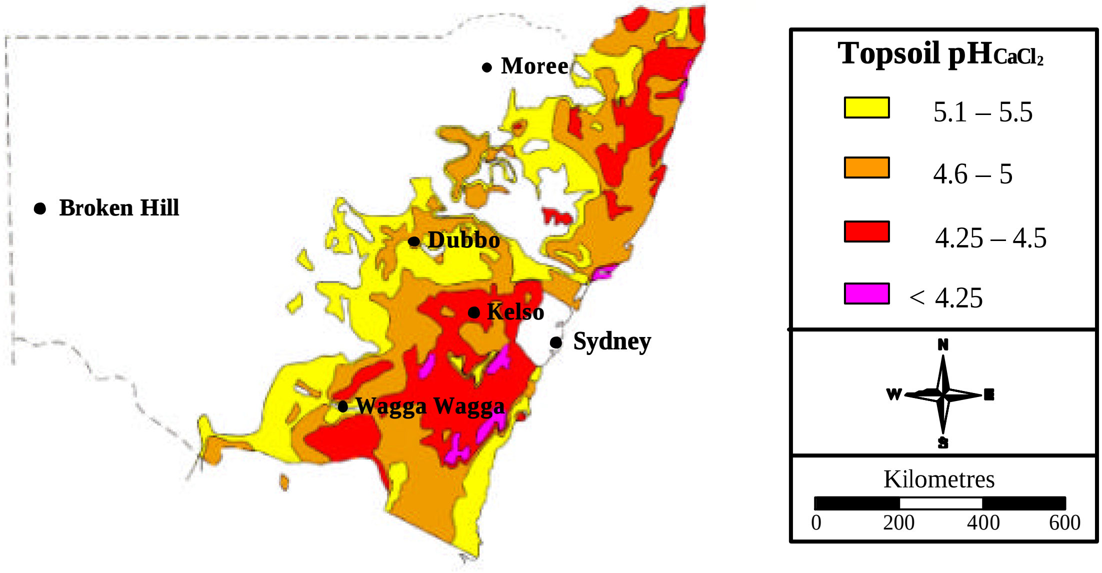

Figure 6.3 Distribution of acid soils (0 – 10 or 0 – 15 cm) in New South Wales. Adapted from Helyar *et al.* (1990).

Areas with mean pH_{CaCl_2} values below 5 extend a further inland and represent soils that may potentially acidify if integrated management systems for acid soil, that include prophylactic liming, are not implemented. It is perhaps this realisation that has prompted a steady increase in the amount of lime usage in NSW. Figure 6.4 shows the trends in agricultural lime use in NSW by region, in the period from 1975 to 1995.

Coinciding with the acid soil regions shown in Figure 6.3, lime usage in central and southern NSW increased significantly over the given period. The trend in total lime usage shows an almost continuous exponential increase in the period from 1985 to 1995 (Figure 6.4).

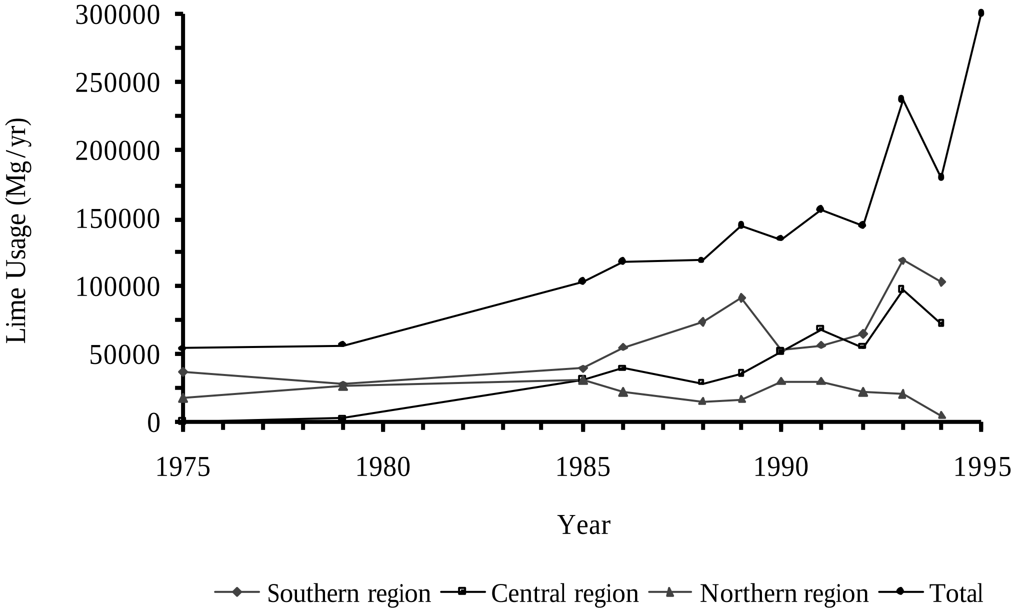

Figure 6.4 Agricultural lime use in New South Wales, 1975 to 1995

6.7 A CONTINUOUS MANAGEMENT SYSTEM FOR ACID SOIL

Conventional agronomic management neglects the fact that soil forms a variable three-dimensional continuum in space (McBratney, 1992). Such blatant disregard for soil variability may be attributed to the historical absence of an accurate positioning system for geo-referencing, suitable statistical methods to quantify spatial variability patterns and technologies to implement spatially variable management (Chapter I). These 'enabling' technologies are now available and are making it increasingly possible to implement variable management in agricultural fields. As was indicated by Figure 4.1 in Chapter IV, the future aim of PA is real-time continuous soil and crop management whereby measurement, decision and implementation of management occurs 'on-the-go' in a single pass over the field.

The unavailability of adequate techniques for 'on-the-go' data collection has resulted in the evolution of interim management systems between uniform and continuous management (Figure 4.1, Chapter IV). Currently, PA is implemented using these interim approaches, where each phase of the PA management system (Chapter II) is conducted independently and at different times. In these circumstances site-specificity relies upon the ability to accurately resolve ground positioning during data collection operations. At a later time the geo-referenced data may be spatially analysed for the formulation of optimal decisions. Accurate ground positioning is then also crucial for navigation when implementing site-specific management.

A real-time continuous management system for the management of acid soil is proposed in Figure 6.5.

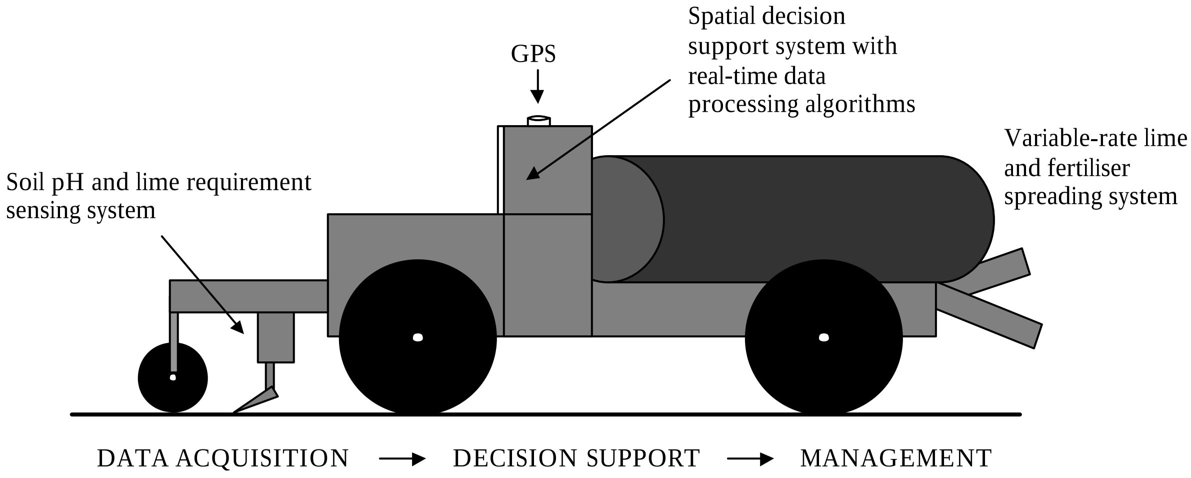

Figure 6.5 A real-time continuous management system for acid soil. The system links data acquisition, spatial decision support and the implementation of optimal management

The system illustrated in Figure 6.5 proposes a system for real-time, continuous soil management. An 'on-the-go' proximal sensing system is used to collect information on the spatial variability of soil pH and lime requirement. For example the sensor may take a pH measurement every five seconds. The data is transferred to the spatial decision support system (SDSS) that contains real-time spatial data processing algorithms, lime requirement models, economic models, and the uncertainties of the models. The SDSS may access a database that contains other spatial, geo-referenced information related to the particular field (*e.g.* crop response to liming, data on exchangeable aluminium, organic matter, texture, general field conditions, etc.). Spatial data processing in real-time may, for example, involve the use of a Kalman filter algorithm (Brown & Hwang, 1992). The algorithm may also incorporate information on the measurement dynamics of the sensing system, a statistical description of the instrumental noises and measurement errors. When the optimal decision is made, a signal is sent to the variable-rate controller for the optimal and timely application of lime. Optimal management may be either single- or variable-rate, or for example, in areas where liming is deemed uneconomical, acid-tolerant varieties may be sown. In this system all operations are conducted in the same pass over the field. Fertiliser management, crop varieties or cultivars to be sown, and sowing densities may be similarly determined. At harvest, the crop may be yield-mapped and the data used in a subsequent season to assess crop response to liming in the particular field. In a real-time system (Figure 6.5), the use of a GPS is not crucial but useful for record keeping. These logged data may then be used as auxiliary information for future management, and may also provide useful information on the temporal variation of soil pH, lime requirement and lime application rates.

6.8 CONCLUDING REMARKS

Acidification of soil in an agricultural production system occurs because of imbalances between the inputs and outputs of the system. Soil acidification has adverse effects on agricultural productivity, mainly due to the increased solubility of phytotoxic elements such as aluminium and manganese when absorbed by plants in high concentrations. Acid soil may also be a precursor to other forms of land degradation such as nutrient depletion and erosion. Human health can also be affected. Thus, soil acidification is considered a form of land degradation that has adverse effects on not only production and soil quality but also society.

This chapter proposes site-specific management of acid soil as a sustainable management system that prevents the adverse economic and environmental consequences of conventional management practices. It also describes a real-time continuous management system for acid soil. Although interim management systems between uniform and site-specific management are currently being implemented, ultimately the objective of precision agriculture is to implement optimal and timely management in real-time using information collected ‘on-the-go’. The development of an ‘on-the-go’ proximal soil pH and lime requirement sensing systems and adequate spatial decision support for optimal predictions of lime requirement are imperative for the development of a real-time continuous management system for acid soil.

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Chapter VII

DEVELOPMENT OF AN ‘ON-THE-GO’ PROXIMAL SOIL pH AND LIME REQUIREMENT SENSING SYSTEM

ABSTRACT

This chapter describes work towards the development of an ‘on-the-go’ proximal soil pH and lime-requirement sensing system, and the components that make up that system. The sensing system will be used for the real-time continuous management of acid soil. Initially the chapter presents an evaluation of four potentiometric pH sensors for ‘on-the-go’ acquisition of field soil pH and lime requirement information. In comparing some of their operational features as well as their accuracy, precision, response time and robustness, the pH ion-sensitive field-effect transistor (ISFET) proved the most suitable. A brief literature review on historical and current developments in pH ISFET technology is presented, as well as approaches to the application of ISFETs in soil science and precision agriculture. Experimental results on the sensitivity, drift, hysteresis and response time behaviour of a pH ISFET indicate that the device is suitable as the sensor component of the sensing system. The sensitivity of the Al_2O_3-gate ISFET was 50.3 mV pH^{-1}, drift was 0.76 mV hr^{-1} in standard pH buffer and 1.7 mV hr^{-1} in lime-requirement buffer. The hysteresis of the device was 1.7 mV. The response time was shortest when the electrolyte was injected directly onto the ISFET surface. Continual measurements showed that the average response time across all measuring solutions ranged from 0.11 s to 4.2 s. Continual pH measurements were accurate when measured in both soil:0.01M $CaCl_2$ and soil:lime-requirement buffer extracts. The quality of the pH ISFET sensor measurements was adequate in terms of accuracy and precision. A literature review is presented on flow injection analysis and sequential injection analysis systems and their use in soil analytical chemistry. Drawing on these concepts, a design for the analytical component of the sensing system is proposed. Results from kinetic experiments are shown that describe the soil:0.01M $CaCl_2$ pH (pH_{CaCl_2}) and soil:lime-requirement buffer pH (pH_{buffer}) reactions. The kinetics of soil:lime-requirement buffer reactions may be successfully characterised using different, though not incompatible, models. First, the reactions were characterised using two separate first-order reactions, each with a single rate coefficient, and second, using a continuous double-exponential function with two rate coefficients. Both models described the sequential, biphasic nature of the soil:lime-requirement buffer reactions. A statistical methodology was devised to predict equilibrium pH_{buffer} measurements at shorter time intervals than those suggested in the literature. The framework for the development of a prototype soil pH and lime requirement sensing system is presented and a

creative design that describes the components of the ‘on-the-go’ proximal soil pH and lime requirement sensing system proposed. Finally, a design for an ‘on-the-go’ soil sampling mechanism is considered and a data processing system described.

7.1 INTRODUCTION

Among the factors that are essential for the implementation of precision agriculture (PA) is a fine-scale characterisation of the degree and extent of the spatial soil variability within the management unit. However, discrete sampling at a spatial resolution of 10 m or less (Whelan *et al.*, 1996) and consequent laboratory analysis is often vexatious and far too costly for broadacre farming (Chapter IV). For many crops, fine-scale yield data is readily attainable using proximal yield-sensing systems (Chapter II). Proximal soil-sensing systems (Viscarra Rossel & McBratney, 1998) that collect data at equivalent or even similar spatial resolutions are unavailable for most agronomically significant soil properties, although some are now beginning to emerge (Chapter II). The literature review presented in Chapter II described currently available proximal soil-sensing systems and some of the possibilities for future development. Soil sampling and analysis and the use and advantages of an ‘on-the-go’ proximal soil electrical conductivity sensing system were shown in Chapter IV.

Chapter VI described a prospective real-time continuous management system for acid soil. Continuous management is the ultimate objective of PA. Continuous management requires the development of ‘on-the-go’ proximal soil-sensing systems that are able to collect variability data accurately, rapidly and economically. These data may be used in real-time to make decisions on the degree of management to implement. Currently, the development of proximal soil-sensing systems lags behind other enabling technologies necessary for the implementation of PA. A premiss for research in PA must be to develop invasive and non-invasive proximal soil sensing systems for agriculturally relevant attributes to meet the demand for fine spatial resolution soil data (Sudduth, *et al.* 1997; Viscarra Rossel & McBratney, 1998).

Research towards the development of proximal sensing systems is ongoing in universities, research organisations and companies in Australia and abroad (Table 2.11 Chapter II). This chapter describes work towards the development of an ‘on-the-go’ proximal soil pH and lime-requirement sensing system, and the components that make up that system. The chapter is composed of six sections whose aims are to:

1. Evaluate the suitability of four potentiometric pH sensors for the 'on-the-go' acquisition of soil pH and lime requirement information
2. Investigate and assess the electrochemical characteristics of a pH ion-sensitive field-effect transistor (ISFET) for its use as the sensor component in the proximal sensing system
3. Design the analytical apparatus of the sensing system for 'on-the-go' field operation
4. Conduct kinetic experiments to describe the soil:0.01M $CaCl_2$ pH (pH_{CaCl_2}) and soil:lime-requirement buffer pH (pH_{buffer}) reactions, and devise a statistical methodology that may be used to predict equilibrium pH measurements at shorter time intervals than those suggested in the literature
5. Outline the framework for the development of a prototype soil pH and lime requirement sensing system
6. Propose the creative design of the 'on-the-go' proximal soil pH and lime requirement sensing system which includes the design for an 'on-the-go' soil sampling mechanism, and the data processing system to be used.

7.2 ASSESSMENT OF FOUR POTENTIOMETRIC SENSORS

The characteristics of the sensor to be used in the proximal soil pH and lime requirement sensing system are important because of the constraints imposed by continual 'on-the-go' field operation. The characteristics to consider include:

- Response time – refers to the time it takes the sensor to produce a stable signal. It is the most critical property because the sensor needs to operate 'on-the-go' and in real-time. For example, if the sensing system were towed by an vehicle travelling at 8 km/hr, measurements would need to be made every 4.5 seconds to characterise the pH of the field at 10 m intervals (similarly sampling and analysis will need to be made at this speed).
- Fragility and durability – the sensor should be robust, durable, and be able to withstand field operation
- Measurement range – should cover the pH range of different soil, *i.e.* 3 - 10
- Measurement resolution – for soil 0.1 pH units will suffice

- Precision – pH measurements should be reproducible
- Sensitivity – depends on the mode of measurement, however it should be as close as possible to an ideal Nernstian response of 59 mV pH^{-1}.
- Drift – refers to the unidirectional change in pH over time, and should be small
- Hysteresis – refers to a delayed reaction to pH changes, and should be small
- Maintenance and storage – the sensor should require minimal maintenance and easy storage
- High signal to noise ratio

Initially, the first four characteristics of sensor operation are dealt with in the evaluation of four potentiometric pH sensors. The remaining characteristics are dealt with in a latter section of the chapter, in the assessment of the most suitable soil pH sensor for the sensing system.

Four potentiometric pH sensors, namely a glass electrode (GE), a glass microelectrode (GME), a metallic (SbE) electrode and a pH ISFET were evaluated for their response time, fragility, resolution and precision. Sensor characteristics and properties are shown in Table 7.1.

Table 7.1 Characteristics and properties of the four sensors evaluated, namely a glass electrode (GE), a glass microelectrode (GME), an antimony electrode (SbE) and an ISFET.

Characteristic/Property	GE	GME	SbE	ISFET
Material	glass	glass	antimony	silicon chip
pH range	0 - 12	0 - 12	2 - 11	0 - 14
Resolution	±0.001	±0.001	±0.01	±0.01
Fragility	high	high	low	low
Mode of measurement	Diffusive processes	Diffusive processes	Electrical Conductivity	Electrostatic interactions

All sensors have appropriate resolution, however only the SbE and the ISFET may be suitably robust (or less brittle) for continual field pH measurements.

7.2.1 COMPARISON OF ACCURACY AND PRECISION

Performing a number of replicated experiments assessed both the accuracy and precision of the four sensors. These are discussed below.

Using a batch-type methodology (Sparks, 1995), 25 ml of standard buffer solutions (pH 4 and 7), 1:5 soil:0.01M $CaCl_2$ and soil:H_2O extracts, and soil:lime-requirement buffer solutions were in-turn placed into 35 ml centrifuge vessels. Each was stirred at a constant rate (400 rpm) using a magnetic stirrer and stirring rod. Initially, the sensor being evaluated was rinsed with deionised water, dabbed dry with soft tissue paper and then dipped into the centrifuge vessel containing each solution or extract. The time taken for a stable reading was automatically recorded. A reading was deemed stable when drift was less than 50 mpH per minute, in which case the result was locked and recorded. These experiments were replicated eight times, and all were conducted at 20° C.

The accuracy and precision of pH measurements for the four sensors is shown in Table 7.2 below.

Table 7.2 Accuracy and precision of pH measurements (pH units) in standard (St.) buffer, soil:0.01M $CaCl_2$, soil:$H_2O$and soil:lime-requirement (LR) buffer extracts, using the glass electrode (GE), glass microelectrode (GM-E), antimony electrode (Sb-E) and ISFET, *n* = 8

	St. buffer		1:5 0.01M $CaCl_2$		1:5 H_2O		LR buffer	
	Mean	S.D.	Mean	S.D.	Mean	S.D..	Mean	S.D.
GE	4.00	0.0058	4.07	0.0019	4.69	0.005	6.51	0.005
GME	3.99	0.0082	4.02^{*}	0.0096	4.62^{*}	0.0013	6.52	0.013
SbE	4.01^{*}	0.0096	4.08	0.0096	4.73	0.0019	5.23^{*}	0.017
ISFET	3.99	0.0058	4.02^{*}	0.0019	4.63^{*}	0.0096	6.47^{*}	0.0082

Note: Significant differences at 5 % probability level are indicated by *.

Although there were some statistically different pH measurement values between the ISFET and the conventional GE (Table 7.2), these differences were not large enough for the sensor to be deemed impractical. The GME and the ISFET provided the most similar values in most of the measurement mediums, indicating some relationship between the small size of the devices. All four sensors appeared reliable, however the glass electrode and the ISFET were generally more precise than the glass microelectrode and antimony electrode. The inaccurate pH reading in lime-requirement buffer obtained by the SbE (Table 7.2), may be attributed to either complexation or oxidation of the antimony by agents present in the lime-requirement buffer (refer to Chapters III, VIII).

7.2.2 COMPARISON OF RESPONSE TIMES

Along with durability, response time will be critical for a sensor to be deemed suitable for use in the sensing system. Mean response times to obtain stable pH readings for each of the four sensors being assessed are shown in Table 7.3.

Table 7.3 Response times (seconds) in standard (St.) buffer, soil:0.01M $CaCl_2$, soil:$H_2O$and soil:lime-requirement (LR) buffer extracts, using the glass electrode (GE), glass microelectrode (GM-E), antimony electrode (Sb-E) and ISFET, *n* = 8

	St. buffer		1:5 0.01M $CaCl_2$		1:5 H_2O		LR buffer	
	Mean	S.D.	Mean	S.D.	Mean	S.D.	Mean	S.D.
GE	30.1	3.9	38.3	2.2	30.3	3.9	39.8	1.9
GME	25.3	2.4	35.5	1.3	25.6	2.4	36.0	1.8
SbE	21.8	1.7	20.0	3.2	21.8	1.7	44.0	9.8
ISFET	5.6	0.4	4.6	0.5	5.6	0.4	4.4	0.3

The ISFET sensor exhibited the fastest and most reliable response times, with a mean response of 5.6 s in the standard buffer, 4.6 s in 0.01M $CaCl_2$, 5.6 s in water, and 4.4 s in lime-requirement buffer (Table 7.3). The considerably longer response times of the ion-selective electrodes may be attributed to the size of the measuring devices in relation to the diffusive processes taking place. The smaller size sensors may induce more localised diffusion and therefore rapid changes in activity may be registered with greater ease. This effect is exemplified in the comparison between the glass electrode and glass microelectrode, where pH response times for the glass electrode are higher than for the glass microelectrode (Table 7.3).

All of the four sensors measure pH in the appropriate range and produce reproducible readings. The antimony electrode and the ISFET are rugged enough to use in low soil to solution mixtures. However, as response time is the critical property the ISFET sensor appears most suitable for adaptation and use in the proposed sensing system. Further experimentation was conducted with the ISFET sensor only.

7.3 ION SENSITIVE FIELD-EFFECT TRANSISTORS

ISFETs are a type of chemically sensitive field-effect transistors that were first described by Bergveld (1972), and later by Matsuo & Wise (1974) and Esashi & Matsuo (1978). As the acronym suggests ISFETs combine two well-established technologies, that of ion selective electrodes (ISE) and field-effect transistors (FET).

The historical development of ISEs and FETs are somewhat interrelated and steps towards their development may be chronologically traced back as early as 1791 with Luigi Galvani’s discovery of the relationship between electric and physiologic processes. Galvani is generally credited with the discovery of electricity, the ‘galvanic cell’ honouring his name. A number of important developments followed, the most remarkable of which are those of Faraday who developed the principles of electrolysis and Arrhenius’ postulation of the conductivity properties of solutions. Thompson discovered the electron in 1898. Consequently, an important step forward was the work of Nernst who pioneered the development of electrochemical theory. In the 1890s Ostwald formulated the concept of membrane semi-permeability and the selective transport of ions. The first glass ion-selective electrode was developed in the 1900s and has since been the subject of much research.

In 1945 William Shockley theorised about and designed what he hoped would be the first semiconductor amplifier, relying on what he called the ‘field-effect’ – it didn’t work. In 1948 Shockley conceived the bipolar junction transistor better known simply as the transistor. During the 1950s, transistors although in their infancy, were being mass-produced (Session & Tuite, 1973). By the late 1960s, manufacturers converted from junction type integrated circuits to field-effect devices.

7.3.1 FROM FET TO ISFET

The ‘field-effect’ device that Shockley theorised about was what he later referred to as a unipolar transistor (Session & Tuite, 1973). One of the major disadvantages of the bipolar transistors was their low input impedance, preventing their application in many electronic circuits (Malmstadt & Enke, 1963). Currently most transistors are FETs that exhibit low output impedance.

A FET consists of a semiconductor, generally silicon, impregnated with impurities. When the tetravalent array of silicon atoms is disrupted by the introduction of impurities (also referred to as doping), electrons may break free leaving behind holes in the structure, which may be filled by electrons from adjacent atoms. An electron donor impurity makes the semiconductor an n-type material, while an acceptor impurity makes it a p-type material. By definition the semiconductor is neither a good conductor nor a good insulator, but when it is doped, the availability of charge carriers makes the material a potentially good conductor. With n-type materials the resulting extrinsic conductivity is due to free negative charges (electrons), while with p-type materials conductivity is due to positive charges (holes). Field-effect transistors are so named because the availability of charge carriers within the semiconductor can be enhanced or depleted by an electric field created within the semiconductor.

Currently, most transistors are IGFETs or Insulated Gate Field-Effect Transistors of which the most common examples are the MOSFETs (Metal Oxide Semiconductor Field-Effect Transistors). Figure 7.1a shows the basic construction of an enhancement mode MOSFET (*c.f.* depletion mode MOSFET, see Janata & Huber (1980)) where the drain and source are n-type regions formed in the p-type silicon substrate. The gate is a metal electrode insulated from the silicon slab by a layer of silicon dioxide (SiO_2) that protects and enhances the electrical properties of the crystal (Session & Tuite, 1973). From Figure 7.1a, supplying a positive voltage on the gate VG with respect to the source makes the device conductive. Hence the electric field of the positive gate repels holes in the p-type substrate away from the insulating SiO_2 layer leaving behind a narrow channel of n-type silicon called an inversion layer. The inversion layer provides a conducting path for the flow of current ID from source to drain as long as the threshold voltage is maintained on the gate. That is, if the voltage is below the threshold level or no voltage is applied the inversion layer is non-existent, as source and drain are insulated from each other. The magnitude of the drain current ID will be determined by the electrical resistance of the inversion layer and the voltage difference VD between the source and drain (Janata & Huber, 1980).

The ISFET shown in Figure 7.1b is based on an enhancement mode MOSFET where the gate metal is replaced by a reference electrode, a chemically sensitive layer, and the solution containing the specific ions, all protected by a suitable encapsulate. The operation of the ISFET is similar to that of a MOSFET described previously. When the ISFET is immersed in solution, the electrical circuit VG is closed with the reference electrode, the $[H^+]$ in solution influencing the source-drain current ID. The electrical resistance of the inversion layer and the voltage difference VD between the source and drain determines the magnitude of the drain current ID. ISFET operation occurs due to the electrostatic control of the current flowing between source and drain as determined by the $[H^+]$ present at the gate. If the pH of the solution changes so does the potential of the gate and hence also the drain current ID. Simultaneously, electronic feedback causes the voltage supply VG to the reference electrode to readjust, maintaining the drain current ID constant. The value of VG is the causal measurement parameter of the system, it being related to pH.

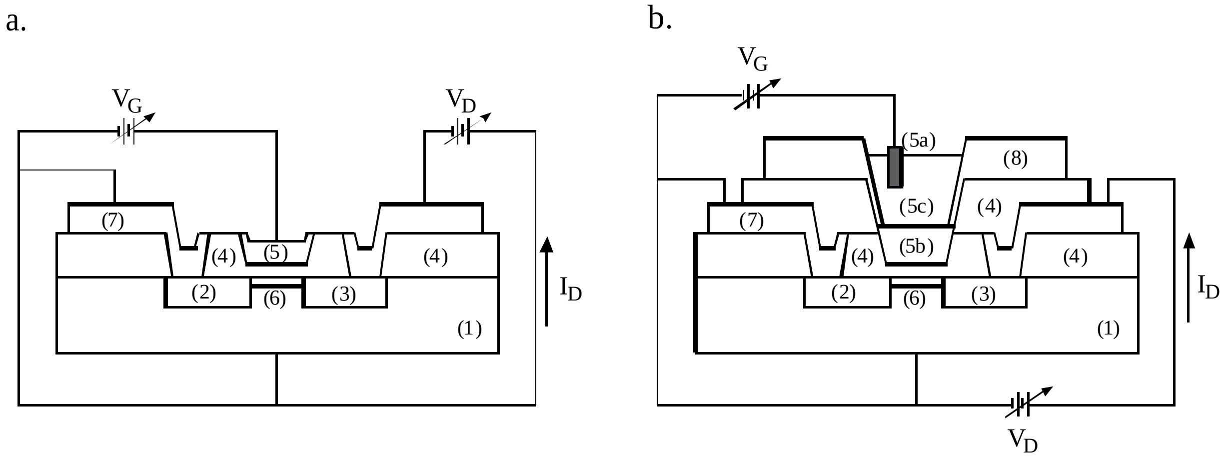

Figure 7.1 Schematic diagrams of the complete electrochemical systems of (a.) a MOSFET and (b.) an ISFET. Both devices share in common a (1) p-type silicon substrate, (2) n-type source, (3) n-type drain, and (4) insulator, (6) conducting channel and (7) metal contacts. The metal gate (5) in the MOSFET, is replaced by a (5a) reference electrode, (5b) membrane and (5c) electrolyte in the ISFET. Furthermore, the ISFET structure has a (8) protective encapsulate (adapted from Covington (1994) - IUPAC recommendations).

7.3.2 DEVELOPMENTS IN pH ISFET TECHNOLOGY

The pioneering work of Bergveld (1972) suggested that ISFET operation without a reference electrode was possible; however Matsuo & Wise (1974) proved otherwise. Bergveld (1972) proposed that SiO_2 gates have ion exchange properties similar to a pH glass electrode. Matsuo & Wise (1974) advised the use of an overlying layer of silicon nitride (Si_3N_4) to improve the stability of the gate insulator. Esashi & Matsuo (1978) examined the mechanism of the ion selective interface potential for Si_3N_4. Abe *et al.* (1979) reported that the Si_3N_4 membrane has greater stability and pH sensitivity than SiO_2, but that Si_3N_4 is prone to deterioration due to oxidation of the Si_3N_4 layer. Matsuo & Esashi (1981) reported similar results for the Si_3N_4 membrane. Niu *et al.* (1996) also alluded to the slow oxidation of Si_3N_4 membranes with time. To overcome this problem Abe et al (1979) used alumima (Al_2O_3) as the inorganic gate membrane sensitive to $[H^+]$ and Matsuo & Esashi (1981) used alumina and tantalum oxide (Ta_2O_5). These authors suggested that Al_2O_3 and Ta_2O_5 are better-suited membrane materials for pH ISFETs than Si_3N_4, their ion sensing performances being most satisfactory for practical use. Liao *et al.* (1998) reported the successful use of a SnO_2-gate membrane for pH measurements.

7.3.3 PROPOSED MECHANISMS OF ISFET OPERATION

Theoretical and experimental research has been conducted to investigate the operating principle and response characteristics of pH-sensitive inorganic-gate ISFETs. Initially, much of the theory of response was thought to be Nernstian as similarities with the glass electrode were recognised. Although the Nernst equation accurately predicts glass electrode response, the pH sensitivity of ISFETs may be below the predicted Nernstian value. The Nernst equation provides no explanation for this behaviour (Bousse *et al.*, 1983a).

There are a number of models of ISFET operation proposed in the literature, these may be classified according to the location where the mechanism of pH sensitivity is presumed to take place (Bousse & Bergveld, 1984). First, as previously mentioned, the Nernstian-type models that imply the movement of ions in the insulating membrane. Second, models based on the modification of the Si/SiO_2 interface through a pH-controlled change in the surface state density via transport of hydrogen-bearing species. Bousse & Bergveld (1984) suggested that this model may be considered as an extreme form of the previous. Third and more acceptably, models based on the site-binding theory of colloidal chemistry suggest that reactivity is purely the result of surface reactions. Fung *et al.* (1986) provided the generalised theory of the mechanism for oxide-gate ISFETs. Bousse & Bergveld (1984) and Meixner & Koch (1992) applied and verified its validity for oxide and nitride-gate ISFETs respectively. Bousse *et al.* (1983b) extended the theory to include the possibility that counter-ion adsorption occurs at different distances from the insulator surface. Fourth, Woias et al (1995) provide a model for the short-time response of ISFETs, proposing an approach that accounts for the kinetics of the electrochemical reactions occurring on the gate-insulator surface. In contrast to the static site-binding theory, this approach was developed to describe the dynamic behavior of Si_3N_4-gate membranes.

The main difference between the models is whether a bulk or surface mechanism is postulated (Bousse & Bergveld, 1984). Information on the characteristics that describe the response of pH ISFETs may provide a general outlook on the roles of the various mechanisms involved. Table 7.4 summarises certain accuracy and precision related characteristics of common gate materials used.

Table 7.4 Reported characteristics of inorganic membrane materials used in pH ISFETs

Author	Membrane	pH range	Sensitivity (mV pH^{-1})	Drift (mV h^{-1})	Hysteresis (mV)
Esashi & Matsuo (1978)	S_iO_2	3-13	30		
	Si_3N_4	3-13	54		
	Al_2O_3	3-13	54		
Abe *et al.* (1979)	S_iO_2	2-13	25 - 35	Unstable	Unstable
	Si_3N_4	2-13	46 - 56	0.6	3
	Al_2O_3	2-13	52 - 58	0.3	0.8
Matsuo & Esashi (1981)	S_iO_2	4-10	25 - 48	Unstable	Unstable
	Si_3N_4	1-13	46 - 56	1	3
	Al_2O_3	1-13	53 – 57	0.1-0.2	0.8
	Ta_2O_5	1-13	56 - 57	0.1-0.2	0.2
Bousse et al (1983a)	Al_2O_3	3-11	52		
Bousse *et al.* (1990a)	Si_3N_4	3-11	57	0.1	7.1
Bousse *et al.* (1990b)	Al_2O_3	3-11	50	0.2	3-6
Garde *et al.* (1995)	Si_3N_4	2-9	41 - 57		
Niu *et al.* (1996)	Si_3N_4	2-13	56		0.08
Shul'ga *et al.* (1996)	Si_3N_4	2-10	55		
Cambiaso *et al.* (1996)	Si_3N_4	6-8	52		
Kwon *et al.* (1996)	Ta_2O_5	2-12	58 - 59		
	S_iO_2	2-10	29		
	Si_3N_4	2-10	49		
Yeow *et al.* (1997)	Si_3N_4	4-10	41		
Liao *et al.* (1998)	SnO_2	2-10	55 - 58	0.13	2.5
	S_iO_2	2-10	34		
	Si_3N_4	2-10	49		

Sensitivity

The sensitivity of SiO_2 is very low compared to the ideal Nernstian response of 59 mV pH^{-1}, it ranging from 25 to 48 mV pH^{-1} (Table 7.4). Bousse & Bergveld (1984) suggested that the decreased sensitivity observed in SiO_2-gate ISFETs is due to the presence of buried OH-groups beneath the SiO_2 surface. These sites show slow pH response exhibit hysteresis and have low sensitivity. Silicon nitride membranes show improved pH sensitivity, it ranging from 41 to 57 mV pH^{-1}. This variation may be explained by the varying concentration of oxygen in the membrane. Niu *et al.* (1996) discussed the characteristics of Si_3N_4-gate pH ISFETs and Woias *et al.* (1998) investigated the pH response of ISFETs with silicon nitride gate insulators. The sensitivities of Al_2O_3 and Ta_2O_5 are much closer to the ideal Nerstian response, they range from 51 to 58 mV pH^{-1} and 56 to 59 mV pH^{-1} respectively (Table 7.4). Kwon *et al.* (1996) described a heat-treated Ta_2O_5 gate ISFET with low drift and high sensitivity, suggesting its superiority over alumina and silicon nitride gate membranes. Liao *et al.* (1998) showed that amorphous tin oxide (SnO_2) gate membrane may be used in pH ISFETs, the material having ideal sensitivity.

Drift

Drift refers to a slow unidirectional and continuous change in voltage (and hence pH) of an ISFET. Esashi & Matsuo (1978) postulated that the occurrence of drift in ISFET membranes may be due to electric field-enhanced gate migration within the insulator and electrochemical imbalances at the insulator-solution interface. Bousse & Bergveld (1984) suggested that drift results from slow surface effects such as the re-hydration of a surface that is partially dehydrated. Bousse & Bergveld (1984) also referred to the postulation of drift by other authors, for example drift caused by injection of electrons from the electrolyte at a strong anodic polarisations creating negative space charge inside SiO_2 films. Bousse *et al.* (1990b) indicated that drift in Al_2O_3-gate ISFETs originates from the bulk of the Al_2O_3 layer and not from the Al_2O_3-electrolyte interface. Jamasb *et al.* (1998) presented a physical quantitative model that accurately described drift behaviour in Si_3N_4 and Al_2O_3-gate ISFETs. Their model suggested the cause of drift to be a temporal decrease of the effective membrane capacitance resulting from slow chemical modification of the pH-sensitive surface, as a result of exposure to the electrolyte. The work by Jasamb *et al.* (1998) provided information that may help to correct, reduce or eliminate voltage instability in pH ISFETs. SiO_2-gate ISFETs are unstable (Table 7.4).

The literature reported on drift characteristics of Si_3N_4-gate ISFETs ranges from 0.1 to 1 mV hr^{-1}, which is roughly equivalent to 0.002 to 0.02 pH units per hour. For Al_2O_3, reported drift is lower and has a much shorter range from 0.1 to 0.3 mV hr^{-1}, which is of the order of 0.002 to 0.006 pH units per hour. Drift for Ta_2O_5 and SnO_2 is also small, it ranged from 0.1 to 0.2 mV hr^{-1} (Table 7.4).

Hysteresis

Hysteresis is a delayed reaction to pH changes, and refers to the reproducibility or precision of pH measurements. Bousse *et al.* (1990a) modelled the time-dependence and hysteresis of Si_3N_4 surfaces. Bousse *et al.* (1990b) indicated that the mechanisms of drift and hysteresis in Al_2O_3-gate ISFETs are quite different, hysteresis being related to the chemical interactions between the Al_2O_3 surface and the electrolyte solution. The review in Table 7.4 shows that hysteresis of Si_3N_4-gate membranes range from approximately 0.002 to 0.15 pH units, while hysteresis of Al_2O_3 membranes range from around 0.02 to 0.12 pH units. The reproducibility of Ta_2O_5 and SnO_2-gate membranes is reported at roughly 0.004 and 0.05 pH units respectively (Table 7.4).

Response Time

The time for an ISFET to produce a stable signal, *i.e.* its response time, is the crucial property considered in this investigation as the proposed sensing system is to operate ‘on-the-go’ in a continual manner as it is towed across a field. Table 7.5 summarises the response time of ISFETs with different gate membranes. Response time for ISFETs with SiO_2-gate coating membranes is greater than for any other type of coating (Table 7.5). For Si_3N_4 coatings, 95 % response is obtained in less than 1 s while 98 % response ranges from 4 to 10 minutes (Table 7.5). Al_2O_3, Ta_2O_5 and SnO_2-gate membranes have faster response, 95 % being obtained in usually much less than 1 s and 98 % in no more than 2 minutes (Table 7.5). The fast response time of ISFET sensors may be attributed to their small surface area.

Table 7.5 Reported time responses of common inorganic membrane materials used in pH ISFETs

Author	Membrane	Measuring condition	Time response	
			95 % (ms)	98 % (s)
Esashi & Matsuo (1978)	Si_3N_4		100*	
Abe *et al.* (1979)	S_iO_2			
	Si_3N_4		100	300-600
	Al_2O_3		100	120
Janata & Huber (1980)	Si_3N_4		< 1	
Matsuo & Esashi (1981)	SiO_2		1	
	Si_3N_4		< 1000	240-600
	Al_2O_3		< 1000	120
	Ta_2O_5		< 1000	60
van der Schoot *et al.* (1983)	Al_2O_3	FI	1	
Bousse & Bergveld (1984)	Al_2O_3		< 1	
Oelβner *et al.* (1995)		F	300	120
Woias *et al.* (1995)	Si_3N_4	FI	1 – 600	
Liao *et al.* (1998)	SnO_2	I		< 1

F = low; I = injection; FI = flow injection
* Authors suggest that an 80 % deflection is obtained in approximately 100 ms.

Drift and hysteresis are the biggest observed limitations on the accuracy of pH ISFETs in biomedical applications, however this literature review suggests that these characteristics are satisfactory for the intended application in soil science and PA. Although the time taken to obtain 95% of the total response is very quick, the response time behaviour needs further investigation if pH ISFETs are to be used in the sensing component of the proposed system. Because ISFETs are electrochemical sensors that sense through electrostatic surface interactions (section 7.3.1), the signal may be improved by altering the flow rate at the sensor surface. In this way response time may be further reduced because the thickness of the diffusion layer depends on the flow rate.

7.3.4 EVALUATION OF A pH ISFET SENSOR

Measurements were made using a SENTRON[7.1] pH ISFET with an Al_2O_3-gate membrane. A schematic representation of the sensor is shown in Figure 2.

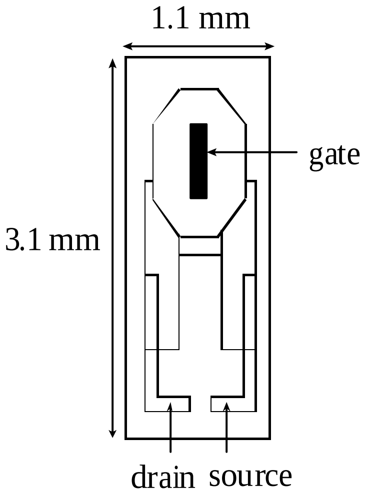

Figure 7.2 Schematic representation of SENTRON ISFET sensor used in experiments

The drain current in the sensor is kept constant by means of electronic feedback.When the pH of the solution is altered, the potential of the gate and hence the drain current also change. At the same time the electronic feedback causes the voltage supply to the reference electrode to re-adjust in such a way, that the drain current is kept constant.

An A/D converter and suitable data logging software were used to register the signals from the sensor. Power was supplied from a regulated source. Static and stirred solution pH measurements were made in 35 ml centrifuge vessels, stirring achieved by using a magnetic stirrer and stirring rod. Injection measurements were made by placing the ISFET inside an enclosed 'injection chamber' (Figure 7.3) with an outlet for waste solution, the ISFET gate being directly under the solution propelled from a syringe. Alonso-Chamarro *et al.* (1992) suggested that a 45° injection flow onto the gate of ISFETs produced best results, while tangential flow is conducive to air bubbles that cause unstable response. In this instance, best results were obtained with 90° injection flow.

[7.1] SENTRON Pty. Ltd. www.sentron.nl

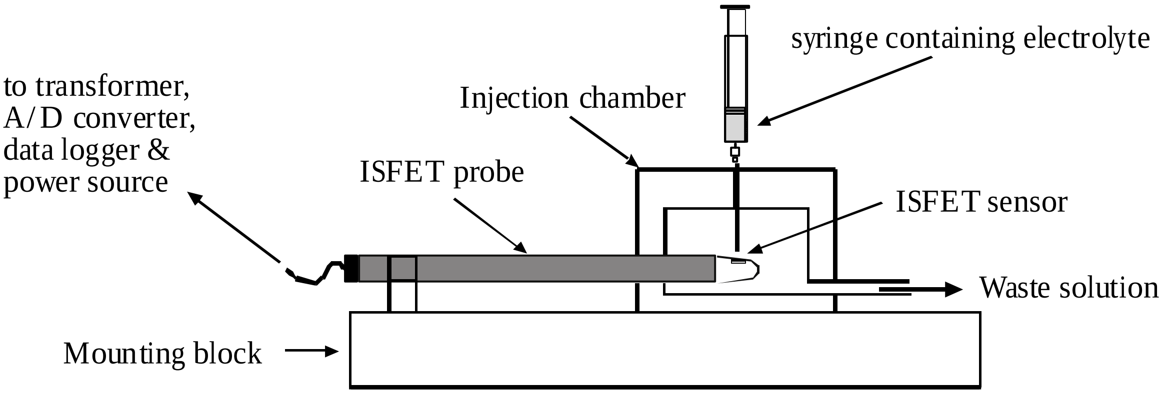

Figure 7.3 Injection chamber with a capacity of 6 ml. Electrolyte solution is injected directly onto the ISFET sensor surface.

Analytical Methodology

The ISFET sensor was calibrated using pH 3, 4, 5, 6, 7, 8, 9 and 10 standard buffer solutions, their preparation is described in Weast (1975). These pH buffers were also used for sensitivity, drift, hysteresis and response time behavior experiments, which are described below. Response time experiments were conducted using ten soil samples from the experimental field in Kelso NSW, (Chapter III). Representative samples were collected along a diagonal transect to a depth of 0.2 metres. Soil pH was measured in 1:5 soil:0.01 M $CaCl_2$ and soil:lime-requirement buffer extracts (Methods are described in Chapter III). The pH of the samples was initially determined using a conventional glass electrode for comparison. pH values in soil:0.01 M $CaCl_2$ ranged from 4.02 to 4.98 and in soil:lime-requirement buffer from 6.62 to 6.75. Note that the relationship between pH_{CaCl_2} and pH_{buffer} is relatively low. The reason for measuring pH_{buffer} is to determine the amount of lime required to ameliorate acid soil (Chapters VI and VIII).

All experiments were conducted at 20°C.

Determination of Drift and Hysteresis

The drift characteristic of the ISFET sensor was determined using standard pH buffer solution pH 7 and lime-requirement buffer solution pH 7. Drift was measured by recording sensor signal every 15 minutes during an eight-hour period using a data logger (see above).

ISFET calibration, sensitivity and hysteresis experiments were conducted using the standard pH buffers. Starting form pH 8, unit pH changes were made in the acid direction (pH 3), then back to pH 8, towards pH 10, and finally back to pH 8. Measurements were made with 2-minute stops at each pH, except at pH extremes and pH 8 (which is expected to be the point of zero charge for Al_2O_3 membrane), where 30-minutes was allowed to elapse. pH measurements were recorded immediately after the pH transition and at 2-minutes or 30-minutes accordingly. Figure 7.4 depicts this process.

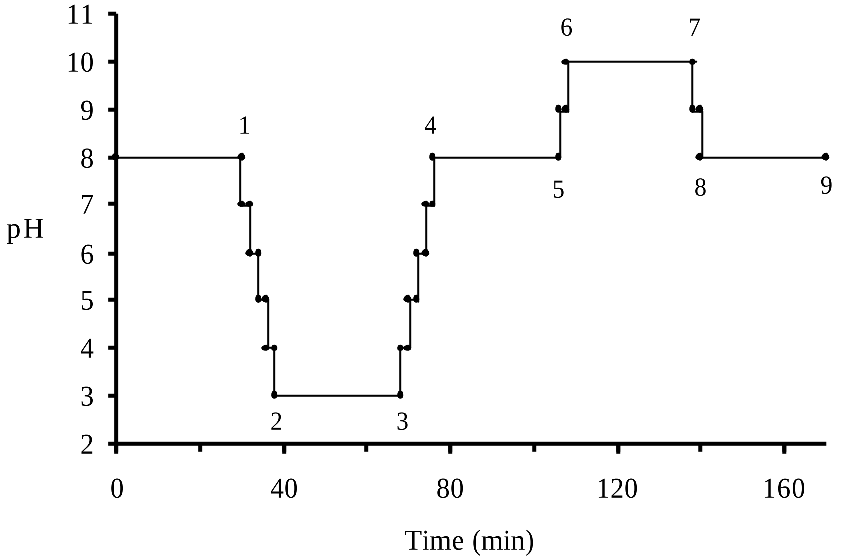

Figure 7.4 The pH measurement process as a function of time for determination of sensor sensitivity and hysteresis. The numbering in the graph will be used to indicate the pH value at corresponding times in equations 7.2 through to 7.6 below.

To present hysteresis data in a meaningful manner Bousse *et al.* (1983b) suggested the use of a reduced interface potential ψ'_0 which removes most of the linear variation expressed in sensitivity curves. The reason for this linearity is that hysteresis represents small proportions of the total response, which is approximately 50 mV pH^{-1}. To demonstrate the second-order effects that are of interest when determining hysteresis, the following reduced response equation was suggested:

$$\psi'_0 = \psi_0 + 50 \times (pH - pH_{PZC}) \qquad (7.1)$$

where ψ'_0 is the reduced response potential (mV), ψ_0 is the potential (mV) and pH_{PZC} is taken as 8, which is expected to be the point of zero charge of Al_2O_3. The reduced pH response is similar to the residuals of a linear regression. An advantage of this method is that measurements are standardised and hence all the ψ'_0 data for all measurements are directly comparable. Hysteresis of the ISFET was determined by:

$$H = \psi'_0(5) - \psi'_0(9) \tag{7.2}$$

Where $\psi'_0(5)$ is the reduced potential at pH 8 after 108 minutes (Figure 7.4), and $\psi'_0(9)$ is the reduced potential at pH 8 after 172 minutes (Figure 7.4). Similarly, the drifts that occurred at pH extremes were determined by:

$$D_A = \psi'_0(3) - \psi'_0(2) \tag{7.3}$$

$$D_B = \psi'_0(7) - \psi'_0(6) \tag{7.4}$$

where; D_A and D_B are the drifts occurring at pH 3, the acidic extreme, and at pH 10, the basic extreme, respectively. Drifts occurring at pH 8 after changes in towards the acidic and basic extremes may be determined by:

$$D_{NA} = \psi'_0(5) - \psi'_0(4) \tag{7.5}$$

$$D_{NB} = \psi'_0(9) - \psi'_0(8) \tag{7.6}$$

where D_{NA} and D_{NB} are the drifts occurring after pH transition in the acidic direction, and basic direction respectively. Equations 7.1 through to 7.6 are similar to those of Bousse *et al.* (1990b)

Determination of Response Time

Response time behaviour of the pH ISFET was recorded by measuring pH changes in a static solution (where the sensor was dipped into the solution), in a solution stirred at 1000 rpm, and in a 6 ml solution jet with a flow rate of 3 ml s^{-1}. Measurements were made in standard pH buffer solutions, 1:5 soil:0.01M $CaCl_2$ and soil:lime-requirement buffer extracts. Experiments were replicated four times rinsing with deionised water and dabbing the ISFET dry between measurements.

Continual time-response measurements using standard buffer, 0.01 M $CaCl_2$ and lime-requirement buffer soil extracts were made in the ISFET chamber (Figure 7.3), all measurements were made starting from and ending in a stable reference pH 7 buffer solution. Sample solutions were jetted directly onto the ISFET chip continually, once the previous signal had stabilised.

Quality Control

Experiments were conducted to verify the quality of continual pH measurements using the ISFET sensor. This was achieved by measuring soil pH measurements in both soil:0.01M $CaCl_2$ and lime-requirement buffer as follows. Nine of the same soil samples were prepared accordingly (as previously described), and continual pH measurements made in the respective solutions, replicating the process thrice. Control charts were drawn up specifying 1 % significance upper and lower control limits (Kreyzig, 1967).

7.3.5 RESULTS

Sensor Characteristics - Sensitivity, Drift and Hysteresis

The Al_2O_3-gate pH ISFET was first calibrated using standard pH buffers and its sensitivity (dmV / dpH) in the pH 3 to 10 range appeared constant and was determined to be 50.3 mV pH^{-1} (Figure 7.5).

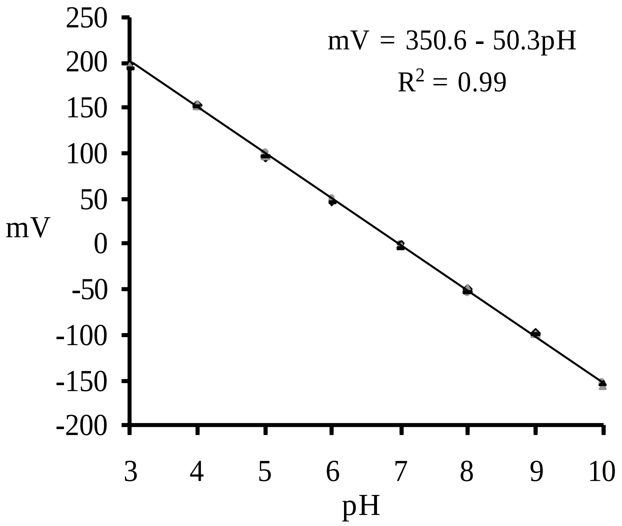

Figure 7.5 Calibration of the Al_2O_3-gate pH ISFET. pH sensitivity of 50.3 mV pH^{-1}.

The sub-Nernstian results (Nernstian response being 59 mV pH^{-1}, see above) obtained in this study represent the lower limit of Al_2O_3-gate pH ISFET sensitivity obtained in other research (Table 7.4).

The voltage instability or drift of the Al_2O_3-gate ISFET in standard buffer and lime-requirement buffer solutions is shown in Figure 7.6.

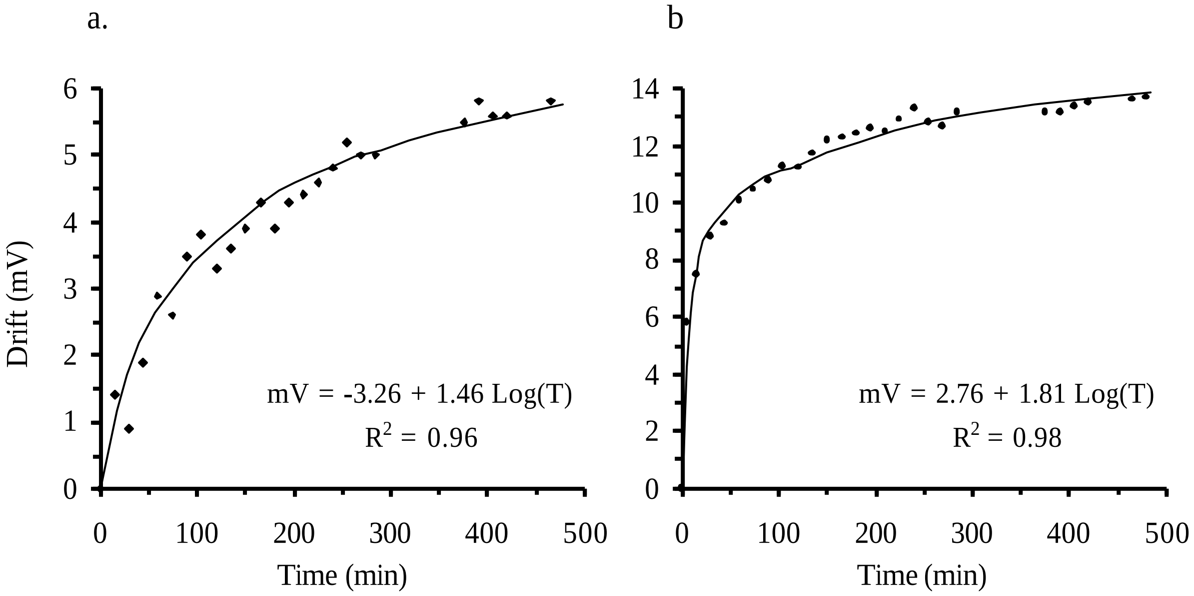

Figure 7.6 Drift characteristics of the Al_2O_3-gate ISFET tested in (a.) standard pH buffer pH 7, and (b.) lime-requirement buffer pH 7

Drift in the standard pH buffer was measured at 0.76 mV hr^{-1}, corresponding to 0.015 pH units hr^{-1}. This result is higher than what is reported in the literature (Table 7.4). Voltage instability in the lime-requirement buffer was measured to be higher at 1.7 mV hr^{-1}, which is approximately equivalent to 0.03 pH units hr^{-1}. Drift in this ISFET may be modelled by a logarithmic function, R^2 in standard pH buffer and lime-requirement buffer being 96 % and 98 % respectively (Figure 7.6). The implication is that drift decreases with time and that it is predictable and hence rectifiable. These results agree with those by van den Vlekkert *et al.* (1986), reported in Bousse *et al.* (1990b).

Hysteresis is observed when an ISFET is exposed to consecutive upward and downward changes in pH, as will be the case in the proposed application. The extent of this behaviour for the Al_2O_3-gate ISFET being tested is shown in Figure 7.7.

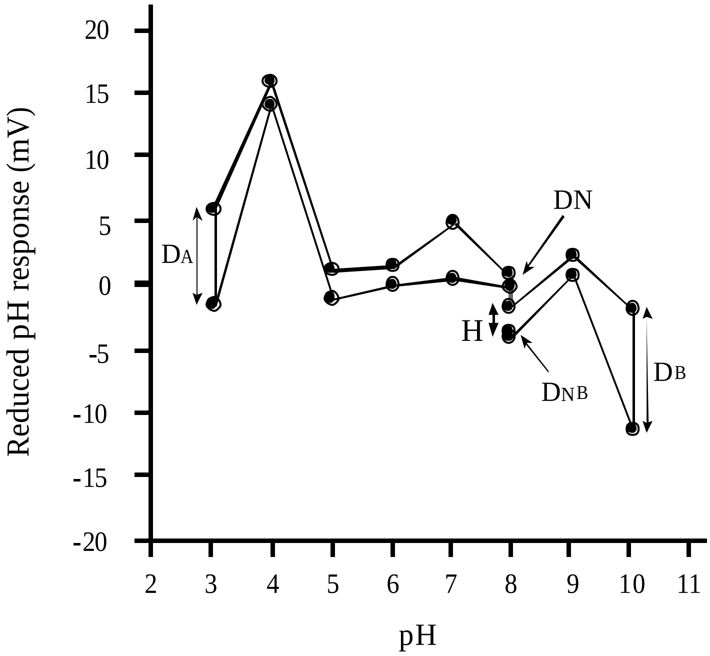

Figure 7.7 A typical hysteresis curve. Readings taken starting from pH 8 towards the acid range then reversing towards basic pHs and finally back to pH 8. The points shown were taken two minutes after a pH step, except at each extreme and at pH 8 where the time spent was 30 minutes (refer to Figure 7.4)

Figure 7.7 shows the hysteresis effect for the SENTRON pH ISFET. The graph may be explained as follows (also refer to Figure 7.4): starting measurements from pH 8 towards pH 3, the ISFET response relative to the starting pH 8 is 241.6 mV. After spending 30 minutes at pH 3 an additional response D_A of 4.6 mV occurs. Likewise, after returning to pH 8 from pH 3, an extra response D_{NA} of –2.2 mV is observed. Similarly, starting measurements from pH 8 towards pH 10 produces D_B and D_{NB} with respective values of –6 mV and 0.3 mV (Figure 7.7). The hysteresis (H) of the ISFET was 1.7 mV, corresponding to approximately 0.06 pH units. This value lies within the range encountered in other studies (Table 7.4). The drift values at pH extremes, D_A and D_B, were 4.6 mV and –6 mV respectively (Figure 7.7). The drift recorded at pH 10 is larger than at pH 3, none of which is recovered in the following 30 minutes at pH 8. Hence the drift in the basic pH region is responsible for a larger proportion of most of the observed hysteresis. These results are in agreement with the work of Bousse *et al.* (1990b).

Response Time of the ISFET Sensor

The response time of the ISFET sensor in static, stirred and injected electrolytes, for the three measuring solutions is shown in Figure 7.8.

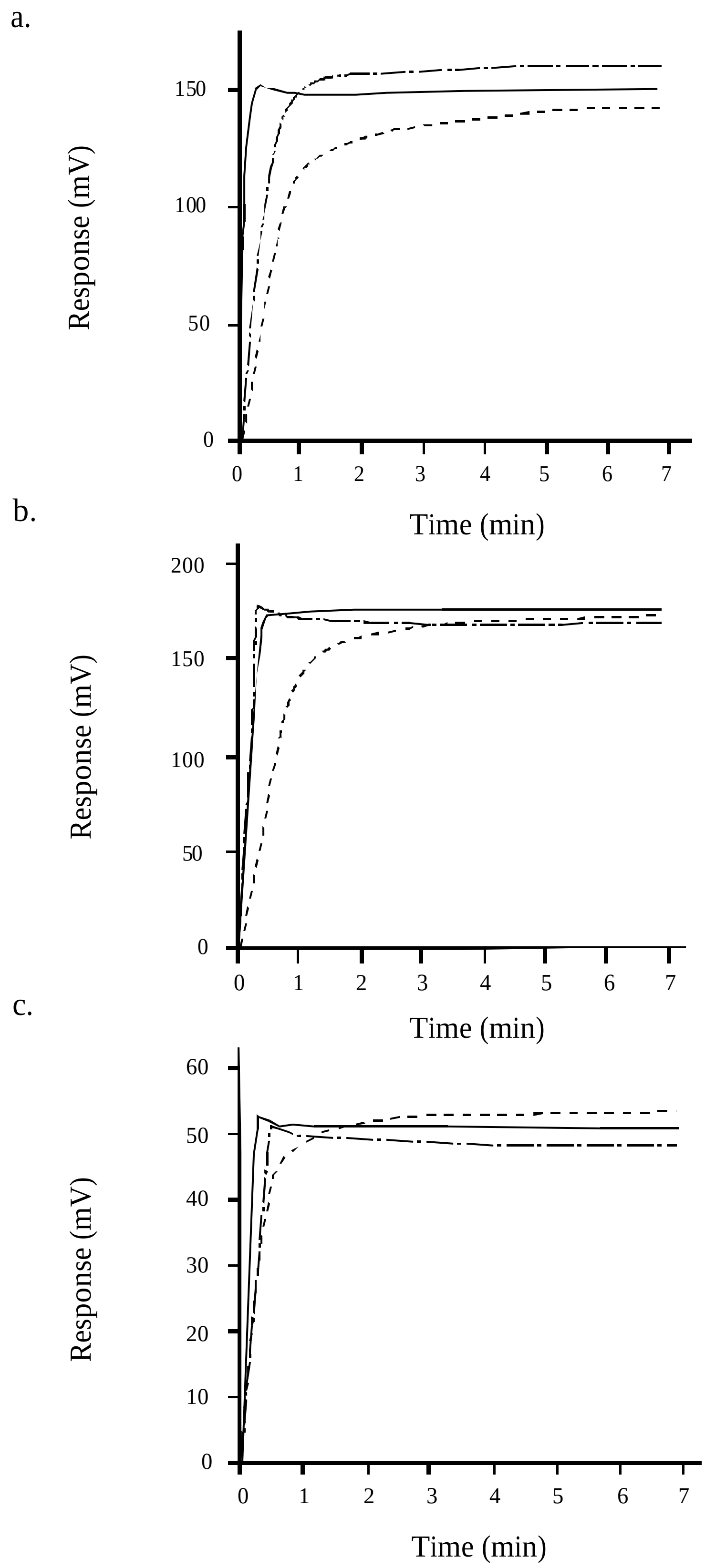

Figure 7.8 ISFET response time in static (fine-dash line), stirred at 1000 rpm (broken line) and injected at 3 ml s^{-1} (solid line) solutions. Response from transitions between standard buffer pH 7 and (a.) standard buffer pH 4, (b.) 1:5 soil:0.01M $CaCl_2$ extract, pH 3.4 and (c.) soil:lime-requirement buffer extract pH 6. Each curve represents the average of four response replicates.

ISFET response to a pH step from 7 to 4 in standard buffer solution, displayed response times of 5.7 s, 3.3 s and 0.7 s under static, stirred and injected conditions respectively (Figure 7.8a). In the same order, response to a pH transition from standard buffer pH 7 to a pH_{CaCl_2} 3.4 extract, was 5 s, 2.4 s and 0.9 s (Figure 7.8b). Similarly, Figure 7.8c. shows response to a pH step from standard buffer pH 7 to a pH_{buffer} 6 soil:lime-requirement buffer extract to be 3.5 s, 3.3 s and 0.9 s under static, stirred and injected conditions respectively. The rapid response of the Al_2O_3-gate ISFET resulting from an injection of electrolyte onto the ISFET membrane justifies the theory that the response mechanism is based on surface reactions rather than on movement (diffusion) of ions in the insulating membrane (section 7.3.3). The response times encountered in this study are similar to those reported in the literature (Table 7.5).

Continually injected measurements in standard pH buffer solutions are shown in Figure 7.9.

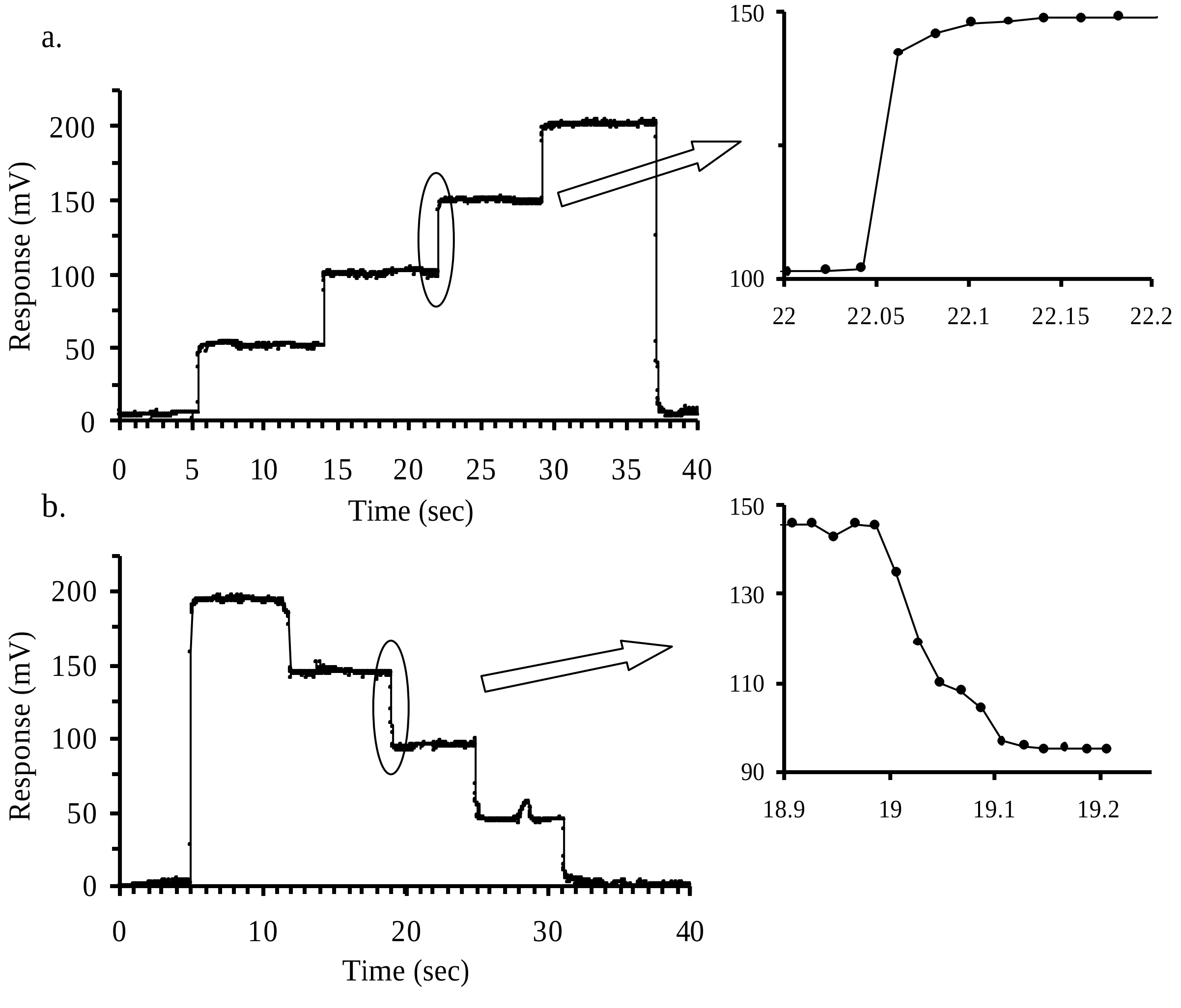

Figure 7.9 Continual pH measurements in standard pH buffers. Each step corresponds to 1 pH unit starting from (a.) pH 7, 6, 5, 4, 3, 7 and (b.) pH 7, 6, 5, 4, 3, 7

The average response time of the pH ISFET sensor was 0.54 s, response ranging from 0.11 s to 1.4 s (Figure 7.9). The magnified response plot in Figures 7.9a and 7.9b shows the almost instantaneous response of the pH ISFET. On Figure 7.9b, the peak at 50 mV may be due to air bubbling on the surface of the ISFET membrane during injection of the pH buffer. Alonso-Chamarro *et al.* (1992) reported that with tangential flow inlet air-bubbles were easily retained on the gate surface, causing unstable response. However, except for this instance, best results were obtained with a 90° injection flow. These response time values are similar to those reported in the literature (Table 7.5).

The response time of three continual soil pH_{CaCl_2} and pH_{buffer} measurements are shown in Figure 7.10.

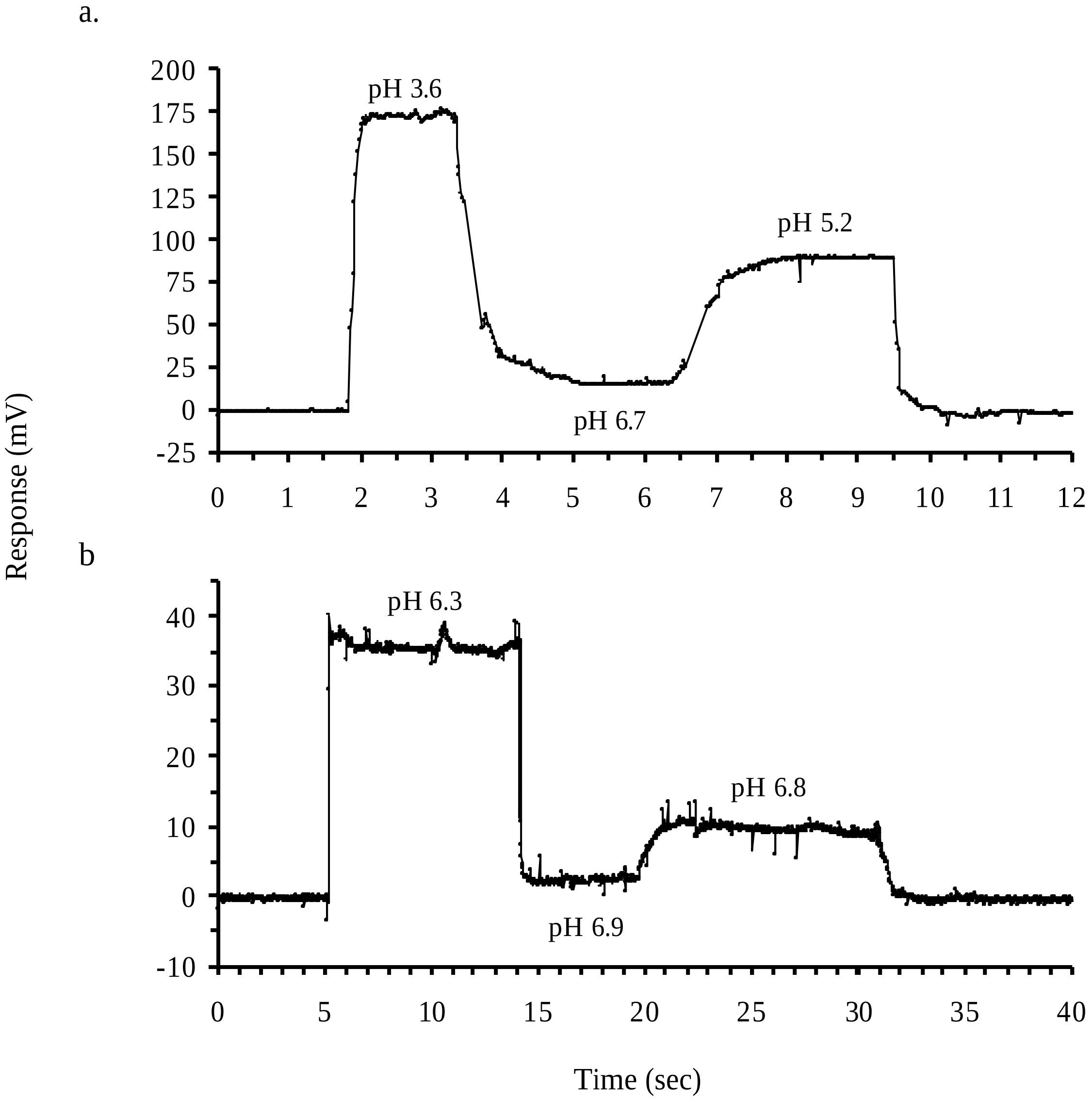

Figure 7.10 Continual pH measurements in (a.) 1:5 soil:0.01M $CaCl_2$ extracts, and (b.) soil:lime-requirement buffer extract

The ISFET response time for transitions between standard pH 7 buffer and pH_{CaCl_2} 3.56 extract was 0.42 s, followed by 1.85 s to pH 6.7, then 1.74 s to pH 5.22 and 0.79s when injected with standard pH buffer 7 (Figure 7.10a). Similarly, response times in the soil:lime-requirement buffer extracts were 1.38 s, 0.82 s, 2.4 s and 1.74 s (Figure 7.10b). The slower response time between low to high pH transitions may be due to the lower $[H^+]$ in the higher pH extracts. The ‘noisier’ signals obtained from measurements in the soil:lime-requirement buffer extracts (Figure 7.10b) may be the result of surface interactions between the buffer’s chemical constituents (Chapters III and VIII) and the ISFET membrane. Longer times were spent at each pH (Figure 7.10b) to see if the signal would become less noisy with time, however this did not happen.

Soil pH_{CaCl_2} and pH_{buffer} measurements of samples collected along the experimental field transect were made to determine response time using a wide range of ‘real’ soil pH values. Measurements pH_{CaCl_2} ranged from 4.02 to 4.98 while pH_{buffer} ranged from 6.62 to 6.75. The continual response time curves are shown in Figure 7.11. The average response time of measurements in soil:0.01M $CaCl_2$ extracts was 1.16 s, response time ranged from 0.55 s to 4.2 s (Figure 7.11a). The fastest response occurred in the transition from 123 mV (pH 4.54) to 115 mV (pH 4.69) while the slowest in the step from 110 mV (pH 4.79) to 132 mV (pH 4.36). The average response time of measurements in soil:lime-requirement buffer extracts was 0.69 s, response ranged from 0.25 s to 1.5 s (Figure 7.11b). The quickest response time occurred in the step from 19 mV (pH 6.61) to 8 mV (pH 6.83), the slowest in the transition from 18.4 mV (pH 6.62) to 16.4 mV (pH 6.66). Shorter response times were obtained by using the lime-requirement buffer. This may have been due to the much narrower pH_{buffer} range than for pH_{CaCl_2}.

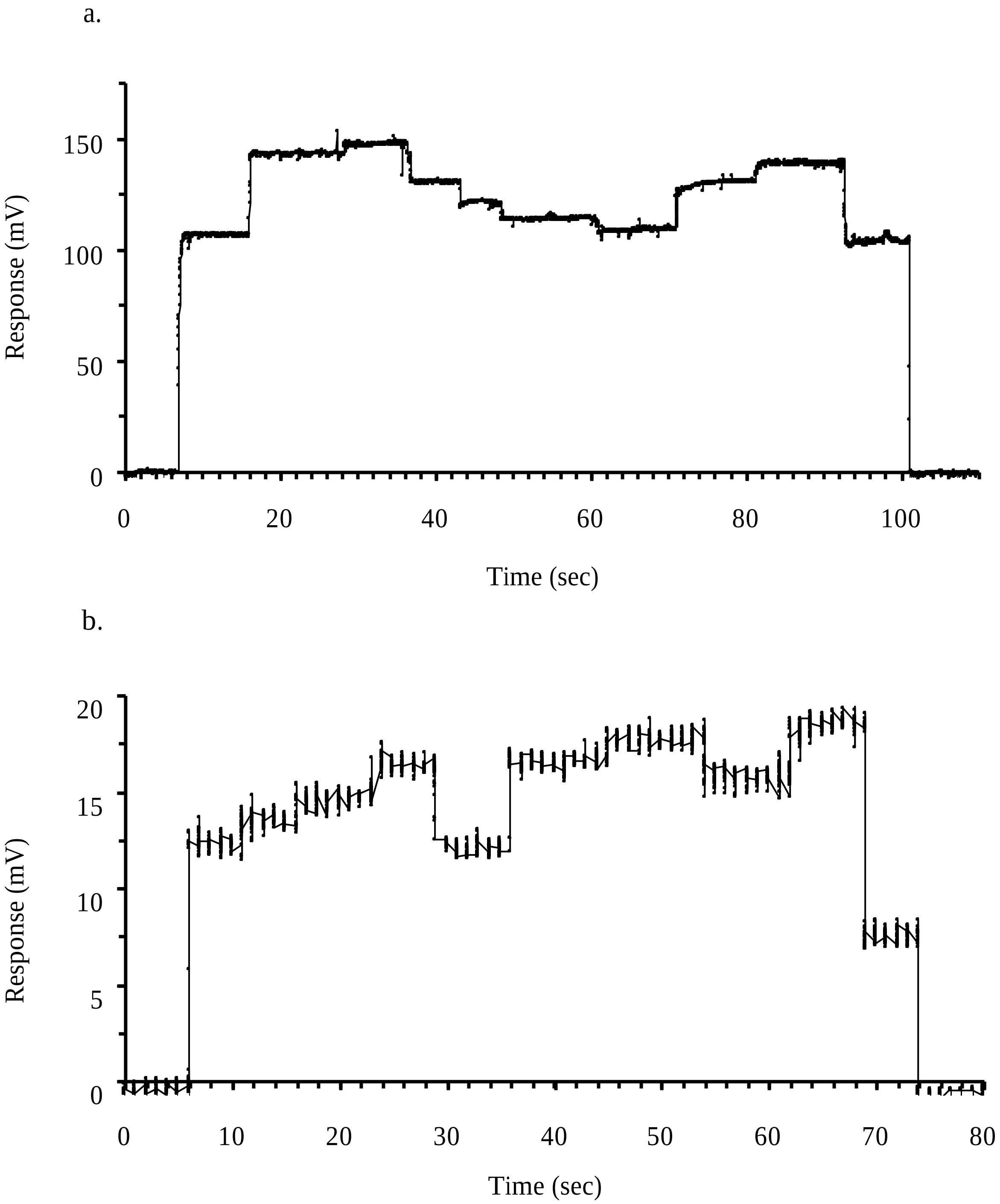

Figure 7.11 Continual response time curves of soil collected from the experimental field. Measurements made in (a.) 1:5 soil :0.01M $CaCl_2$ and (b.) soil:lime-requirement buffer extracts

The accuracy of these measurements is shown in Figure 7.12.

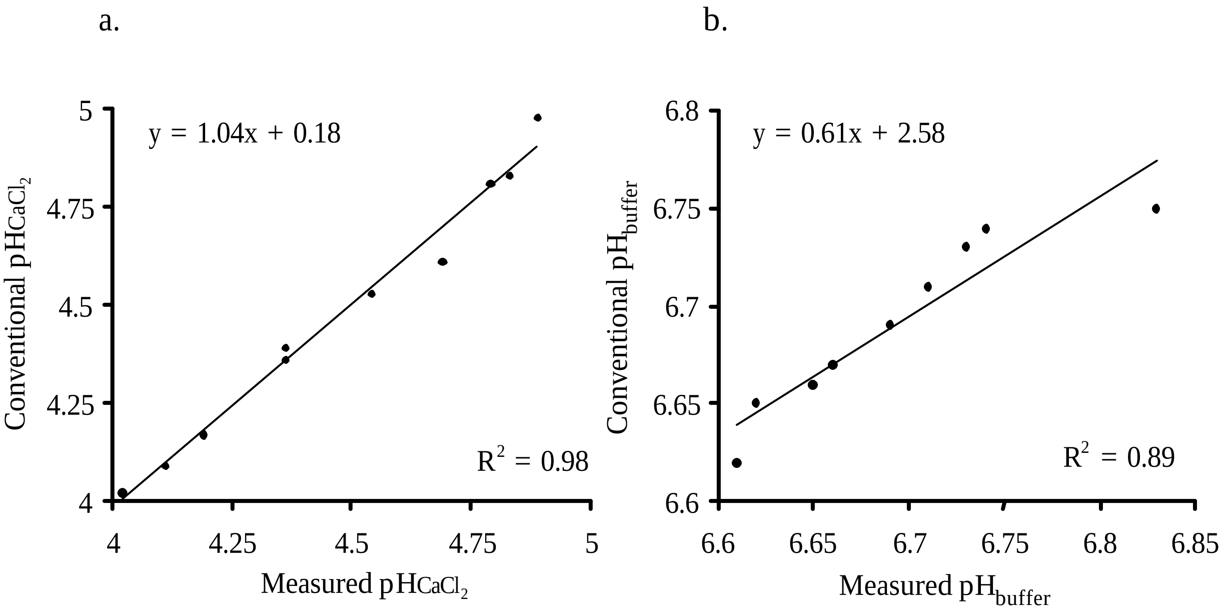

Figure 7.12 Comparison between the continually measured (a.) pH$_{\mathrm{CaCl_2}}$ and (b.) pH$_{\mathrm{buffer}}$ values (Figure 7.11) and pH measured using conventional methods

There is a good correlation between the continually measured and conventionally determined pH$_{\mathrm{CaCl_2}}$ values, the slope of the relationship being near 45° (Figure 7.12a). Continual pH$_{\mathrm{buffer}}$ measurements using the injection chamber were also well correlated to the conventional methods of measuring pH$_{\mathrm{buffer}}$, but for a slight underestimation of pH$_{\mathrm{buffer}}$ values (Figure 7.12b).

ISFET Quality Control

Having established the adequacy of the pH ISFET in terms of its robustness, sensitivity, drift, hysteresis and response time, control charts (Kreyzig, 1967, pp. 808-811) were drawn to illustrate the quality of its measurements. These charts for pH$_{\mathrm{CaCl_2}}$ and pH$_{\mathrm{buffer}}$ measurements are shown in Figures 7.13a and 7.14a respectively. Figures 7.13b and 7.14b show the range (R) of the samples, where R is a measure of the precision of measurements. In quality control, R replaces the sample variance, as it is an easier measurement that corresponds to the differences between the largest sample value minus the smallest sample value. Although the sample variance is a better estimate of σ than R (because R does not use all information contained in the sample, but depends on only two sample values), it was used to illustrate common quality control practice. In a normal distribution, the random variable R^* for which R is an observed value, is proportional to σ by $E(R^*) = \lambda_n\sigma$, where λ is a proportionality factor which depends on the n number of observations (Kreyzig, 1967).

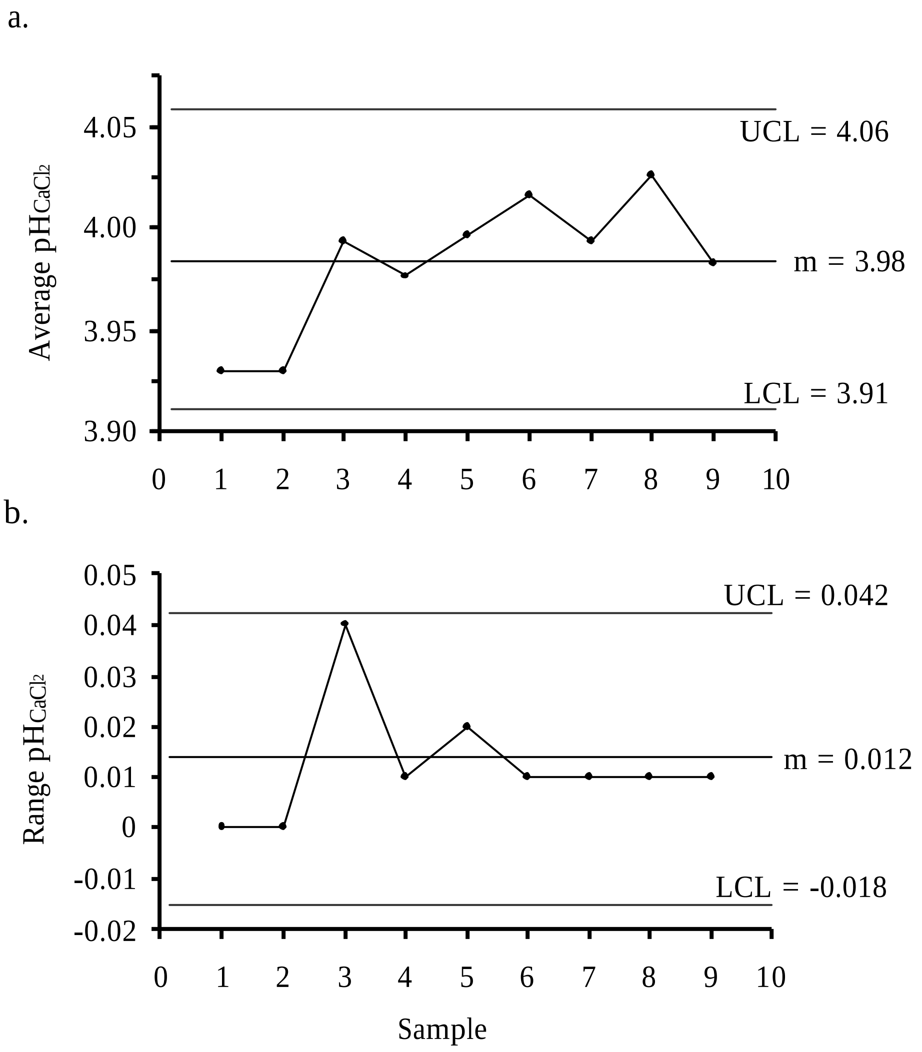

Figure 7.13 (a.) Average and (b.) range control charts for the continual soil pH measurements in soil:0.01M CaCl$_2$ extracts, using the ISFET sensor

In Figures 7.13 and 7.14, the line (m) represents the average pH measurements, and (ULC) and (LCL) the upper and lower confidence limits. ULC and LCL correspond to the critical values above or below which the quality of measurements is deemed insufficient. All ISFET pH$_{CaCl_2}$ measurements were accurate and precise. Similarly, Figure 7.14 shows that pH$_{buffer}$ measurements were accurate and precise.

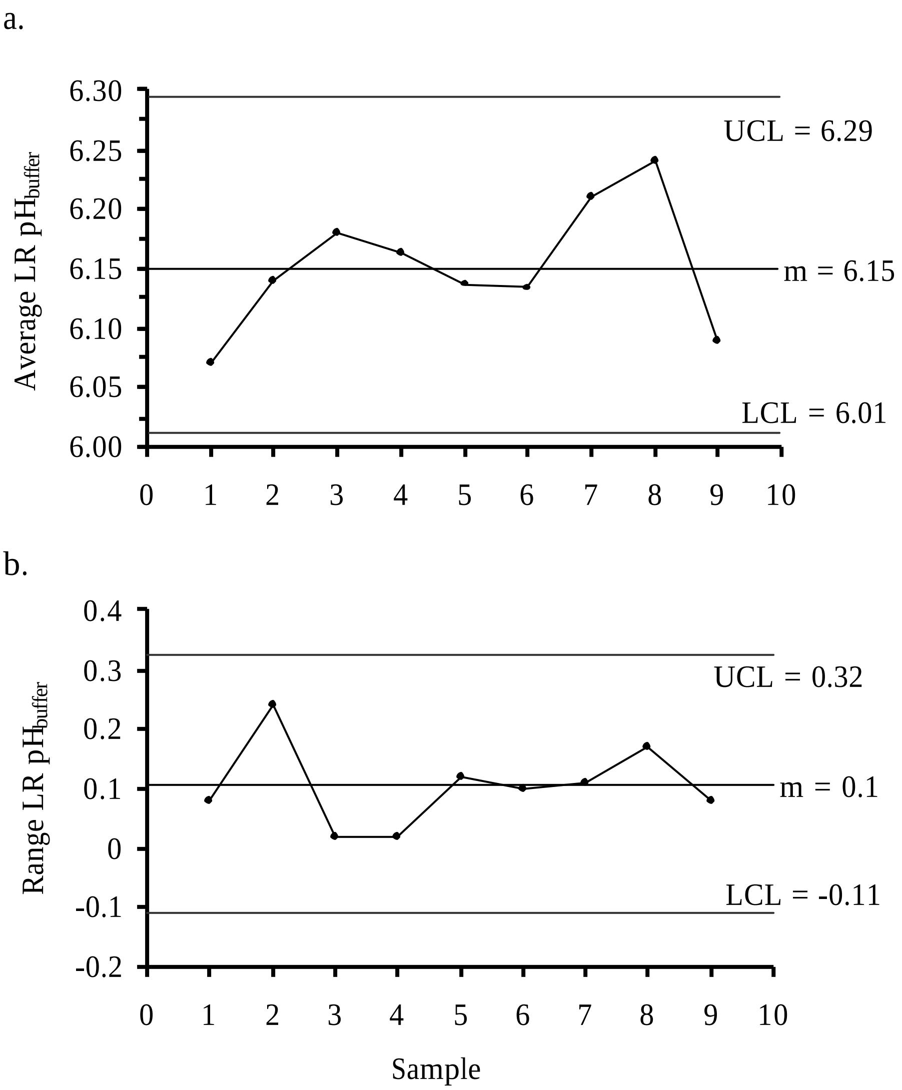

Figure 7.14 (a.) Average and (b.) range control charts for the continual soil pH measurements in soil:lime-requirement buffer, using the ISFET sensor

7.4 THE ANALYTICAL SYSTEM

Classical methods of soil analysis are generally labour intensive, time consuming and expensive. Soil analysis involves five main procedural stages: soil sampling, preparation (drying, grinding, sieving and sub-sampling), extraction, preparation of extract for measurement (involving dilution, addition of reagent, etc.), and measurement of the analyte. The first three stages are difficult to automate because of the need to handle solid soil samples. Latter sections of this chapter will suggest mechanisms for their automation. The last two stages however, may be performed automatically using continuous/continual flow methods such as flow injection analysis (FIA) or sequential injection analysis (SIA).

Classical procedures used to measure soil pH (pH_{CaCl_2} and pH_{H_2O}) and lime requirement pH_{buffer} consist of weighing a specified mass of dry, sieved soil, adding the extracting or buffered reagent, shaking and standing the mixture for predetermined periods before measurements may be made (Chapter III). The shaking and standing times are found in the literature, however they may be determined experimentally from chemical kinetic experiments. Such batch-type methodologies may be adequate for laboratory experimentation but are much too slow and awkward for 'on-the-go' field measurements. Field-deployed soil chemical analysis needs to be rapid and accurate. Flow injection analysis or SIA systems provide simple, rapid, accurate, and convenient methods of analysis, which may be adapted for 'on-the-go' field operation.

7.4.1 FLOW INJECTION ANALYSIS SYSTEMS

Ruzicka & Hansen (1975) first defined FIA. The technique has since generated a lot of interest in different fields of analytical chemistry including agricultural (McLeod, 1992b), soil (McLeod, 1992a; Zhi *et al.*, 1994) and environmental (Luque de Castro & Valcárcel, 1990) chemistry. Attesting to this interest are the large number of papers that have been published in many international journals as well as in the International Journal of Flow Injection Analysis which is totally devoted to the methodology. Several books have also been published on the technique (*e.g.* Valcárcel & Luque de Castro, 1987; Ruzicka & Hansen, 1988). The successful use of the procedure lies in its simplicity, its relative low cost, high sampling rate, and low sample reagent and composition (Ruzicka & Hansen, 1988).

A typical FIA manifold is made up of a bi-directional pump, injection valve, reactor, detector, and tubing manifold (Ruzicka, 1992) (Figure 7.15).

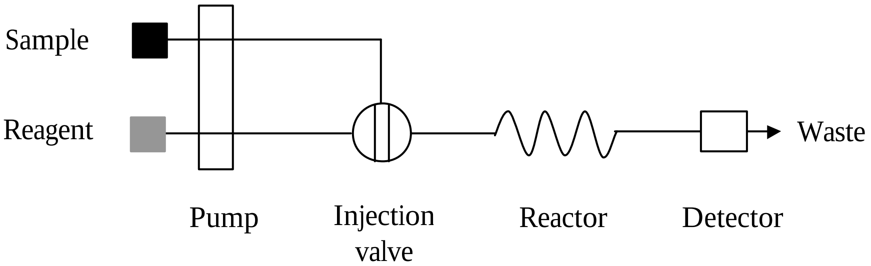

Figure 7.15 A simple flow injection analysis system manifold

From Figure 7.15, the sample and reagent are pumped separately into the injection valve, which injects the sample and reagent into the carrier stream (thus the name flow injection analysis). The sample and reagent are then processed in the reactor and transformed into a species (*i.e.* the analyte) that can be measured by the detector. The fluid dynamics of the flow through the reactor disperses the sample, mixing it with the reagent and leading to chemical reaction and sample dilution. This process is referred to as controlled dispersion in FIA (Ruzicka & Hansen, 1988). The analyte then passes through to the detector, which in turn generates a quantifiable signal. The detector may be an ISE, ISFET, UV, visible, infrared, or a variety of other sensors. Hence FIA combines three operations: sample injection, controlled dispersion, and reproducible timing of its movement from the injection point to the detector (Ferreira *et al.*, 1998).

Dispersion is one of the fundamental processes in FIA, and its theory is dealt with by a number of publications. For example, Ruzicka & Marshall (1990) suggested that the random walk model might provide a theoretical description of dispersion. The model allows one to view the element of fluid as being displaced during the dispersion process in any direction by a step of fixed length, where the direction of the step is determined entirely by chance. Paiton & Mottola (1983) and Ruzicka & Hansen (1988) also provided some theory.

Generally, dispersion may be defined as the dynamic but reproducible intermixing of sample and reagent caused by flow patterns created by the dynamics of fluid flow through narrow bore tubing (Ruzicka & Hansen, 1988). While the dispersion is dynamic and never reaches steady-state before the sample arrives at the detector, it is reproducible if the factors that affect dispersion are held constant. These factors include sample volume, flow rates, tubing length and internal diameter, type of reactor (*e.g.* straight, coil, knotted, serpentine), and internal arrangement of components such as valves, connectors and detectors, all of which can be readily controlled. Therefore the degree of chemical reaction and sample dilution caused by dispersion during transport of the sample-reagent mixture from injector to detector can be controlled so that it is reproducible - hence ‘controlled dispersion’. This allows calibration of the system and use of the calibration to quantitate samples.

However dispersion must be controlled using a set of conditions that depend on the application the analyst requires, since on the one hand dispersion promotes chemical reaction between sample and reagent, while on the other it causes dilution. Generally, following injection of the sample chemical reaction predominates leading to a net increase in sensitivity with increased dispersion, however beyond a certain point, dilution has the predominant effect and sensitivity decreases. The dispersion coefficient D may be used to classify the degree of dispersion and hence for the design of FIA systems. The coefficient $D = K^0 / K$, where K^0 is the original sample concentration prior to injection and K is the concentration of the sample in the dispersed sample zone from which the analytical readout is to be obtained (Ruzicka & Hansen, 1984). Dispersion may be classified as limited (D = 1 – 3), medium (D = 3 – 10), or large (D = > 10). Limited dispersion will merely transport samples through the system to the detector, medium dispersion will provide a suitable mixing ration between sample and reagent and large dispersion will result in extensive sample dilution (Ruzicka & Hansen, 1984). For soil pH and measurements medium dispersion would be suitable.

Dispersion in FIA may be either axial or radial (Ruzicka & Hansen, 1988). Axial dispersion predominates in a straight tube and occurs in the direction of the stream flow, causing greater dilution than radial dispersion. Radial dispersion is caused by circular flow patterns (or eddies) in the flow stream that cause effective mixing with minimal dilution. Frequent and sharp turns in the flow path (*e.g.* coiling the tubing) promote radial dispersion.

7.4.2 FLOW INJECTION ANALYSIS SYSTEMS FOR SOIL ANALYSES

Flow injection analysis methods have been employed in soil science laboratories for quite some time. The procedures were introduced to replace more established yet sometimes tedious and time-consuming manual methods of soil analysis. Examples of FIA for a number of agriculturally important properties are given in Table 7.6. Generally, the flow injection techniques tested (Table 7.6) proved more efficient, accurate and reliable than their manual counterparts. Moreover, their implementation raised sample throughput three to four-fold without an increase in the number of laboratory personnel. Fang (1986) indicated that rather than handling soil samples in batches of six to ten, a single operator may process large batches of 50 to 100 samples using FIA. For example Fang (1986) reported 120 soil pH measurements per hour with a flow injection system using a pH electrode as detector. Hongbo *et al.* (1985) reported 110 soil pH measurements per hour and Edmonds & Coutts (1983) 90 measurements per hour. Clearly these analytical rates are much greater than what is currently accomplished using conventional manual laboratory techniques.

These features make the technique attractive for ‘on-the-go’ field operation and encourage research towards the development of fully automated field-deployed analytical systems for a variety of soil properties that require wet-chemistry for the acquisition of results.

Table 7.6 Flow injection analysis (FIA) system application to soil analysis

Soil property (analyte)	Detector	Reference
Aluminium	UV / Visible	Reis *et al.*, 1979
Calcium	UV / Visible	Jacintho, *et al.*, 1981
	AAS	Ferreira *et al.*, 1995
Magnesium	AAS	Ferreira *et al.*, 1995
Total-N	Visible	Mcleod, 1992b
	Potentiometry	Ferreira *et al.*, 1996
Nitrate-N	ISFET	Birrell & Hummel, 1997
Phosphorus	UV / Visible	Garcia *et al.*, 1991
Potassium	FES	Ferreira *et al.*, 1995
pH	Potentiometry	Edmonds & Coutts, 1983
	Potentiometry	Hongbo, *et al.*, 1985

Note: atomic absorption spectrophotometry (AAS); flame emission spectrometry (FES)

7.4.3 SEQUENTIAL INJECTION ANALYSIS SYSTEMS

Ruzicka & Marshall (1990) first described Sequential Injection Analysis (SIA). The technique arose from a need to simplify FIA manifolds and make them more versatile and robust. Sequential injection analysis is similar to FIA however it uses a piston (rather than bi-directional peristaltic) pump, a selector (rather than injection) valve, a holding coil, a reactor and detector (Ruzicka, 1992) (Figure 7.16).

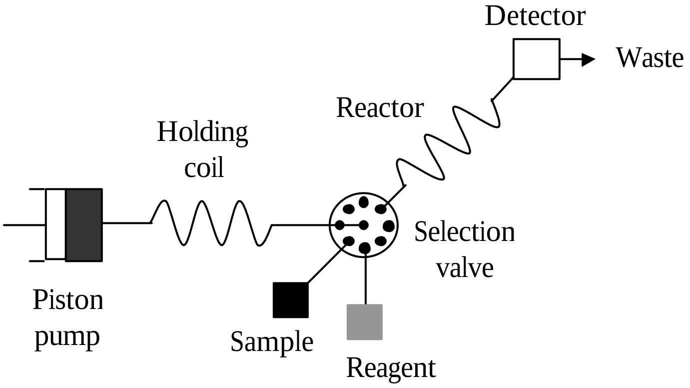

Figure 7.16 A simple sequential injection analysis system manifold

From Figure 7.16, through the selection valve, precisely measured volumes of sample and reagent solutions are aspired into a holding coil by means of a piston pump that is capable of precise and controlled movements. The selection valve is then advanced to the port that is connected to the detector and the analyte is pumped through the reactor to the detector, as with the FIA technique described above. However instead of aspiring both sample and reagent simultaneously into the holding coil, SIA allows them (and any other solutions) to be loaded separately. Thus with SIA it is possible to construct a stack of well-defined ‘zones’ which can be mixed together to give rise to the detectable analyte. Unlike FIA that needs re-plumbing when more complex chemistry is required, all that is needed with SIA is a change to the flow program while the manifold may remain the same (Ruzicka & Marshall, 1990). Additional ports may be used for calibration standards or additional reagents.

Dispersion in SIA begins during aspiration of the sample and reagents into the holding coil (Ruzicka, 1992). The flow reversal that takes place when the sample is directed towards the reactor and detector provides effective mixing of the sample and reagents. Following from the brief description of the random walk model given in section 7.6.1, moving the solution forward and backward in several steps of sufficient length, ensures efficient mixing of sample and reagents. By selecting the step length and number of flow reversals, any degree of mixing and any desired length of reaction time can be obtained simply through flow reversal (Ruzicka & Marshall, 1990). The one-directional flow of classic FIA systems is thus only required because the sample needs to be transported through the manifold to the detector, to waste.

The advantages of SIA over FIA systems include simpler flow manifolds that are versatile and robust; reduced reagent use; more efficient mixing; a means for selecting different samples, reagents and calibrants, and option for automated calibration. Thus SIA manifolds may be more amenable to field operation.

7.4.4 AN ANALYTICAL SYSTEM FOR FIELD OPERATION

Birrell & Hummel (1997) were the first to design an ISFET-FIA system for ‘on-the-go’ measurements of soil, in that instance, nitrate-nitrogen. Their analytical system was described in Chapter II. This section will describe the design of an analytical system for the soil pH and lime-requirement sensing system, using the FIA/SIA techniques previously outlined. The proposed design of the analytical manifold consists of three piston pumps, a peristaltic bi-directional pump, a selector valve, mixing coils, inert plastic tubing, a reactor and a pH ISFET detector (Figure 7.17).

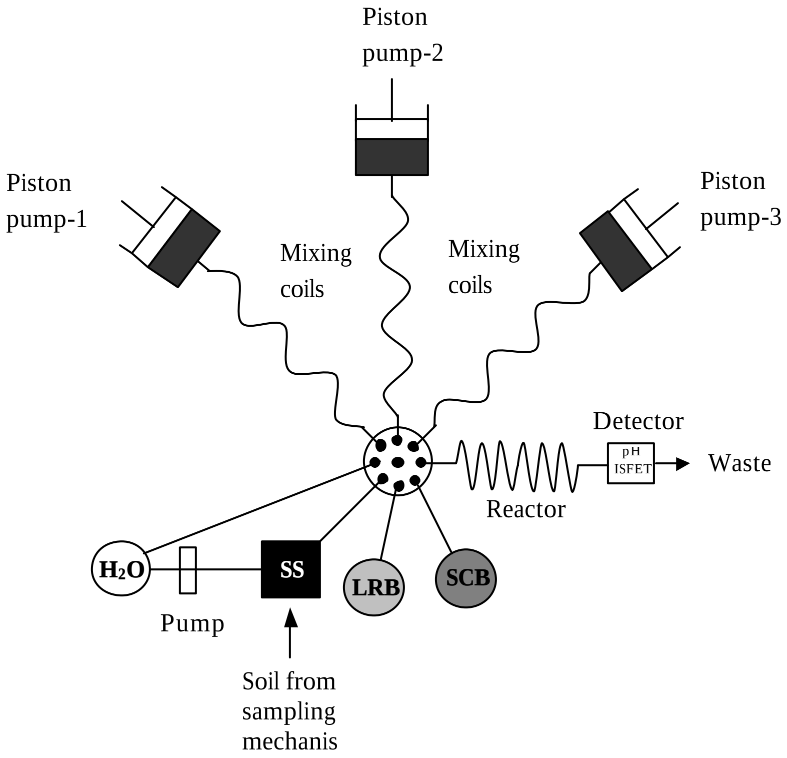

Figure 7.17 Analytical manifold for 'on-the-go' soil pH and lime requirement measurements. Where SS represents the soil sample compartment where soil is initially introduced into the analytical manifold; LRB the reservoir containing the lime-requirement buffer solution, and SCB the reservoir with the standard calibration buffer solutions.

From Figure 7.17, coinciding with continual aspiration of 5 g of soil by the sampling mechanism (section 7.7.1), into the soil sample (SS) compartment of the manifold, soil is mixed with 5 ml of deionised water and is drawn up by a piston pump. Deionised water is pumped into the SS compartment from the H_2O reservoir using a calibrated bi-directional peristaltic pump. The analytical system (Figure 7.17) may then operate in either of two different modes depending on their experimentally determined timeliness of operation:

First, continual, cyclical operation of the analytical manifold would encompass the following steps:

1. Initially, the soil slurry sample is drawn up by piston pump-1 into its mixing coil together with 5 ml of lime-requirement buffer from the LRB reservoir (Figure 7.17).
2. Piston pump-2 then draws up the next soil slurry sample into its mixing coil together with 5 ml of lime-requirement buffer.

3. The selection valve advances to the ports connected to piston pump-1 and the detector, and the soil-analyte mixture is pumped through the reactor to the pH ISFET for measurements, then to waste. The reversal of flow that occurs when the samples is drawn and pumped ensures adequate mixing of the soil slurry and the lime-requirement buffer for adequate chemical reaction and measurement (refer to section 7.4.3).
4. Using piston pump-1 water is flushed through the system to wash the pump, tubing manifold and detector.
5. Immediately, piston pump-3 draws the next soil sample and 5 ml of lime-requirement buffer into its mixing coil.
6. The selection valve advances to the ports connected to piston pump-2 and the detector, and the soil-analyte mixture is pumped through the reactor to the pH ISFET for measurements, then to waste. The reversal of flow ensures mixing of both zones for adequate chemical reaction and measurement.
7. Using piston pump-2 water is flushed through the system to wash the pump, tubing manifold and detector.
8. Step 1 is repeated.
9. The selection valve advances to the ports connected to piston pump-3 and the detector, and the soil-analyte mixture is pumped through the reactor to the pH ISFET for measurements, then to waste. The reversal of flow ensures adequate mixing.
10. Using piston pump-3 water is flushed through the system to wash the pump, tubing manifold and detector.

Steps 2 to 10 are repeated continually as soil samples are introduced into the SS compartment. It will be possible to including more piston pumps in the design if it is deemed necessary to increase the analysis and measurement rates.

The second mode of operation is also continual but may be more straight forward:

1. Initially, the soil slurry sample is drawn up by piston pump-1 into its mixing coil together with 5 ml of lime-requirement buffer from the LRB reservoir (Figure 7.17). The selection valve advances to the ports connected to piston pump-1 and the detector, and the soil-analyte mixture is pumped through the reactor to the pH

ISFET for measurements, then to waste. The reversal of flow that occurs when the samples is drawn and pumped ensures adequate mixing of the soil slurry and the lime-requirement buffer for adequate chemical reaction and measurement (refer to section 7.6.3).

2. Water is flushed through the system to wash the pump, tubing manifold and detector.

These two steps are repeated for each piston pump in a continual manner.

The pH ISFET may be calibrated using standard calibration buffer solutions (pH 4 and 7) from the SCB reservoir (Figure 7.17), after an experimentally determined number of analytical cycles. The most efficient mode of operation will depend on the timeliness of sample throughput, which needs to be determined experimentally using various pumps, flow rates, conduit diameters, etc. For example, as previously suggested, if a vehicle travelling at 8 km/hr towed the sensing system, sampling, analysis and pH measurements would need to be made every 4.5 seconds to characterise the soil of the field at ten metre intervals.

As the manifold needs to handle solid particles in the soil-analyte mixture, the architecture of the manifold will also need to be determined experimentally. For example, various conduit diameters, s-bend positions and the degree of bending of the conduits (mixing/holding coils and the reactor) will need to be tested so that the fluid dynamics of the flow ensure appropriate mixing of the soil and analyte. Similarly, various materials may need to be trialled.

7.5 KINETICS OF ION EXCHANGE REACTIONS

The chemical reactions that occur when soil is mixed with a solution of 0.01M-$CaCl_2$, or with a lime-requirement buffer, involve ion exchange reactions. Soil pH_{CaCl_2} measures the activity of H^+ present in solution, and pH_{buffer} the exchangeable acidity by way of cation displacement. When such reactions reach equilibrium, a measure of their pH_{CaCl_2} or pH_{buffer} can provide information on the H^+ activity in the soil solution, or the amount of base needed for the amelioration of the exchangeable acidity (Chapter VI). With the lime-requirement buffers, the measurement pertains to the change in pH_{buffer} caused by soil-buffer interaction (refer to Chapters VI and VIII). The more the pH_{buffer} is depressed by the addition of the acid soil, the less completely the soil is titrated by the buffer and consequently, the greater the lime requirement of the soil.

Successful 'on-the-go' field operation of the soil pH and lime requirement sensing system is time-dependent, thus the time-dependency of the mentioned chemical reactions (*i.e.* their kinetics) needed to be investigated. Section 7.3.5 concluded that the pH ISFET sensor has a sufficiently rapid response for 'on-the-go' field operation, and section 7.4.4 indicated that rapid sample throughput rates using a modified FIA/SIA system can also be achieved for continual 'on-the-go' operation. However the time scale for ion exchange reactions are varied and may range from microseconds to hours (Amacher, 1991). Therefore the objectives of this section are to (i) determine how quickly the soil:0.01 M $CaCl_2$ and soil:lime-requirement buffer reactions reach equilibrium (or quasi-state equilibrium), (ii) investigate the reaction mechanism of soil:lime-requirement buffer reactions and (iii) suggest how their equilibrium state may be accurately predicted from pH_{buffer} measurements of the reacting solution at time periods that satisfy the operational requirements of the sensing system (*i.e.* a few seconds). The lime-requirement buffer tested was the Mehlich buffer (Mehlich, 1976).

7.5.1 METHODOLOGY

Nine agricultural surface soil samples (0 – 200 mm) with widely varying properties were collected from the southwestern wheat-belt of NSW, Australia (refer to Figure 8.2 of Chapter VIII for their locations). The soils were analysed for pH_{CaCl_2}, pH_{buffer}, organic carbon (OC), cation exchange capacity (CEC), clay content, and lime requirement (LR), using methods described in Chapter III.

Kinetic Methodology

Kinetics is the generic name referring to the study of time dependent or non-equilibrium processes that occur in heterogeneous systems (Sparks, 2000). The kinetic experiments for both soil:0.01M-$CaCl_2$ and soil:lime-requirement buffer were conducted using a batch technique discussed in Sparks (1989, pp. 41-46) and Amacher (1991). It involved placing both soil and solution into 35 ml centrifuge tubes and stirring the suspension at 1000 rpm using a magnetic stirrer and stirring rod. A pH ISFET connected to an A/D converter and data logging software were used to measure pH_{CaCl_2}/pH_{buffer} changes at predetermined time intervals, and to detect reactions equilibriums.

Soil pH_{CaCl_2} measurements were made at 0, 0.5 s, 1 s, from 2 s to 5 s every second, from 5 s to 20 s every 5 s, from 20 s to 60 s every 10 s, from 1 min to 2 min every 30 s, from 2 min to 5 min every minute and from 5 min to 30 min every 5 min. These measurements were replicated twice for each soil sample and their average pH_{CaCl_2} plotted against time.

Changes in $\mathrm{pH}_{\mathrm{CaCl_2}}$ (*i.e.* $\delta\,\mathrm{pH}_{\mathrm{CaCl_2}}$) over time were plotted to determine the time at which the reactions reached equilibrium.

Soil $\mathrm{pH}_{\mathrm{buffer}}$ measurements were made at 0, 0.5 s, 1 s, 2 s, 3 s, 5 s, 15 s, 30 s, 60 s, from 2 min to 14 min every 2 min, from 15 min to 40 min every 5 min and from 40 min to 60 min every 10 min. Measurements were replicated four times for each soil sample and the average $\mathrm{pH}_{\mathrm{buffer}}$ plotted against time. Changes in $\mathrm{pH}_{\mathrm{buffer}}$ (*i.e.* $\delta\mathrm{pH}_{\mathrm{buffer}}$) over time were also plotted to determine the time at which the reactions reached equilibrium.

Description of the Kinetics of $\mathrm{pH}_{\mathrm{buffer}}$ Reaction

The $\mathrm{pH}_{\mathrm{buffer}}$ kinetic data were characterised using first-order kinetic equations similar to those described by Martin & Sparks (1983) and Jardine & Sparks (1984):

$$\ln\left(1-\frac{\mathrm{pHb}_e}{\mathrm{pHb}_t}\right)=\ln\left(\mathrm{pHb}_e\right)-k_t \qquad (7.7)$$

where pHb_e is the equilibrium $\mathrm{pH}_{\mathrm{buffer}}$; pHb_t is the $\mathrm{pH}_{\mathrm{buffer}}$ at time t; and k is the rate coefficient for a single reaction.

In an attempt to learn more about the reaction mechanism, a two constant rate equation was also fitted to the data using non-linear least-squares regression. The equation was a double exponential model with the following form:

$$a_0+a_1\times\mathbf{e}^{-k_1t}+a_2\times\mathbf{e}^{-k_2t} \qquad (7.8)$$

where a_0 is the predicted equilibrium $\mathrm{pH}_{\mathrm{buffer}}$, *i.e.* the asymptote; a_1 and a_2 are parameters of the model; k_1 and k_2 are the two rate coefficients; and t represents reaction time in minutes.

Prediction of Equilibrium $\mathrm{pH}_{\mathrm{buffer}}$ Values

Prediction of the equilibrium $\mathrm{pH}_{\mathrm{buffer}}$ comprised three steps:

1. Transforming the elapsed soil:lime-requirement buffer reaction time to a log scale.
2. Fitting a linear regression to only initial $\mathrm{pH}_{\mathrm{buffer}}$ values and corresponding 0.5 s, 1 s, 2 s and 3 s measurements.

3. Using the linear regression equation to predict the pH_{buffer} at which the reaction reached equilibrium.

The method is illustrated graphically in the Results section. Predictions were made for the nine soil samples used in the study.

Finally, predictions were assessed using the relationship between inaccuracy, bias and imprecision (equation 4.1, Chapter IV). The root–mean square-error (RMSE) (Equation 5.16, Chapter V) quantified the inaccuracy of predictions while the mean error $ME = \frac{1}{n}\sum_{j=1}^{n}[predicted - observed]$, quantified their bias. Their respective lime requirements were also calculated and compared.

7.5.2 RESULTS

A statistical description of the different soils used for the chemical kinetic experiments is given in Table 7.7.

The soil properties had wide ranging values and relatively high coefficients of variation (Table 7.7). These statistics verify the diversity of the samples. Their heterogeneity will help to demonstrate the range in responses, reaction equilibration times, reaction rates, and hence the robustness of the proposed prediction method for estimating reaction equilibrium using only initial pH_{buffer} values.

Table 7.7 Descriptive statistics of pH in 0.01M-$CaCl_2$ (pH_{CaCl_2}), pH in lime-requirement buffer (pH_{buffer}), organic carbon (OC), cation exchange capacity (CEC), clay content and lime requirement (LR) for the nine soil samples used in the experiments

Soil Property	Mean	S.D.	CV %	Minimum	Median	Maximum
pH_{CaCl_2}	4.75	0.77	16	3.69	4.80	6.20
pH_{buffer}	5.74	0.48	8	4.83	5.99	6.22
OC dag/kg	1.3	0.6	43	0.6	1.4	2.3
CEC mmol(+)/kg	88.4	59.0	67	23.0	61.0	175.2
Clay Content dag/kg	27.3	11.3	41	14.0	21.7	45.0
LR Mg/ha	7.1	5.3	74	0	5.1	15.8

Kinetics of Soil:0.01M-Calcium Chloride (pH_{CaCl_2}) Reactions

The soil:0.01M-$CaCl_2$ reactions for eight different soil types are depicted in Figure 7.18a. The reactions of all the soils tested were rapid. The largest changes in pH_{CaCl_2} over time (*i.e.* $\delta pH_{CaCl_2}/t$) occurred during the first 30 s of reaction, after which only small changes of less than 0.1 pH_{CaCl_2} units were observed (Figure 7.18b).

Section 7.2 suggested that a pH sensor with a resolution of 0.1 pH units would suffice for field measurement of soil pH_{CaCl_2} or pH_{H_2O}. The reaction time required to achieve a measurement accuracy of 0.1 pH_{CaCl_2} units was approximately 20 s (Figure 7.18b). These changes over the 20 s period were somewhat erratic and varied for the eight different soil types. Further experimentation is needed to model and more comprehensively describe the kinetics of pH_{CaCl_2} reactions.

Although a 20 s to 30 s reaction time to equilibrium is much shorter than the suggested 30 min reaction time for laboratory measurements of soil pH_{CaCl_2} (Chapter III), it is too long for continual field measurements. Using the three-pump analytical system previously outlined in section 7.6.4, or a similar system with four- or five-pumps, all operating in a sequential manner, may account for the 20 to 30 second reaction time required for measurements of soil pH_{CaCl_2}.

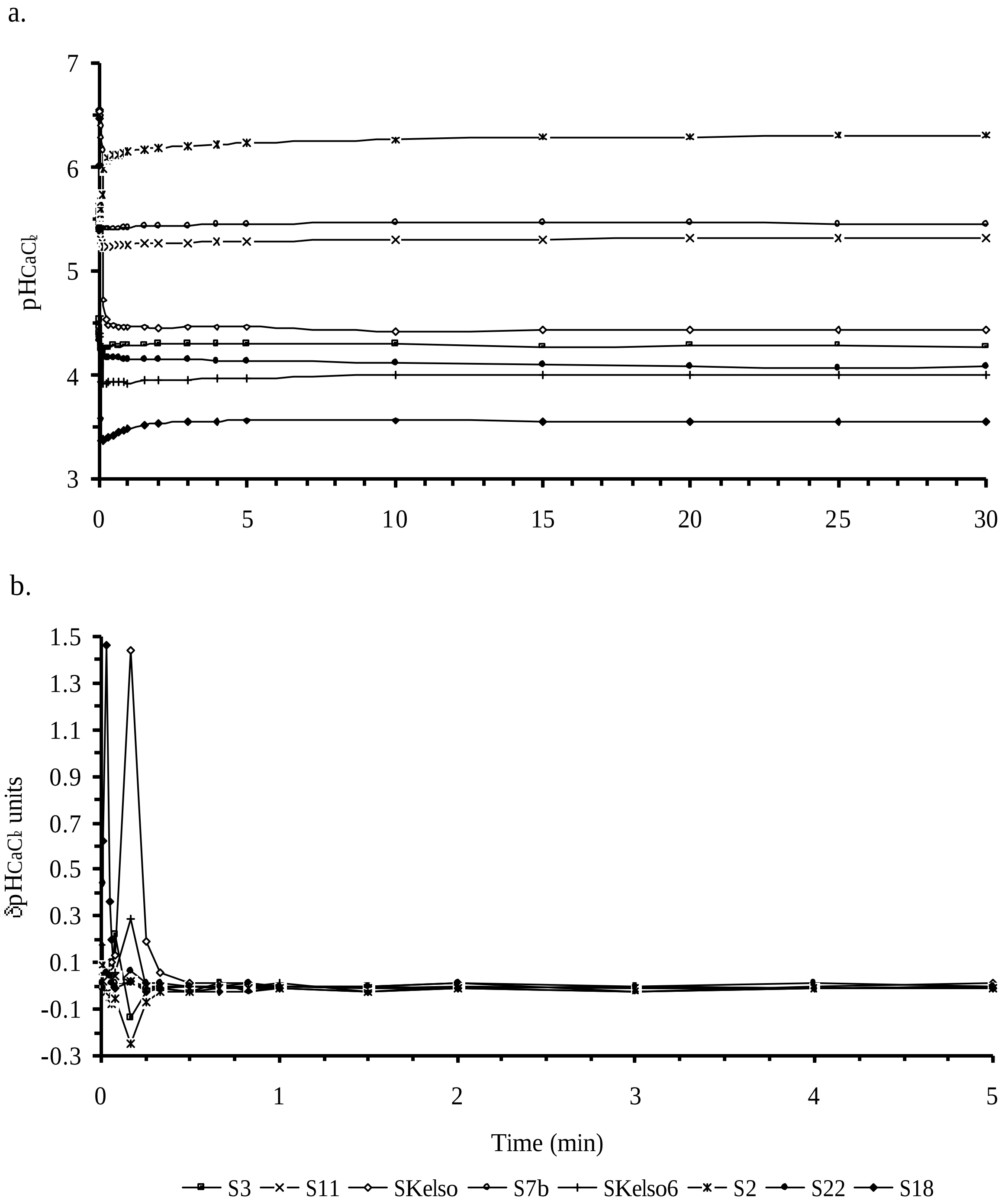

Figure 7.18 (a.) pH measurements during the soil:0.01 M $CaCl_2$ reactions at various time intervals over a 30 minute period, and (b.) changes in pH during the first five minutes of the reactions, for eight different soil types. Both (a.) and (b.) correspond to the average of two replicates.

Kinetics of Soil:Lime-Requirement Buffer (pH_{buffer})Reactions

The average soil:lime-requirement buffer reactions for each of the nine different soil types are shown in Figure 7.19a, while changes in pH_{buffer} over time (*i.e.* δ pH_{buffer}/t) are shown in Figure 7.19b.

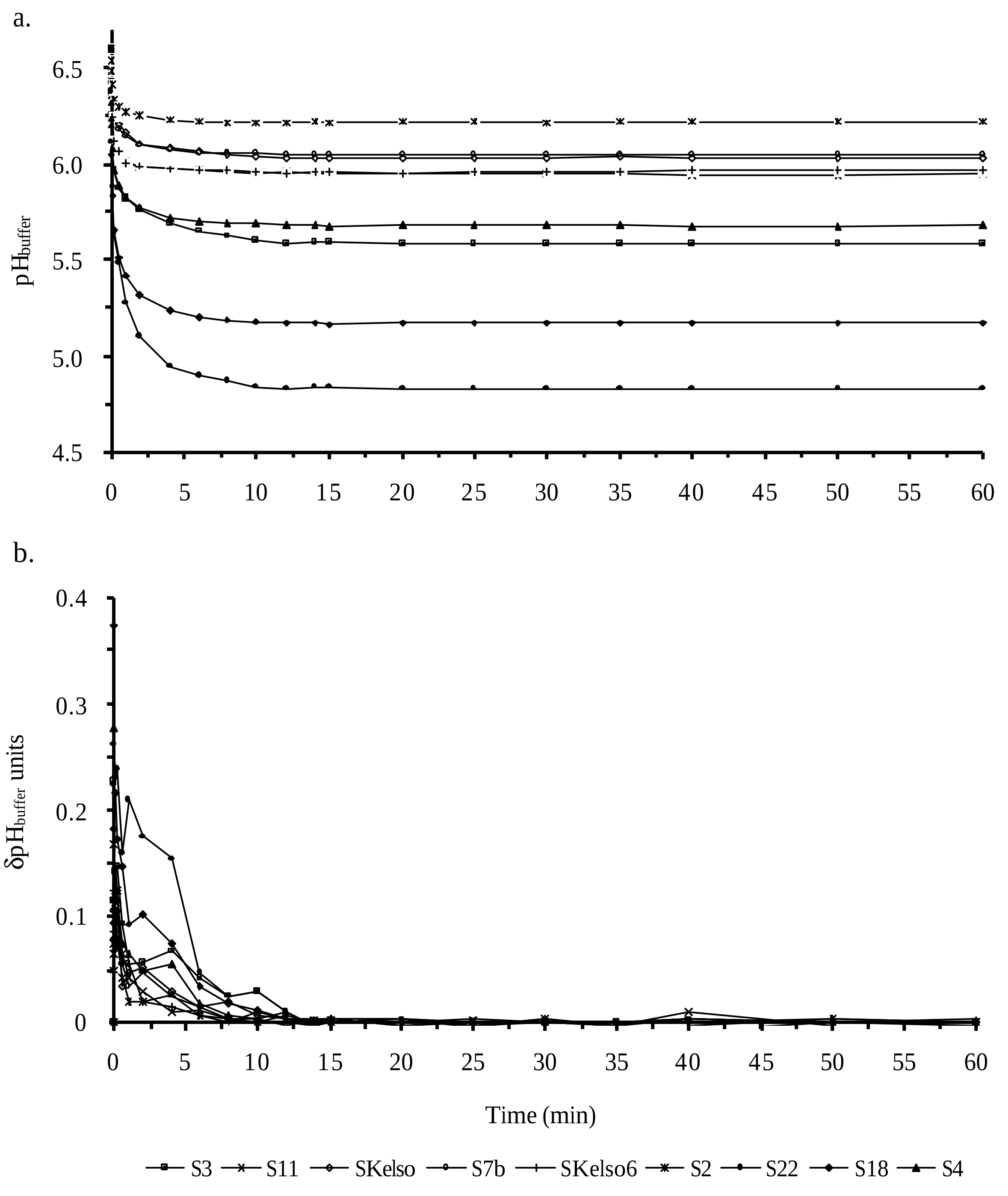

Figure 7.19 (a.) pH_{buffer} measurements during the soil:lime-requirement buffer reactions at various time intervals over a 60 minute period, and (b.) changes in pH_{buffer} during the reactions, for nine different soil types. Both (a.) and (b.) correspond to the average of four replicates.

For all nine soils, the largest changes in pH_{buffer} over time occurred during the first six minutes of reaction. At eight minutes, sample S3 displayed a change in pH_{buffer} of 0.03 units, samples S18, S22 and SKelso registered changes of 0.02 units and samples S4 and S7b changes of 0.01 pH_{buffer} units (Figure 7.19b). At ten minutes, samples S3 and S22 registered changes in pH_{buffer} of 0.03 units while samples S7b, S18 and SKelso registered changes of 0.01 pH_{buffer} units (Figure 7.19b). At 12 minutes, only soil samples S3 and S22 registered changes of 0.01 pH_{buffer} units (Figure 7.19b). A change of 0.03 pH_{buffer} units is equivalent to a change in lime requirement of approximately 0.4 Mg/ha; a change of 0.02 pH_{buffer} units is equivalent to a change of approximately 0.3 Mg/ha; and a change of 0.01 pH_{buffer} units is equivalent to a change in lime requirement of approximately 0.1 Mg/ha (refer to Chapter VII). Therefore, a reaction time of 12 minutes was deemed to encompass and apply to the range of soils used in this study.

Clearly, an equilibrium reaction time of 12 minutes is much too long for continual field pH_{buffer} measurements. However, it is shorter than the suggested 60 minute reaction time suggested for laboratory determinations of pH_{buffer} (Mehlich, 1976). The development and use of a technique for the prediction of the equilibrium pH_{buffer} using only 0.5 s, 1 s, 2 s and 3 s measurements is presented in a latter sub-section of this chapter.

Description of the Kinetics of pH_{buffer} Reaction

During the first 12 min of reaction, the pH_{buffer} reactions of all nine soils reached an asymptote (Figure 7.19a). First-order kinetic equations (similar to equation 7.7) fitted by linear regressions were used to describe the soil:lime-requirement buffer reactions. Their first-order graphs and equations are shown in Figure 7.20. Values of pHb_e were estimated from the data used in Figure 7.19b.

The plots in Figure 7.20 were fitted with two separate linear regressions, as the experimental data displayed two clear and distinct slopes. The linearity of the regressions (supported by their high R^2 values) indicated that the exchange reactions were first-order.

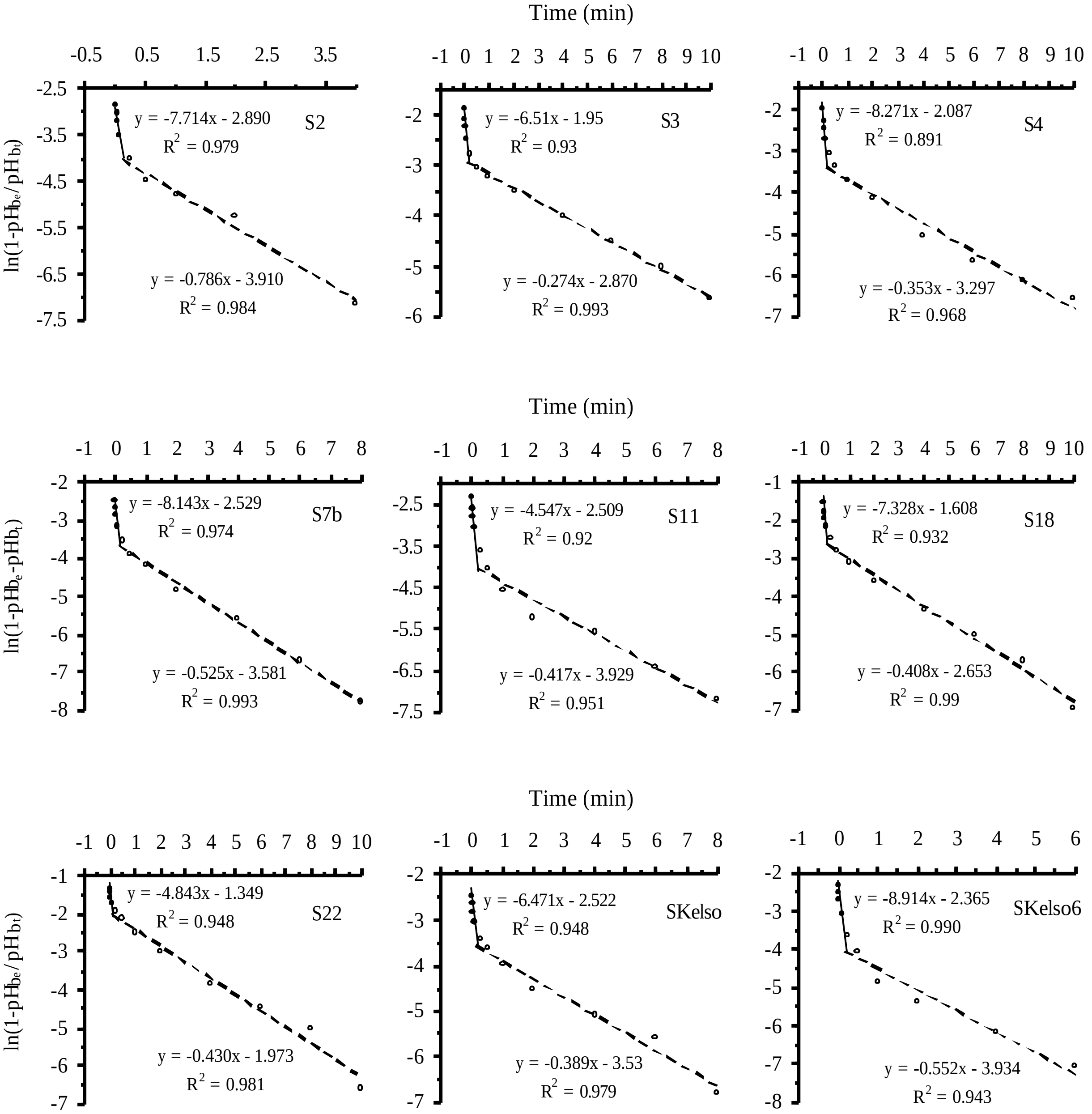

Figure 7.20 First-order biphasic kinetic plots used to $\mathrm{pH}_{\mathrm{buffer}}$ reactions of all of the soils tested. Points were averaged from four replicates.

The split of the plots at time t_i into two separate lines suggested that the soil:lime-requirement buffer reaction occurred sequentially and in two stages. It was assumed that the initial fast reaction was completed at the point of inflection t_i, where the second slower reaction commenced. Therefore, such apparent biphasic kinetics had two reaction rate coefficients, kt_{fast} and kt_{slow} (shown in Figure 7.20 and Table 7.8).

Table 7.8 Apparent rate coefficients kt_{fast} and kt_{slow} for the pH_{buffer} reactions whose first-order kinetic plots are shown in Figure 7.20

Sample	kt_{fast}	kt_{slow}	kt_{fast}/kt_{slow}
S2	7.71	0.79	9.8
S3	6.51	0.27	23.8
S4	8.27	0.35	23.4
S7b	8.14	0.53	15.5
S11	4.55	0.42	10.9
S18	7.33	0.41	18.0
S22	4.83	0.43	11.2
SKelso	6.47	0.39	16.6
Skelso6	8.91	0.55	16.1
Mean	6.97	0.46	16.16

The apparent reaction rate coefficients for the fast (kt_{fast}) and for the slower (kt_{slow}) reactions were similar in magnitude for all the soil tested (Table 7.8), *i.e.* the slopes of the linear plots in Figure 7.20 were similar. This provided further indication that the reactions were first-order under the imposed experimental conditions.

Martin & Sparks (1983) and Jardine & Sparks (1984) observed similar biphasic kinetics for desorption of potassium, and Jopony & Young (1987) for desorption of copper.

Characterisation of the pH_{buffer} Reactions using Double Exponential Models

The soil:lime-requirement buffer reactions may also be characterised using continuous double exponential expressions, similar to that shown in equation 7.8. The fitted models for each of the nine soils are shown in Figure 7.21.

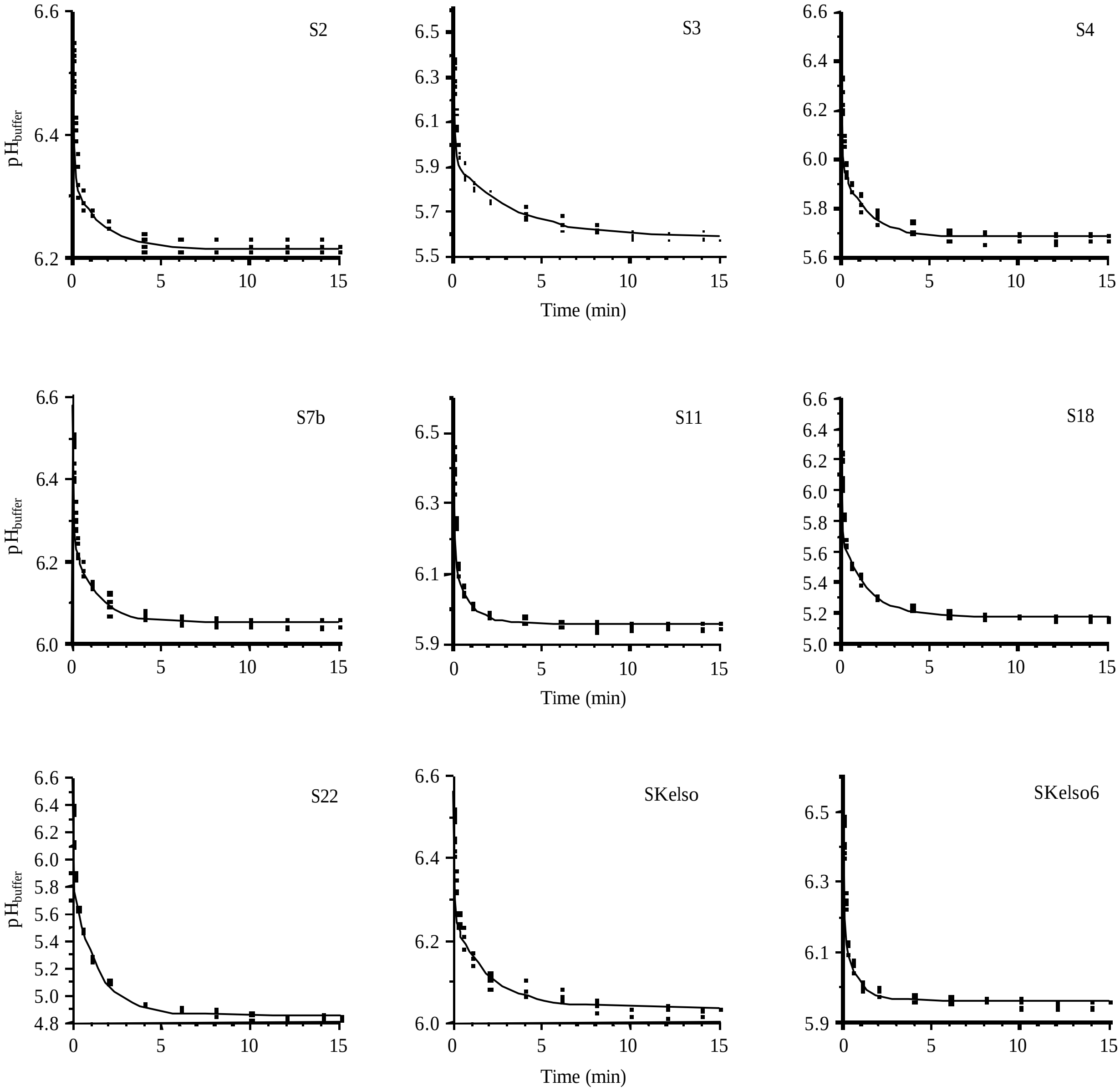

Figure 7.21 Plots of double exponential models used to describe the pH_{buffer} reactions of all of the soils tested. Four pH_{buffer} replicates for each time shown.

Figure 7.21 shows that the double exponential functions, each having two rate coefficients k_1 and k_2, were appropriate for describing the range of soils in the study. The parameters of the models and the rate coefficients for each of the nine soils are given in Table 7.8 below.

Table 7.9 Apparent exponential model parameters and rate coefficients $k_{(1)\,fast}$ and $k_{(2)\,slow}$ for the pH_{buffer} reactions shown in Figure 7.21

Sample	pH_{buffer}	a_0	a_1	$k_{(1)fast}$	a_2	$k_{(2)slow}$	$k_{(1)\,fast}$ / $k_{(2)\,slow}$
S2	6.22	6.22	0.26	12.9	0.12	0.66	19.5
S3	5.59	5.59	0.54	12.68	0.35	0.32	39.6
S4	5.68	5.68	0.43	16.42	0.3	0.69	23.8
S7b	6.05	6.05	0.32	15.75	0.2	0.71	22.2
S11	5.95	5.96	0.37	11.4	0.17	0.99	11.5
S18	5.17	5.18	0.74	17.7	0.52	0.7	25.3
S22	4.83	4.85	0.85	18.68	0.9	0.67	27.9
SKelso	6.03	6.03	0.31	13.42	0.22	0.48	28.0
SKelso6	5.95	5.96	0.43	13.93	0.19	1.17	11.9
Mean				14.76		0.71	23.3

As shown by the a_0 asymptotic parameter in Table 7.9, the exponential models accurately predicted the equilibrium pH_{buffer} of the reactions. The models also characterised the kinetic nature of the soil:lime-requirement buffer reactions as being made up of two sequentially occurring reactions with two distinct rate coefficients. First an apparently fast reaction characterised by the rate coefficient $k_{(1)fast}$ followed by an apparently slower reaction with rate coefficient $k_{(2)slow}$ (Table 7.9).

Comparison between the Kinetic Models

From the precedent, it is evident that the kinetics of soil:lime-requirement buffer reaction may be successfully characterised using different, though not necessarily incompatible, models. First, the reaction of each of the soils tested was characterised by two linear regressions depicting two separate first-order reactions, each with a single rate coefficient. Second, using a continuous double exponential function with two rate coefficients. Both models illustrated the sequential, biphasic nature of the kinetics of soil:lime-requirement buffer reactions.

On average, the two first-order models described the initial fast reaction as being 16 times faster than the slower reaction (coefficients kt_{fast}/kt_{slow}) (Table 7.8), while the exponential models parameters suggested that the fast reaction was 23 times faster than the slower one (coefficients $k_{(1)fast}/k_{(2)slow}$) (Table 7.9). The correlation of kt_{fast}/kt_{slow} to $k_{(1)fast}/k_{(2)slow}$ was $\rho = 0.56$, suggesting reasonable agreement in the relative differences between the reaction coefficients of two models.

Interpretation of the Biphasic Kinetics of pH$_{\mathbf{buffer}}$ Reactions

Before delving into an interpretation of the kinetics of pH$_{buffer}$ reactions, it will be useful to briefly recall and describe some of the principles of soil acidity and lime-requirement buffer methodology.

In very acidic soils (pH < 4) the main culprit in soil acidity is H^+. However in the majority of acid agricultural soils (pH > 4 < 7) Al^{3+} is the major acidic cation. As leaching occurs, basic cations are removed from the cation exchange complex of the soil and are replaced by Al^{3+}. The H^+ in solution, whose activity is measured by pH is in most cases derived from the hydrolysis of the monomeric exchangeable and nonexchangeable forms of aluminium, as well as from various acidic sources such as CO_2 in the air and that respired by plant roots and microorganisms. Hydrogen ions are adsorbed onto the soil's exchange complex and are hence present in the soil as exchangeable acidity. Build up of this exchangeable acidity lowers the pH of the soil and consequently mineral crystals are broken down releasing more aluminium ions. A portion of these aluminium ions add to the exchangeable acidity of the soil, while others form hydroxy-aluminium ions, which are chelated by organic matter or polymerised on cation exchange sites of the mineral surfaces (Chapter VI). In these latter forms, soil acidity is said to be non-exchangeable. Both exchangeable and non-exchangeable forms of soil acidity need the addition of base for neutralisation and hence add to the soil's lime requirement. Acidity associated with the soil's cation exchange complex is referred to as the capacity factor of soil acidity, while the fraction that exists as H^+ in solution is referred to as the intensity factor (Chapter VI). In soil, both capacity and intensity factors are in equilibrium.

Adsorption of ions occurs not only on permanent charge surfaces of the soil, but also on the pH-dependent charge of soil organic matter, clay mineral crystals (the edges of phyllosilicates), and/or pH-dependent charge of polymerised hydroxy-aluminium associated with the clay minerals (McLean, 1978). These ions dissociate from the various types of pH-dependent charges, thereby providing most of the buffering capacity of soils. Thus a soil may be viewed as a buffer system because it is a weak acid having most of the acidic cations adsorbed to, polymerised on, or chelated to the cation exchange complex. It is also a salt of a weak acid because the basic cations are also adsorbed on the exchange complex (McLean, 1978).

As previously mentioned, detection of a soil's lime requirement using the lime-requirement buffer methods involves a measure of the change in pH_{buffer} with the addition of acidity added by the soil. For most of the lime-requirement buffers this change in pH_{buffer} is directly proportional to the amount of acid added by the soil. All lime-requirement buffers are mixtures of individual buffers, which are combined to strengthen the buffering capacity in a given pH range and to extend their linearity through a wider pH range.

The Mehlich lime-requirement buffer is made up of sodium glycerophosphate ($Na_2C_3H_5(OH)_2PO_4 \cdot 5.5H_2O$); ammonium chloride ($NH_4Cl$); triethanolamine (TEA) ($C_6H_{15}NO_3$); barium chloride ($BaCl_2 \cdot H_2O$); and acetic acid ($C_2H_4O_2$) (Mehlich, 1976). Sodium glycerophosphate was used in the buffer mixture as it has a well-defined buffer range in NH_4Cl between pH 7 and 5.2. Titration of acetic acid with triethanolamine was linearly related to pH within the range 3.8 to 5.2. These mixtures were used as complements in the final Mehlich buffer. NH_4Cl served the dual purpose of reducing the pH of the unbuffered portion of the sodium glycerophosphate and in the replacement of exchangeable soil acidity. $BaCl_2$ was included to supplement the replacement of exchangeable acidity and to function as a preservative against decomposition of the buffer during prolonged storage (Mehlich, 1976).

Characterisation of the kinetics of the soil:lime-requirement buffer reactions in a buffered soil system is relatively complex and clear conclusions are difficult to draw. However, from the modelling of the kinetics of reactions (using both types of models - first-order and double exponential), and the elucidation of two distinct reaction coefficients, two types of reactions were recognised for the range of soils tested. First, reactions on external, readily accessible cation exchange sites. These occurred within the first 5 s to 15 s of the reactions for the nine different soil types (Figures 7.20). During this time, NH_4^+ and Ba^{2+} were the main cations in the buffer mixture replacing the readily accessible exchangeable soil acidity (*i.e.* exchangeable H and Al ions). These reactions were characterised by fast reaction rate coefficients (Tables 7.8 and 7.9) and rapid drops in pH_{buffer} (Figures 7.20 and 7.21). Second, reactions with the residual exchangeable soil acidity and reactions on less accessible sites, occurring immediately after the first reactions and lasting between 8 min to 12 min for the range of soils tested (Figure 7.19, 7.20 and 7.21). During this time Ba^{2+} was the main cation in the buffer mixture replacing the residual exchangeable soil acidity and that on less accessible exchange sites such as interlayer sites of clay minerals. Other reactions occurring simultaneously may have involved the buffer solution and the pH-dependent acidity of soil organic matter, clay minerals, and polymerised hydroxy-aluminium associated with the clay minerals. These reactions were characterised by slower rate coefficients (Tables 7.8 and 7.9) and hence slower, asymptotic drops in pH_{buffer} (Figures 7.20 and 7.21).

Prediction of Equilibrium pH_{buffer} Values

Previously (in sections 7.2 and 7.6.4) it was suggested that to characterise field soil pH at 10 m intervals, the sensing system operating at a ground speed of 8 km/hr, needs to measure pH every 4.5 s. A reaction time of 12 min to attain an equilibrium pH_{buffer} measurement is practically much too long for continual 'on-the-go' field operation. Therefore a technique was developed to predict the equilibrium pH_{buffer} that occurs at the maximum reaction time of 12 min (Figure 7.19b), using only the initial 0.5 s, 1 s, 2 s and 3 s pH_{buffer} measurements. The technique will now be presented and illustrated graphically using all nine soils used in the study:

1. Figure 7.22 shows the pH_{buffer} plotted against the $\log_{10}$ of the reaction times. The graphs for each of the nine soil types show a reasonably linear section of constant decreases in pH_{buffer} and a section of no pH_{buffer} change. This latter portion of the plot corresponds to the pH_{buffer} reaction equilibrium (also shown in Figure 7.19b).

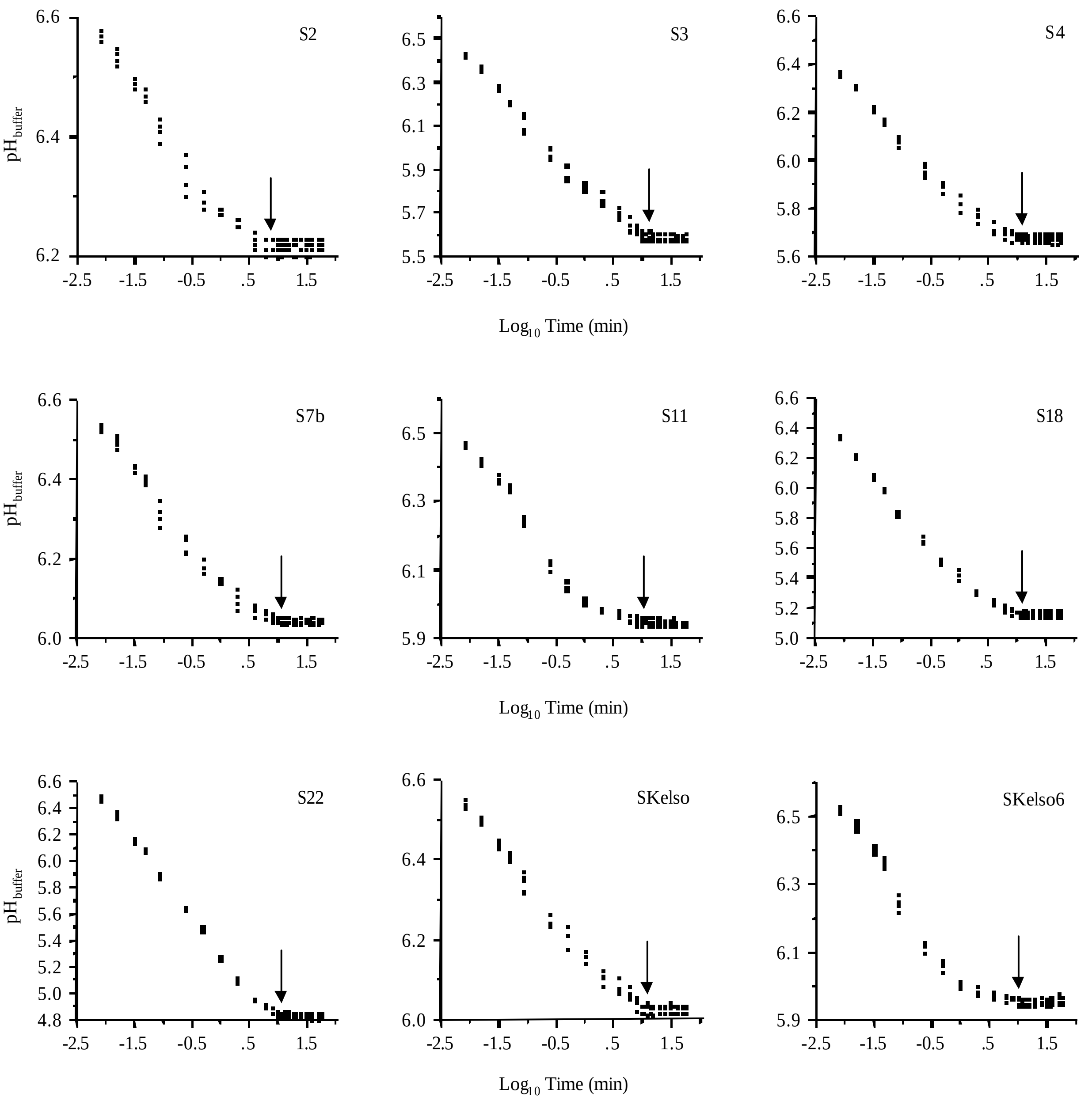

Figure 7.22 Measurements of pH$_{buffer}$ plotted against the log$_{10}$ of their corresponding reaction times. Four pH$_{buffer}$ replicates for each time shown.

The linear portions of constant decreases in pH$_{buffer}$ (on a log time scale), up to the point where equilibrium was attained in the reactions (shown by the arrows in Figure 7.22) were fitted with linear regressions (Table 7.10). Samples S11 and SKelso6 displayed slightly Gaussian shapes (Figure 7.22), however they were justly represented by linear fits ($R^2 = 0.95$) (Table 7.9).

Table 7.10 Linear regressions fitted to the linear portions of the graphs in Figure 7.22 and Respective R^2 values. Their predicted pH_{buffer} values are also shown and compared with actual, equilibrium pH_{buffer} values

Sample	Linear regression (all points)	R^2	Predicted pH_{buffer} (all points)	pH_{buffer} (equilibrium)
S2	$6.29-0.13\log_{10}Time$	0.96	6.14	6.22
S3	$5.85-0.27\log_{10}Time$	0.98	5.55	5.59
S4	$5.86-0.24\log_{10}Time$	0.98	5.60	5.68
S7b	$6.17-0.17\log_{10}Time$	0.97	5.98	6.05
S11	$6.07-0.19\log_{10}Time$	0.95	5.96	5.95
S18	$5.48-0.39\log_{10}Time$	0.98	5.06	5.17
S22	$5.33-0.55\log_{10}Time$	0.99	4.74	4.83
SKelso	$6.18-0.17\log_{10}Time$	0.98	6.00	6.03
SKelso6	$6.06-0.21\log_{10}Time$	0.95	5.83	5.95

The fitted linear regressions were reasonable predictors of the equilibrium pH_{buffer} values (Table 7.10).

2. The linearity of the plots (Figure 7.22), their well-fitted regressions and reasonably accurate predictions of pH_{buffer} equilibrium (Table 7.10) pointed to the possibility of predicting reaction equilibrium values (shown by the arrows in Figure 7.22) using only a few pH_{buffer} measurements at the beginning of the pH_{buffer} reactions. The method is illustrated using sample S22, in Figure 7.23.

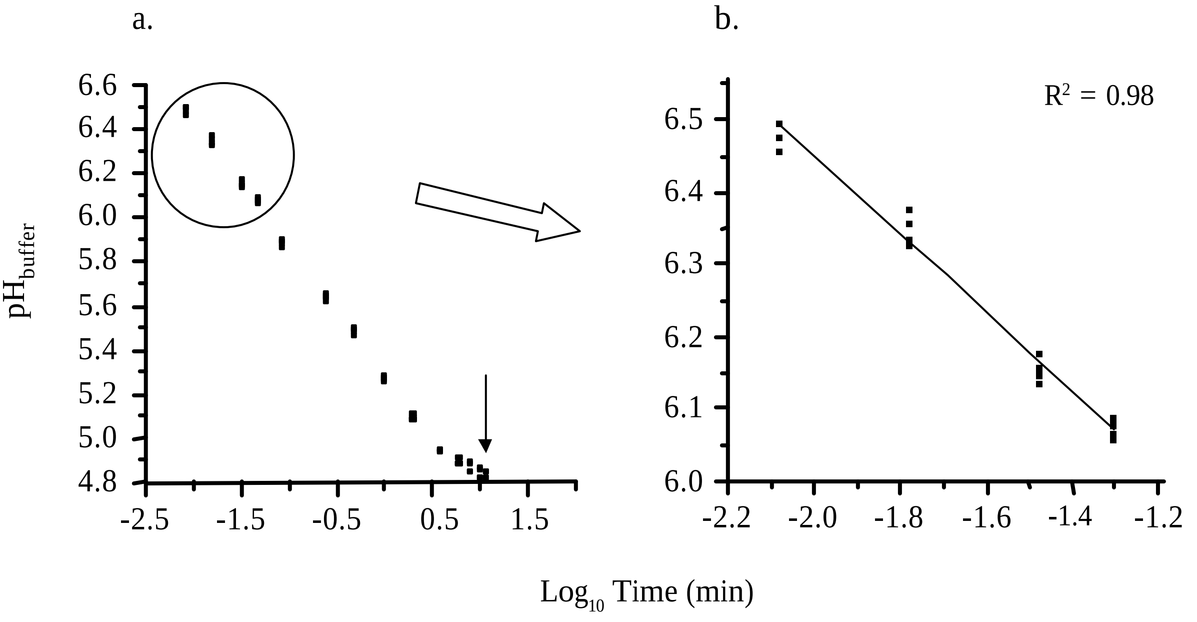

Figure 7.23 Prediction of reaction equilibrium using only initial pH_{buffer} values and according 0.5 s, 1 s, 2 s and 3 s measurements for sample S22

For sample S22, Figure 7.23a shows the plot the linear portion of constant decreases in pH_{buffer} (on a log time scale), up to the point where reaction equilibrium is attained (small black arrow). Taking the initial four pH_{buffer} measurements corresponding to the 0.5 s, 1 s, 2 s and 3 s (circled points Figure 7.23a) and fitting a linear regression to them (Figure 7.23b) allows predictions of pH_{buffer} equilibrium at the equilibrium time of 12 minutes (shown by the small black arrow on Figure 7.23a).

In an operational sensing system, it may not be possible to obtain four replicates during 'on-the-go' field operation. However it will be possible to collect data at much shorter intervals, thereby obtaining more points to which a linear regression may be fitted (*e.g.* collection of pH_{buffer} data at 100 μs intervals up to three seconds would result in a total of 30 pH_{buffer} measurements). To demonstrate the technique, the replicated data will continue to be used.

3. Therefore for each of the nine samples, the equations of the linear regression fitted to the 0.5 s, 1 s, 2 s and 3 s pH_{buffer} measurements were used to predict equilibrium pH_{buffer} values at 12 min reaction time. The predictions are shown in Table 7.11. Because of the linearity of the reacting soil-buffer systems (Figure 7.22), these regression equations were very similar to those fitted to all points (Table 7.10). Hence predictions of pH_{buffer} were also similar (compare Table 7.10 with Table 7.11).

Table 7.11 Linear regressions fitted to the first four initial pH_{buffer} points of all each of the nine soils and their R^2. Equilibrium pH_{buffer} values with corresponding lime requirements are shown and compared with predicted pH_{buffer} equilibrium values and respective lime requirements

Sample	Linear regression (four points)	R^2	Equilibrium pH_{buffer}	LR(6.5) Mg/ha	Predicted pH_{buffer}	LR(6.5) Mg/ha
S2	$6.3-0.13\log_{10}$Time	0.95	6.22	1.4	6.16	2.2
S3	$5.85-0.29\log_{10}$Time	0.97	5.59	9.8	5.54	10.4
S4	$5.84-0.26\log_{10}$Time	0.98	5.68	8.6	5.56	10.1
S7b	$6.18-0.17\log_{10}$Time	0.95	6.05	3.8	5.99	4.5
S11	$6.13-0.17\log_{10}$Time	0.97	5.95	5.0	5.95	5.0
S18	$5.41-0.45\log_{10}$Time	0.99	5.17	15.0	4.93	17.8
S22	$5.37-0.54\log_{10}$Time	0.98	4.83	19.0	4.78	19.6
SKelso	$6.19-0.17\log_{10}$Time	0.97	6.03	4.0	6.01	4.2
SKelso6	$6.1-0.21\log_{10}$Time	0.96	5.95	4.9	5.88	6.0

The RMSE for the pH_{buffer} predictions was 0.1 units, and the ME was –0.07 units. Prediction errors ranged from 0.01 to 0.24 pH_{buffer} units (Table 7.11), with an average of 0.08 pH_{buffer} units and a median value of 0.06 units. Respectively, the range in errors for lime requirements was from 0 to 2.85 Mg/ha (Table 7.11), with an average error of 0.94 Mg/ha and a median of 0.68 Mg/ha. Therefore, the technique was relatively successful for the prediction of equilibrium pH_{buffer} and hence may be useful for incorporation into the data acquisition and data handling algorithms of the sensing system.

To better illustrate the correlation between equilibrium pH_{buffer} with predicted pH_{buffer} using the previously outlined methodology, these were plotted and are shown in Figure 7.24a. Figure 7.24b illustrates the correlation between respective lime requirements.

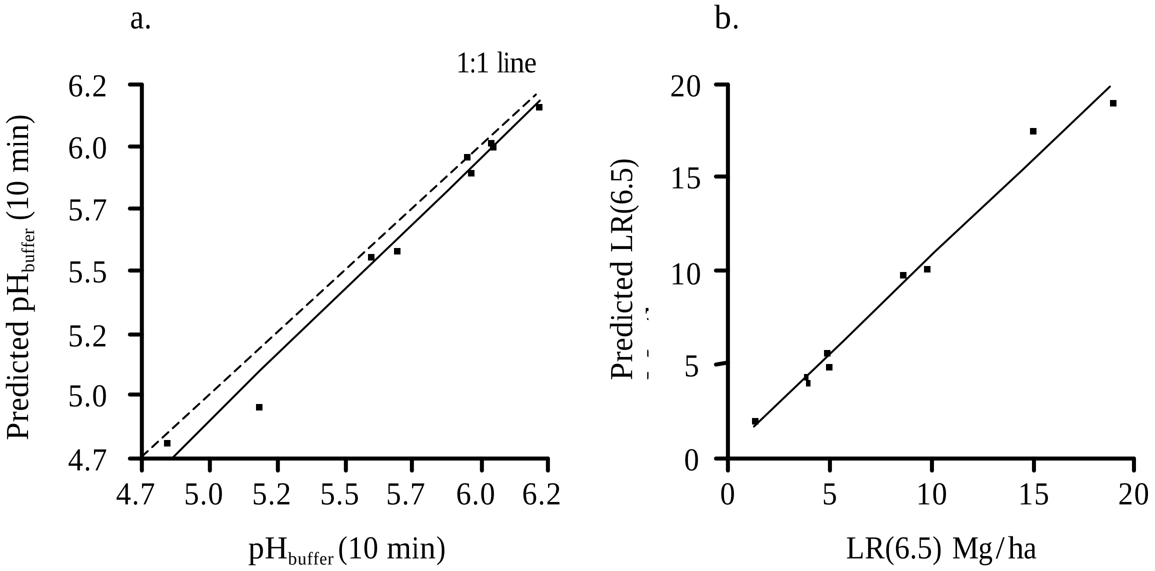

Figure 7.24 Plot of (a.) predicted equilibrium pH_{buffer} values versus actual equilibrium pH_{buffer} values and (b.) plot of respective lime requirements. $R^2 = 0.98$

On average, the prediction method tended to underestimate the reaction equilibrium of soils with lower pH_{buffer} values (*i.e.* higher lime requirements) while predictions of reaction equilibrium for soils with higher pH_{buffer} (*i.e.* lower lime requirements) tended to be less biased (Figure 7.24a and 7.24b).

7.6 FRAMEWORK FOR THE DEVELOPMENT OF THE SENSING SYSTEM

The development of the soil pH and lime requirement sensing system prototype requires research in both soil science and mechatronic engineering. Figure 7.25 illustrates the framework for research and development of the sensing system prototype that combines both disciplines. The flow chart on Figure 7.25 is recursive. At each step in the design and development process, the specifications and engineering feedback loops of the sensing system ensure that both the soil science and engineering particulars, and the design and development of the sensing system are optimised.

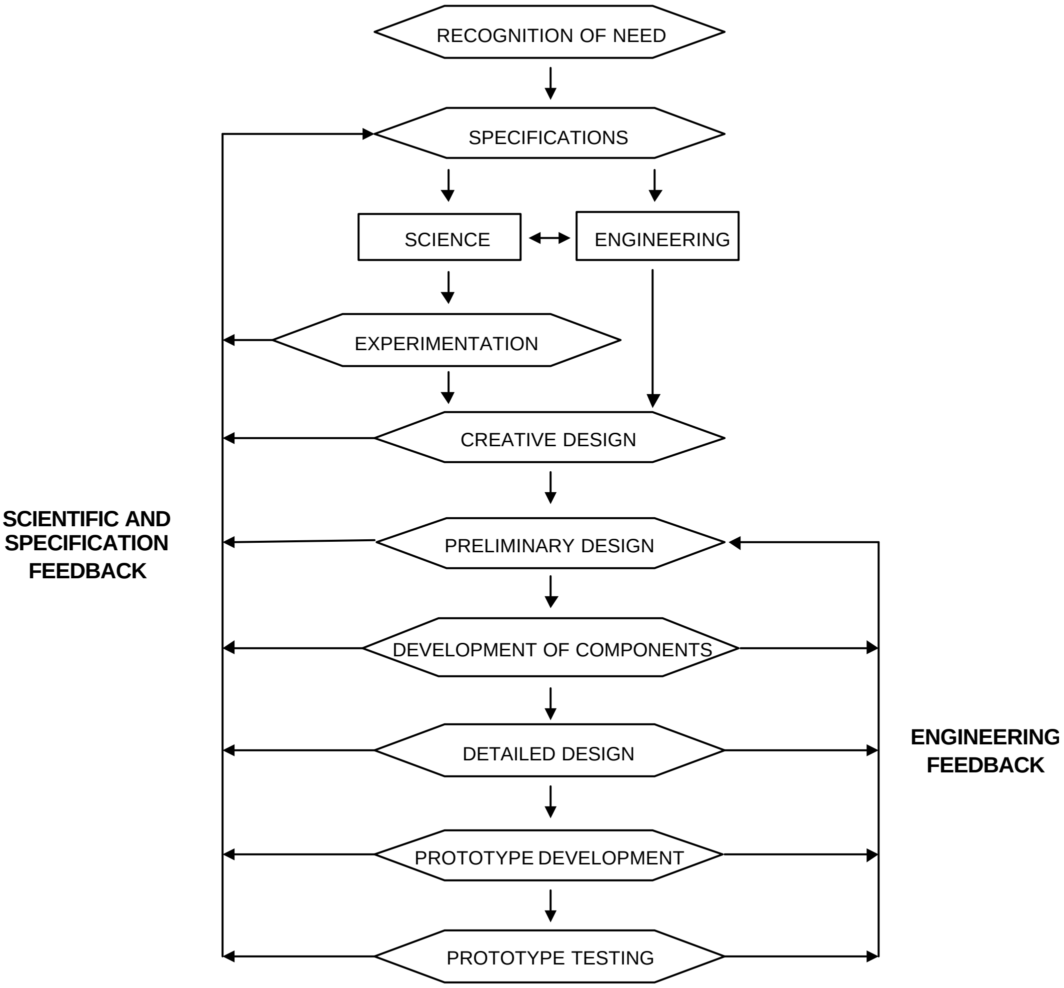

Figure 7.25 Flow chart for the optimal design and efficient development of an 'on-the-go' proximal soil pH and lime requirement sensing system prototype.

So far, this chapter has described the specifications of the system, evaluated suitable pH sensors, designed the analytical component of the sensing system, described the kinetics of soil pH_{CaCl_2} and pH_{buffer} reactions and suggested how pH_{buffer} measurements may be predicted during continual pH_{buffer} measurements. The development of a real-time spatial decision support system (SDSS) and the data processing algorithms for real-time predictions of lime requirement are also needed. Chapter VIII deals with the development suitable models for prediction of lime requirement, which may be incorporated into the real-time SDSS. All of these constitute the experimentation step in Figure 7.25. A creative design of the sensing system is illustrated in the following section, and briefly, a possible sampling mechanism and data processing system are described. Future work will involve further (engineering) specifications, design, development and testing of the prototype, as well as the development of the real-time SDSS and spatial data processing algorithms.

7.7 CREATIVE DESIGN OF THE SENSING SYSTEM

Implementation of a real-time continuous management system for acid soil (Chapter VI, section 6.4) necessitates the development of an 'on-the-go' proximal soil pH and lime requirement sensing system. A creative design for the 'on-the-go' proximal soil pH and lime requirement sensing system, and each of its components, is illustrated in Figure 7.26.

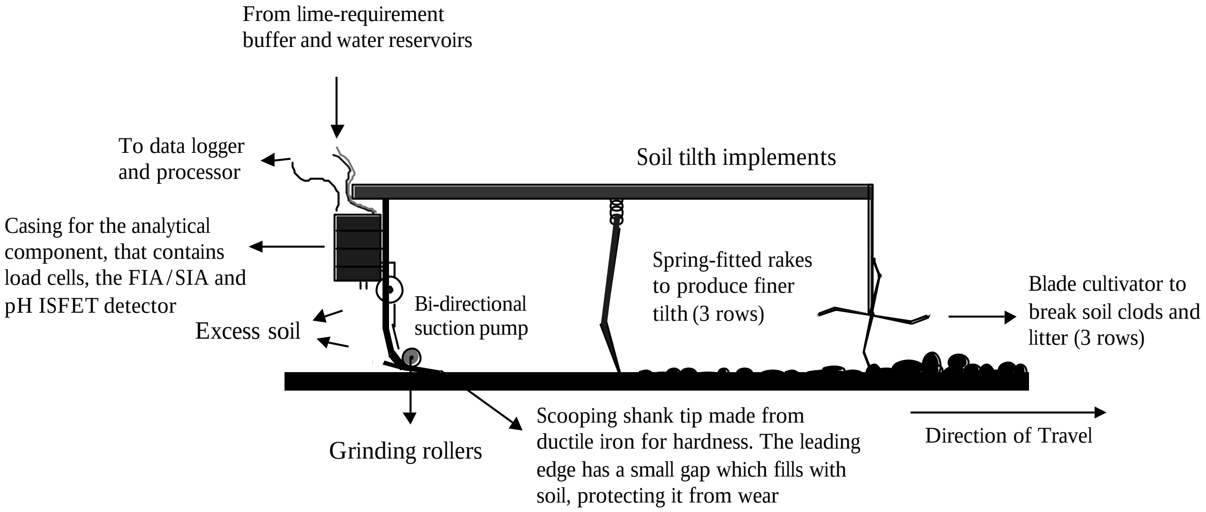

Figure 7.26 Creative design of the 'on-the-go' proximal soil pH and lime requirement sensing system showing soil tilth implements, the sampling, analytical and sensing components of the system

As the vehicle (*e.g.* see Figure 6.7, Chapter VI) traverses the field, the cultivating implements will break soil clods and produce a finer soil tilth (Figure 7.26). The grinding rollers will ensure that smaller soil particles are used for analysis (Figure 7.26). Once in the analytical component of the sensing system, the soil will be continually analysed and measured for pH as previously described (section 7.4.4). The following sections describe the possible sampling component of the sensing system (Figure 7.26), and the data processing system.

7.7.1 SAMPLING COMPONENT

The sampling component of the 'on-the-go' sensing system must be capable of continual field operation, albeit under certain environmental constraints related to field soil condition. Mostly, these constraints will be related to soil water content. As with most agricultural operations and due to these constraints, use of the sensing system will need to be timely. However a slight advantage in Australia is that most acid soils (where the sensor will be most useful) are medium to coarser textured (sandy) soils. These soils may be less problematic in terms of continual sampling with a sampling mechanism, as they are much less ‘sticky’ when moist.

The sensing system must sample field soil and transfer it into the analytical component of the sensing system (section 7.4.4) for analysis and measurement. Conceptually, the sampling component will consist of soil tilth implements to break soil clods and to displace large stones and plant material; and grinding rollers to grind the soil to a finer size so that it may be drawn onto a load cell by an air operated bi-directional suction pump (Figure 7.26). The mass of the soil used for analysis will depend on the size of the tubing manifold of the analytical system. The advantages of using such a soil-sampling pump are: the bi-directional action will alternately clear itself and the grinding rollers of remaining soil once a sample has been aspired; the sampler will not wear easily as it is not in continuous contact with the abrasive soil; it may sample only discrete amounts of soil depending on the diameter of the suction tube; and it may be relatively simple to construct. The sampled soil may subsequently be mixed with water to produce a slurry, and pumped into the analytical equipment using a peristaltic pump (section 7.4.4). Once the soil is in the analytical component and the soil mixed and filtered, an electronic signal will be sent to the sampling mechanism to take the next soil sample. This sampling mechanism will operate continually at a rate that will depend on the speed of soil analysis and pH measurement, and/or the chosen sampling interval. The sampling speed of the continual soil sampling mechanism will be one of the most important factors in the design.

7.7.2 DATA PROCESSING SYSTEM

The aim is to use the sensing system for the continuous management of acid soil (Section 6.4, Figure 6.7, Chapter VI). A possible data processing system is illustrated in Figure 7.27. The system in Figure 7.27 has no moving parts and is suitable for field operations. As the sensed data is tagged with geographical position using a GPS, the CPU (central processing unit) will mirror the GPS signal so that other sensors and equipment in the vehicle may use it. In the post-processing stage of development and for record keeping, the data will be stored in a PCMCIA card (flash card) or a laptop (Figure 7.27). Using the latter, the data may be viewed in the field during data collection. Ultimately the data is to be used in real-time to control variable-rate application equipment, *e.g.* a variable-rate lime spreader.

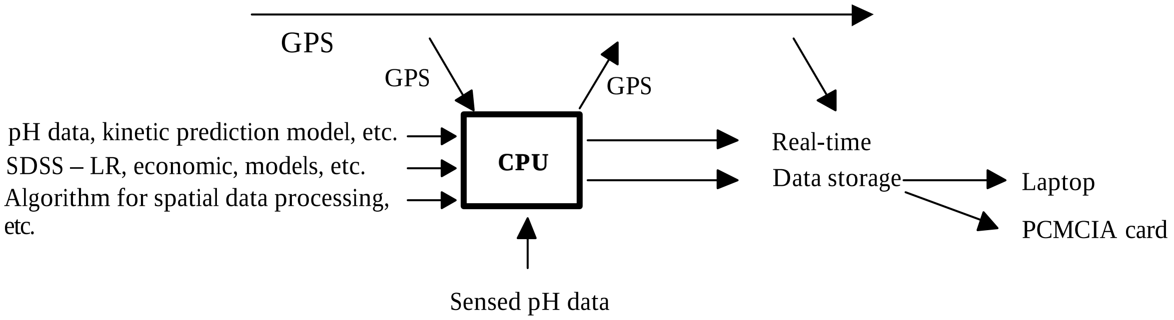

Figure 7.27 The operating system for the 'on-the-go' proximal soil pH and lime requirement sensing system showing data inputs and outputs

For real-time predictions of lime requirement, a versatile calibration model was developed (Chapter VIII). The model may be incorporated into the SDSS of the sensing system together with economic and uncertainty models (*e.g.* Chapter X), and real-time, recursive spatial data processing algorithms such as the Kalman filter (Brown & Hwang, 1992) (Figure 7.27). The Kalman filter incorporates all information it receives for estimation, *e.g.* it may process pre-sensed pH measurements to estimate current values as the system traverses the field using information from the system, its measurement dynamics, a statistical description of the system noises, measurement errors and uncertainty in the models. The filter might also use any previously acquired information about initial pH and lime requirement and other auxiliary data such as field moisture conditions, temperature, terrain attributes, etc.

7.8 CONCLUDING REMARKS

This chapter described the initial experimentation required for the development of an 'on-the-go' proximal soil pH and lime requirement sensing system to be used for the real-time continuous management of acid soil.

Results from the assessment of four potentiometric sensors showed that the pH ISFET was the most suitable sensor for inclusion into the proposed sensing system. A literature review on the state of ISFET technology was presented, accentuating the characteristics that are of interest to this research. The review showed the superior characteristics of Al_2O_3 and Ta_2O_5-gate membranes for pH ISFETs. Experimentally, pH sensitivity was determined to be 50.3 mV pH^{-1}, which is below the Nernstian value for glass electrode response of 59 mV pH^{-1}. However, Nernstian-type models do not define ISFET response. The more acceptable models are based on the site-binding theory of colloidal chemistry, suggesting that reactivity is purely due to surface reactions. Drift was 0.015 pH units hr^{-1} in standard pH buffer, and 0.03 pH units hr^{-1} in lime-requirement buffer. These results are slightly higher than those reported in the literature but they are satisfactory for the intended application in soil science and precision agriculture. A logarithmic model of drift was presented that allows drift rectification. Hysteresis was 1.7 mV or approximately 0.06 pH units. ISFET response time was measured under static, stirred and injected flow conditions. The response time was shortest when the electrolyte solution was injected onto the ISFET surface at approximately 3 ml s^{-1}. Continual injection measurements were made using standard pH buffer solutions and soil:0.01M $CaCl_2$ and soil:lime-requirement buffer extracts to determine the response time using various pH transitions. The average times of response were 0.84 s in standard pH buffer solutions, 1.2 s in soil:0.01M $CaCl_2$ and 1.6 s in soil:lime-requirement extracts. Average response time of continual injections using nine field soil:0.01M $CaCl_2$ and soil:lime-requirement buffer extracts were 1.16 s and 0.69 s respectively. The faster response times of the lime-requirement buffer extracts were due to the much shorter pH transitions between samples. The tested pH ISFET has all the desirable characteristics required for inclusion in an ‘on-the-go’ proximal soil pH and lime requirement sensing system. It is small, accurate and precise, responds rapidly to wide pH changes and may be used in an integrated sensor array containing ISFETs sensitive to various other ions important for plant growth. All of these features make ISFETs attractive for use in PA.

A literature review was presented on flow injection analysis and sequential injection analysis systems and their use in soil analytical chemistry. Using these concepts, a design for the analytical component of the sensing system was proposed. The proposed analytical system is composed of three piston pumps, one peristaltic bi-directional pump, a selector valve, mixing coils, a reactor, the pH ISFET detector and tubing manifold. Two different modes of operation were described.

Kinetic experiments that characterise the soil:0.01M $CaCl_2$ pH and soil:lime-requirement buffer pH reactions were described. Experiments were conducted using nine different soil types with widely varying properties collected from southwestern NSW. Results showed that the kinetics of soil:lime-requirement buffer reactions may be distinguished using different, though not incompatible, models. First, the reactions were characterised using two separate first-order reactions, each with a single rate coefficient. Second, using a continuous double-exponential function with two rate coefficients. Both models described the sequential, biphasic nature of the soil:lime-requirement buffer reactions. A possible explanation of the biphasic nature of the reactions was given. A statistical methodology was devised to predict equilibrium pH_{buffer} measurements at shorter time intervals than those suggested in the literature. Predictions of equilibrium pH_{buffer} using only initial soil:lime-requirement buffer reaction measurements at 0.5 s, 1 s, 2 s and 3s were made using the devised method for the nine soil samples. The accuracy of predictions was 0.1 pH_{buffer} units and the bias was low.

The framework for the development of a prototype soil pH and lime requirement sensing system was presented and a creative design that describes the components of the 'on-the-go' proximal soil pH and lime requirement sensing system proposed. The design for an 'on-the-go' soil sampling mechanism and the data processing system were described.

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SECTION IV

Chapter VIII

EMPIRICAL DETERMINISTIC RESPONSE SURFACE MODELS FOR REAL-TIME PREDICTIONS OF LIME REQUIREMENT

ABSTRACT

This chapter describes the derivation of empirical deterministic models that may be used in conjunction with the lime-requirement buffer methods for predictions of the amount of lime required to attain any target pH. The models may be used to produce variable-rate lime-requirement maps, and ultimately may be incorporated into the spatial decision-support system of the proposed real-time continuous system for the management of acid soil. As well as single-factor response surfaces, two-factor models were derived that encompass both soil pH measurements in 1:5 soil:0.01M$CaCl_2$ (pH_{CaCl_2}) and soil:lime-requirement buffer (pH_{buffer}) in their predictions of lime requirement. The predictions from both of these were compared to those obtained from buffer methods calibrated using conventional linear regressions and multivariate functions. The multivariate functions describe lime requirement as a function of a number of soil variables. All of the models were validated against soil:$CaCO_3$ incubations using a statistical jackknifing procedure for the estimation of error and bias. The Akaike Information Criterion (AIC) was used to ascertain the best models. The two-factor response surface models produced the best predictions of lime requirement followed by the single-factor models, the conventional linear regressions and finally the multivariate functions. The advantages of the response surface models are their improved prediction accuracy and their flexibility in the choice of any target pH (from pH 5.5 to 7) without the need for excessive calibrations. The most suitable buffers were the Woodruff and Mehlich buffers. The field precision of these techniques was assessed using data from the experimental site in Kelso, NSW. Spatial analysis of lime requirements, exchangeable aluminium and exchangeable calcium was conducted to show some field relationships between these properties. Finally the economic and agronomic benefits of site-specific liming were considered.

8.1 INTRODUCTION

Soil pH as a single measure is perhaps the most informative and influential property of agricultural soil (Chapter VI). By measuring how acid or alkaline a soil is information can be obtained for example, on the solubility and hence availability of various plant nutrients for uptake, the activities of microorganisms (*e.g.* pH-dependent symbiotic interactions of *Rhizobia* and host legumes), etc. Thus in agriculture, the important consideration regarding pH is the maintenance of a suitable pH range to achieve near-optimal crop growth and yield potential. As a general guideline, the optimal range for most crop species varies from pH 5.5 to 7.

Helyar (1991) reviewed conventional agronomic techniques used to manage acid soil, which included the use of tolerant plant species, careful management of carbon and nitrogen cycles, rotations, enterprise diversification and lime applications. Liming acid soil has been suggested as the best method to attain and maintain a suitable pH for the growth of a variety of crops (Coventry *et al.*, 1997; Moody *et al.*, 1993; Slattery & Coventry, 1993; Ridley & Coventry, 1992). The lime requirement of acid soil is defined as the amount of $CaCO_3$ needed to raise the pH of the top 200 mm of the profile from an initial acid state to a pre-determined higher pH for near-optimal crop growth. The higher the selected target pH, the greater the amount of lime needed to be applied. Lime requirement may also be defined as the amount of lime needed to neutralise the exchangeable acidity of the top 200 mm of soil. Using either definition, the amount of lime applied will depend on the reason for liming, the initial soil pH and the buffering capacity of the soil. The quality of the liming material used must also be considered (Merry *et al.*, 1995). Chapter VI provided a description of the reactions and processes involved.

Single-rate applications of lime over an entire management unit disregard the spatial variation of soil pH (Chapter II) and lime requirement (Linsley & Bauer, 1929; Borgelt *et al.*, 1995; Evans *et al.*, 1997; Gustafsson, 1999; Chapter III). Single-rate applications of input resources (e.g. lime, fertilisers) do not optimise crop productivity or the efficiency of resource use. Site-specific applications of input resources aim to overcome these problems (Chapters I, II, VI). Therefore, site-specific liming is the most effective and efficient technique to attain and maintain a suitable pH for crop growth. Site-specific applications of fertiliser, irrigation and more effective crop choice and rotations may also be integrated into the management of acid soil (Chapter VI).

The objectives of this chapter are to:

- Derive models for site-specific field predictions of lime requirements, using the four most commonly used lime-requirement buffers.
- Compare their predictions to those obtained from various other methodologies that are conventionally used to estimate the lime requirement of acid soil.
- Validate the models against soil:$CaCO_3$ incubations using statistical jackknifing and resolve their accuracy and precision for predicting field lime requirements.

- Select the model that best achieves a balance between goodness of fit and parsimony.
- Quantify the spatial variability of field lime requirements and related properties.

A further criterion to consider is that the model to be incorporated into the spatial decision-support-system (SDSS) of the continuous management system (Chapter VI) must be flexible and allow the choice of any target pH for 'on-the-go' and real-time predictions of lime requirement.

8.2 A BRIEF REVIEW OF THE LITERATURE ON LIMING

There are various methods that may be used to determine the lime requirement of acid soil. Most commonly, these include; soil:$Ca(OH)_2$ titrations (Dunn, 1943; Alley and Zelazny, 1987); soil:$CaCO_3$ incubations; buffer pH (pH_{buffer}) procedures (*e.g.* Woodruff, 1948; Shoemaker *et al.*, 1961; Mehlich, 1976; Brown & Cisco, 1984), multivariate functions that resolve lime requirement as a function of a number of soil variables including pH, exchangeable aluminium (Al), organic matter (OM), clay content, etc. (*e.g.* Keeney and Corey, 1963; Pionke *et al.*, 1968; Gustafsson, 1999), and measures of exchangeable aluminium (*e.g.* Aitken, 1992; Kamprath, 1970). Soil:$Ca(OH)_2$ titrations and soil:$CaCO_3$ incubations are the most accurate laboratory procedures for determining lime requirements. However they are time consuming and labour intensive, and are generally only used for validation studies and for model calibrations (*e.g.* Shoemaker *et al.*, 1961; Aitken *et al.*, 1990). The main criticism against multivariate functions is their additional requirement for predictor variables, and the extra cost and effort required for their collection and measurement. The pH_{buffer} procedures are deemed the most effective methods for rapid and accurate estimations of field lime requirements (Tran and van Lierop, 1981). Aitken *et al.* (1995) conducted a field calibration of soil lime requirement methods and also concluded that the pH_{buffer} methods were good predictors of lime requirement. Both multivariate and buffer methods are reviewed below.

8.2.1 PREDICTIONS OF LIME REQUIREMENT USING MULTIVARIATE FUNCTIONS

Field predictions of lime requirement using multivariate functions are based on resolving the soil's lime requirement as a function of one or more soil properties either through simple or multiple regressions. Keeney & Corey (1963) measured a variety of soil properties that were reported to affect the lime requirement of soil. Their findings indicated that OM was significantly correlated with lime requirement, while aluminium was not an important contributor, particularly in soils with low inherent aluminium content. Keeney & Corey (1963) suggested that where OM is routinely measured, a function relating pH and organic matter to lime requirement could be used to predict the amount of lime needed to raise acid soil pH to a desired target pH. The proposed Keeney & Corey function is:

$$\mathrm{LR} = (\mathrm{pH}_{\mathrm{target}} - \mathrm{pH}) \times \mathrm{OM} \tag{8.1}$$

where LR is the lime requirement of the soil, $\mathrm{pH}_{\mathrm{target}}$ is the desired (or target) soil pH after the application of lime, and pH is the measured soil pH of the acid soil.

Keeney & Corey (1963) compared the predictions of Equation 8.1 to those derived from $\mathrm{pH}_{\mathrm{buffer}}$ methods and concluded that the latter are more accurate in predicting field lime requirements.

Pionke *et al.* (1968) found that OM, exchangeable and non-exchangeable Al and clay content were good predictors of lime requirement and proposed a multiple regression equation for its prediction. The function they proposed has the following form:

$$\mathrm{LR} = 0.47 + 0.97(\mathrm{pH}_{\mathrm{target}} - \mathrm{pH}) \times \mathrm{OM} + 0.03(\mathrm{pH}_{\mathrm{target}} - \mathrm{pH}) \times \mathrm{CC} + 1.73\mathrm{Al}_{\mathrm{exch.}} + 0.53\mathrm{Al}_{\mathrm{non\text{-}exch.}} \tag{8.2}$$

where $\mathrm{Al}_{\mathrm{exch.}}$ refers to exchangeable Al, and $\mathrm{Al}_{\mathrm{non\text{-}exch.}}$ to non-exchangeable Al.

Pionke *et al.* (1968) reported that the $\mathrm{pH}_{\mathrm{buffer}}$ methods produced far superior predictions of lime requirement.

Gustafsson (1999) proposed two functions for the prediction of field lime requirements. The first relates pH, OM and clay content to lime requirement, while the second function uses pH, OM and HCl-soluble potassium. The reason for their derivation of the second function and the use of HCl-soluble potassium data instead of clay content is that clay content is not part of routine soil analysis in Sweden, while HCl-soluble potassium is a routinely measured soil property. The equations they proposed are:

$$\mathrm{LR} = (\mathrm{pH}_{\mathrm{target}} - \mathrm{pH}) \times (1.9 + (3.5 \times \mathrm{OM} + \text{clay content}) / 3.8) \tag{8.3}$$

or

$$\mathrm{LR} = (\mathrm{pH}_{\mathrm{target}} - \mathrm{pH}) \times (2.2 + (0.85 \times \mathrm{OM} + \mathrm{HCl\text{-}K}) / 28) \tag{8.4}$$

Where HCl-K refers to HCl-soluble potassium. Gustafsson (1999) used the latter model to calculate the site-specific lime requirement of a 30 ha field in Sweden and produced variable-rate application maps.

8.2.2 PREDICTIONS OF LIME REQUIREMENT USING BUFFER METHODS

The more rapid methods used to estimate the liming needs of acid soil are the lime-requirement buffer methods (*e.g.* Tran and van Lierop, 1981, 1982; Aitken *et al.*, 1990; Aitken *et al.*, 1995). Examples include those buffers developed by Woodruff (1948) (WRF), Shoemaker *et al.* (1961) (SMP), Adams & Evans (1962) (A&E), Yuan (1974) (Yuan-DB), Mehlich (1976) (MCH), and Brown & Cisco (1984) (NWRF). Essentially the buffer procedures determine the lime requirement of acid soil by measuring the proportional change in pH_{buffer} that is brought about by the buffer's reaction with acid soil. Woodruff (1948) and McLean (1978) provided reviews of the principles underlying lime requirement buffer preparation and practice. The methods that were used in this work are reviewed below, together with other significant research from around the world.

The Woodruff Buffer (WRF)

C.M. Woodruff developed the Woodruff buffer in 1948, prior to which lime requirements were generally estimated by soil:$Ca(OH)_2$ or soil:Ca(OAc) titrations. A number of researchers have since found the WRF buffer method to underestimate the lime requirement of acid soil *e.g.*, Shoemaker *et al.* (1961) and Fox (1980) both suggested that it underestimated the lime requirement to pH 6.8 and 7.0 respectively, by approximately 50 %. Tran & van Lierop (1981) also found that on average, the Woodruff buffer tended to underestimate the lime requirement to a target pH of 6.5. Keeney & Corey (1963) suggested that this method overestimated low lime requirement soils while underestimated high lime requirement soils. Keeney & Corey (1963) and later Tran & van Lierop (1981) indicated that a curvilinear fit for lime requirements to a target pH of 6.5 might be more appropriate than the commonly used linear fit. However, Tran & van Lierop (1982) found that a quadratic regression between soil:buffer equilibrium pH values and lime requirements to target pH 6.0 did not improve the accuracy of the relationship. However they suggested that a quadratic relationship would probably be more accurate for calculating the lime requirement of soils with either very high or very low lime requirements.

The Shoemaker, McLean and Pratt Buffer (SMP)

The SMP lime-requirement buffer was developed by Shoemaker *et al.* (1961) and has since been modified by a number of researchers. For example, McLean (1972) attempted to improve the SMP buffer by incorporating a double-buffer and quick-test feature into the method, however the procedure had little success. Tran & van Lierop (1981, 1982) suggested that an initial SMP buffer pH of 7.5 would allow estimates of lime requirement over a wider range of soils. Furthermore the authors indicated that rather than linear regressions, quadratics fitted to the SMP pH_{buffer} and incubation lime requirement data produced for more accurate predictions of lime requirement. Tran & van Lierop (1981) and Aitken *et al.* (1990, 1995) found that a curvilinear relationship increased the goodness of fit for predicting lime requirements to target pH 6.5.

The Mehlich Buffer (MCH)

Mehlich (1976) took a slightly different approach to the previous two methods when he developed the MCH lime-requirement buffer. The basis for the development of this buffer resulted from a comparative assessment of buffer methods by Mehlich *et al.* (1976). These authors found that buffer methods, although practical and acceptable as lime requirement indices, tend to be somewhat limited to the range of soils with characteristics for which they were developed. Hence the MCH pH_{buffer} was developed principally on the basis that salt exchangeable acidity, and particularly exchangeable Al^{3+} was of primary importance in the liming of soils.

Tran & van Lierop (1981) found that on average the MCH buffer underestimated the lime requirement to pH 6.5 of some light textured Canadian soils. Tran & van Lierop (1982) indicated that the MCH buffer was the most accurate method for predicting lime requirements to a target pH of 5.5, indicating that its results should be comparable to those from the SMP and WRF methods.

The New Woodruff Buffer (NWRF)

Brown & Cisco (1984) re-evaluated the use of a modified WRF buffer method. The method described by Brown & Cisco (1984) endeavoured to improve the WRF buffer by changing the composition of the buffer mixture. They called it the New Woodruff lime-requirement buffer (NWRF). Brown & Cisco (1984) compared the SMP and WRF buffers to the NWRF buffer procedure, and reported that it was a the best predictor of lime requirement when compared to $Ca(OH)_2$ titrations.

Previous Comparative Research on Lime-Requirement Buffers

A number of researchers have adapted and attempted to improve either the methods or statistical calibration regressions used for predictions of lime requirement. Some of these were mentioned above. Other examples include the work by Tran & van Lierop (1981, 1982) who evaluated and improved the calibrations of the SMP, WRF, MCH and Yuan buffers by fitting quadratic rather than linear regressions to the calibration data.

Some researchers have also conducted comparative studies to determine the best, most accurate method to use. Such studies have been conducted over the last fifty years. Table 8.1 reviews some of these and their findings. For example, Tran & van Lierop (1981, 1982) compared a number of buffers for their ability to predict the lime requirement of Canadian soils. They concluded that the SMP method was most accurate. Similarly Fox (1980) found the SMP buffer to be most accurate for agricultural soils in Pennsylvania. Alabi *et al.* (1986) compared several buffer methods on coarse-textured soils of Nebraska, finding that both the A&E and SMP buffers predicted lime requirement most accurately. Aitken *et al.* (1990) compared various methods for predicting the lime requirement of Queensland soils, concluding that the Mehlich buffer needed more attention since it, together with the SMP method produced the most accurate predictions. Aitken *et al.* (1995) conducted a field calibration of soil lime requirement methods concluding that the pH_{buffer} methods were good predictors of lime requirement. Aitken *et al.* (1995) also suggested that improvements in predictions might be obtained by combining soil pH with pH_{buffer} measurements in a multiple regression.

The above studies were made on a wide range of geographic positions from Canada, the USA and Australia, and using individual calibrations to target pH values of 5.5, 6.0, 6.5 and 6.8. It is important to realise that the regressions used for predictions of lime requirement are empirical functions that need to be calibrated locally, using soils with similar properties to the ones that are to be limed.

Table 8.1 Literature review of methodologies used to determine the lime requirement of soil.

Author	LR methods evaluated	Target pH	Best methods
Dunn (1943)	pH values, $Ca(OH)_2$ titration		$Ca(OH)_2$ titration
Peech & Bradfield (1948)	pH, $Ca(OH)_2$ and Ca(OAc) titration, exchangeable-Ca and Al		Titration most common
Woodruff (1948)	WRF buffer	6.5	WRF
Shoemaker et al.(1961)	SMP, WRF, MCH and incubation	6.8	SMP
Adams & Evans (1962)	A&E, $Ca(OH)_2$ titration	6.5	
Keeney & Corey (1963)	SMP, WRF, MF & incubation	6.5	SMP
McLean et al. (1966)	SMP, WRF, MCH, A&E, & Peech	6.5	SMP
Pionke et al. (1968)	SMP, WRF, MF & incubation	6.0	SMP
Reeve & Sumner (1970)	Exchangeable Al		Exch.-Al
Kamprath (1970)	Exchangeable Al	5.6	Exch.-Al
Yuan (1974)	Yuan-DB, $Ca(OH)_2$ titration, $BaCl_2$-TEA		Yuan-DB
Mehlich et al. (1976)	SMP, A&E, $BaCl_2$, BaCl2-TEA, Yuan-DB	Various	SMP, A&E, Yuan-DB
Mehlich (1976)	MCH		MCH
Webber et al. (1977)	Peech, Schofield, WRF, SMP & incubation	5.5 & 6.0	WRF, SMP
McLean et al. (1978)	SMP-DB & $Ca(OH)_2$ titration		SMP

Table 8.1 Continued

Author	LR methods evaluated	Target	Best methods
Fox (1980)	SMP, WRF, A&E, SMP-DB, Yuan-DB, BaCl$_2$-TEA, Ca(OH)$_2$ & incubation	7.0 (A&E 6.5)	SMP
Tran & van Lierop (1981)	WRF, SMP, A&E, MCH, Yuan-DB, SMP-DB & incubation	6.5	SMP
Tran & van Liertop (1982)	SMP, WRF, MCH, Yuan-DB, SMP-DB & incubation	5.5 & 6.0	SMP
Follet & Follet (1983)	SMP, WRF, A&E, Dunn, BaCl$_2$-TEA, MCH, MF, BS & incubtion		
Brown & Cisco (1984)	WRF, NWRF, SMP, Ca(OH)$_2$ & incubation	7.0	NWRF
Alabi et al. (1986)	WRF, A&E, Peech, SMP, SMP-DB, Yuan-DB, NWRF, Ca(OH)$_2$ & incubation	6.5	SMP, A&E
Aitken et al. (1990)	Exchangeable Al, Ca(OH)$_2$, SMP, SMP-DB, Yuan-DB, MCH & incubation	5.5 & 6.5	MCH, SMP
Bailey et al. (1991)	MF requiring soil pH and sample bulk density.	<7.9	MF
Aitken (1992)	Extractable Al using various salt solutions	5.5 & 6.5	Al$_{La}$ and Al$_{Cu}$
Aitken et al. (1995)	Exchangeable -Al, Ca(OH)$_2$, SMP, SMP-DB, Yuan-DB, MCH, MR(pH$_{H_2O}$)	5.5 & 6.5	Yuan-SB, MR(pH$_{H_2O}$)

Note: The Shoemaker, McLean & Pratt buffer (SMP), and double buffer (SMP-DB); Woodruff (WRF); Mehlich (MCH); New Woodruff (NWRF); Adams & Evans (A&E); Yuan single buffer (Yuan-SB); Yuan double buffer (Yuan-DB); Multivariate Function (MF).

8.2.3 LIME REQUIREMENT BASED ON EXCHANGEABLE ALUMINIUM

Kamprath (1970) suggested an approach to liming acid soil based on the neutralisation of exchangeable Al. He indicated that additions of lime to raise the initial acidic soil pH to pH_{CaCl_2} values in the range of 5.2 to 5.4 resulted in only slight increases in CEC, while greater amounts of lime applied to raise soil pH_{CaCl_2} well above 5.4 were more advantageous. Kamprath (1970) indicated that a reason for this may be that a proportion of the lime added reacted with other forms of soil acidity and the neutralisation of appreciable amounts of non-exchangeable acidity. Hence the author proposed the use of a liming factor of 1.5 or 2 depending on soil type.

Similarly, Reeve & Sumner (1970) used an extractable aluminium index (EAI) for liming acid soil. They suggested that response of sorghum (*Sorghum sudanese* L.) be attributed to the elimination of aluminium toxicity. Reeve & Sumner (1970) showed that maximum growth was obtained when EAI was below 2 mmol(+)/kg soil and 87 % of the EAI and 42 % of other forms of acidity where neutralised. Reeve & Sumner (1970) suggested that on average only one-sixth as much lime as that determined using the SMP buffer to a target pH of 6.5 was necessary to eliminate aluminium toxicity.

Although liming to a target pH of 5.5 may eliminate the risks of toxicity, a better practice is to lime soil according to crop requirements, which may require lime applications to target pH values greater than 5.5. The choice of a fixed chemical criterion for liming is not in accordance with the chemical nature of acid soil or the nutritional requirements and phytotoxic tolerances of different plant species. These factors needs to be considered when liming, particularly when liming rates are lowered due to financial and other constraints (van Raij, 1991).

Analytical techniques used to determine the lime requirement of soil using exchangeable Al concentrations as indicators have been criticised. Oates & Kamprath (1983) evaluated the use of various chloride salts for the extraction of aluminium and the determination of lime requirement. They concluded that aluminium extracted using $LaCl_3$ was a good indicator of the amount of lime required to neutralise exchangeable Al, while $CuCl_2$ produced better estimates when liming to a target pH of 6.0. Aitken (1992) indicated that the lime requirement to reduce exchangeable Al to a predetermined level far exceeded that calculated from the exchangeable Al (using 1 M KCl) value, even when multiplied by the liming factor suggested by Kamprath (1970). However, Aitken (1992) found that lime requirements based on the neutralisation of exchangeable Al using $LaCl_3$ was sufficient to raise pH_{H_2O} to 5.5 while $CuCl_2$ gave reasonable estimations to a target pH_{H_2O} of 6.5.

The lime requirement of soil depends on the initial soil pH, the buffering capacity (which in itself results from a combination of chemical reactions) of the soil and the reasons for liming. It is unlikely that measures of exchangeable Al alone will provide an adequate prediction of lime requirement. Obviously the standardisation of the methodologies is also important.

8.2.4 SITE-SPECIFIC PREDICTIONS OF LIME REQUIREMENT

Linsley & Bauer (1929) described the earliest variable-rate lime application map. The authors noted that "…soils, often within a single field, vary widely in their need for limestone". They suggested that systematic and detailed tests are needed so that lime may be applied according to the need for it. The researchers went on to describe a soil sampling procedure for geo-referencing (counting foot-paces in the east-west and north-south directions). After chemical determination of lime requirement Linsley & Bauer (1929) produced a variable-rate application map (Figure 8.1).

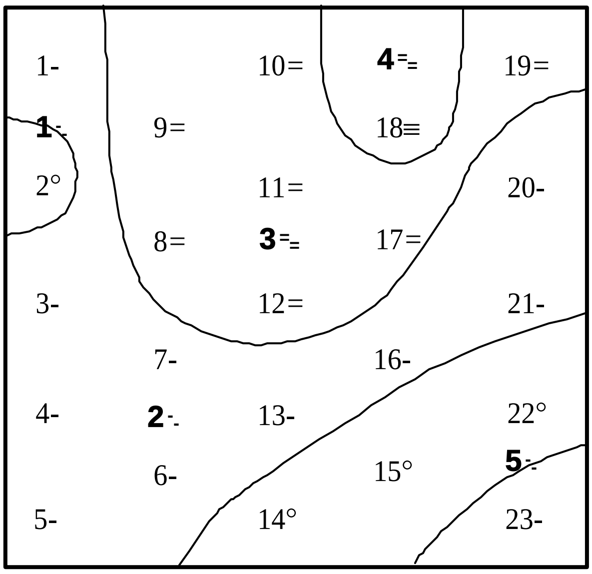

Figure 8.1 Variable-rate liming map adapted from Linsley & Bauer (1929). Numbers indicate locations of 23 surface samples. Larger bold numbers show the location of five subsurface and subsoil samples. Symbols represent the degree of soil acidity and the amount of lime to add for amelioration: ° indicates neutral or basic soil, no lime required; - slightly acidic soil, two tons of lime/acre; = medium acidity, three tons of lime/acre; ° strongly acidic soil, four tons of lime/acre. Symbols in superscript correspond to subsurface samples and symbols in subscript to subsoil samples. Boundary lines separate different areas of the map for differential liming.

Linsley & Bauer (1929) indicated that the change in acidity of the field (Figure 8.1) is gradual, hence the boundary lines where drawn so that no one line meets or touches another at any point on the map. Since this pioneering work by Linsley & Bauer (1929), the spatial variability of lime requirement has not been widely researched.

Although much attention has been given to the use buffers for lime requirement determinations in agriculture research, endorsement of their use for site-specific applications of lime is sparse. Borgelt *et al.* (1995) examined the spatial variability of soil pH and lime requirement. Lime requirements were the determined using the A&E buffer and a pH-texture index method for liming recommendations. They concluded that the method had potential for managing acid soils in East Texas.

Other than the mentioned, little research has been conducted on the field variability of lime requirements. Some examples were described in previous sections, and include Evans *et al.* (1997) and Gustafsson (1999). Even less has been conducted on the use of lime-requirement buffers for site-specific predictions of lime requirement. Obviously more attention needs to be given to the use of lime-requirement buffers and the quantification of lime requirement variability in agricultural fields.

8.3 METHODOLOGY

Twenty-two agricultural surface soils (0 – 200 mm) from the south-western wheat-belt of NSW, Australia (Figure 8.2) were collected to determine their lime requirement using a number of laboratory and statistical techniques.

8.3.1 ANALYTICAL METHODS

Relevant soil properties were measured prior to incubations and lime requirement determinations. Soil properties were analysed using procedures described in Chapter III.

Soil:$CaCO_3$ Incubations

After drying, 200 g sub-samples of each of the twenty-two soils were ground and sieved to a size fraction smaller than 2 mm. These sub-samples were incubated for twelve months with amounts of analytical grade CaCO3 (99.9 % pure) corresponding to 0, 2.5, 5, 10, 15, 20, 25, 30, 40 and 50 Mg of lime per ha. Conversions to Mg $CaCO_3$ per ha were made using an average bulk density of 1.3 $g^{-1}cm^{-3}$ and assumed incorporation to a depth of 200 mm. Soils were then wet to field capacity and the incubation period comprised of four wetting / drying cycles. On each cycle after drying, the soils were ground (< 2 mm), mixed and re-moistened to field capacity.

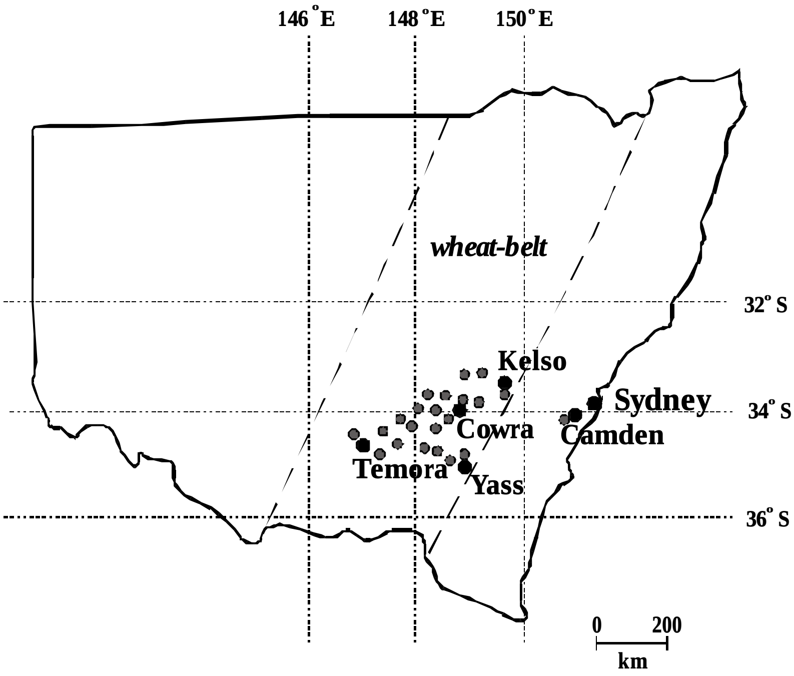

Figure 8.2 Soil sampling sites across the southwestern wheat-belt of NSW, Australia

pH_{buffer} measurements

The pH_{buffer} methods tested were the WRF, NWRF, MCH and SMP buffers. Equilibrium pH_{buffer} measurements were made using the authors' suggestions, as follows: the WRF and NWRF buffers were made up to an initial pH of 7.0 ± 0.05. pH_{buffer} determinations were made in a 1:2 soil:buffer mixture after shaking for 15 minutes. SMP buffer was made up to an initial pH of 7.5 ± 0.05. pH_{buffer} measurements were made in a 1:1:2 soil-$CaCl_2$:buffer mixture after it had been shaken for 10 minutes and allowed to stand for an additional 15 minutes. MCH buffer was made up to an initial pH of 6.6 ± 0.05. pH_{buffer} readings were obtained from a 1:1:1 soil:H_2O:buffer mixture after being shaken for 10 minutes and allowed to stand for 30 minutes.

Essentially the pH_{buffer} procedures resolve the lime requirement of acid soil by measuring the proportional change in pH_{buffer} that is brought about by the buffer's reaction with acid soil. The procedures account for the initial soil pH, the buffering capacity (BC) of the soil, the amount of base required to raise the initial soil pH to a desired level and hence neutralise the exchangeable acidity present.

8.3.2 STATISTICAL METHODS

Incubation Lime Requirements

Soil pH_{CaCl_2} was measured at the start, middle and end of the incubation period, when pH values stabilised. These stable values were used to determine each soil's titration curve (similar to the one shown in Figure 8.3), from which incubation lime requirements necessary to raise initial pH_{CaCl_2} to target pH values of 5.5 [LR(5.5)], 6.0 [LR(6.0)], 6.5 [LR(6.5)] and 7.0 [LR(7.0)] were obtained. For example, from Figure 8.3, the amount of lime needed to raise the soil pH of that particular soil to 6.5 is approximately 4 Mg $CaCO_3$/ha.

The pH buffering capacity (BC) of each of the twenty-two soils was calculated as the inverse of the linear gradient of each curve. For example in Figure 8.3 the buffering capacity of the Kelso soil sample (calculated for the linear portion between pH_{CaCl_2} 4.5 and 7) was 3.5 Mg $CaCO_3$/200 mm soil/unit pH.

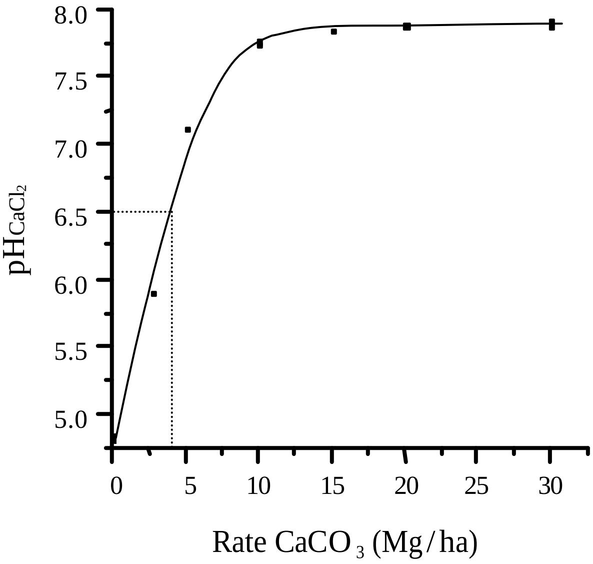

Figure 8.3 Soil buffer (titration) curve for the Kelso field sample

Multivariate Functions

In this instance, the multivariate models used to predict lime requirement were those proposed by Keeney and Corey (1963), Pionke *et al.* (1968) and Gustafsson (1999). The Keeney and Corey (1963) method resolved the soil's lime requirement as a function of the initial soil pH_{CaCl_2}, the desired target pH and the OM content of the soil (Equation 8.1). Pionke *et al.* (1968) used a regression of the initial soil pH_{CaCl_2}, the target pH, OM, clay content and the aluminium concentration, to predict lime requirements (Equation 8.2). Gustafsson (1999) suggested that site-specific lime requirements may be predicted as a function of the initial soil pH_{CaCl_2}, the target pH, OM and clay contents (Equation 8.3).

Conventional Calibrations

The WRF, SMP, MCH, and NWRF lime-requirement buffers were calibrated by fitting linear regressions to relationships between the lime requirement of soils (determined from soil:$CaCO_3$ incubations) and equilibrium pH_{buffer} values. For each buffer method four regression equations were derived to calculate the amount of lime required to attain target pH values of 5.5, 6, 6.5 and 7.

Single-Factor Response Surface Models

Response surface models of target pH and measured pH_{buffer} values (for each buffer method), were fitted to the LR(5.5), LR(6.0), LR(6.5) and LR(7.0) incubation lime requirement data. Therefore lime requirement calibration equations were constructed using parameter estimates from the fitted models. The equations were of the form:

$$\text{LR (Mg/ha)} = b_0 + b_1x + b_2y + b_3x^2 + b_4xy + b_5y^2 + e \qquad (8.5)$$

where b_n are parameters of the model; x is the equilibrated pH_{buffer}, y is the selected target pH post-liming, and $e \sim N(0, \sigma^2)$ is a normally distributed error term with zero mean and variance σ^2. When Equation 8.5 is used, the lime requirement of acid soil may be predicted with the selection of any target pH in the range from pH 5.5 to 7.

Two-Factor Response Surface Models

The two buffers with the best fitting single-factor response surface models were selected, and a two-factor response surface model was derived, to gauge whether to gauge whether pH_{CaCl_2} measurements would significantly improve lime requirement predictions from those of a single-factor model that uses pH_{buffer} measurements only (described above), without the risk of over-parametisation. The two-factor response surface models had the following form:

$$\text{LR (Mg/ha)} = b_0 + b_1x + b_2y + b_3z + b_4x^2 + b_5xy + b_5y^2 + b_6y^2 + b_7xz + b_8yz + b_9z^2 + e \qquad (8.6)$$

Where b_n are parameters of the two-factor response surface model; x is the pH_{buffer}, y is the pH_{CaCl_2} value, z is the desired target pH and ε is a normally distributed error term with zero mean and variance σ^2.

Comparison and Validation of Lime Requirement Predictions

The multivariate models, conventional buffer regressions and the response surface models were validated against lime requirements determined by the incubation experiment. The procedure employed for the quantification of prediction biases and errors was that of 'leave-one-out' jackknifing, described by Efron & Tibshirani (1993). The validation of predictions involved running each of the predictive models using (n - 1) soil samples and predicting the lime requirement of the soil removed. The leave-one-out then replace jackknife procedure was repeated until every soil's lime requirement was predicted for all four target pH values, namely 5.5, 6, 6.5 and 7. Statistics that relate the accuracy of predictions to their precision and bias were used to compare the quality of lime requirement predictions. The relationship was of the form given in Equation 4.1 of Chapter IV. Bias was quantified by the mean error (ME):

$$ME = \frac{1}{n}\sum_{j=1}^{n}\left(LR_{Predicted} - LR_{Incubation}\right) \qquad (8.7)$$

where the model-predicted lime requirement is denote $LR_{Predicted}$ and that determined from the soil:$CaCO_3$ incubation experiment by $LR_{Incubation}$.

Inaccuracy was measured by the root mean square error (RMSE):

$$RMSE = \sqrt{\frac{1}{n}\sum_{j=1}^{n}\left(LR_{Predicted} - LR_{Incubation}\right)^2} \qquad (8.8)$$

Therefore imprecision was determined from their difference (rearranging Equation 4.1, Chapter IV):

$$Imprecision = \sqrt{RMSE^2 - ME^2} \qquad (8.9)$$

The Akaike Information Criterion (AIC) (Akaike, 1973) (Equation 2.19, Chapter II) was used to determine the method that most satisfactorily compromised between goodness-of-fit and parsimony. The equation for the residual sum of squares (RSS), used to determine the AIC is given in Equation 5.17 of Chapter V.

8.3.3 SPATIAL METHODS

For the spatial analysis of lime requirement, samples were collected from the experimental field at Kelso NSW (Chapter III). Soil preparation and chemical analysis is described in Chapter III. The lime required to attain a target pH of 6.5 was predicted using the best two lime requirement models.

Uncertainty of Response Surface Models

The uncertainty of the best two response surface models was determined using field estimates of lime requirement and their upper and lower 95% confidence intervals. These confidence intervals were derived for the lime requirements to a target pH of 6.5 by:

$$95\%\ \text{CI LR}(6.5) = \text{LR buffer RS model} \pm 2\sigma_E \qquad (8.10)$$

where σ_E is the model predicted standard error. That is, the 95% confidence intervals of the lime requirement predictions to target pH 6.5 correspond to twice the standard error of the model and hence represent its uncertainty. The confidence intervals also demonstrate the spatial distribution of limits for LR(6.5).

Geostatistical Analysis of Lime Requirements, Aluminium and Calcium

Semi-variograms fitted with either exponential or double-exponential functions were used to quantify the spatial dependence of the pH_{buffer} and derived lime requirements.

Chapter II provides a review of the fundamental concepts in geostatistics. The exponential semi-variogram model is given in Equation 2.15 of Chapter II, and the double-exponential semi-variogram in Equation 4.2 of Chapter IV. Here it will suffice to review their parameters: $g(h)$ is the semi-variance at lag h, C_0 is the nugget variance, C_1 and C_2 are components of the sill variance and a_1 and a_2 are their respective effective ranges.

The corresponding variogram models were used to block krige the pH_{buffer} and respective lime requirements data onto a 2.5 m grid. Interpolations were averaged over 15 m blocks, 15 m being the spreading width of variable-rate lime spreaders. A minimum of 100 data points were used for each estimation and kriged maps of pH_{buffer} values, and respective lime requirements to target-pH 6.5 were contoured. Block kriged maps of exchangeable aluminium and exchangeable calcium were also produced for comparison. Their methods of analysis and semi-variogram data is given in Chapter III. The resulting maps served to show the spatial distribution of these properties in the field at Kelso.

Comparison between Single-Rate and Site-Specific Liming

Two scenarios, namely single-rate liming and site-specific liming, were compared to consider the possible advantages of site-specific lime applications for the amendment of soil acidity. For both scenarios, Equation 8.6 was rearranged so to derive the pH_{CaCl_2} of the field post-liming (*i.e.* the target pH) such that:

$$\text{Target } pH_{CaCl_2} = f(pH_{CaCl_2}, pH_{buffer}, LR) \qquad (8.11)$$

where $f(\cdot)$ is a response surface model of the acidic soil pH_{CaCl_2}, the pH_{buffer}, and the lime requirement (LR).

For the single-rate liming case, an average lime requirement of 7.46 Mg/ha was used in Equation (8.11). This value was the average from 17 duplicate samples corresponding to one duplicate sample per hectare. The differences between single-rate and site-specific liming were then calculated and inferences were made on the consequences of each scenario.

8.4 RESULTS AND DISCUSSION

Descriptive statistics of some relevant properties for the soils used in this study, together with their lime requirements as determined from incubations are given Table 8.2. The summary on Table 8.2 emphasises the variation in lime requirements and related soil properties over the sampled area (Figure 8.2), indicating that the soils used were suitable for the research. They also highlight the need for an accurate and precise predictive analytical test for lime requirement to replace the more common predictions based on either farmer knowledge or intuition, or pH tests alone. Chapters IV suggested that the evolution of PA into a real-time continuous management system requires the development of analytical techniques that are rapid, less labour-intensive, and no less accurate and precise than current methods. Incubation lime requirements to target pH values of 5.5, 6.0, 6.5 and 7.0 were selected for comparative purposes and to provide flexibility in the selection of target pH values deemed optimal for plant growth.

Table 8.2 Soil property statistics for soils used in incubation, *n* = 22

Soil property	Mean	S.D.	Median	Range	CV
pH_{CaCl_2}	4.60	0.80	4.65	3.60 – 6.20	17.3
pH_{H_20}	5.48	0.66	5.35	4.70 – 7.20	12.1
SMP pH_{buffer}	6.28	0.48	6.47	5.02 – 6.81	7.6
MCH pH_{buffer}	5.79	0.41	5.95	4.84 – 6.29	7.1
WRF pH_{buffer}	6.59	0.26	6.71	5.98 – 6.88	4.0
NWRF pH_{buffer}	6.76	0.24	6.86	6.14 – 7.01	3.7
OC dag/kg	1.23	0.54	1.28	0.40 – 2.40	44.0
Clay content dag/kg	25.0	11.8	19.8	14.0 – 49.2	47.2
CEC mmol(+)/kg	63.4	56.3	42.6	13.0 – 203.4	88.9
Al mmol(+)/kg	6.6	12.0	0.80	0.01 – 53.6	182.9
Ca mmol(+)/kg	30.0	26.6	23.5	2.0 – 106.0	88.5
BC Mg $CaCO_3$/200 mm soil/unit pH	4.16	1.78	3.69	1.81 – 8.84	42.8
Incubation LR(5.5) Mg/ha	3.7	4.0	2.6	0 – 12.6	108.4
Incubation LR(6.0) Mg/ha	5.1	4.7	3.6	0 – 15.3	92.2
Incubation LR(6.5) Mg/ha	7.0	5.4	5.0	0 – 18.7	77.4
Incubation LR(7.0) Mg/ha	9.7	6.2	7.1	2.2 – 23.7	64.5

Note: pH measured in 1:5 soil:0.01M $CaCl_2$, ($pHCaCl_2$) and in 1:5 soil:H_2O (pHH_2O); Shoemaker, McLean & Pratt buffer (SMP), Woodruff buffer (WRF); Mehlich buffer (MCH); New Woodruff buffer (NWRF); organic carbon (OC); cation exchange capacity (CEC); exchangeable aluminium (Al); exchangeable calcium (Ca); buffering capacity (BC); lime requirements to a target pH (LR(target pH))

8.4.1 PROPERTIES AND LIME REQUIREMENTS OF INCUBATED SOILS

Soil pH_{CaCl_2} or pH_{H_2O} are poor predictors of a soil's lime requirement. A number of researchers have also inferred similar findings, *e.g.* Keeney & Corey (1963); Ross *et al.* (1964); Pionke *et al.* (1968); Aitken *et al.* (1990); Aitken *et al.* (1995). These findings are not peculiar, and although pH is used as an indicator of whether or not a soil should be limed, measurements of soil pH and lime requirement are dependent on some different soil properties. Soil pH measures the hydrogen ion activity in soil while lime requirement depends on, amongst other properties, soil pH, the BC of the soil, the reason for liming and the amount of exchangeable acidity in the soil solution. Figures 8.4a and 8.4b show the regressions between pH and incubation determined lime requirements to pH 6.5.

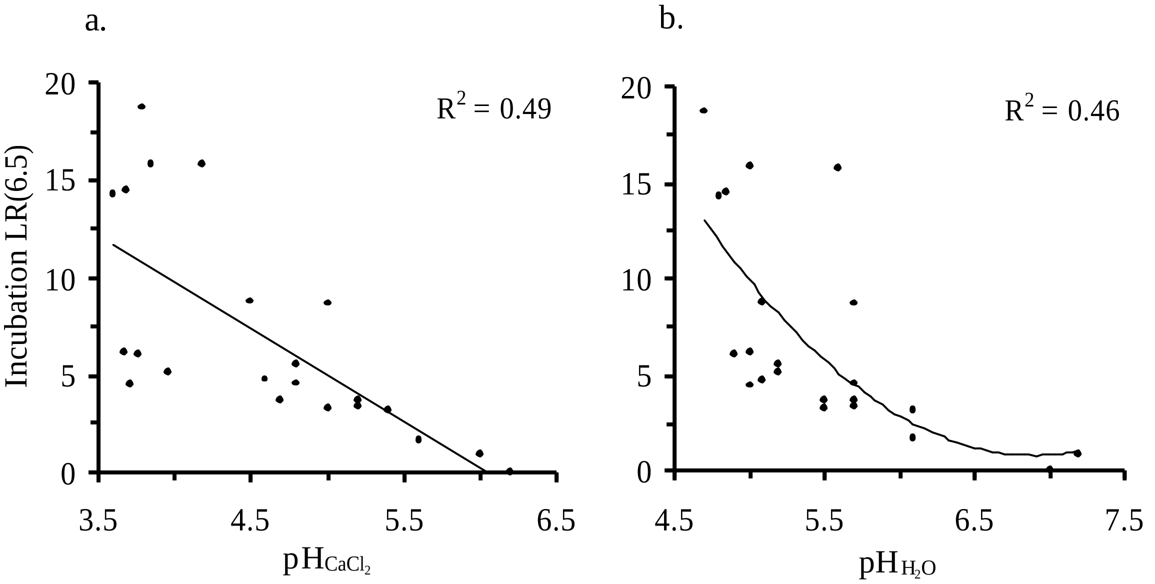

Figure 8.4 Relationships between (a.) soil pH_{CaCl_2}, (b.) pH_{H_2O} and lime requirement to a target pH of 6.5

Soil pH_{CaCl_2} accounted for 49 % of the variation in lime requirement while pH_{H_2O} accounted for 46 % (Figure 8.4a and b, respectively). Hence soil pH alone is not a good predictor of lime requirement. Figure 8.5 shows relationships between exchangeable calcium, exchangeable aluminium, BC and lime requirements to target pH 6.5.

Exchangeable calcium accounted for 31 % of the variation in lime requirements (Figure 8.5a) and exchangeable aluminium for 53 % of the variation in lime requirements (Figure 8.5b). From Figure 8.5, at high lime requirements the concentration of aluminium in the soil solution is high while the concentration of calcium is low. Conversely when lime requirements are low, calcium levels are high and the aluminium concentration in soil is low. The antithetic influence of increasing concentrations of aluminium on calcium levels in the soil is demonstrated and discussed in Chapter IX. Figure 8.5c illustrates the non-linear relationship between the BC of the soils used in the incubation experiment and their respective lime requirements. The graph shows that poorly buffered soils required smaller amounts of lime for the amelioration of acidity than soils with higher BCs. Figure 8.6 shows the titration curves of six of the twenty-two soils used in the incubations and their buffering capacities.

Soil sample S2 (Figure 8.6b) was the most highly buffered soil *i.e.*, large additions of base cause only small increases in pH, while sample S6 (Figure 8.6d) had the lowest BC *i.e.* small additions of lime caused large changes in pH. Generally the soils in this study were more highly buffered at pH values greater than 7 than in the mid-range between pH 4.5 to 7. Magddoff & Bartlet (1985) reported similar findings *i.e.*, that soils have a higher BC at low (<4) and high (>7) pH values than in the mid-range. At pH values greater than 7.5 high lime application rates caused either small or no changes in pH (Figure 8.6), implying that the incubation period allowed adequate time for the dissolution of lime in the soil.

Table 8.3 shows some of the linear correlations between the soil properties used in the experiments.

Table 8.3 Correlation matrix for incubation lime requirements and soil properties: incubation lime requirements (LR_{INC}), pH_{CaCl_2}, organic carbon (OC), clay content (CC), cation exchange capacity (CEC); exchangeable calcium (Ca), exchangeable aluminium (Al) and buffering capacity (BC). *n* = 22

Variable	LR_{INC}	pH_{CaCl_2}	OC	CC	CEC	Ca	Al	BC
LR_{INC}	1							
pH_{CaCl_2}	-0.63	1						
OC	0.31	0.09	1					
CC	-0.23	0.7	0.05	1				
CEC	-0.11	0.61	0.26	0.82	1			
Ca	-0.47	0.88	0.29	0.73	0.79	1		
Al	0.68	-0.46	-0.09	-0.35	0.12	-0.4	1	
BC	0.39	0.12	0.53	0.51	0.56	0.45	0.36	1

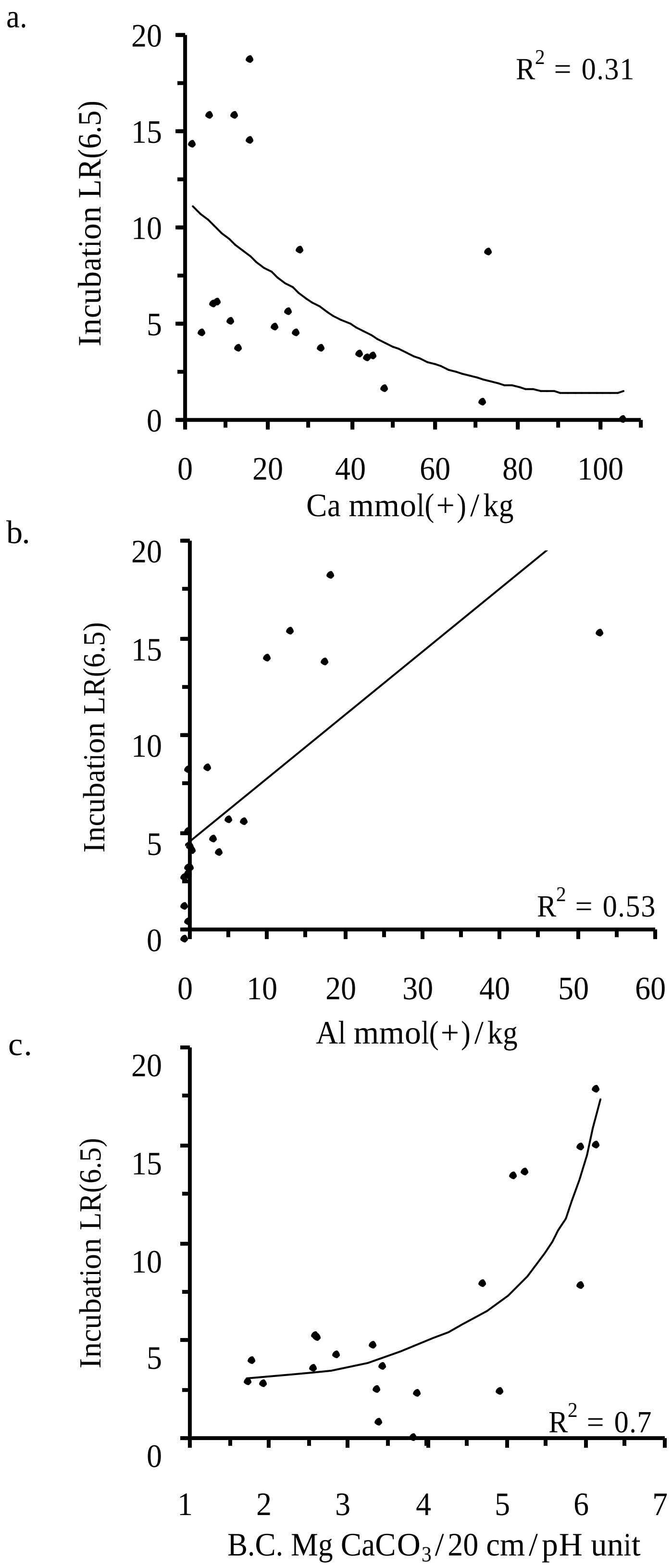

Figure 8.5 Relationships between (a.) exchangeable calcium, (b.) exchangeable aluminium and (c.) buffering capacity and lime requirement to a target pH of 6.5

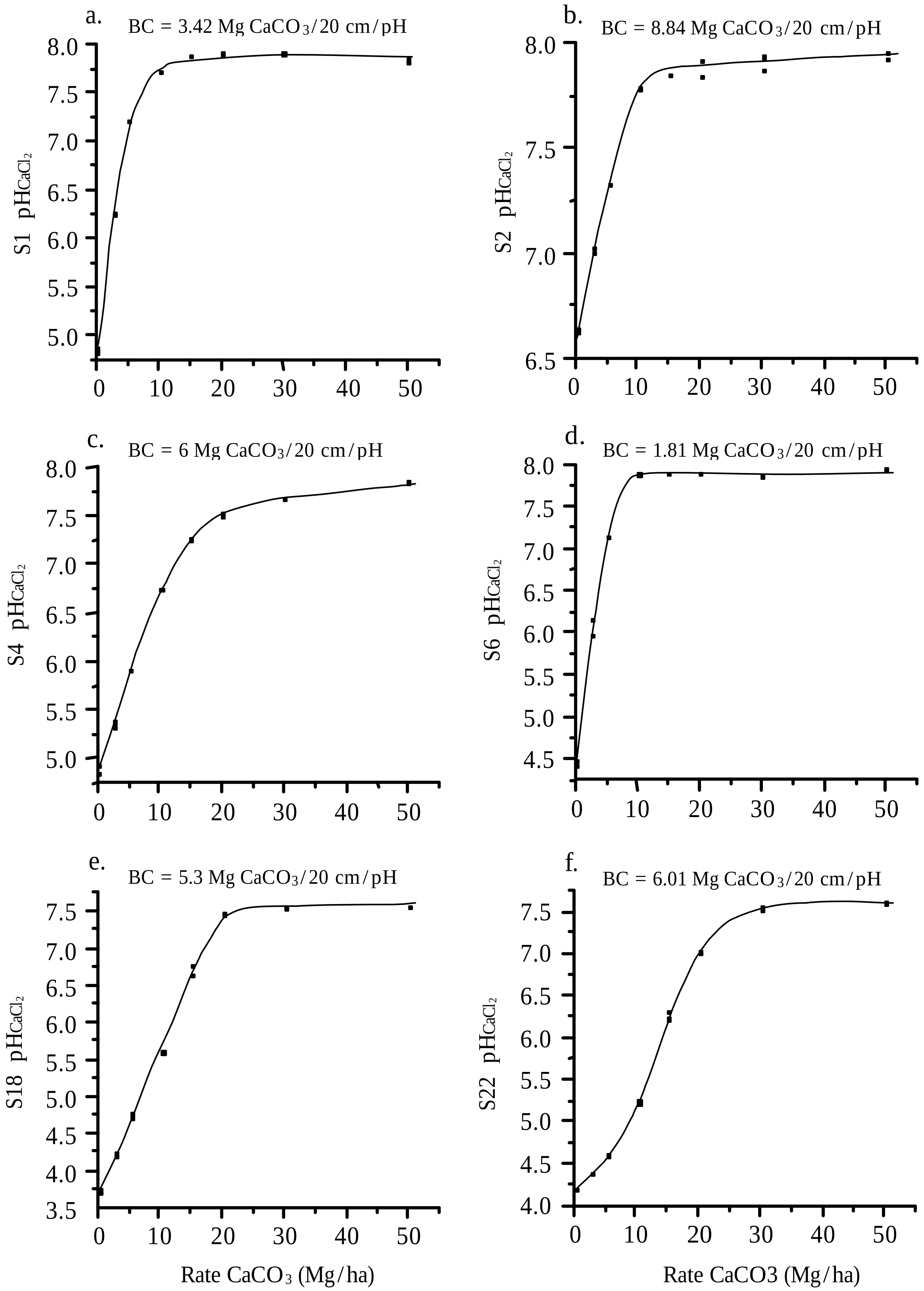

Figure 8.6 Soil titration curves showing the range in buffering capacities of the soils used in the incubation experiment

Lime requirement is well correlated to soil pH_{CaCl_2}, exchangeable calcium and exchangeable aluminium (Table 8.3). The linear relationship between lime requirement and soil BC was relatively low, however as previously described their relationship is non-linear (Figure 8.5c). Similar to the findings by Aitken *et al* (1990) for a number of acidic Queensland soils, BC was well correlated with organic carbon, clay content and cation exchange capacity. However Table 8.3 confirms that none of these relationships is strong enough to justify estimations of lime requirement based on only these properties.

8.4.2 CONVENTIONAL REGRESSION EQUATIONS

The SMP, WRF, NWRF and MCH buffers with given linear or quadratic regressions are commonly used to predict lime requirement to target pH values of 5.5, 6 and 6.5 (refer to Table 8.1). In this instance linear regressions fitted all of the data more aptly than quadratics. Table 8.4 shows the equations required to realise target pH values of 5.5, 6 and 7 for each of the buffers tested.

Table 8.4 Lime requirement regressions to attain target pH values of 5.5, 6 and 7

Target pH	Equation	R^2
WRF LR(5.5)	$102.4 - (14.9 \times \text{buffer-pH}_{WRF})$	0.95
WRF LR(6.0)	$120.4 - (17.5 \times \text{buffer-pH}_{WRF})$	0.96
WRF LR(7.0)	$161.7 - (23 \times \text{buffer-pH}_{WRF})$	0.94
SMP LR(5.5)	$52.1 - (7.7 \times \text{buffer-pH}_{SMP})$	0.85
SMP LR(6.0)	$62.6 - (9.2 \times \text{buffer-pH}_{SMP})$	0.88
SMP LR(7.0)	$86.3 - (12.2 \times \text{buffer-pH}_{SMP})$	0.88
MCH LR(5.5)	$58.2 - (9.4 \times \text{buffer-pH}_{MCH})$	0.93
MCH LR(6.0)	$69.4 - (11.1 \times \text{buffer-pH}_{MCH})$	0.95
MCH LR(7.0)	$94.1 - (14.6 \times \text{buffer-pH}_{MCH})$	0.94
NWRF LR(5.5)	$109.6 - (15.7 \times \text{buffer-pH}_{NWRF})$	0.93
NWRF LR(6.0)	$128.6 - (18.3 \times \text{buffer-pH}_{NWRF})$	0.93
NWRF LR(7.0)	$174.5 - (24.4 \times \text{buffer-pH}_{NWRF})$	0.94

Figure 8.7 shows the regressions for each of the four buffer methods, to attain a target soil pH of 6.5.

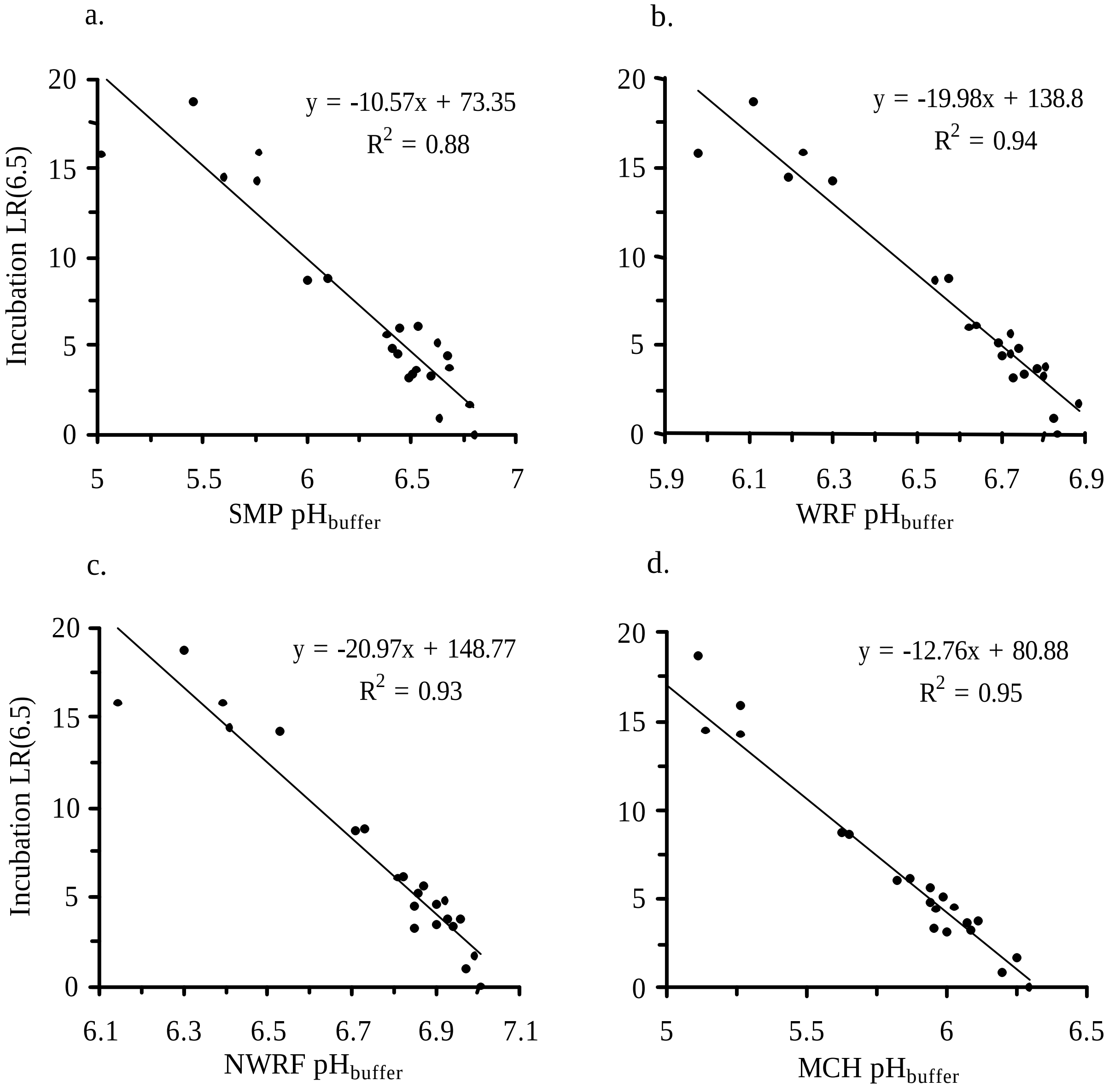

Figure 8.7 Relationships between soil pH_{buffer} and lime requirements, to attain a soil pH_{CaCl_2} of 6.5 for (a.) the Shoemaker, McLean & Pratt (SMP) buffer; (b.) the Woodruff (WRF) buffer; c. the New Woodruff buffer (NWRF); and d. the Mehlich (MCH) lime-requirement buffers.

Generally the WRF buffer regressions produced higher coefficients of determination than the other methods used, although the MCH and NWRF buffer methods had comparable results (Table 8.4). The MCH buffer regression produced the highest R^2 for lime requirements to a target pH of 6.5 (Figure 8.7d). These linear regressions (Table 8.4

and Figure 8.7) can only be used to derive lime requirements to their corresponding predefined target pH. For example using any of the regression in Figure 8.7 only permit predictions of lime requirement to a target pH of 6.5, and will need derivations of other independent regression for liming predictions to target pH values of 5.5, 6 and 7 (given in Table 8.4).

8.4.3 SINGLE-FACTOR (PH$_{BUFFER}$) RESPONSE SURFACE MODELS

The statistical calibration of the lime-requirement buffers was modified using response surface regressions rather than single linear or quadratic regression for each target-pH value. The purpose of the modification was to add versatility and flexibility to the selection of target pH values without the need for excessive calibration curves, while maintaining or improving the precision of lime requirement predictions. One such model may be more suitable than those described in the preceding section, as a component of the SDSS for the real-time continuous management of acid soil (Chapter VI). The SDSS would use pH$_{buffer}$ (and pH$_{CaCl_2}$) data collected by the soil pH and lime requirement sensing system (Chapter VII), for predictions of the amount of lime needed to raise to pH of field soil to site-specific target pH values. The form of the deterministic response-surface models is given by Equation 8.5. The derived response-surfaces and corresponding whole model fits for each of the buffers used are shown in Figures 8.8 to 8.11 below.

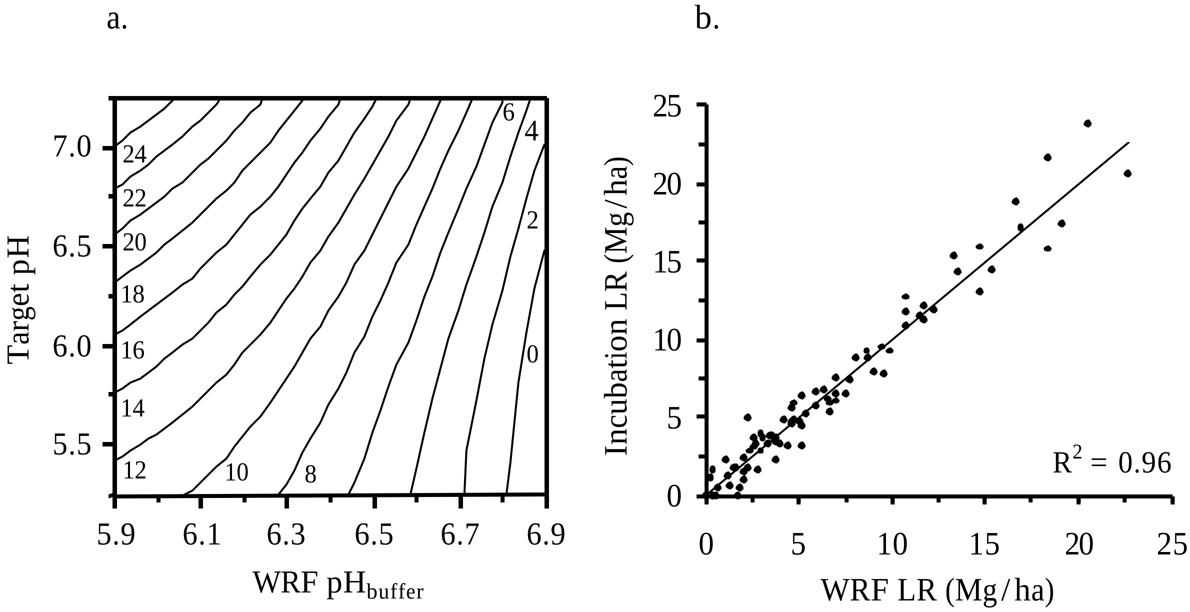

Figure 8.8 (a.) The Woodruff (WRF) buffer single-factor response surface. Lime Requirements (LR) in Mg/ha, and (b.) WRF model fit

The fitted WRF buffer single-factor response surface model is shown in Figure 8.8a, and the whole model fit is shown in Figure 8.8b. The fitted line has unit gradient and a R^2 value of 0.96, depicting a good fit. Figure 8.9a shows the response-surface model fitted to the SMP data.

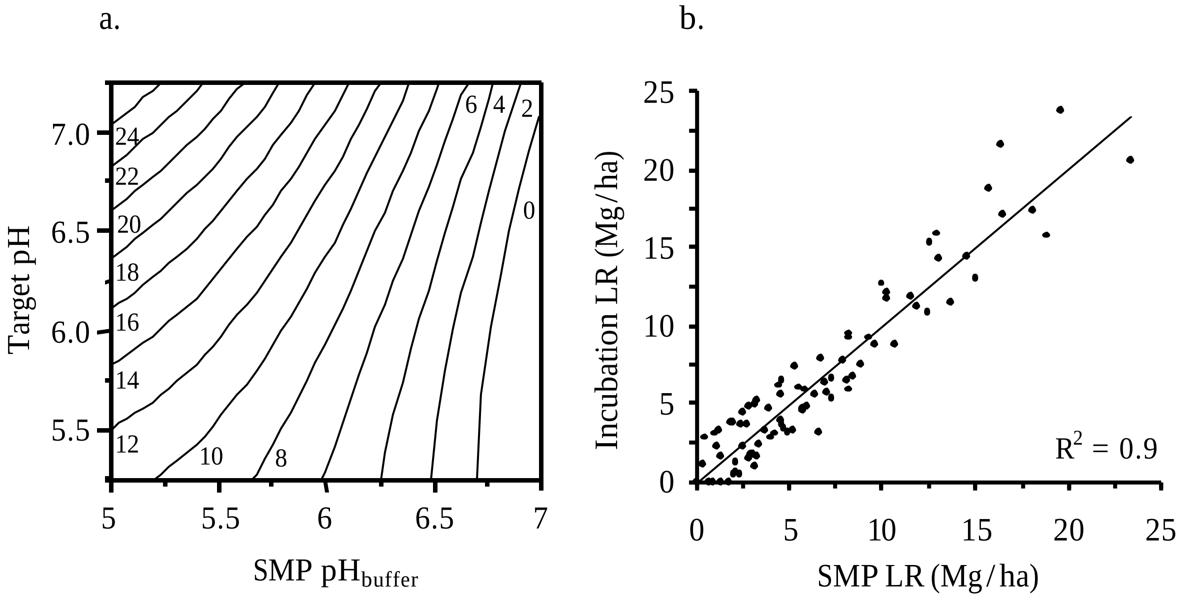

Figure 8.9 (a.) The Shoemaker, McLean & Pratt (SMP) buffer single-factor response surface. Lime requirements (LR) in Mg/ha, and (b.) SMP model fit

The comparison between the lime requirements predicted using the SMP response surface (Figure 8.9a.) and the reference incubation lime requirements is shown in Figure 8.9b. The NWRF response surface is given in Figure 8.10a.

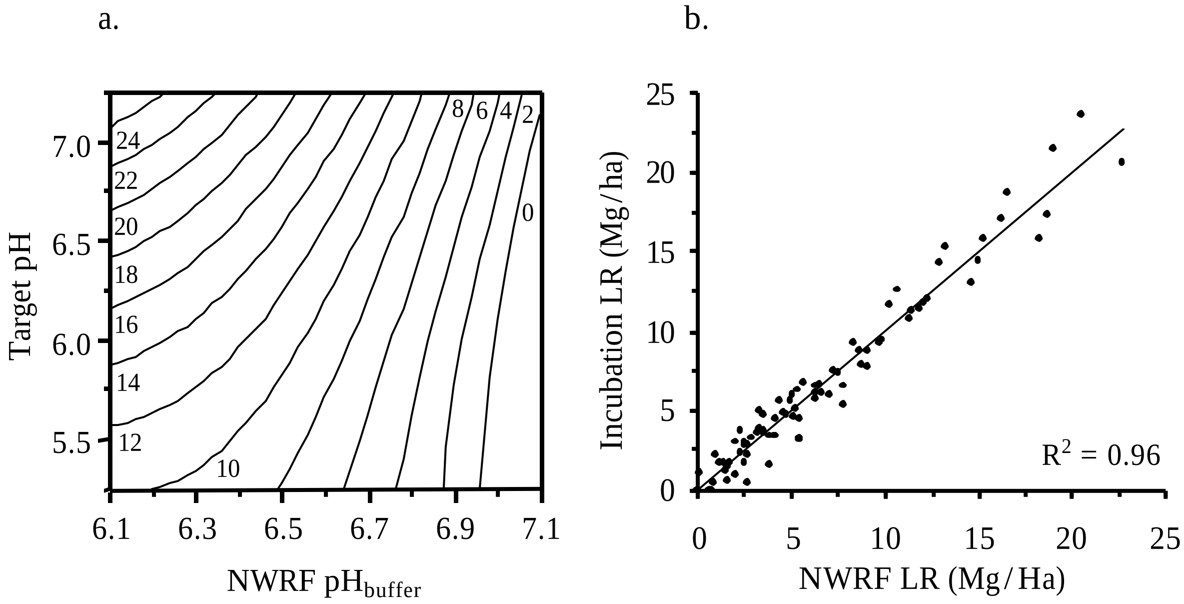

Figure 8.10 (a.) The New Woodruff (NWRF) buffer single-factor response surface. Lime requirements (LR) in Mg/ha, and (b.) NWRF model fit

The model fit for the NWRF predicted lime requirements is shown in Figure 8.10b. Both the WRF and NWRF buffers yielded equivalent model R^2 values, confirming the similarity in buffer composition and reaction.

A feature of the WRF, SMP and NWRF response surface models (Figures 8.8 to 8.10) is the curvilinearity of the response at lower pH$_{buffer}$ and lower target pH values. For example the WRF buffer surface shown in Figure 8.8a shows that where pH$_{buffer}$ values are lower than 6.4 and the selected target pH is below 6.5, response is curvilinear. The reason for these curvilinearities may be that the buffers measure a greater proportion of soil acidity from soils with low lime requirements than from soils with high lime requirements. Section 8.2.2 indicated that a number of other authors have found this feature with conventional regressions. The model for the SMP buffer (Figure 8.9) did not fit the incubation data as well as the other buffer models. The NWRF response surface model produced an almost identical fit to its original counterpart (Figures 8.10 and 8.8 respectively). Due to this similarity and the likeness in their chemical composition, in this work they are considered to be analogous.

Unlike the other buffer models, the response surface of the MCH buffer (Figure 8.11) appears to be linear and relatively constant for the range of pH$_{buffer}$ values measured.

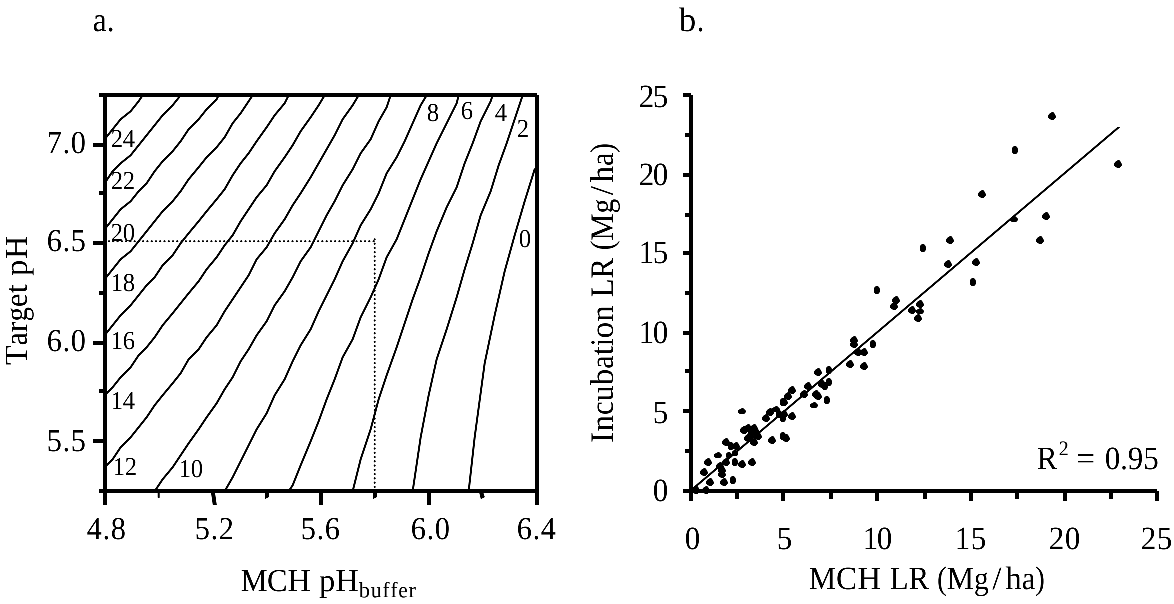

Figure 8.11 (a.) The Mehlich (MCH) buffer single-factor response surface. Lime requirements (LR) in Mg/ha, and (b.) MCH model fit

The relationship between the MCH buffer predicted lime requirements and the incubation lime requirement is shown in Figure 8.11b. The fitted line has unit gradient and an R^2 value of 0.95.

Graphically, lime requirements may be estimated by simply reading of the graph, or more precisely by using the model as follows: *e.g.* using the MCH single-factor response surface, liming to a target pH of 6.5 may be desirable if an acid intolerant crop such as canola (*Brassica napus*) is to be grown. If the measured field MCH $\mathrm{pH_{buffer}}$ at the site or management unit is 5.8, then the lime requirement at that site is calculated from Figure 8.11a and using Equation 8.12 (which is similar in form to Equation 8.5):

$$\text{MCH LR Mg/ha} = -49.34 - 19.19(5.8) + 7.38(6.5) - 0.87(5.8)^2 - 3.43(5.8 \times 6.5) + 1.32(6.5)^2 \tag{8.12}$$

$$= 7.04 \text{ (result shown by dashed line in Figure 8.11a)}$$

The WRF and MCH buffers respectively, produced the best fitting single-factor response surface models.

8.4.4 TWO-FACTOR ($\mathrm{pH_{BUFFER}}$ AND $\mathrm{pH_{CaCl_2}}$) RESPONSE SURFACE MODELS

Soil pH is a routinely measured soil property that may not add to the laboratory work required when estimating lime requirements, hence response surface models that include both pH_{buffer} and pH_{CaCl_2} values were built for both the WRF and MCH buffers. The addition of the extra variable was made to further improve the accuracy of lime requirement predictions. The two-factor response surfaces for target pH values of 5.5, 6, 6.5 and 7, using the WRF buffer are shown in Figures 8.12a to 8.12d respectively.

Graphically lime requirement estimates can be taken as follows: *e.g.* if a soil needs to be limed to a target pH of 6.5 and it has an acidic pH_{CaCl_2} of 4.5 and a WRF pH_{buffer} value of 6.6, then the amount of lime needed for amelioration is approximately 7.4 Mg of lime per hectare (dashed line Figure 8.12c). The model is of the form given in equation 8.6. Using the same example, the lime requirement may be predicted using parameters of the fitted model by:

$$\begin{aligned}\text{WRF LR}(\text{Mg/ha}) &= -287.28 + 113.03(6.6) - 48.7(4.5) + 25.03(6.5) - 10.11(6.6)^2 + 8.77(6.6\times4.5) - \\ &\quad 1.3(4.5)^2 - 5.88(6.6\times6.5) + 0.27(4.5\times6.5) + 1.32(6.5)^2 \\ &= 7.39 \text{ (dashed line in Figure 8.12c)}\end{aligned} \tag{8.13}$$

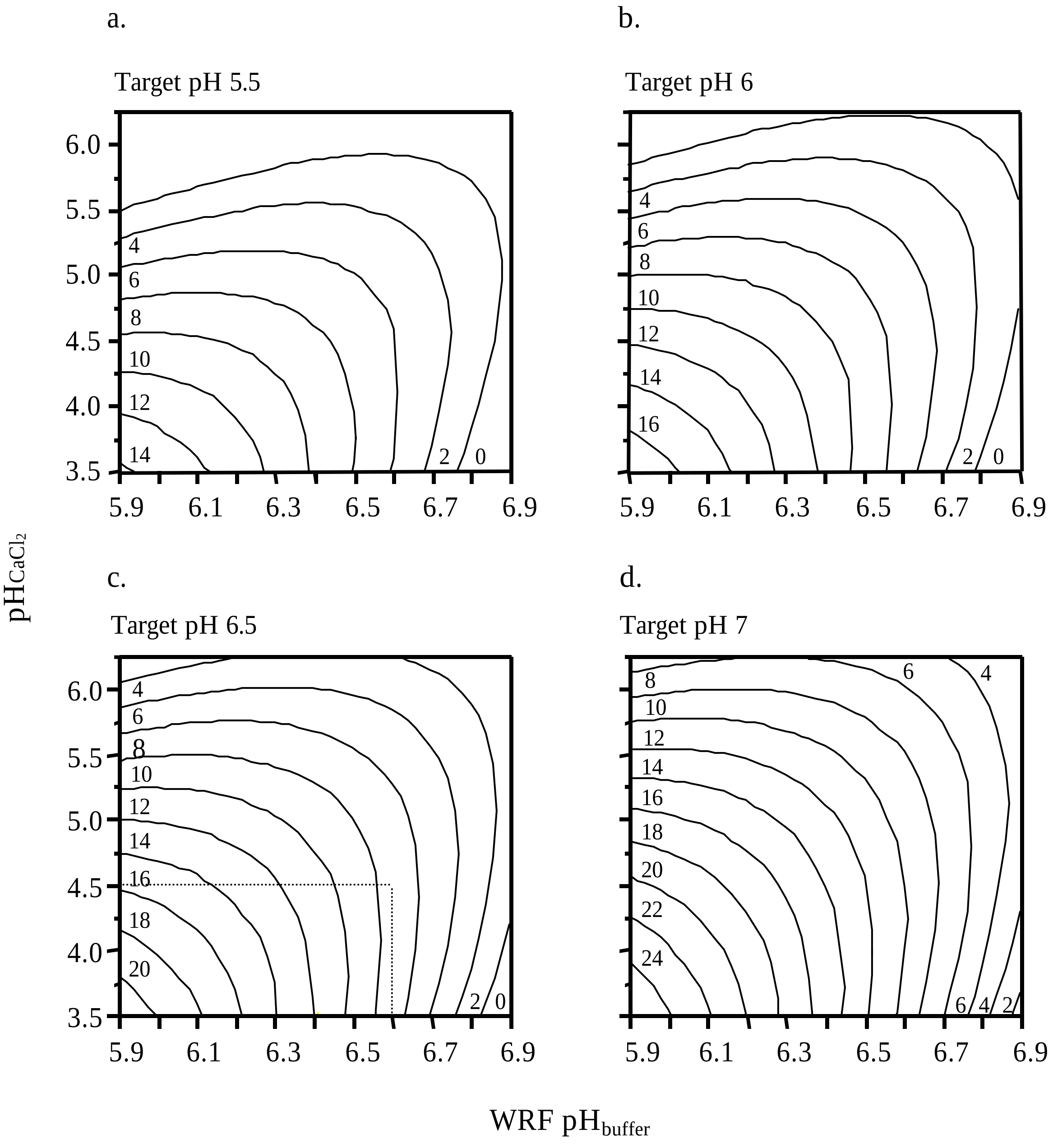

Figure 8.12 Woodruff (WRF) buffer two-factor (pH_{buffer} and pH_{CaCl_2}) response surface. The contours represent lime requirements in Mg / ha. The R^2 of the model was 0.98

Response-surfaces for the MCH buffer are shown in Figures 8.13a to 8.13d. Using the MCH buffer response-surfaces (Figure 8.13); for example if the soil pH_{CaCl_2} is 4.5 and buffer-pH_{MCH} is 5.8, then the lime requirement may be calculated using:

$$\begin{aligned}\text{MCH LR (Mg/ha)} &= 8.31 + 17.31(5.8) - 26.09(4.5) + 8.41(6.5) - 2.35(5.8)^2 + 5.35(5.8\times4.5) - 0.94(4.5)^2 - \\ &\quad 3.9(5.8\times6.5) + 0.36(4.5\times6.5) + 1.32(6.5)^2 \\ &= 6.88 \text{ (dashed line in Figure 8.13c)}\end{aligned} \tag{8.14}$$

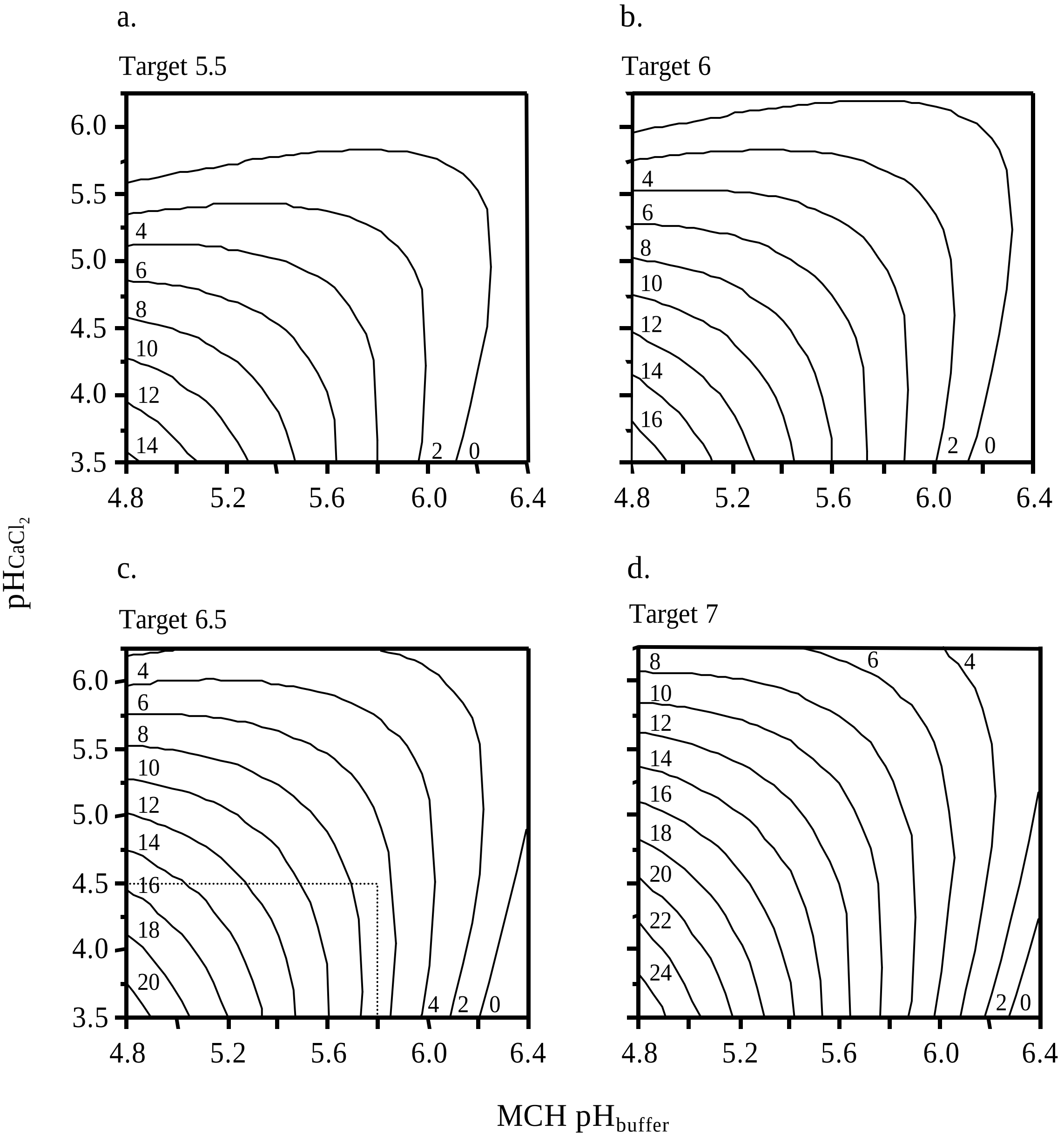

Figure 8.13 Mehlich (MCH) buffer two-factor (pH_{buffer} and pH_{CaCl_2}) response surface. The contours represent lime requirements in Mg/ha. The R^2 value of the model was 0.97

These more complex models provide versatile and flexible methods for predicting lime requirement when soil pH_{CaCl_2} data is readily available or easily acquired. The inclusion of pH_{CaCl_2} in the two-factor response surface models produced higher coefficient of determination (Figures 8.12 and 8.13) than single-factor models (Figures 8.8b and 8.11b).

8.4.5 COMPARISON AND VALIDATIONS OF LIME REQUIREMENT PREDICTIONS

Three multivariate functions used to predict lime requirements (section 8.21, Equations 8.1, 8.2 and 8.3) were included in the comparison between model-based lime requirement predictions and those determined from incubations. Table 8.5 shows the descriptive statistics of the incubation-determined and model-predicted lime requirements, and compares the quality of their predictions. The methods with the most efficient compromise between prediction accuracy and parsimony (lower AIC values) are ranked (last column in Table 8.5).

Predictions of lime requirement using the multivariate methods were highly biased, either under estimating (Keeney & Corey, 1963) or overestimating (Pionke *et al.*, 1968; Gustafsson, 1999) the amount of lime required to raise the initial soil pH to a desired level (Table 8.5). Of the multivariate techniques, the multiple-regression that Pionke *et al.* (1968) suggested produced the more accurate predictions of lime requirement. This result was expected because Pionke *et al.*'s regression uses the greatest number of auxiliary soil variables for predictions of lime requirement. An important drawback to consider when using multivariate techniques is their additional requirement for predictor variables, for example organic carbon, clay content, exchangeable and non-exchangeable aluminium, etc. This feature makes the use of such techniques inefficient for precision agriculture because of the extra cost effort and resources required to collect and measure the additional soil variables, some of which are not measured in routine analysis.

Generally, conventional lime requirement buffer predictions were more accurate, precise and less biased than those derived from the multivariate techniques. Various researchers reported similar findings (Table 8.1). The single-factor response surface models improved the prediction accuracy of all lime-requirement buffer methods (Table 8.5). As for conventional linear regressions, the WRF buffer and its modified compeer the NWRF buffer fitted with single-factor response surface models produced similar results and were considered analogous. Therefore, the WRF and MCH buffers respectively, produced the best predictions. Contrary to much of the reported literature (refer to Table 8.1), the SMP buffer produced the least accurate predictions of lime-requirement buffer method.

Table 8.5 Comparison between incubation lime requirements and model-based predictions of lime requirements to target pH values of 5.5, 6, 6.5 and 7, expressed in Mg/ha. The number of samples *n* = 88 (4×22)

LR method	p	v	Mean	St.Dev.	Med.	Min.	Max.	RSS	RMSE	ME	Imprecision	AIC	Rank
Incubation LR			*6.34*	*5.52*	*4.79*	*0*	*23.72*						
R.S. (pH$CaCl_2$) WRF LR	10	2	6.34	5.46	4.73	-1.55	21.61	92	1.02	0.004	1.01	418	1
R.S. WRF LR	6	1	6.35	5.45	4.69	-1.5	23.63	135	1.24	-0.0056	1.12	445	3
R. WRF LR	2	1	6.38	5.48	4.59	-0.69	25.41	185	1.46	-0.0399	1.22	467	6
R.S. (pH $CaCl_2$) MCH LR	10	2	6.34	5.43	4.76	-1.27	21.71	125	1.19	-0.0005	1.19	444	2
R.S. MCH LR	6	1	6.34	5.44	4.92	-1.45	24.15	172	1.4	-0.0003	1.18	465	5
R. MCH LR	2	1	6.35	5.45	4.97	-1.18	24.7	203	1.52	-0.0138	1.24	474	7
R.S. NWRF LR	6	1	6.35	5.45	4.93	-1.27	23.9	138	1.25	-0.0089	1.12	446	4
R. NWRF LR	2	1	6.39	5.52	4.69	-0.19	27.11	247	1.68	-0.0507	1.32	491	8
R.S. SMP LR	6	2	6.36	5.33	4.82	-1.22	25.16	311	1.88	-0.0189	1.38	517	9
R. SMP LR	2	1	6.39	5.44	4.8	-0.35	27.7	415	2.17	-0.0527	1.49	535	11
Pionke et al. (1968)	5	5	5.29	3.53	4.57	-2.16	13.3	356	2.01	-1.0789	1.76	527	10
Kenney & Corey (1963)	2	2	3.49	2.79	2.57	-1.93	11.85	1826	4.56	2.8483	1.31	667	12
Gustafsson (1999)	3	3	11.25	7.92	11.54	-9.86	29.37	5000	7.54	-4.8806	3.52	756	13

Note: p is the number of parameters in the models and v is the number of soil variables used in the predictions. R. buffer-name LR = conventional regression-type predictions; R.S. buffer-name LR = single-factor response surface; R.S. (pH $CaCl_2$) buffer-name LR = two-factor response surface. The buffers are the Shoemaker, McLean & Pratt (SMP), the Woodruff (WRF), the Mehlich (MCH) and the New Woodruff (NWRF). The indices used to quantify the comparisons are the residual sum of squares (RSS), the root-mean square-error (RMSE), the mean error (ME) and the Akaike Information Criterion (AIC).

Two-factor response surface models improved the WRF and MCH buffer's lime requirement predictions significantly, in terms of their accuracy and parsimony. The bias of the predictions were virtually zero for most of the response surface models tested, hence the RMSE produced a measure that described both the accuracy and precision of predictions. Models with the smaller AIC present the best compromise between goodness of fit and parsimony, *i.e.* the better models (Table 8.5). The two-factor response surface models fitted to the WRF and MCH buffers, respectively, yielded the best predictions of lime requirement. Most of the response surface models (single- and two-factor) fitted the data well and produced precise and unbiased predictions. It is recommended that the two-factor model be used when pH_{CaCl_2} is readily available or easily acquired.

8.4.6 UNCERTAINTY OF THE RESPONSE SURFACE MODELS

The upper and lower 95 % confidence intervals of field-estimated lime requirements provide a measure of the uncertainty in the model predictions. In this way, the WRF and MCH buffers with their respective two-factor response surface models were assessed for their ability to predict the lime requirements of the experimental field. Table 8.6 shows the descriptive statistics for the WRF and MCH lime requirements to attain a target pH of 6.5, together with their respective upper and lower 95 % confidence intervals.

Table 8.6 Statistical description of the Woodruff (WRF) and Mehlich (MCH) pH_{buffer} data, corresponding lime requirements to target pH 6.5 (LR(6.5)) and 95 % confidence intervals (CI) data for the soil in the field at Kelso

	Mean	S.D.	Median	Range
WRF LR(6.5) Mg/ha	7.13	1.58	7.13	3.76 – 12.07
Lo. 95% CI WRF LR(6.5) Mg/ha	6.72	1.55	6.73	3.37 – 11.55
Up. 95% CI WRF LR(6.5) Mg/ha	7.55	1.60	7.54	4.15 – 12.58
MCH LR(6.5) Mg/ha	6.39	1.33	6.34	3.13 – 10.99
Lo. 95% CI MCH LR(6.5) Mg/ha	5.93	1.33	5.89	2.69 – 10.46
Up. 95% CI WRF LR(6.5) Mg/ha	6.85	1.34	6.78	3.58 – 11.52

For the WRF buffer model the uncertainty of field predicted lime requirements to a target pH of 6.5 was 0.42 Mg/ha, while for the MCH model it was 0.46 Mg/ha (Table

8.6). As well as presenting the precision of the models, Table 8.6 also displays the range of limits for the lime requirements of the field. Note this data gives only the error of the response surface models. Chapter X illustrates the use of a geostatistical modelling technique to measure the production and economic risks of liming. The method accounts for both the local uncertainty about soil properties and uncertainty about the parameters of two models: a response surface regression (a rearranged form of Equation 8.5) used to derive pH_{CaCl_2} values post-liming; and a crop model (derived in the proceeding Chapter IX).

8.4.7 SPATIAL ANALYSIS OF LIME REQUIREMENT, ALUMINIUM AND CALCIUM

The semi-variogram models and parameters for the MCH and WRF field buffer-pH values, and corresponding lime requirements to a target pH of 6.5, predicted using the two-variable response-surface models are given in Table 8.7.

Table 8.7 Semi-variogram models and parameters for the Woodruff (WRF) and Mehlich (MCH) pH_{buffer} values, and corresponding lime requirement estimates to a target pH of 6.5 (LR(6.5))

Variable	Model	C_0	C_1	C_2	$C_0/\ C_0 + C_1$	a_1(m)	a_2 (m)
WRF pH_{buffer}	Exponential	0.0012	0.0044		0.23	39	
WRF LR(6.5)	Exponential	0.46	2.05		0.18	38	
MCH pH_{buffer}	Double-exponential	0.0019	0.0083	0.76	0.19	26	10000
MCH LR(6.5)	Double-exponential	0.15	0.67	26.73	0.18	24	10000

Note: C_0 is the nugget variance, C_1 and C_2 are the sill variances, and a_1 and a_2 are the range parameters in metres

Double exponential semi-variogram models (Table 8.7) fitted the MCH data better than single exponential or spherical models (AIC values not shown), indicating the presence of a slight trend in the data. As expected, the ranges of spatial dependence for both the pH_{buffer} and lime requirement data are similar since lime requirement is a function of pH_{buffer}. The ratio of nugget to sill variance of both the WRF and MCH pH_{buffer} data and respective lime requirements is low (Table 8.7). This proportion represents the short-range variability of soil lime requirement as well as the inaccuracies of the sampling and analytical methods (Chapter IV).

Figures 8.14 and 8.15 show maps of WRF and MCH pH_{buffer} and respective lime requirements, produced by block kriging using the variogram parameters given in Table

8.6. Although the WRF buffer predicts higher lime requirements (4.42 to 10.85 Mg/ha) than the MCH method (3.7 – 10.14 Mg/ha), they are comparable in their predictions (ρ = 0.9). The very high lime requirements of the field are explained by the very low pH_{CaCl_2} values and by the fact that the field has not been previously limed. A pH_{CaCl_2} map of the field is shown in Figure 5.8d of Chapter V. Descriptive statistics for pH_{buffer} values and lime requirements to pH 6.5 across the experimental field, for the kriged WRF and MCH methods are given in Table 8.8.

As well as pH, calcium and aluminium were the properties that were moderately correlated with lime requirement (Table 8.3). These properties influence the amount of lime needed to amend acid soil, and liming obviously affects their concentration in the soil solution. Figure 8.16 shows the spatial distribution of exchangeable aluminium and exchangeable calcium concentrations in the soil of the experimental field.

In the northwestern portion of the field, concentrations of exchangeable aluminium in the soil are high (Figure 8.16a), while concentrations of exchangeable calcium are low (Figure 8.16b). The correlation matrix shown in Table 8.3 hinted at this antagonistic reaction between aluminium and calcium (ρ = -0.4) (also reported in Chapters VI and IX, the latter providing evidence of the behaviour). Statistics of the kriged aluminium and calcium concentrations in the field are given in Table 8.8.

Table 8.8 Descriptive statistics of the kriged Woodruff (WRF) and Mehlich (MCH) pH_{buffer} and lime requirement to target pH of 6.5 (LR(6.5)) data, as well as exchangeable calcium and exchangeable aluminium. *n* = 28 869

Property	Mean	S.D.	Median	Range
WRF pH_{buffer}	6.61	0.04	6.61	6.43 – 6.73
WRF LR(6.5) Mg/ha	7.12	0.91	7.16	4.42 – 10.85
MCH pH_{buffer}	5.85	0.06	5.85	5.56 – 6.04
MCH LR(6.5) Mg/ha	6.39	0.79	6.36	3.7 – 10.14
Exchangeable Al mmol(+)/kg	1.72	0.89	1.37	0.77 – 6.47
Exchangeable Ca mmol(+)/kg	23.91	4.82	22.83	16.32 – 38.07

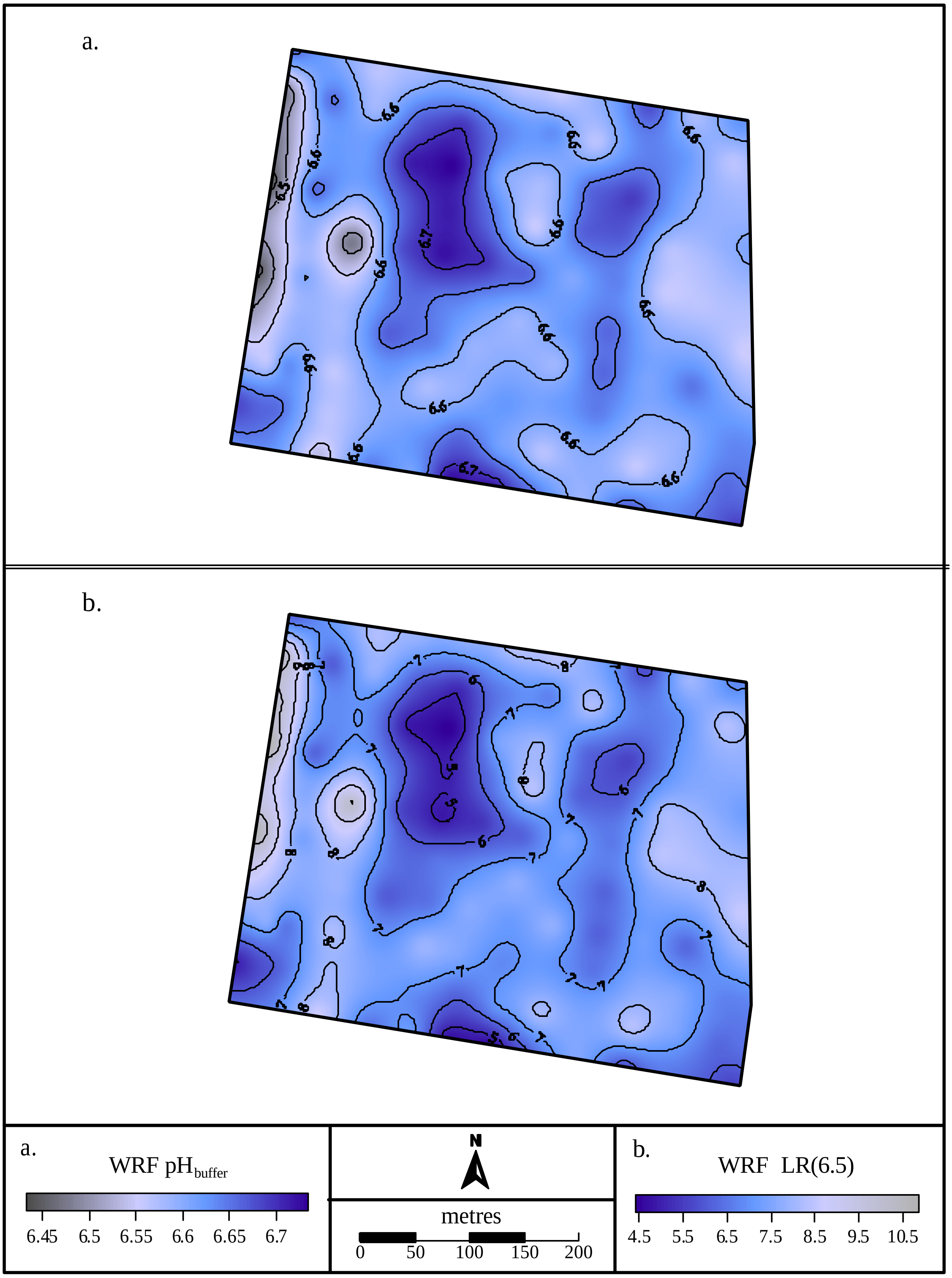

Figure 8.14 Block kriged (a.) Woodruff (WRF) pH_{buffer} and (b.) lime requirement map to a target pH of 6.5 (LR(6.5)), in Mg/ha

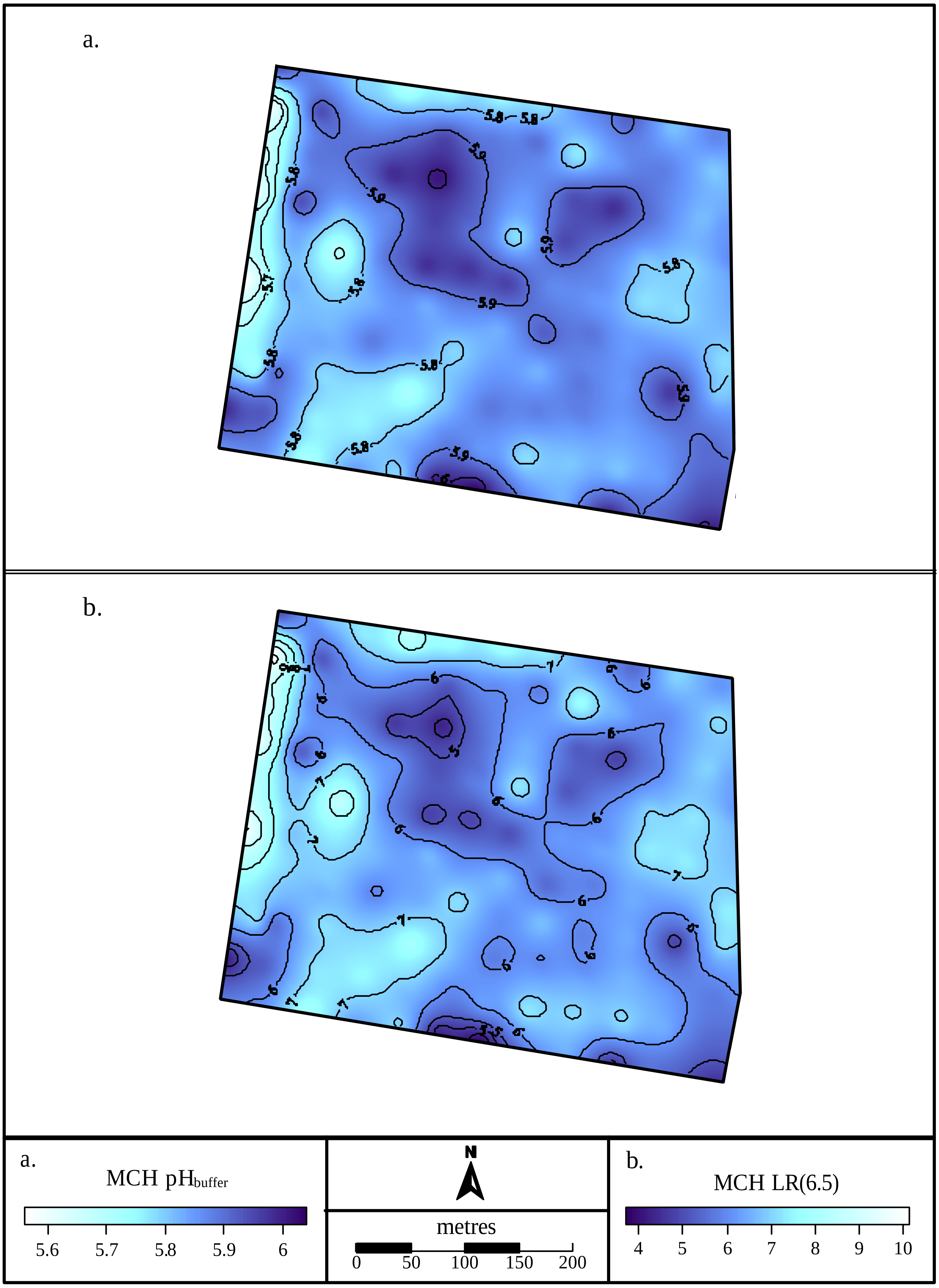

Figure 8.15 Block kriged (a.) Mehlich (MCH) pH$_{buffer}$ and (b.) lime requirement map to a target pH of 6.5 (LR(6.5)), in Mg/ha

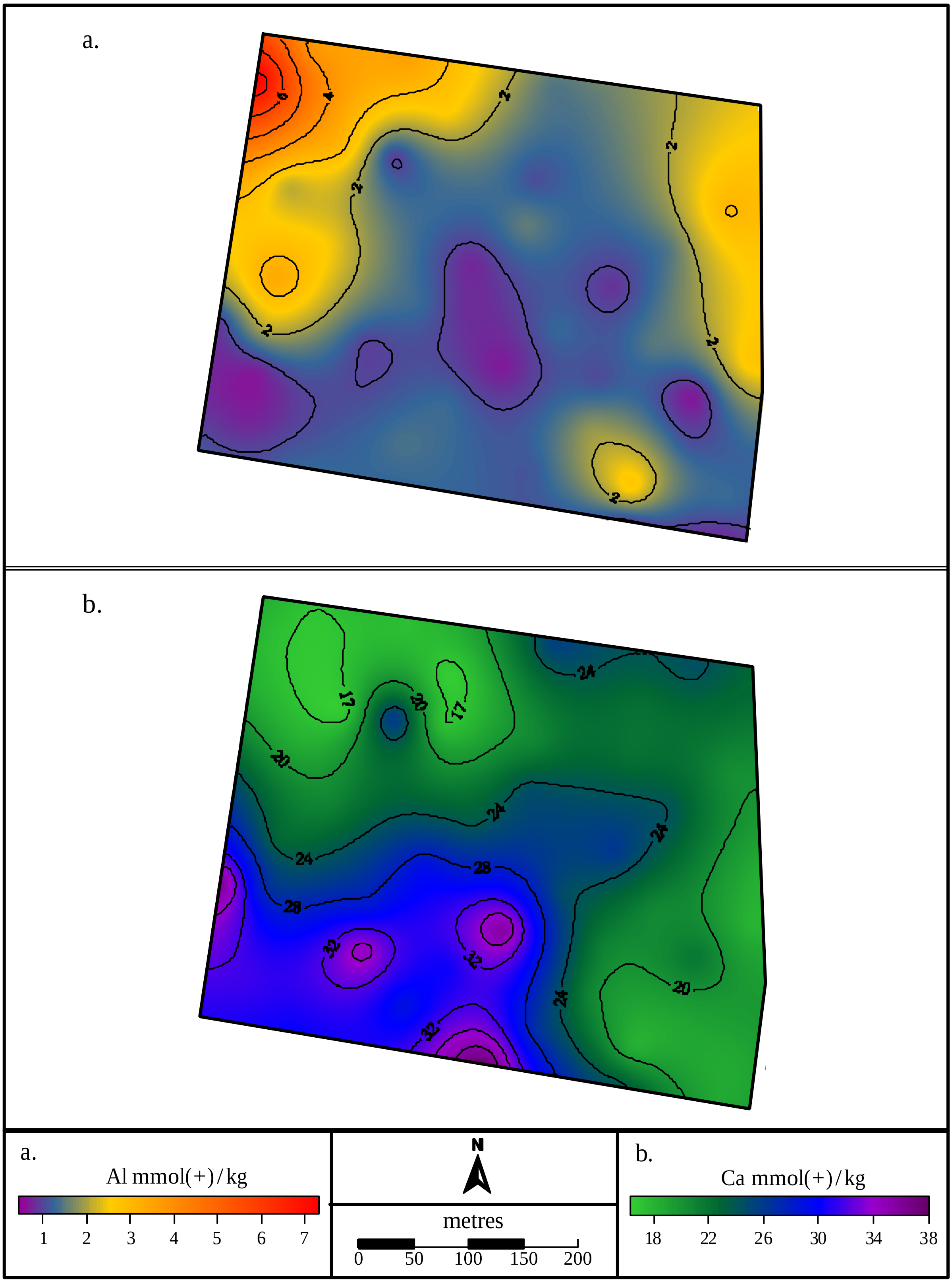

Figure 8.16 Maps of (a.) exchangeable aluminium (Al) and (b.) exchangeable calcium (Ca), in mmol(+)/kg soil

8.4.8 COMPARISON BETWEEN SINGLE-RATE AND SITE-SPECIFIC LIMING

The resultant field soil target pH values for a single-rate lime application of 7.46 Mg/ha are shown in Figure 8.17.

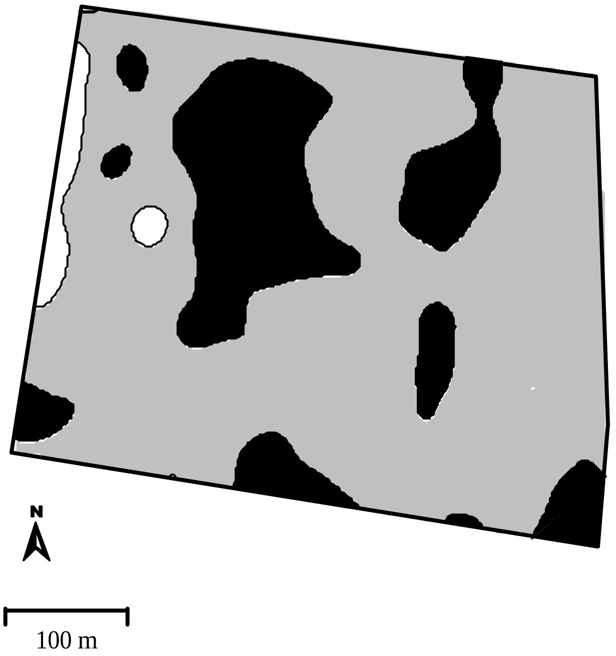

Figure 8.17 Resultant $\mathrm{pH_{CaCl_2}}$ values if lime is applied uniformly across the field at a rate of 7.46 Mg/ha. ▒ represent resultant $\mathrm{pH_{CaCl_2}}$ values between 6.25 and 6.75; □ represent areas where $\mathrm{pH_{CaCl_2}}$ values < 6.25; ■ represent areas where $\mathrm{pH_{CaCl_2}}$ values > 6.75

The range in $\mathrm{pH_{CaCl_2}}$ post-liming resulting from the single-rate application of lime was 5.78 to 7.19 with an average $\mathrm{pH_{CaCl_2}}$ of 6.58 units (Figure 8.17). If a 7.46 Mg/ha blanket rate of lime to pH 6.5 were applied, target soil pH values may be expected to deviate from the target pH by some margin. An acceptable deviation may be 0.25 pH units, i.e. $6.25 \geq \mathrm{LR}(6.5) \leq 6.75$. If the mean liming rate is applied uniformly across the field, 22 % of land will have $\mathrm{pH_{CaCl_2}}$ values over 6.75 and 3% $\mathrm{pH_{CaCl_2}}$ values under 6.25 (Figure 8.17). These areas of the field show where lime has been inefficiently applied. In comparison, resultant target pH values for the site-specific liming case ranged from 6.38 to 6.58, with an average of 6.5.

Applying the average lime requirement over the entire field would result in areas of over- and under-application, ranging from 3 to -3.5 Mg/ha, respectively. Single-rate application of lime will have both economic and physiologic consequences, *e.g.* significant resource misallocation and the risk of hindered crop production. Hence these results demonstrate the rationale behind site-specific liming using a lime requirement buffer and response surface methodology.

8.5 CONCLUDING REMARKS

A soil's lime requirement is influenced mainly by its buffering capacity and the amount of exchangeable acidity in the soil solution. As such soil pH and aluminium explained only moderate proportions of the variation in lime requirements. These properties alone do not provide accurate estimates of a soil's lime requirement.

Multivariate functions that used other soil properties (*e.g.* pH, organic matter, aluminium, clay content, etc.) as predictive variables were inaccurate and highly biased, either underestimating or overestimating the amount of lime needed for the amelioration of acid soil. The lime requirement buffer procedures, which in a single measurement account for the initial soil pH, the buffering capacity of the soil and the amount of base required to neutralise the exchangeable acidity present, were more accurate.

Conventional lime requirement buffer calibrations were less accurate and less versatile than the developed single- and two-factor response surface models. These type of models were developed to facilitate the choice of target pH without the need for excessive calibrations. These models are more accurate and more practical than conventional techniques, and may be more suitably incorporated into the spatial decision-support system of the proposed real-time continuous system for the management of acid soil. Initially, the response surface methodology may be used to produce variable-rate lime requirement maps to guide variable-rate lime applicators. In a real-time continuous system, the data collected by the 'on-the-go' proximal soil pH and lime requirement sensing system would be used in the response surface models to predict lime requirements for real-time applications of lime.

It is important to note that the model, being empirical, will only make accurate predictions when it is applied to the range of soils that were used in its formulation. In this instance, the range of soils used was collected from across the southern wheat-belt of New South Wales. Hence the model may only be used for predictions of lime requirement in these regions. However the methodology may be widely and easily applied on a regional basis.

The Woodruff, New Woodruff and Mehlich buffers produced the most accurate estimates of lime requirement, respectively. Unlike previous findings, the Shoemaker, McLean & Pratt buffer was the least accurate buffer method. Due to the similarity in chemical composition between the Woodruff and New Woodruff buffers only the original Woodruff and the Mehlich buffers were considered when deriving two-factor response surface models. The two-factor methodology incorporated soil pH_{CaCl_2} and pH_{buffer} measurements in the models. The models produced the most accuracy and parsimonious predictions of lime requirement. Therefore when pH_{CaCl_2} is available or easily acquired, it should be included as a secondary variable in the response surface. If soil pH_{CaCl_2} values are unavailable or too costly to acquire, then the single-factor model with either the Woodruff or Mehlich buffers may be used. Although the single-factor models were found to be slightly inferior to the two-factor models, they fitted the data well and produced precise and relatively unbiased predictions.

Field lime requirements were predicted using the Woodruff and Mehlich buffers calibrated using the two-factor models. Spatial analysis of field pH_{buffer} values and respective lime requirements showed that both techniques are suitable for field predictions of lime requirement and for the production of variable-rate liming maps. The variable-rate maps to target pH 6.5 showed that lime requirements in the experimental field ranged from approximately 3.5 Mg/ha to 11 Mg/ha. The very low soil pH_{CaCl_2} values and the fact that the field had not been previously limed may explain the very high lime requirements. One may argue that this was a rather high, intangible range of lime requirements for most producers. However, such high applications may be expected to occur only once, followed by lower rates of prophylactic liming in subsequent years. Otherwise, the response surface technique is flexible and the farmer may choose lower target pH values depending on the crop grown and the economic outlook. Also, the methodology allows different areas of the field to be limed to different target pH values depending on the yield potentials of different areas in the field, thereby reducing the liming costs.

Maps of exchangeable aluminium and exchangeable calcium showed that in areas where aluminium is present in high phytotoxic concentrations, calcium deficiencies occur. Conversely, where high levels of calcium predominate, the aluminium concentration in the soil solution is low. This is one of the main reasons for liming acid soil. However their spatial distribution showed only small correlation with lime requirements.

A post-lime application map of (target) pH_{CaCl_2} for a single-rate liming scenario, together with quantification of the differences between single-rate and site-specific lime requirements demonstrated the inefficiency of using a mean, blanket application rate. Over- and under-application, ranged from 3 to -3.5 Mg/ha, respectively.

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Chapter IX

A GLASSHOUSE LIMING EXPERIMENT

ABSTRACT

Soil acidity in Australia is an extensive problem that threatens agricultural production. Liming is a rapid and direct method of amelioration. Growing a wheat crop under controlled conditions corroborated the response surface calibration model derived in Chapter VIII for the estimation of lime requirement. The model might be incorporated into the spatial decision-support system (SDSS) of the proposed real-time continuous management system for acid soil, that uses data collected by the 'on-the-go' proximal soil pH and lime requirement sensing system. Soil and soil plant interactions in acid soil were determined and the dynamics of soil interactions at low pH highlighted. The benefits of liming acid soil were clearly illustrated. Comparisons of yield resulting from untreated acid soil, that amended using a single-rate of lime and acid soil amended using variable-rate applications, verified the benefits of liming and showed the advantages of variable-rate liming. While it is acknowledged that glasshouse experiments are beset with some problems, they prove useful in an exploratory and theoretical sense.

9.1 INTRODUCTION

Soil acidity in Australia is an insidious problem affecting a large portion of agriculturally productive land (Chapter VI). Much of this acidification may be attributed to the long-term removal of produce and the application of ley farming practices that use legumes in the rotation sequence. The literature contains many examples that discuss the effect of soil acidity ameliorates and their effect on plant growth (*e.g.* Coventry *et al.*, 1997a, b; Moody *et al.*, 1995; Conyers *et al.* 1991; Coventry *et al.*, 1989; Fox *et al.*, 1985). Some studies attempt to identify soil property interactions that are of consequence (*e.g.* Aitken *et al.*, 1998; Aitken, 1992; Fox *et al.*, 1991; Ritchie, 1989; Adams, 1984), but few propose specific explanations for acid soil infertility. The difficulties in specific diagnosis of the problem may arise from the complexity of the processes involved, *i.e.* it is very difficult to alter one property without simultaneously altering others. Soil property dynamics in an acidic environment and the effects of amelioration on soil quality and plant growth (Chapter VI) cannot be deduced from the analysis of a single soil parameter, *e.g.* pH or cation exchange capacity (CEC) or aluminium (Al) or calcium (Ca). It must come from the interactions between them.

To improve productivity on acid soil, lime applications have been recommended as an effective and direct means of amelioration (Chapter VI). Chapter VIII describes various procedures that have been developed to estimate the lime requirement (LR) of acid soil. It also describes the development of calibration models for rapid and accurate predictions of lime requirement. The models provide versatility and flexibility in the decision of target pH to satisfy specific crop requirements. Important also are their perceived functionality for incorporation in the spatial decision-support system (SDSS) of the proposed real-time continuous management system for acid soil (Chapter VI) that uses information collected 'on-the-go' by the proximal soil pH and lime requirement sensing system (Chapter VII).

The basis for precision agriculture (PA) as site-specific soil and crop management has been identified as that of maximising economic returns whilst concurrently minimising the environmental impact of crop production systems (Chapter I, II). In terms of liming this entails site-specific applications based on not only soil property status but also the agronomic requirements of the crop grown (Chapter VI). Under-applications of lime may result in incomplete amelioration of elemental toxicities and other impeding factors that give rise to less-than-optimal crop growth. Conversely, over-applications may effect nutrient unavailability, which also result in reduced plant growth. The emergence of variable-rate technology and the development of variable-rate lime spreaders (Chapter II) that can vary application rates as the equipment moves over the field have enabled site-specific liming.

The primary objective of this chapter is to use the single-factor response surface lime requirement calibration model with the Mehlich buffer (Chapter VIII) and verify its predictions by growing a wheat crop using selected soil samples from the experimental field (Chapter III), under controlled greenhouse conditions. In this way, the predictions of lime requirement are verified with the responsiveness of the crop. A secondary aim is to determine some of the soil and crop interactions in acid soil and deduce the most limiting factors to plant growth. A third objective of the experiment is to ascertain the benefits of liming acid soil and compare conventional single-rate lime applications with variable-rate (or site-specific) liming. A final but no less important aim was to peruse the null hypothesis of PA proposed by McBratney *et al.* (1997), *i.e.*, that '… the optimal risk aversion strategy is uniform management'. This final aim is developed further in Chapter X.

9.2 METHODS

The soil used in the trial was collected from the experimental field at Kelso during the sampling effort (refer to Chapter III). The crop grown was wheat (*Triticum aestivum* L.).

9.2.1 SAMPLE SELECTION AND ANALYSES

To obtain a good representation of the acidic field soil for the pot trial, measured field pH_{CaCl_2} values where grouped into the quartiles of the sample distribution, and four samples were randomly selected from each class. A total of sixteen samples resulted. The field position and pH_{CaCl_2} values of the samples used in the experiment are shown in Figure 9.1.

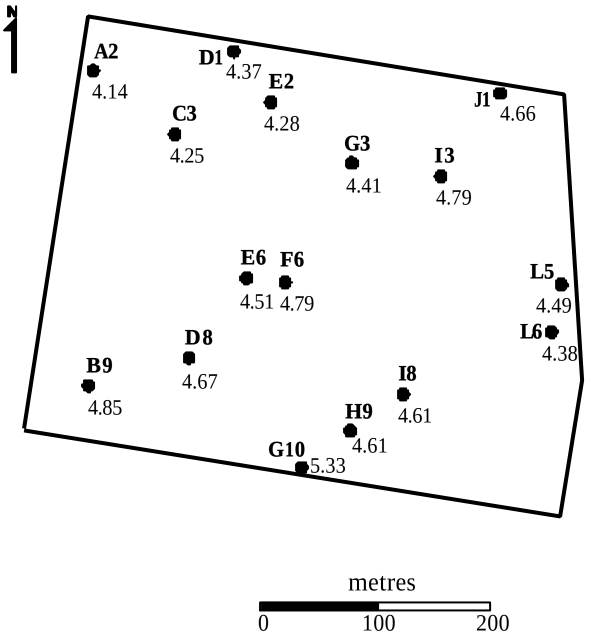


Figure 9.1 Field location and pH_{CaCl_2} values of soil samples used in the pot trial

Soil pH in a 1:5 soil:0.01 M $CaCl_2$ (pH_{CaCl_2}) and 1:5 soil:H_2O (pH_{H_2O}), organic carbon (OC), electrical conductivity (EC), Al (extracted using 1 M KCl), CEC, basic cations and nutrients (N, P, K) were determined using the methods described in Chapter III. Lime requirements were estimated using the Mehlich lime-requirement buffer (pH_{buffer}) with the corresponding single-factor response surface model (Chapter VIII).

The soil was analysed after the liming treatment applications to establish some of the relationships between acid soil and ameliorated soil properties, and to demonstrate their respective effects on soil quality and plant growth.

9.2.2 EXPERIMENTAL DESIGN AND TRIAL PREPARATION

The experimental design consisted of dividing the sixteen samples into three replicated groups: a control group where no lime was applied (NL), one where an averaged single-rate of lime (SRL) was applied to all pots, and one where the measured LR was differentially applied to each pair of replicates in the group (VRL). Table 9.1 shows the design.

Table 9.1 Pot trial design consisting of three treatments, no-lime (NL), single-rate lime (SRL) and variable-rate lime (VRL) applications

Treatment 1 NO-LIME (NL)		Treatment 2 SINGLE-RATE LIME (SRL)		Treatment 3 VARIABLE-RATE LIME (VRL)	
Rep. 1	Rep. 2	Rep. 1	Rep. 2	Rep. 1	Rep. 2
16 pots	16 pots	16 pots	16 pots	16 pots	16 pots
		Equal total amounts of $CaCO_3$ added to SRL and VRL treatments			
All Pots N, P, K fertilised, and watered to maintain field capacity					

There was a total of 16 replicated samples per group (Table 9.1). Each group contained 32 pots.

Fertilisation

The degree of N, P, K fertilisation required was based mainly on soil chemical fertility levels, which were estimated using the analytical techniques previously described. For each of the 16 soil samples, the resultant values were entered into the Nutrient Advantage Software[9.1], which derived fertiliser recommendation rates for an achievable grain yield of 2.8 Mg/ha. The suggested rates of fertiliser application, the degree of Al saturation, and comments on general fertility characteristics of the soil are given in Table 9.2.

Di-ammonium phosphate (DAP) granular fertiliser was deemed suitable to supply the N and P requirements of the soil used in the pot trial. Soil tests results and ensuing recommendations are given in Table 9.2. The elemental analysis of DAP was 19 % N, 20

% P and 3 % S. Fertiliser applications consisted of mixing DAP with the air-dry samples before potting to supply the required amounts of nitrogen to the soil. Phosphorus was supplied in excess amounts. Although Nutrient Advantage suggested that the K status of most samples was satisfactory, Muriate of potash was applied to all samples at 50 Kg/ha. Soil samples from each group were analysed two weeks after fertilising.

Apart from fertiliser recommendations, Table 9.2 provides an indication of the degree of Al saturation and Ca and Mg status of the soil. Medium to high Al saturation and low Ca and Mg are indicative of the need for $CaCO_3$ applications.

Table 9.2 Recommended rates of fertiliser application (Nutrient Advantage Software[9.1])

Soil sample	N (kg/ha)	P (kg/ha)	K (kg/ha)	Al_{sat}	Comments
A2	55	18	50	High	N deficient; P, K, Ca, Mg low
B9	50	18	-	Med.	N deficient; P low
C3	40	18	-	High	N, P, Ca, Mg low;
D1	40	23	-	High	P deficient; N, Ca, Mg low
D8	35	23	-	Med.	P deficient
E2	55	18	-	High	N deficient; P, Ca, Mg low
E6	40	23	-	High	P deficient; N low
F6	50	23	-	Med.	P, N deficient
G3	40	18	50	Med	N, P, K, Ca, Mg low
G10	50	23	-	Low	N, P deficient
H9	50	18	-	High	N deficient; P low
I3	55	23	-	High	N, P deficient; Ca low
I8	50	23	-	High	N, P deficient; Ca, Mg low
J1	45	23	-	High	P deficient; N low
L5	55	23	50	High	N, P deficient; K, Ca, Mg low
L6	50	18	50	High	N deficient; P, K, Ca low

[9.1] INCITEC Fertilisers

Mass of Soil used in Each Pot and Lime Requirement

The gravimetric water content w of each of the sixteen air-dry soil samples was determined. A total of ninety-six pots were prepared each having the capacity to hold 1300 g of soil at Field Capacity (FC). The amount of air-dry soil needed was calculated by:

$$\text{Mass OD soil required (g)} = \frac{\text{Mass of Soil Solids at FC}}{1 + w_{FC}}$$
$$\therefore \text{Mass AD soil required (g)} = \text{ g OD soil } \times \left(1 + w_{AD}\right) \tag{9.1}$$

where w_{FC} is the averaged FC water content (~ 0.15 g g^{-1}) and w_{AD} is the air-dry water content of the soil sample (g g^{-1}).The air-dry water content and corresponding mass of soil for each sample is given in Table 9.3. OD represents oven-dry and AD air-dry.

Field-based estimates of LR assume the incorporation of $CaCO_3$ to a soil depth of 0.2 m, so LR is actually expressed as Mg of lime per 2000 m^3 volume of soil (Chapter VI). In the trial, the volume of potted soil was calculated using:

$$V_P = \frac{m_P}{\text{BD}} \tag{9.2}$$

where m_P is the mass of potted air-dry soil in grams, and BD is the average bulk density of the samples, calculated as 1.67 g cm^{-3} (Chapter III). The volume of soil in each pot V_P is shown in Table 9.3. The conversion of lime requirement Mg/ha to lime requirement g/mass AD soil was made using the following equation:

$$LR_P = \frac{V_P \times LR_F}{V_F} \tag{9.3}$$

where LR_P is the lime requirement in grams, per AD mass of potted soil (g), V_P is the volume of potted soil (cm^{-3}), LR_F is the field lime requirement (Mg/ha) and V_F is the volume of field soil in which incorporation of lime is assumed, *i.e.* 2000 m^3. Table 9.3 shows the Mehlich pH_{buffer} and corresponding lime requirement of each soil in the VRL treatment group (needed to raise its acidic pH to the target pH of 7). The last row of Table 9.3 shows the average lime requirement to pH 7 applied to each pot in the SRL group.

Analytical grade $CaCO_3$ (99% pure) was applied to the air-dry soil by placing corresponding soil samples and amounts of lime in a plastic bag. The bag was vigorously shaken to ensure adequate soil-$CaCO_3$ mixing.

Watering

Before potting, water was sprayed on to each soil to raise their water content from air-dry to half w_{FC} (*i.e.* 0.24 g g^{-1}), where soils had a 'crumbly' consistency. The volume of water required to raise the air-dry soil to half w_{FC} was calculated using:

$$V_W = \frac{\left(\frac{1}{2} w_{FC} - w_{AD}\right)}{1 + w_{AD}} \qquad (9.4)$$

where V_W is the volume of water to be added in ml g^{-1} soil. The pots were packed with the half FC soil, when the bulk density of the soil was assumed to be approximately 1.0 gcm^{-3}. The limed soil was left to stand for a period of two weeks, watering regularly to ensure adequate $CaCO_3$ dissolution.

Planting and Harvesting

Approximately two thousand wheat seeds were germinated on moist cotton fibres and filter paper. After six days 75 % of the seeds had germinated. Seedlings were randomly picked and planted into the pots of each group (Table 9.1) at a density of 15 plants per pot. The germinated seedlings were sown at a depth of 2 to 2.5 cm. Once the seeds were planted, the soil was watered to FC. A silicon-bead mulch was spread on each pot to reduce evaporative water loss. The pots were placed in a glasshouse and watered to FC (by loss in mass) every four to seven days.

Eight weeks after planting the number of plants in each pot was reduced to ten per pot, to reduce competition between plants for nutrients and space. The matured wheat plants were harvested after 22 weeks when the plants had senesced. Yield was measured by cutting the whole grain-filled heads off the plants and cumulatively weighing them for each replicate in each separate treatment group. Statistical comparisons were made on these pooled yield measurements.

Table 9.3 Factors used to determine the amount of soil and lime to use in the pot trial. w_{AD} is the air-dry water content, m_P the mass of potted air-dry soil, V_P the volume of potted soil, pH_{buffer} refers to the Mehlich lime requirement buffer and LR(7.0) to the lime requirement needed to raise the acidic soil pH to a target pH of 7

Pot label	w_{AD} gg^{-1}	m_P g	V_P cm^{-3}	Mehlich pH_{buffer}	LR(7.0) Mg/ha	LR(7.0) g /pot
A2	0.024	1158	702	5.54	13.5	4.7
B9	0.024	1157	701	5.94	7.6	2.7
C3	0.036	1171	710	5.90	8.1	2.9
D1	0.020	1152	698	5.69	11.4	4.0
D8	0.030	1164	706	5.78	10.0	3.5
E2	0.018	1151	697	5.96	7.3	2.5
E6	0.024	1158	702	5.82	9.4	3.3
F6	0.027	1161	704	5.87	8.7	3.1
G3	0.031	1165	706	5.85	9.0	3.2
G10	0.026	1159	703	6.08	5.5	1.9
H9	0.027	1161	704	5.76	10.3	3.6
I3	0.031	1165	706	6.00	6.6	2.3
I8	0.028	1162	704	5.87	8.6	3.0
J1	0.032	1167	707	5.79	9.7	3.4
L5	0.036	1171	710	5.83	9.2	3.3
L6	0.034	1169	708	5.77	10.1	3.6
			Average	5.84	9.1	3.2

9.3 RESULTS AND DISCUSSION

Descriptive statistics for the soil chemical properties of the soil used in the experiment, prior to the application of treatments are given in Table 9.4. The soil property statistics of the samples used in the trial, are representative of those in the populations described in Chapter III.

Table 9.4 Soil chemical property description prior to the application of treatments, *n* = 16

Soil property	Mean	S.D.	Median	Range
pH_{CaCl_2}	4.57	0.29	4.56	4.14 – 5.33
pH_{H_2O}	5.54	0.35	5.51	5.07 – 6.50
OC dag/kg	1.40	0.30	1.40	0.92 – 1.98
Clay dag/kg	14	3	14	8 – 22
CEC mmol(+)/kg	39.9	13.8	35.0	24.3 –72.1
Al mmol(+)/kg	2.18	1.72	1.71	0.70 – 7.70
Al_{Sat} %	6.6	5.9	4.8	1.5 – 23.3
Mehlich pH_{buffer}	5.84	0.13	5.83	5.54 – 6.08
LR(7.0) Mg/Ha	9.0	1.9	9.1	5.5 – 13.5
NO_3 mg/kg	6.2	5.0	4.5	1.0 – 15.0
P(Colwell) mg/kg	13.1	4.5	13.0	6.0 – 21.0
Na mmol(+)/kg	0.73	0.29	0.7	0.4 – 1.4
K (exch.) mmol(+)/kg	6.2	3.0	5.5	2.0 – 13.0
Ca mmol(+)/kg	23.6	9.9	20.0	11.0 – 42.0
Mg mmol(+)/kg	6.6	3.4	5.5	3.0 – 14.0

All three groups of pots corresponding to the NL, SRL and VRL were fertilised according to soil analysis results (Table 9.4) and assumed an achievable grain yield of 2.8 Mg/ha. Ample amounts of N, P and K fertilisers were applied to the soil in each group to remove effects related to the infertility of soil. Table 9.5 shows the soil test results of the three groups after the application of fertiliser. There were no significant fertility differences in the soils from each treatment group at a 5 % probability level (Table 9.5). Adequate amounts of fertiliser were applied to each group, and the adverse effects on plant growth resulting form nutrient infertility were successfully prevented.

Table 9.5 Soil nutrient status post-fertilisation (and pre-liming) for the pots in each of the three treatment groups

Group treatment	NO_3-N (mg/kg)		Pcol (mg/kg)		Kexch. (mmol(+)/kg)	
	Mean	S.D	Mean	S.D	Mean	S.D
NL	78.5	9.1	62.4	10.9	13.9	2.6
SRL	80.1	7.5	60.9	7.7	13.8	2.7
VRL	77.9	8.6	63.4	8.4	13.4	2.3
p- value	0.75		0.74		0.82	

The reaction rate of the lime is thought to have been influenced by the presence of high levels of fertiliser salts in the soil, resulting in greater displacement of exchangeable Al and H^+ into the soil solution. Adams (1984) has reported this effect.

9.3.1 SOIL PROPERTY COMPARISONS BETWEEN TREATMENTS

The effects of NL, SRL and VRL on relevant soil properties are compared in Table 9.6.

Table 9.6 Descriptive statistics for soil properties in each of the three treatment groups after the application of lime

Treatment group	pH_{CaCl_2}		Ca (mmol(+)/kg)		Al (mmol(+)/kg)		CEC (mmol(+)/kg)	
	Mean	S.D	Mean	S.D	Mean	S.D	Mean	S.D
NL	4.57	0.29	23.6	9.9	2.18*	1.72	39.9	13.8
SRL	5.94*	0.56	44.0*	7.8	0.42	0.15	72.6*	11.1
VRL	6.81*	0.21	57.1*	4.8	0.27	0.12	89.1*	6.0

Note: * indicate significant differences between the treatment groups at 5 % probability level.

The three treatments produced significantly different soil pH_{CaCl_2}, calcium and CEC property values (Table 9.6). SRL and VRL produced similar mean Al values, which were significantly different to NL (Table 9.6). The pH_{CaCl_2} of the soil in the VRL samples were closest to the pre-determined target value of 7.0, which estimated pot-specific lime requirements. This result highlights the advantage of VRL. The standard deviations of

pH_{CaCl_2} values, and the other soil properties in the VRL treatment tended to be narrower than for the distributions of SRL and NL (Table 9.6). This suggests that the soil samples were to some extent homogenised by the variable-rate lime applications.

The magnitude of the cations contributing to the CEC is particularly relevant to plant growth. Table 9.7 shows the percent cation saturation of the CEC for the two management treatments and the unlimed soil. It also indicates the desirable ranges for optimal plant growth.

Table 9.7 Cation saturation of the CEC after no lime applications (NL), single-rate liming (SRL) and variable-rate liming (VRL). Desirable levels for plant growth taken from Hazelton & Murphy (1992)

Cation Saturation		Actual range of soil		Desirable range for
% CEC	NL	SRL	VRL	plant growth
Ca	45 – 68*	73 – 94	68 - 96	60 – 80
Mg	9 – 22*	4 – 13	4 - 12	10 – 15
K	7 – 25	13 – 29	13 - 23	1 – 5
Na	0.7 – 4.8*	0.5 – 1.7	0.5 – 1.8	0 – 1
Al	1.5 – 23.3*	0.3 – 1.1	0.1 – 0.5	< 5
Ca:Mg	2 - 7*	4 - 18	6 - 20	4 - 6

Note: * Indicates significant differences between the treatment groups at 5 % probability level.

There were no significant differences between the soil's cation saturation levels after SRL and VRL (Table 9.7). Liming generally lowered the Na and Al saturation of the CEC to more desirable levels. The proportion of Mg^{2+} decreased with increasing rates of liming, suggesting its displacement by Ca^{2+}, and subsequent leaching. Further comments and graphical interpretations of the comparisons are provided in the following section.

9.3.2 IMPORTANT SOIL PROPERTY INTERACTIONS IN ACID SOIL

The dynamics of soil property interactions in acid soil and the effects of amelioration on soil quality and plant growth demand investigation of a number of pertinent soil parameters and their interactions. The difficulties encountered in diagnosing the specific cause of acid soil infertility may arise from the complexity of the processes involved. Before looking at soil-plant interactions and the pot trial itself, soil chemical property relationships will be ascertained in an attempt to establish interactions and deduce the most limiting factors to plant growth in the acid soil of the experimental field.

Soil Property Correlations

Correlations between pairs of soil variables were used to summarise the strength of the linear relationships amid relevant properties of the soils used in the experiment. The correlations were calculated before the application of treatments. These are shown in Table 9.8. Both soil pH_{CaCl_2} and pH_{H_2O} were well correlated with CEC (and its individual constituent cations), pH_{buffer} and lime requirement. As expected, the soil's CEC showed good correlations to OC and Clay content. The lime requirement of the soil was negatively correlated to pH_{CaCl_2} and pH_{H_2O} and positively correlated with exchangeable Al, correlation coefficients were –0.64, -0.75 and 0.66, respectively.

Soil pH and Lime Requirement

The first relationship considered (Figure 9.2) is that between soil pH and the lime requirement of each of the 16 soil samples used in the pot experiment.

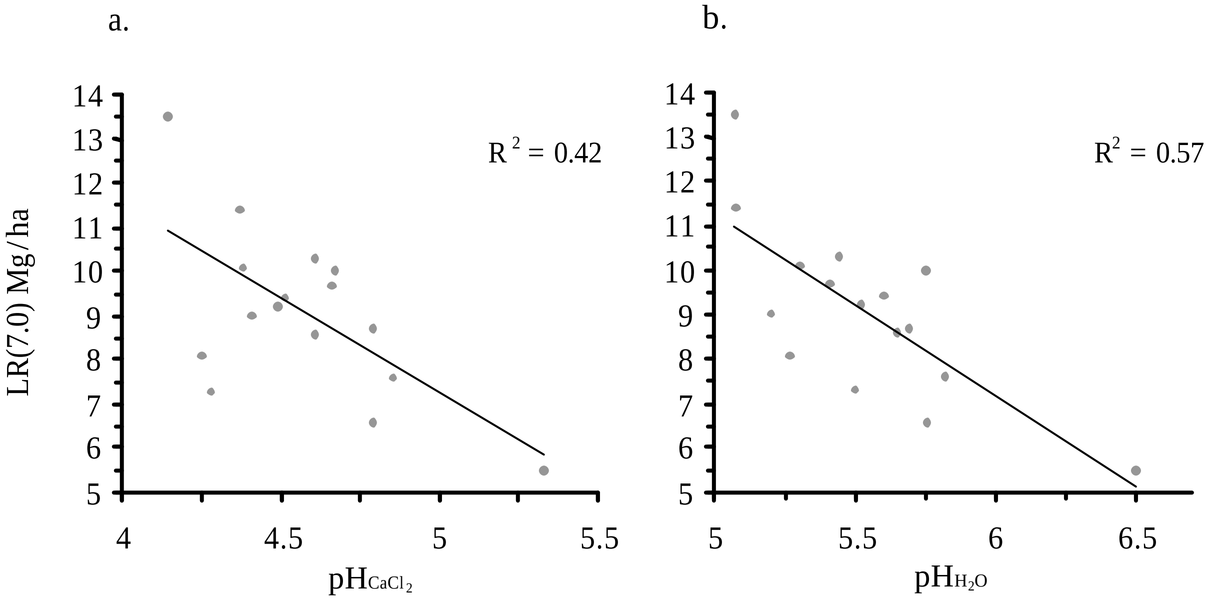


Figure 9.2 Relationships between (a.) pH_{CaCl_2} and lime requirement to a target pH_{CaCl_2} of 7.0 (LR(7.0)), and (b.) pH_{H_2O} and LR(7.0)

pH_{CaCl_2} accounted for 42 % of the variation in lime requirement and pH_{H_2O} accounted for 57 % (Figure 9.2). Soil pH alone poorly defines the amount of lime needed to amend acid soil. These findings are not unusual, *e.g.* Pionke *et al.* (1968), Aitken *et al.* (1990) (Chapter

Table 9.8 Correlations between soil properties for the soils used in the experiment

Soil property	pH_{CaCl_2}	pH_{H_2O}	OC	Clay	Al	CEC	pH_{buffer}	LR(7.0)	NO_3-N	P(Col.)	K(exch.)	Ca	Mg
pH_{CaCl_2}	1												
pH_{H_2O}	0.91	1											
OC %	0.38	0.4	1										
Clay %	0.3	0.26	0.46	1									
Al mmol(+)/kg	-0.64	-0.57	0.07	-0.28	1								
CEC mmol(+)/kg	0.77	0.77	0.71	0.69	-0.46	1							
pH_{buffer}	0.64	0.75	-0.09	-0.29	-0.66	0.26	1						
LR(7.0) Mg/Ha	-0.64	-0.75	0.08	0.3	0.66	-0.26	-1	1					
NO_3-N mg/kg	-0.14	-0.14	0.2	0.22	-0.21	0.25	-0.11	0.11	1				
P (Colwell) mg/kg	-0.54	-0.48	-0.03	-0.08	0.3	-0.36	-0.31	0.31	0.07	1			
K (exch.) mmol(+)/kg	0.69	0.67	0.57	0.37	-0.53	0.73	0.4	-0.4	0.06	-0.21	1		
Ca mmol(+)/kg	0.81	0.79	0.65	0.6	-0.5	0.96	0.31	-0.31	0.25	-0.42	0.65	1	
Mg mmol(+)/kg	0.59	0.61	0.62	0.83	-0.41	0.94	0.07	-0.07	0.35	-0.31	0.56	0.92	1

VIII). Although pH is commonly used as an indicator of whether or not a soil should be limed, measurements of soil pH and lime requirement are dependent on different soil properties. Soil pH depends on and measures the hydrogen ion activity in soil while lime requirement depends on the buffering capacity of the soil, the soil pH, the reason for liming and the amount of exchangeable Al in the soil solution (Chapter VIII).

Soil pH and Aluminium

It is well known that Al^{3+} is the aluminium species that is phytotoxic, while Al complexed with organic ions, SO_4^{2-} and F^- are not (Cameron *et al.*, 1986; Chapter VI). Describing the relative toxicities of Al^{3+}, $AlOH^{2+}$ and $Al(OH)_2^+$ is difficult but it has been shown that at potentially toxic levels, the activity of Al^{3+} is seven to ten times greater than that of the hydroxy-monomers (Helyar & Conyers, 1987).

As soil pH decreases the solubility of aluminium in the soil solution increases exponentially (Figure 9.3), and at pH_{CaCl_2} values below 5, its concentration in soil increases to levels that adversely affect plant growth (Foy, 1984; Kamprath, 1970). Helyar & Conyers (1987) indicated that the rate at which toxic aluminium levels are reached depends on the initial soil pH, the soil's buffering capacity and the rate of H^+ addition. Hence aluminium phytotoxicity may occur at various pH levels depending on soil type and the plant species grown.

Although the symptoms of aluminium toxicity in crops are varied and complex, much of the literature suggests that aluminium toxicity is primarily associated with alterations in root physiology and function (Kochian & Shaff, 1991; Ritchie, 1989; Cameron *et al.*, 1986). These effects will be discussed in a later section of this chapter. Relationships between pH_{CaCl_2} and pH_{H_2O} and each of exchangeable Al and Al saturation of the CEC for NL, SRL and VRL simultaneously, are given in Figure 9.3a through to Figure 9.3d.

Both SRL and VRL raised soil pH and consequently lowered exchangeable Al and Al saturation of the CEC to safe levels for plant growth (Figure 9.3). At pH_{CaCl_2} values above 5 ($pH_{H_2O} > 6$) negligible levels of Al were present. There is documented evidence suggesting that in acid soils, the beneficial effects of liming (Chapters VI and VIII) are partly due to the inactivation of exchangeable Al (*e.g.* Kamprath, 1970; Reeve & Sumner, 1970). However due to the variation in soil types, methods of Al extraction and levels of tolerance by different crops there isn't a widely accepted critical indicator value below which it may be assumed that there is little or no exchangeable Al in the soil. Sometimes a pH_{CaCl_2} of 4.5 ($pH_{H_2O} < 5.5$) is used as the somewhat 'fuzzy' rule-of-thumb value below which aluminium phytotoxicity is less likely to occur (Hazelton & Murphy, 1992; Juo, 1977). Reeve & Sumner (1970) suggested that maximum crop response may be observed when exchangeable Al falls below 2 mmol(+)/kg soil. Figure 9.3a and Figure 9.3b indicate that for the Kelso soil used in the pot trial, a pH_{CaCl_2} value of 4.5 corresponds to 2.2 mmol(+)/kg of exchangeable Al and 5 % Al saturation, respectively (dashed lines). Corresponding pH_{H_2O} values are shown in Figures 9.3c and 9.3d. Using this rule-of-thumb value, approximately half of the unlimed samples fall below the exchangeable Al threshold.

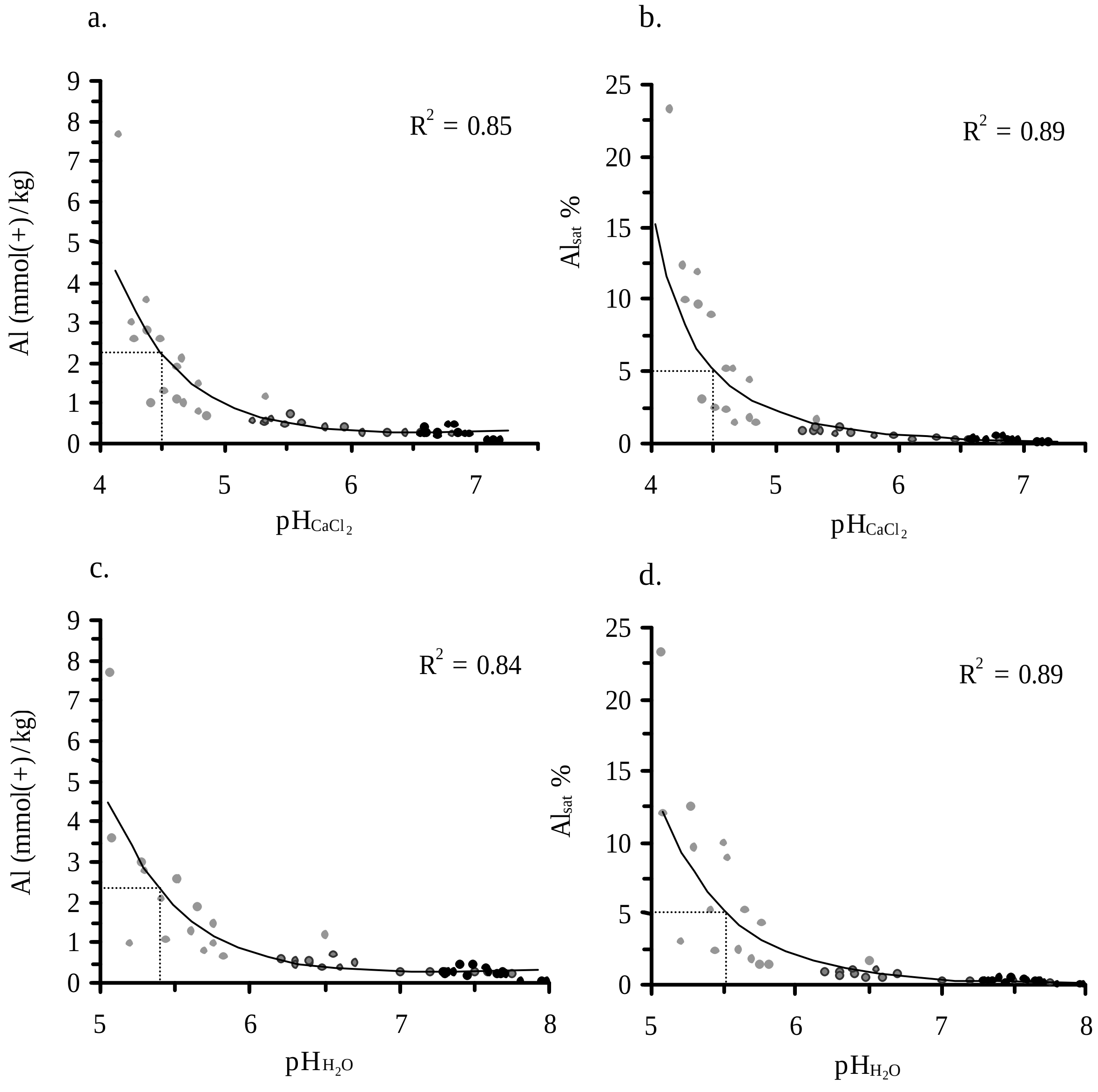


Figure 9.3 Relationships between (a.) pH_{CaCl_2} and exchangeable Al, and (b.) pH_{CaCl_2} and Al saturation of the CEC. (c.) and (d.) illustrate corresponding relationships between pH_{H_2O} and aluminium. Light grey points represent the no lime group, grey points represent single rate and solid black points represent variable-rate liming.

Aluminium and Lime Requirement

There has been much research supporting the proposition that lime requirements could be based on solely the inactivation of exchangeable Al, and some strong statements have been made suggesting its advantages. For example, Reeve & Sumner (1970) indicated that on average only one-sixth as much lime as that determined using the Shoemaker, McLean and Pratt (SMP) lime-requirement buffer to a target pH of 6.5 was necessary to eliminate aluminium toxicity and promote maximum crop growth. Chapter VIII describes some of the methods used to determine the liming needs of acid soil based on estimates of exchangeable Al. However, because the lime requirement of acid soil also depends on the initial soil pH, the buffering capacity of the soil (which in itself results from a combination of chemical reactions), and the reasons for liming, it is unlikely that exchangeable Al alone will provide an adequate estimation of lime requirement. As was previously suggested, the lime-requirement buffer methods take these factors into account and provide more reliable predictions of lime requirement (Chapter VIII). In the context of this work, the buffer methodology used with the response surface models derived in Chapter VIII, may be better incorporated into the SDSS of the continuous management system proposed in Chapter VI.

Figures 9.4a and b, respectively, show the relationships between exchangeable Al and lime requirement, and Al saturation and lime requirement for the 16 soil samples used in the pot trial.

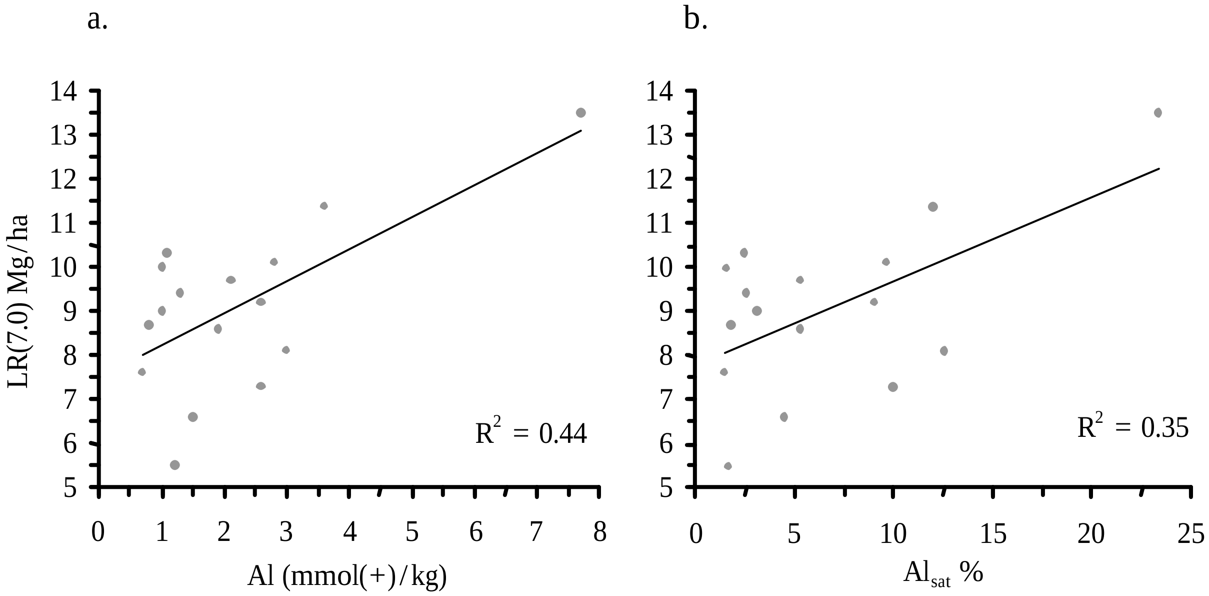


Figure 9.4 Relationships between (a.) exchangeable Al and lime requirement to a target pH of 7 (LR(7.0)), and (b.) Al saturation and LR(7.0).

The lack of a clear relationship in Figure 9.4 suggests the inappropriateness of lime requirement calculations based on solely exchangeable Al. As previously indicated, there are other important factors to consider when determining the lime requirement of acid soil (Figure 9.4). Aitken (1992) and Aitken *et al.* (1995) reported similar results, and indicated that liming rates required to reduce exchangeable Al to a predetermined level were far in excess of the rates calculated from the exchangeable Al values, even when a liming factor of two (suggested by Kamprath, 1970) was used.

Soil pH, Aluminium and CEC

The ability of the soil to hold and exchange cations has obvious implications on its elemental properties, its pH, nutrient availability, and its reactions to lime and fertiliser applications. The relationships between pH_{CaCl_2} and CEC, and Al saturation and CEC are shown in Figures 9.5a and 9.5b respectively. These figures are used to illustrate the effect of acidic sandy soil on the CEC in a temperate region (refer to Chapter III).

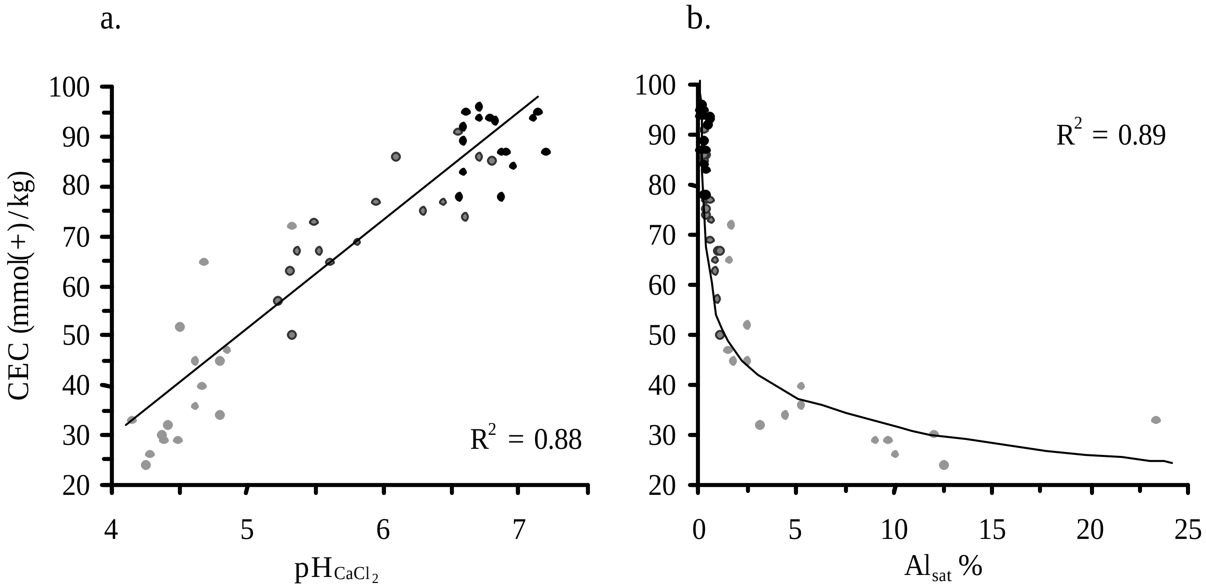


Figure 9.5 Relationships between (a.) pH_{CaCl_2} and CEC, and (b.) Al saturation and CEC. Light grey points represent the no lime group, dark grey points represent single-rate and solid black points represent variable-rate liming. The means for each group are given in Table 9.6

The CEC values of acidic, unlimed soil samples (light grey points in Figure 9.5) were extremely low, ranging from 24 to 72 mmol(+)/kg of soil (also Table 9.6). Although SRL and VRL supplied adequate amounts of Ca that contributed to the CEC (Figure 9.5), CEC values remained lower than the moderately typical levels of 120 to 250 mmol(+)/kg (Hazelton & Murphy, 1992). The increase in CEC due to liming is accomplished by the change in pH and the deprotonation of the surfaces of variable charge minerals and functional groups of humic compounds caused by Ca^{2+}. The greater amount of negative charge available on the surfaces of these minerals results in the increase in CEC (Figures 9.5a).

As the soil becomes more acidic and exchangeable Al increases, the CEC decreases (Figure 9.5). The reason for this may be that the solubility or availability of certain basic cations (*e.g.* calcium) that have a greater contribution to the CEC, are antagonised by increasing levels of soluble Al, lowering basic cation uptake (Sumner *et al.*, 1991). Applications of dolomite (*i.e.* $CaMg(CO_3)_2$) may have been more beneficial in this experiment to augment the magnesium levels of the soil and further raise the CEC of the soil to achieve a more balanced Ca:Mg ratio (Table 9.7). Magnesium levels decreased after liming (Table 9.7). Edmeades (1982) and Edmeades *et al.* (1985) also reported decreases in exchangeable Mg with increasing rates of liming and suggested that the displacement of Mg by Ca caused an increased concentration of Mg in solution, and its potential for leaching. Aitken *et al.* (1998) also suggested that applications of lime at rates greater than 4 Mg/ha effectively reduced exchangeable Mg due to the ease of displacement of the cation by Ca from the exchange complex.

Both the amounts of clay and organic matter in soil affect the CEC. Soils with high clay content and organic matter usually have a high CEC. Organic complexes are potentially large repositories for basic cations in soil, and particularly Ca, when soils are limed (Sumner *et al.*, 1991). In this instance, the low levels of clay and organic carbon in the soil samples (Table 9.4), and their relatively high correlation with the CEC (r = 0.69 and 0.71, respectively (Table 9.8)), may provide an explanation for the very low CEC values.

Despite the low CEC values after lime applications, the increase in CEC per unit pH_{CaCl_2} increase due to liming was calculated as at 22 mmol(+)/kg per pH unit (Figure 9.5a). This considerable increase is the often-ignored beneficial effect of liming on the CEC of acid soil. Variable-rate liming resulted in higher mean CEC values than SRL and NL (Table 9.6).

Soil pH, Aluminium and Calcium

Calcium is the dominant exchangeable basic nutrient cations in the majority of agricultural soils (Dolling & Ritchie, 1985). The main equilibria determining the solubility of Ca in soil involves $CaCO_3$, soil-Ca and simple cation exchange (Sumner *et al.*, 1991). In acid soil the amount of Ca in the soil solution is low (Figure 9.6a) and when lime is applied it dissolves readily producing Ca^{2+} (Chapter VI), which is held on cation exchange sites. Changes in exchangeable Ca and Ca saturation of the CEC with pH_{CaCl_2} for the 16 soils before and after SRL and VRL, are shown in Figure 9.6.

Both SRL and VRL applications raised the exchangeable Ca of the soil to optimal levels (Figure 9.6a), however there were no statistically significant differences in the Ca saturation of the CEC between SRL and VRL (Table 9.7). A pH_{CaCl_2} value of 4.5 has been suggested as the critical pH_{CaCl_2} below which Al phytotoxicity occurs. The corresponding values for exchangeable Ca and Ca saturation of the CEC are in turn, 23 mmol(+)/kg of soil and 54 % (Figures 9.6a and 9.6b respectively).

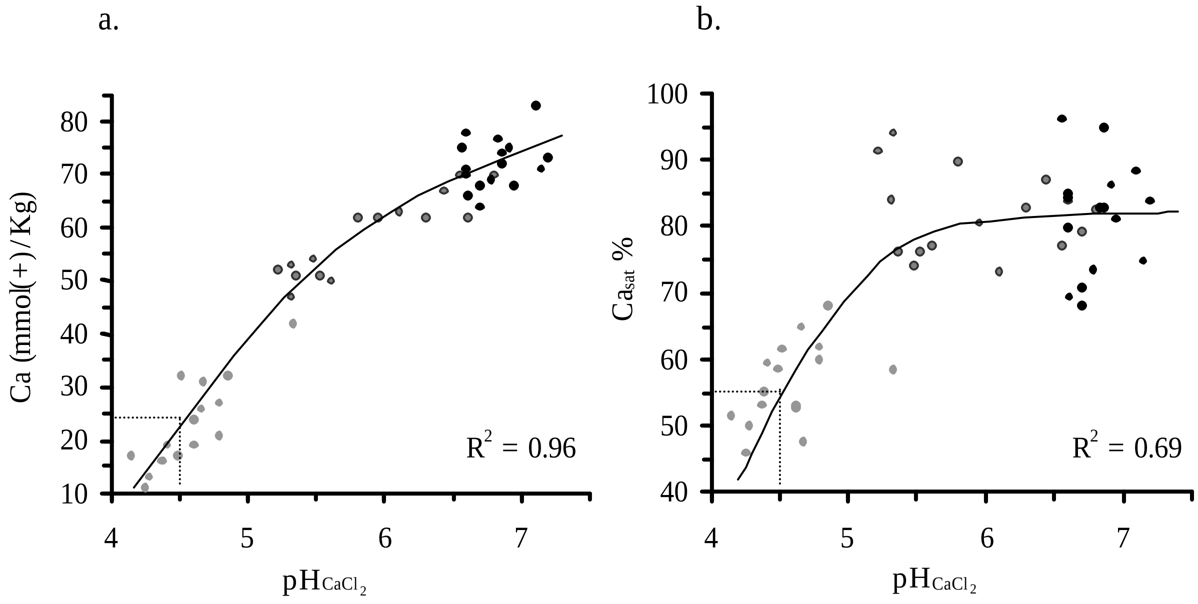


Figure 9.6 Relationships between (a.) pH_{CaCl_2} and exchangeable Ca and (b.) pH_{CaCl_2} and Ca saturation. Light grey points represent the no lime group, dark grey points represent single-rate and solid black points represent variable-rate liming. The means for each group are given in Table 9.6

These values are similar to critical values for Ca-deficient soil suggested by Hazelton & Murphy (1992) for soil types that occur in NSW. The authors indicated that Al phytotoxicity is most likely to affect crop production when exchangeable Ca levels fall below 25 mmol(+)/kg and the Ca saturation below 60 %.

Calcium deficiency is often associated with Al toxicity in acid soils because of the excessive leaching of Ca^{2+} and the higher relative exchange power of Al^{3+} (Norton & Zhang, 1998). Considerable amounts of evidence also exists suggesting the physiological antagonistic effect of Ca on Al in plants, (*e.g.* Foy, 1984; Alva *et al.*, 1986; Noble *et al.*, 1988; Edmeades *et al.*, 1991). That is, when Ca^{2+} levels are high Al^{3+} is reduced to non-toxic levels, and the opposite is true when Ca^{2+} levels are low. Figure 9.7 illustrates this effect.

Figure 9.7a shows that as Al saturation increases the concentration of exchangeable Ca decreases rapidly to levels that are deemed insufficient to maintain healthy plant growth. In Figure 9.7a, the critical exchangeable Ca levels (below which Al toxicity is most likely to occur) of 25 mmol(+)/kg suggested by Hazelton & Murphy (1992) corresponds to an Al saturation of approximately 5 % (dashed line in Figure 9.7a). Accordingly in Figure 9.7b, an Al saturation of 5 % corresponds to a Ca saturation of 58 % (dashed line), which is approximately the critical level (60 %) for sub-optimal plant growth. Figure 9.7 shows that both SRL and VRL raised the Ca concentration of the soils used in the pot trial to levels well above those that may hinder crop growth.

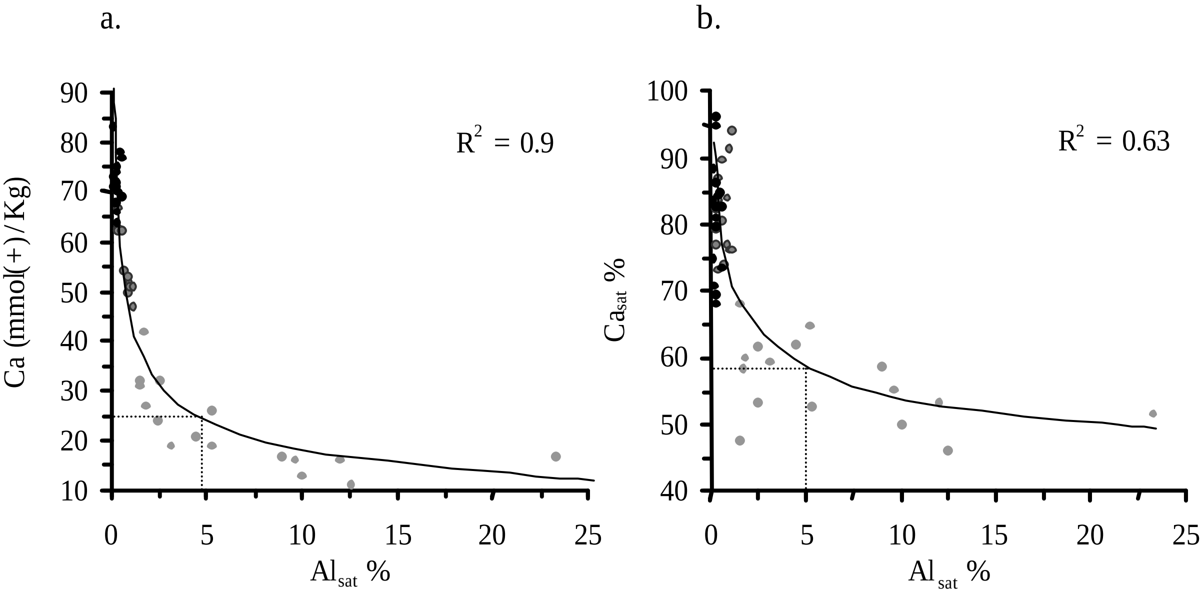
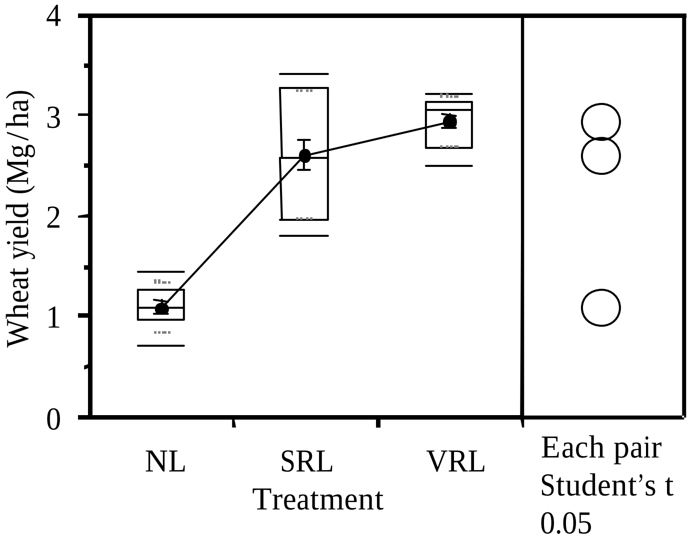


Figure 9.7 Relationships between (a.) Al saturation and exchangeable Ca and (b.) Al saturation and Ca saturation of the CEC. Light grey points represent the no lime group, dark grey points represent single-rate and solid black points represent variable-rate liming. The means for each group are given in Table 9.6

9.3.3 CROP YIELD COMPARISONS BETWEEN LIMING TREATMENTS

Reduced productivity in acid soils and crop response to liming (for a variety of crops) in eastern Australia have been widely reported. For example, wheat (Coventry *et al.*, 1997a; and Coventry *et al.*, 1997b), wheat (*Triticum aestivum*), barley (*Hordeum vulgare*), triticale (*Triticosecale*) and canola (*Brassica napus*) (Slattery & Coventry, 1993), maize (*Zea mays*) (Moody *et al.*, 1995), and barley (Conyers *et al.*, 1991). Having established some of the important soil property interactions in acid soil, the focus of the chapter will now be directed towards a comparison of the effects on crop yield of no lime application, single-rate and variable-rate liming (Table 9.1). The effects of NL, SRL and VRL on wheat yield are summarised by the analysis-of-variance (ANOVA) in Figure 9.8.



ANOVA

Source	**DF**	**SS**	**MS**	**F-ratio**
Model	2	31.1	15.5	84.5
Error	45	8.3	0.18	**Prob. > F**
Total	47	39.3	0.84	< 0.0001

Figure 9.8 Analysis of variance between no lime (NL) application, single-rate liming (SRL) and variable-rate liming (VRL). Quantile boxes showing minimum, 10 %, 25 %, median (50 %), 75 %, 90 %, and maximum values of each treatment, mean dots and error bars, standard deviation lines (dashed lines) and means comparison circles are shown.

The soil elemental toxicity and nutrient deficiency effects on crop growth are clearly illustrated by the NL treatment group (Figure 9.8). The unlimed acid soil (NL) rendered significantly lower wheat yield than that which was amended using SRL which in-turn yielded significantly less than the soil corrected using VRL applications (Figure 9.8). The implications of these results are that liming acid soil (be it SRL or VRL) raises soil pH, increases crop yields and hence improves the economics of crop production. Furthermore, VRL improves resource allocation and crop production by preventing under and over applications. The economic implications of SRL and VRL are dealt with a simulation study in Chapter X.

The connected treatment means (Figure 9.8) provide an indication of the shape of the response function for soil pH and lime requirement. Remember that to both SRL and VRL treatments, the same total amount of lime was applied. The means comparison circles for each treatment group do not intersect, or intersect slightly (between SRL and VRL) suggesting that the means of each treatment are significantly different at 5% level of significance (Figure 9.8). The descriptive statistics for each treatment are given in Table 9.9.

Table 9.9 Wheat yield comparisons (Mg/ha) between the three treatments, *n* = 16

Treatment	Mean	S.D	Min.	Med.	Max.	CV %
NL	1.11*	0.26	0.46	1.11	1.47	23
SRL	2.62*	0.64	1.76	2.6	3.51	25
VRL	2.96	0.27	2.48	3.07	3.31	9

Note: * Indicates significant differences between the treatment groups at 5 % probability level.

Variable-rate liming resulted in a narrower yield distribution than that from SRL and NL (Figure 9.8 and Table 9.9). As with soil (section 9.3.1), yields were homogenised by the VRL applications. This response is shown by the much smaller coefficient of variation of the VRL treatment group (Table 9.9). The heterogeneity in wheat yields resulting from SRL may be attributed to the non-specific averaged 9.1 Mg/ha lime applications to the 16 pots, where misapplications of lime were inevitable. Under- and over-applications in the pots ranged from approximately -4.5 Mg/ha to +3.6 Mg/ha respectively (Table 9.9).

9.3.4 AGRONOMIC INTERACTIONS IN ACID SOIL

Soil nutrient infertility and its adverse effects on plant growth were 'blocked' by the provision of plentiful amounts of fertiliser to the three liming treatment groups (Table 9.1). Similarly, adequate amounts of water were supplied throughout the growing season; hence crop response to liming may be primarily attributed to the neutralisation of aluminium and hydrogen toxicities (pH), the provision of Ca and the consequent increase in the soil's CEC. The following sections will describe how these factors and their interrelations contribute to increases in crop response.

Yield Response to Soil pH

The aim of liming is to adjust acidic soil pH values to near-neutral or neutral levels (refer to Chapter VI), depending on not only soil, but crop requirements and the differing tolerances of crop varieties to pH, elemental toxicities and the previously mentioned factors associated with soil acidity. For example, in regions with granitic soils and approximately 500 mm average annual rainfall (refer to Chapter III), acid-sensitive crops like canola, certain wheat varieties and barley will not yield well below $\mathrm{pH_{CaCl_2}}$ 5.0, while tolerant crops like triticale and oats may still render at $\mathrm{pH_{CaCl_2}}$ values below 4.7. Wheat yield response to pH as effected by NL, SRL and VRL are shown in Figure 9.9.

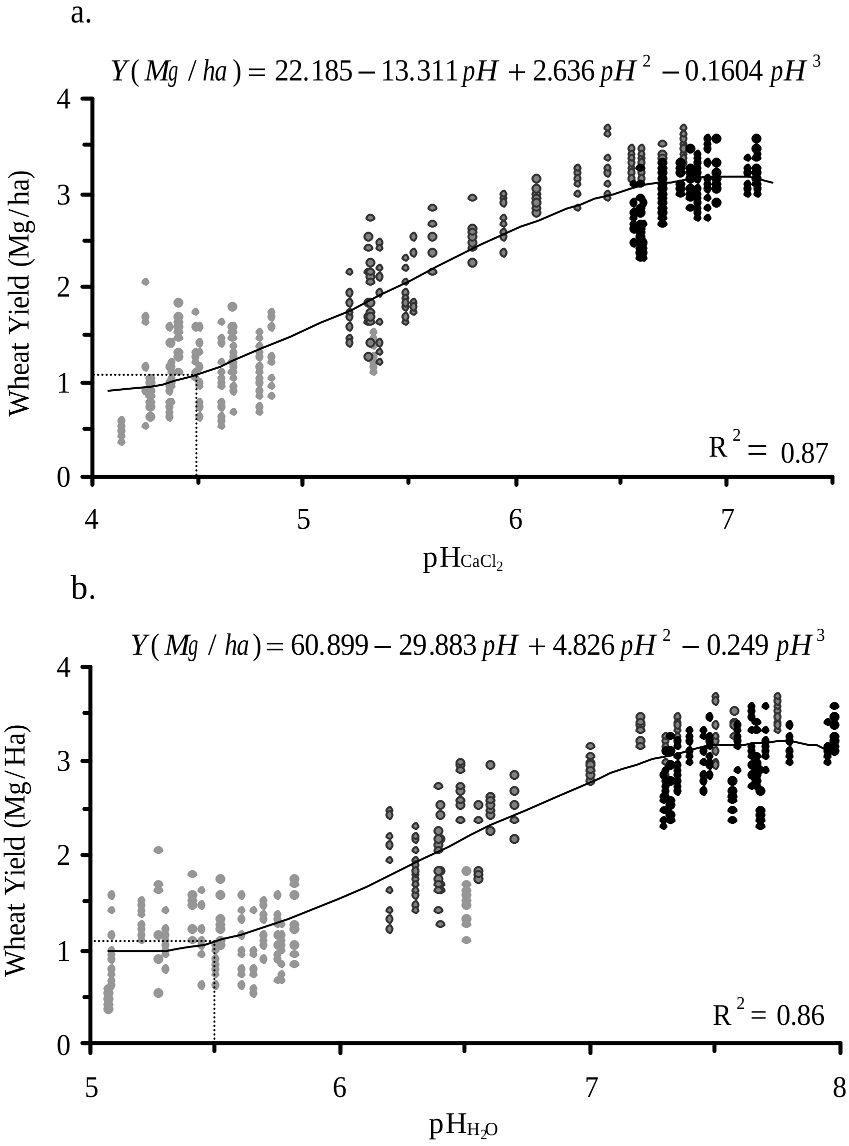


Figure 9.9 Wheat yield as a function of (a.) $\mathrm{pH_{CaCl_2}}$ and (b.) $\mathrm{pH_{H_2O}}$. Light grey points represent the no lime, dark grey points represent single-rate and solid black points represent variable-rate liming. The means for each group are given in Table 9.9.

The yield data points for the three treatment groups are shown in Figures 9.9a and 9.9b. A critical pH_{CaCl_2} value of 4.5 (pH_{H_2O} 5.5) below which adverse effects on plant growth may be experienced, corresponds to an average wheat yield of approximately 1.1 Mg/ha, which is the average yield of the NL treatment group. This result supports previous critical soil property values for plant growth in acid soil.

The heterogeneity in wheat yields resulting from SRL portrays the inefficiency of averaged lime applications where optimal pH values after liming, and hence wheat yields are not achieved. Conversely, the beneficial effects of VRL are clear (Figure 9.9). Optimal yields are achieved near the selected target pH of 7. Cubic polynomials adequately describe the yield response to pH.

Yield Response to Aluminium

Aluminium rhizotoxicity is one of the major constraints to crop production on acid soil (Foy, 1984). Large amounts of research have been conducted to elucidate the physiological and cellular basis of the mechanisms involved in the toxicity and tolerance of plants to high concentrations of Al (Huang *et al.*, 1995; Zeigler *et al.*, 1995; Parker, 1995; Cameron *et al.*, 1986). Typical symptoms of Al rhizotoxicity include damage to plant roots, which are typified by reductions in root length and necrosis of the root tip meristems caused by disturbances of the structure and function of the plasmalemma (Runge & Rode, 1991). The damage caused has obvious implications on crop growth and yield, producing a negative relationships between exchangeable Al and crop production (Soon, 1995). Relationships between wheat yield and exchangeable Al and Al saturation of the CEC for the soils in each treatment group are shown in Figure 9.10.

The yield from the NL treatment group was much lower than those from SRL or VRL (Figure 9.10a). For values of exchangeable Al greater than 2.2 mmol(+)/kg, the critical value for uninhibited crop growth, indicated by the dashed line in Figure 9.10a, yields may be expected to fall below the average NL yield of 1.1 Mg/ha. Similarly, Figure 9.10b, shows that when Al saturation is greater than 5% yields may be expected to fall below the average NL yields.

Exchangeable Al levels have been used as criterion for liming acid soil (Chapter VIII). However Figure 9.10 shows that higher yields may be expected from SRL and particularly VRL, both of which lime to pH values well above the critical aluminium levels. In this instance, lime was applied to attain a target pH_{CaCl_2} of 7. The higher yields may be due to the provision of nutrients such as Ca to the deficient soil as well as the amelioration of the antagonistic behaviour of Al on Ca uptake (refer to 9.3.3). van Raij (1991) reported similar results, indicating that highly profitable yield increases for a variety of crops were achieved by liming acid soil to pH values greater than 6, and commented on the benefits of liming well above critical aluminium levels. Coventry *et al.* (1989) concluded that exchangeable Al did not provide a useful diagnosis for liming acid soil and for wheat yield response.

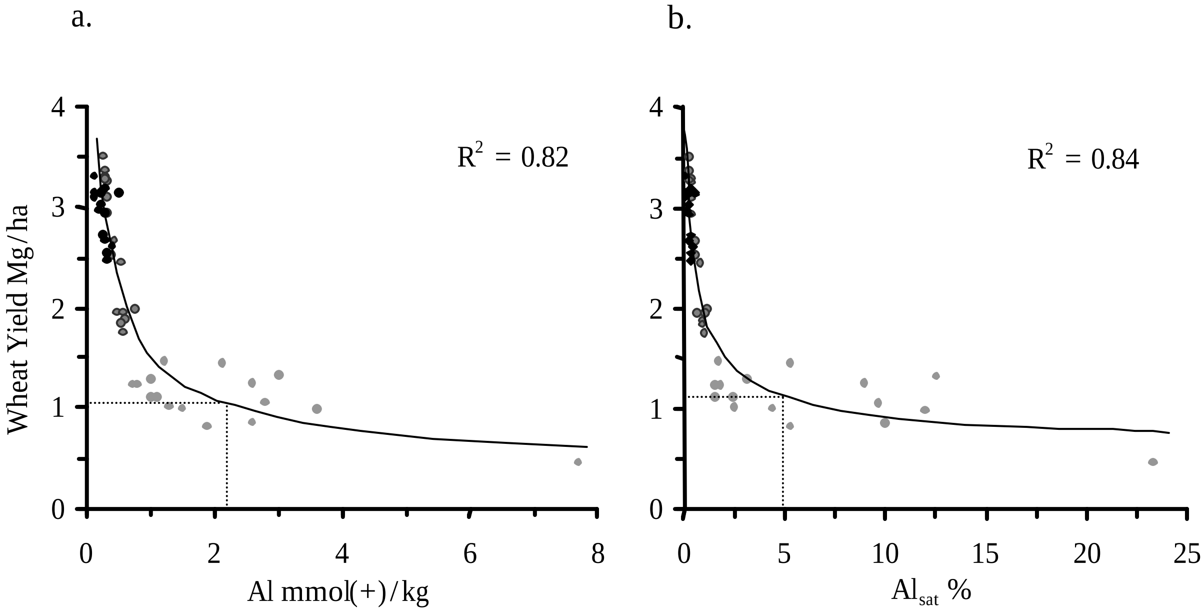


Figure 9.10 Wheat yield as a function of (a.) exchangeable Al and (b.) Al saturation. Light gray points represent the NL, dark gray points represent SRL and solid black points represent VRL. The means for each group are given in Tables 9.6 and 9.9.

Yield Response to Calcium and CEC

Calcium is absorbed by plants in relatively large amounts, so it is regarded as a macro-nutrient. It is necessary for cell growth and cell division, and also plays an important role in plant metabolism (Clark, 1984) and the regulation of plant cellular processes (Huang *et al.*, 1995). For example, Ca is required on the exterior surface of the plasmalemma where it plays a structural role in cell membranes; it is involved in the formation of ionic bridges in cell walls; it prevents membrane damage; and reduces water permeability (Clark, 1984).

Problems with Ca solubility or availability are rarely encountered in soil with near-neutral, neutral or alkaline pH values. However acid soil may be deficient in Ca or deficiency may be instigated by the presence of high concentrations of hydrogen (H) (that is non-exchangeable) and aluminium which depress calcium uptake (Sumner *et al.* 1991; Runge & Rode, 1991). This antagonistic effect of H^+ and Al^{3+} on Ca^{2+} uptake has been interpreted as evidence of the specific requirement for Ca (hence liming) to increase soil pH and reduce Al toxicity (Runge & Rode, 1991; Noble et al, 1988). When the concentration of Ca^{2+} in soil is low, continuous H^+ and Al^{3+} disruption of Ca^{2+} uptake and translocation in the plant may cause Ca deficiency, thus altering Ca^{2+} homeostasis and provoking metabolic malfunctions in cells that inhibit plant growth (Huang *et al.*, 1995). Relationships between Ca saturation, CEC and wheat yield are shown in Figure 9.11.

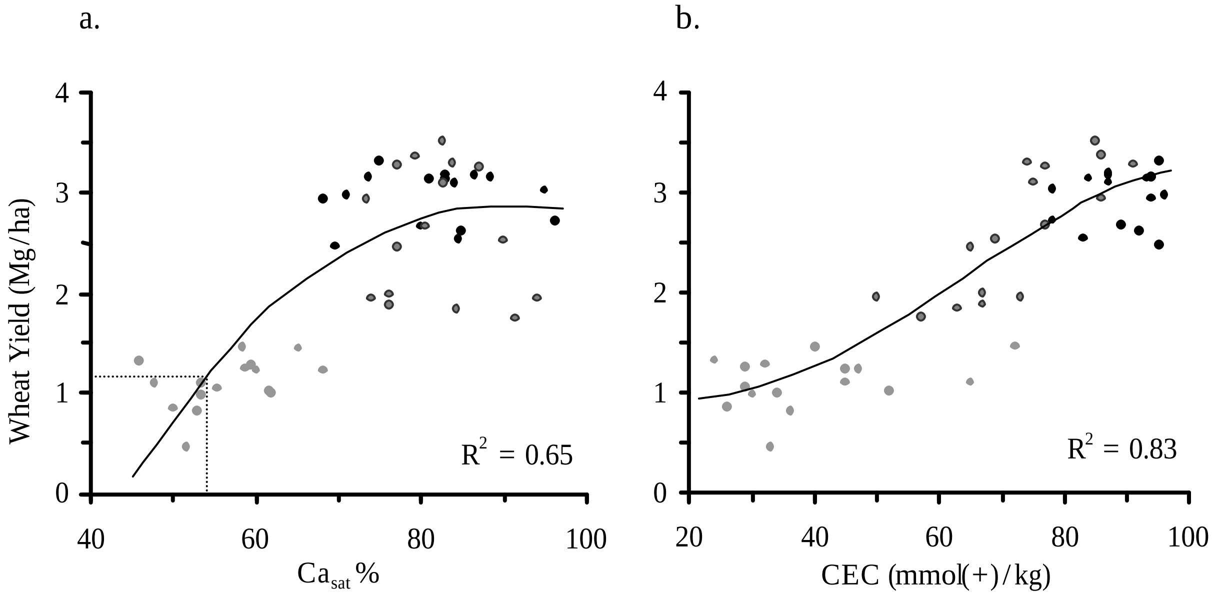


Figure 9.11 Wheat yield as a function of (a.) Ca saturation and (b.) CEC. Light grey points represent the no lime, dark grey points represent single-rate and solid black points represent variable-rate liming. The means for each group are given in Tables 9.6 and 9.9.

A value of 54 % Ca saturation was identified in section 9.3.2 as the critical level below which Ca deficiency and Al phytotoxicity are most pronounced. In accordance with previous results, Figure 9.11a shows that this value (dashed line) corresponds to the average yield for the NL treatment group. Optimal Ca saturation levels (between 60 % and 90 %) were achieved by both SRL and VRL, contributing to the production of optimal yields (Figure 9.11a).

Relatively moderate increases in the amount of lime applied (and thus pH) caused rapid increases in Ca and CEC, indicating the presence of mostly pH-dependent charge and a soil with very low CEC. Both SRL and VRL raised the soil's CEC to levels that produced higher yields than NL (Figure 9.11b). VRL produced a higher and narrower CEC range (Table 9.6) than SRL. These effects were reflected by their contribution to the higher wheat yields.

9.4 CONCLUDING REMARKS

The significance of this chapter in the context of the work lies in its authentication of the methodology developed in Chapter VIII – the derivation of a suitable method that may be incorporated into the spatial decision-support system of the continuous system for the management of acid soil (Chapter VI).

The glasshouse experiment was also conducted to study soil property interactions and soil-plant relationships in acid and ameliorated soil, to compare the effects of no lime applications, single-rate and variable-rate liming. The results accentuate the dynamics of soil interactions at low pH and the difficulty in deriving one specific cause for acid soil infertility. As in other studies, aluminium was found to be a limiting factor for plant growth below pH_{CaCl_2} 4.5. The antagonistic effect of aluminium on calcium was demonstrated and critical values were identified. The CEC of the soil was initially very low, however considerable increases resulted from liming, this being an often overlooked benefit of amelioration by lime. All of these properties and their interactions were determined in the study and all were found to contribute to acid soil infertility. Relationships between soil properties (before and after liming) and crop yields were established by looking at yield response as functions of pH, aluminium, calcium and CEC. The benefits of liming acid soil were clearly illustrated in all examples, as well as the significant advantages of variable-rate liming.

In all of the relationships drawn, the untreated soil, that amended using a single-rate application of lime and that using a variable-rate liming were graphically differentiated. The benefits of liming acid soil were confirmed. Results from the yield comparison between the three treatments also provided the theoretical basis for VRL in the experimental field. That is, results from the controlled experiments presented in this chapter suggest that the null hypothesis of PA may be rejected in favour of differential liming. However this may be a premature conclusion because no field experiments and no economic analysis were conducted. Chapter X explores these points further by means of a simulation study that also presents an economic sensitivity analysis for liming in southeastern Australia.

It is acknowledged that while glasshouse experiments are cheaper and more convenient than field trials, they are beset with some additional problems. For example the plant rooting volume is limited, only one soil horizon is usually examined, etc., hence the response observed from pot trials may not accurately relate to field situations. Although glasshouse experiments are useful in an exploratory and theoretical sense, confirmations of results by field trials are essential.

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Chapter X

GEOSTATISTICAL ASSESSMENT OF THE PRODUCTION AND ECONOMIC RISKS OF SITE-SPECIFIC LIME APPLICATIONS

ABSTRACT

Precision agriculture offers the potential to improve the efficiency and environmental impact of conventional crop production systems. However, its implementation will depend on the farmer's perception of how the adoption of technology will increase his yields and gross margins, and lower production risk. This chapter presents an approach to deal with this type of decision making. The consequences of three management scenarios (no lime, single-rate liming and site-specific lime applications to acidic field soil) were assessed in terms of production and economic risks. The methodology involved modelling the uncertainty in wheat yield, accounting for the local uncertainties in soil pH and lime requirement determinations, and the uncertainties in the crop model parameters used in the simulations. Indicator kriging was used together with Latin Hypercube Sampling of the probability distributions of variables and model parameters for the propagation of uncertainties through to the output yield and net profit maps. These maps together with a sensitivity analysis were used for decision making. Comparison of the three scenarios showed that under the economic conditions of the analysis, the optimum was reached for a single-rate application of 3.5 Mg/ha over the entire field instead of site-specific lime applications. Finally, a sensitivity analysis is presented for the adoption of site-specific lime applications in the experimental field.

10.1 INTRODUCTION

Throughout most of the 20th Century conventional agricultural land management at the field-scale consisted of simple, homogeneously applied input and output systems (Chapter I). Such 'uniform' management neglected the spatial and temporal variability of base resources, primarily soil and water, and ignored the energy and material flows within such systems. As such, significant resource misallocation may well have occurred causing adverse environmental conditions and socio-economic problems (Chapter I). Hence in agriculture, the management principle for the 21st Century must be to manage land by considering its heterogeneity in both space and time. This is the rationale behind PA (Chapters I, II, IV, and VI). If PA is to have a sound scientific basis and be successfully implemented, then the null hypothesis that remains to be tested is: 'given the variation in yields relative to the scale of a single field, then the optimal risk aversion strategy is uniform management' (McBratney *et al.*, 1997).

PA as site-specific management requires vast amounts of information to delineate the variation of relevant soil and crop properties within a field (Chapters II and IV). In the absence of field-deployed 'on-the-go' proximal soil sensing systems that can efficiently and economically collect high spatial resolution information (*e.g.* Chapter VII), the reliability of management decisions depends on the sampling strategy and analytical methodology (Chapter IV), the geostatistical techniques used for map production (Wollenhaupt *et al.*, 1997; Chapter V), and the uncertainty of the system (McBratney, 1992).

Geostatistics in soil science has been used for the quantification of geo-referenced spatial data and interpolation by kriging (Chapter II). Similarly, in PA kriging is used to enhance sparse soil information and to provide a detailed representation of the spatial variation of the desired properties for site-specific management (Chapter II, IV and V). However it is important to keep in mind that kriging estimates are not true values. The prediction error, or more generally the uncertainty about the soil attribute at an unsampled location, must be assessed and accounted for in any decision-making process. Geostatistics provide tools for deriving the set of possible outcomes at any single location as well as the associated probability of occurrence (Goovaerts, 1999).

Even if actual soil property values were known everywhere, the prediction of yield would still be uncertain because of our imperfect knowledge of underlying mechanisms. Therefore, the uncertainty about crop yield arises from both the uncertainty about the soil properties and the uncertainty about the parameters of the models used to derive crop yield. For example, in determinations of lime requirement (LR) within a field, even if actual $\mathrm{pH}_{\mathrm{buffer}}$ values were known everywhere, the amount of lime required to reach a target $\mathrm{pH}_{\mathrm{CaCl_2}}$ would still be uncertain because of our imperfect knowledge of the exact impact of liming on acid soil. Similar uncertainties affect the prediction of crop yield from only soil pH. Therefore, the uncertainty about crop yield arises from both the uncertainty about the soil properties and the uncertainty about the parameters of the models used to derive crop yield. While this concept of propagation of uncertainty is well known for GIS operations (Heuvelink *et al.*, 1989), it has only recently received attention in soil science (Pebesma & Heuvelink, 1999; van Meirvenne & Goovaerts, 2001; Hansen *et al.*, 1999).

This chapter presents a procedure whereby indicator kriging (IK) (Journel, 1983) and Latin Hypercube Sampling (LHS) (McKay *et al.*, 1979) of the resultant probability distributions are used together with regression functions for the propagation of uncertainties about crop response to uniform and site-specific management. To illustrate the technique, the production and economic risks of two liming management scenarios (single-rate and site-specific liming) and no lime application were assessed for the soil in the experimental field (described in Chapter III). Indicator kriging of Mehlich pH_{buffer} values was followed by LHS of the probability distributions to generate a set of possible pH_{buffer} values at each location. These simulated pH_{buffer} values were used in two regression models to derive resultant distributions of pH_{CaCl_2} post-liming (Chapter VIII) and wheat yield (Chapter IX), respectively. Net profit for each management scenario was computed as the difference between the expected revenue and the cost of liming. Finally, a sensitivity analysis for the adoption of site-specific liming in the experimental field was conducted.

10.2 THEORY

10.2.1 MODELLING LOCAL UNCERTAINTY USING INDICATOR KRIGING

Consider the problem of modelling the uncertainty about the value of a soil attribute s at the unsampled location $\mathbf{u}$ that is conditional to the set of n observations $\{s(\mathbf{u}_\alpha), \alpha = 1, 2,\ldots, n\}$. The probabilistic way to model uncertainty consists of viewing the unknown value $s(\mathbf{u})$ as a realization of the random variable $S(\mathbf{u})$ that is characterised by its conditional cumulative distribution function (*ccdf*):

$$F(\mathbf{u}; s|(n)) = Prob\{S(\mathbf{u}) \leq s|(n)\} \tag{10.1}$$

where (n) denotes the set of conditional data. The ccdf fully models the uncertainty at $\mathbf{u}$ since it gives the probability that the unknown is no greater than any given threshold s.

In this research, the *ccdf* (10.1) has been modelled using the non-parametric technique of indicator kriging (IK) (Journel, 1983). IK estimates the value of the *ccdf* for a series of K threshold values s_k, discretising the range of variation of s:

$$F(\mathbf{u}; s_k|(n)) = Prob\{S(\mathbf{u}) \leq s_k|(n)\}, \quad k = 1,2,\ldots,K \tag{10.2}$$

The resolution of the discrete *ccdf* is then increased by interpolation within each class $[s_k, s_{k+1}]$ and extrapolation beyond the two extreme threshold values s_1 and s_K.

Implementation of IK is discussed in length in Goovaerts (1997, 1999) and only the key steps are presented here:

Each observation $s(\mathbf{u}_a)$ is coded into a vector of binary indicator values defined as:

$$i(\mathbf{u}_a ; s_k) = \begin{cases} 1 & \text{if } s(\mathbf{u}_a) \leq s_k \\ 0 & \text{otherwise} \end{cases} \qquad a = 1,\ldots,n \tag{10.3}$$

When an excessive number of threshold values are chosen the inference and computation becomes unnecessary and tedious, while with too few thresholds the details of the distribution are lost.

For each threshold value s_k, an indicator semi-variogram is calculated as:

$$\widehat{g}_I(\mathbf{h}; s_k) = \frac{1}{2N(\mathbf{h})} \sum_{a=1}^{\mathbf{N(h)}} [i(\mathbf{u}_a ; s_k) - i(\mathbf{u}_a + \mathbf{h}; s_k)]^2 \tag{10.4}$$

where $\mathbf{h}$ is the lag distance.

The set of indicator semi-variograms are modelled and used to derive the set of kriging weights that allow the computation of each *ccdf* value $F(\mathbf{u};s_k\,|\,(n))$ as a linear combination of surrounding indicator data:

$$F(\mathbf{u}; s_k|(n)) = E\{I(\mathbf{u}; s_k|(n))\} = i^*(\mathbf{u}; s_k), k = 1,2,\ldots,K \tag{10.5}$$

Once IK has been conducted for each threshold s_k, order-relation deviations are corrected using the techniques described in Deutsch & Journel (1998).

The value of s at location $\mathbf{u}$ can be estimated by the mean of the *ccdf*, called the E-type estimate, which is defined as:

$$s_E^*(\mathbf{u}) = \int_{-\infty}^{+\infty} s\, dF(\mathbf{u}; s|(n)) \tag{10.6}$$

In practice, equation 10.6 is approximated by the following discrete sum:

$$s_E^*(\mathbf{u}) \approx \sum_{k=1}^{K+1} \bar{s}_k \left[F(\mathbf{u}; s_k|(n)) - F(\mathbf{u}; s_{k-1}|(n))\right] \tag{10.7}$$

where s_k, $k = 1,\ldots,K$ are the K threshold values, and $\bar{s}_k$ is the mean of the class $[s_{k-1}, s_k]$.

The conditional variance $\sigma^2(\mathbf{u}\,|\,(n))$, which measures the spread of the *ccdf* around its mean $s_E^*(\mathbf{u})$, is respectively defined and approximated by:

$$
\begin{aligned}
s^{2}(\mathbf{u}) &= \int_{-\infty}^{+\infty} \left[s - s_{E}^{*}(\mathbf{u})\right]^{2} \times f\left(\mathbf{u}; s|(n)\right) ds \\
&\approx \sum_{k=1}^{K+1} \left[\bar{s}_{k} - s_{E}^{*}(\mathbf{u})\right]^{2} \times \left[F\left(\mathbf{u}; s_{k}|(n)\right) - F\left(\mathbf{u}; s_{k-1}|(n)\right)\right]
\end{aligned}
\qquad (10.8)
$$

10.2.2 PROPAGATION OF UNCERTAINTY

Consider the problem of assessing the uncertainty attached to the response value *y* (*e.g.* pH, crop yield) of a model, such as a regression used to determine resultant pH_{CaCl_2} values after liming, or a crop model. Two sources of uncertainty may be distinguished: uncertainty arising from the incomplete knowledge of the value of the input variable *s* at **u**, and uncertainty about the parameters of the function itself, say:

$$y(\mathbf{u}) = f(s(\mathbf{u})) = a + b \cdot s(\mathbf{u}) + \varepsilon$$

Where a and b are model parameters and ε Nor(0,σ^2). The uncertainty about the input variable is modelled by the *ccdf* $F(\mathbf{u};s\,|\,(n))$ while the uncertainty about the parameters may be modelled by building for each parameter *a* and *b* a probability distribution that is assumed to be Gaussian. If the model is a regression function, the mean and variance of each probability distribution, as well as the covariance between parameters, are determined automatically. Both sources of uncertainty can then be incorporated numerically by sampling randomly the different distributions of input values, model parameters and regression errors and feeding each combination of sampled values ($s^{(l)}(\mathbf{u})$, $a^{(l)}$, $b^{(l)}$, $e^{(l)}$) into the function *f*(.) to retrieve the corresponding *y*-value $y^{(l)}(\mathbf{u})$.

Practical implementation of the so-called Monte-Carlo simulation faces two problems. First, the random sampling of probability distributions is not very efficient and the total number of combinations required to sample the full space of uncertainty becomes prohibitive as more parameters are considered. Second, the probability distributions of correlated parameters cannot be sampled independently. Latin Hypercube Sampling (LHS) is an efficient way to generate random samples that include all the range of possible values (McKay *et al.*, 1979; Iman & Conover, 1980). The LHS procedure involves stratifying the probability distribution into *M* disjunct equiprobable classes, then drawing randomly a value within each class. In this way, the input distributions (in particular the lower and upper tails) are represented in their entirety. The process requires a much smaller sample than the Monte Carlo approach for a given degree of precision. Recent applications of LHS to soil science can be found in Pebesma & Heuvekink

(1999), van Meirvenne & Goovaerts (2001), Hansen *et al.* (1999) and Minasny & McBratney (2000).

If only two parameters are considered and M = 100, then 10 000 combinations of possible values can be created. If the parameters are correlated, such correlation should be reproduced by the 10 000 pairs of simulated values. This is performed by the following procedure (Davis, 1987):

1. Sample the standard normal probability distribution (zero mean and unit variance) using LHS (M = 100 classes). Repeat the procedure, as many times as there are parameters. In the above example, one would need to repeat the procedure twice, yielding two sets of 100 random numbers that can be combined into 10 000 pairs, $[v^{(l)}, w^{(l)}]$, l = 1,…,10 000.
2. Decompose the variance-covariance matrix of parameters, **C**, into the product of a lower and an upper triangular matrix: **C** = **L U** (lower-upper decomposition).
3. Premultiply each vector of two random numbers $[v^{(l)}, w^{(l)}]$ by the lower triangular matrix **L**, and add the vector of means of the two parameters $[m_a, m_b]$:

$$\begin{bmatrix} a^{(l)} \\ b^{(l)} \end{bmatrix} = \begin{bmatrix} \mathbf{L}_{11} & 0 \\ \mathbf{L}_{12} & \mathbf{L}_{22} \end{bmatrix} \cdot \begin{bmatrix} v^{(l)} \\ w^{(l)} \end{bmatrix} + \begin{bmatrix} m_a \\ m_b \end{bmatrix}$$

The assumption here again is that the parameters follow a Gaussian distribution. The two sets of 10 000 values $[a^{(l)}, b^{(l)}]$, l = 1,…,10 000 will be such that the mean of each parameter as well as their variance and correlation coefficient are reproduced.

10.3 MATERIAL AND METHODS

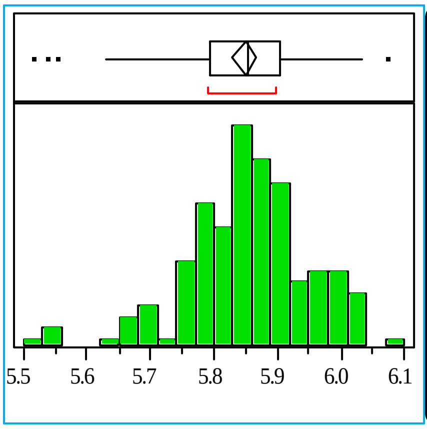
The field site for the research is described in Chapter III.

10.3.1 ANALYTICAL METHODOLOGY

Samples in duplicate were collected at 122 nodes of an approximately 40 m regular grid as described in Chapter III. For each of the 244 samples, soil $\mathrm{pH_{CaCl_2}}$ and $\mathrm{pH_{buffer}}$ were measured as described in Chapter III, and paired measurements were averaged, resulting in 122 observations. Chapter VIII described the derivation of a one-factor response surface model for predictions of LR. The empirical deterministic model predicted lime requirement using $\mathrm{pH_{buffer}}$ and target $\mathrm{pH_{CaCl_2}}$ values. Rewriting this model allowed derivation of the target soil pH_{CaCl_2} after certain amounts of lime were considered for application.

10.3.2 GEOSTATISTICAL METHODOLOGY

The *ccdf* of pH_{buffer} was derived at the nodes of a 40 × 50 grid (with 10 m spacing) using IK. The pH_{buffer} data (Fig. 10.1) were discretised into 20 classes of equal frequency, that is nineteen threshold values were considered corresponding to the 0.05, 0.1, 0.15,…,0.95 quantiles of the sample histogram. For each threshold, the indicator semi-variogram (Equation 10.4) was computed and the fitted models were used for ordinary IK.



Quantiles

maximum	100.0%	6.08
	99.5%	6.08
	97.5%	6.03
	90.0%	5.99
quartile	75.0%	5.91
median	50.0%	5.85
quartile	25.0%	5.79
	10.0%	5.74
	2.5%	5.56
	0.5%	5.52
minimum	0.0%	5.52

Moments

Mean	5.85
Std Dev	0.10
Std Error Mean	0.01
Upper 95% Mean	5.87
Lower 95% Mean	5.83
N	122.00
Sum Weights	122.00
Sum	713.67
Variance	0.01
Skewness	-0.56
Kurtosis	1.06
CV	1.73

Figure 10.1 Histogram of pH_{buffer} and descriptive statistics

At each node, 100 pH_{buffer} values were generated using the LHS procedure: the *ccdf* was discretised into 100 equiprobable classes and one value was then randomly drawn from within every class. The set of 100 values were fed into the following equation that regressed soil pH_{CaCl_2} as a function of pH_{buffer} and the amount of lime applied:

$$pH_{CaCl_2} = 35.532 - 12.815q - 0.379p + 1.282q^2 + 0.124qp - 0.004p^2 + e \qquad (10.9)$$

where q is the equilibrated Mehlich pH_{buffer}, p is the amount of lime applied, and $e \sim \mathrm{Nor}(0,\sigma^2)$. Equation 10.9 was derived by rewriting the one-factor Mehlich lime requirement response surface model (Chapter VIII), for predictions of lime requirement. Twenty-one rates of lime, ranging from no lime to 5 Mg/ha (0.25 Mg/ha increments) were considered. This is a realistically estimated range of lime requirements that may be uniformly applied to acid soil in agricultural fields of southeastern Australia. Equation

10.9 assumes that the target pH is attained after lime is applied and incorporated, usually three to six months prior to planting.

The six distributions of regression parameters and the error term (ε) (in equation 10.9) were jointly sampled using LHS and 5 equiprobable classes, leading to 78 125 (5^7) possible combinations of simulated parameters. Each of these combinations was used to propagate the uncertainty about the pH_{buffer} values, as represented by the distribution of 100 simulated values, through Equation 10.9. Hence the result at each node was a distribution of 7 812 500 simulated pH_{CaCl_2} values for each amount of lime. To reduce the computational time in subsequent calculations, the distribution of simulated pH_{CaCl_2} was partitioned into 100 classes and re-sampled using LHS as previously described for pH_{buffer}.

The 100 re-sampled values were then fed into the following production function to derive wheat yield:

$$Y(\mathrm{Mg/ha}) = -10.411 + 3.648w - 0.246w^2 + e \qquad (10.10)$$

where w is the pH_{CaCl_2}, and $e \sim \mathrm{Nor}(0,\sigma^2)$. Equation 10.10 was is a simpler form of a function derived from the wheat trial described in Chapter IX. In this instance a quadratic function was fitted to the data instead of a cubic polynomial. The R^2 of Equation 10.10 was 0.85. As for Equation 10.9, the distributions of regression parameters in Equation 10.10 were jointly sampled using LHS and eight equiprobable classes, leading to 4 096 (8^4) possible combinations of simulated parameters and regression errors.

The uncertainties were propagated by using the 100 pH_{CaCl_2} values as input into Equation 10.10 for all 4 096 combinations of the simulated parameters, producing at each node and for each amount of lime applied (0 - 5 Mg/ha) a distribution of 409 600 simulated wheat yield values.

10.3.3 PROFITABILITY

The profitability of lime application at each node was determined by considering the cost of lime and its application, and the price for wheat in Australia. Information and lime application costs were not considered as the study was conducted to provide an basic insight into the current economic effects of site-specific liming. For a solely economic analysis of site-specific agriculture and liming, the reader is directed to Bongiovanni &

Lowenberg-DeBoer (1998) and Lowenberg-DeBoer & Aghib (1997). The cost of lime used in the study was A$55 per Mg/ha applied (cost of lime and transport A$45 and application AUD$10). The price for wheat was valued at A$200 /Mg. The equation for net profit (NP) was:

$$NP = (Y \times 200) - (p \times 55) \tag{10.11}$$

For each amount of lime *p*, the probability distribution of the net profit was numerically approximated by the distribution of 409 600 NP values obtained from the set of simulated wheat yield (*Y*)values. The probability of making a positive NP was estimated, for each management scenario, by the proportion of 409 600 wheat yield values that provides a revenue exceeding the cost of liming.

10.3.4 OPTIMISATION OF SITE-SPECIFIC LIME REQUIREMENT

For the site-specific management scenario, lime requirement was optimised either in terms of expected NP or the probability of making a profit for a minimum application. The first criterion amounts at selecting at each node the lime requirement category that yields the NP probability distribution with the largest mean. The second criterion involved increasing the lime requirement progressively (up to five Mg/ha) until the probability of a positive NP reached 100 %, that is until none of the 409 600 simulated NP values was negative.

10.3.5 SENSITIVITY ANALYSIS

A number of economic scenarios were quantitatively considered for the present and future implementation of site-specific liming in the experimental field. The monetary advantages and disadvantages of adoption were assessed by calculating various cost/price scenarios. The costs of lime and liming considered ranged from A$35/Mg/ha to $60/Mg/ha while the farm-gate price of wheat ranged from A$170/Mg to $210/Mg.

For clarity, a flowchart of the entire process is given in Figure 10.2.

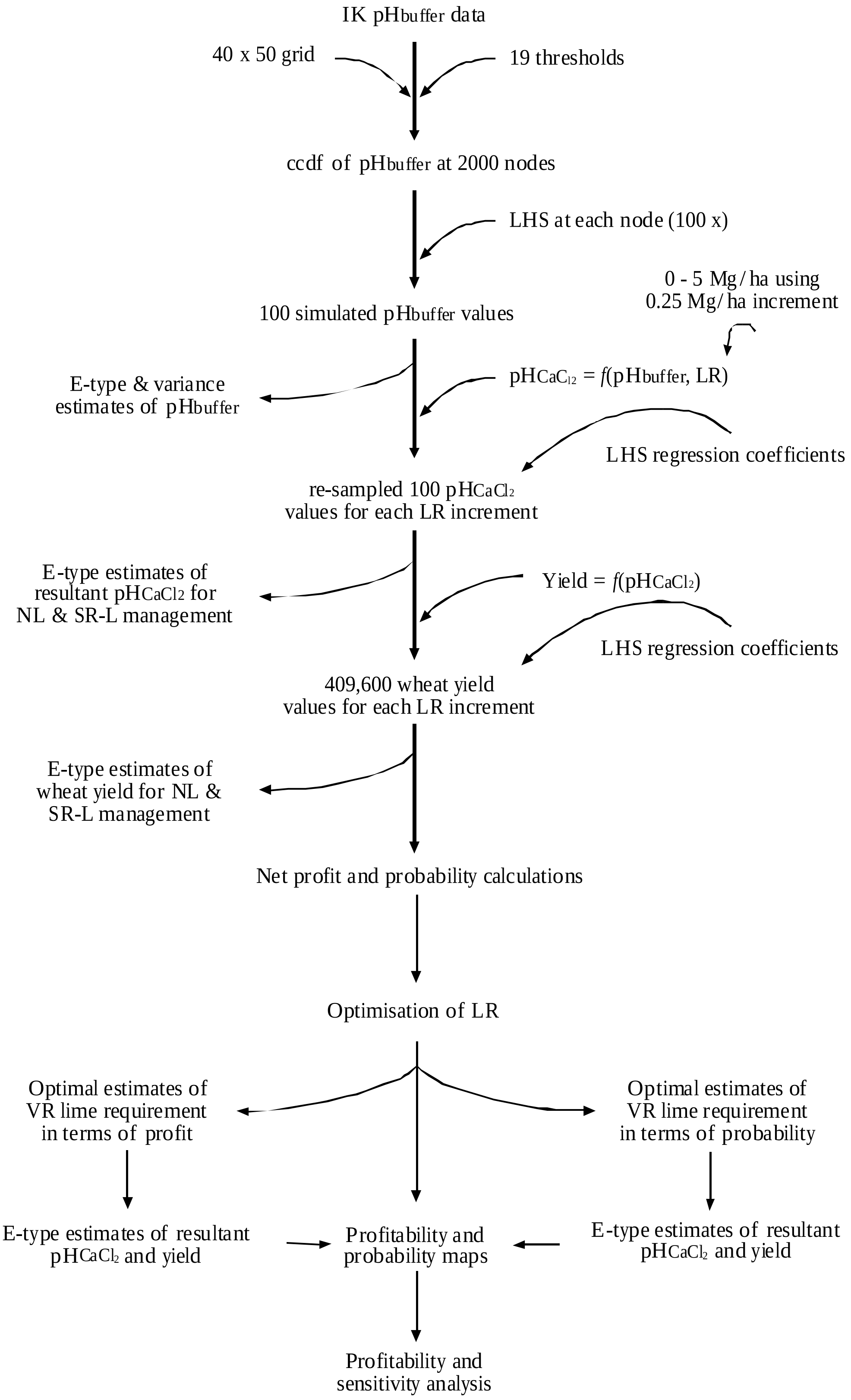
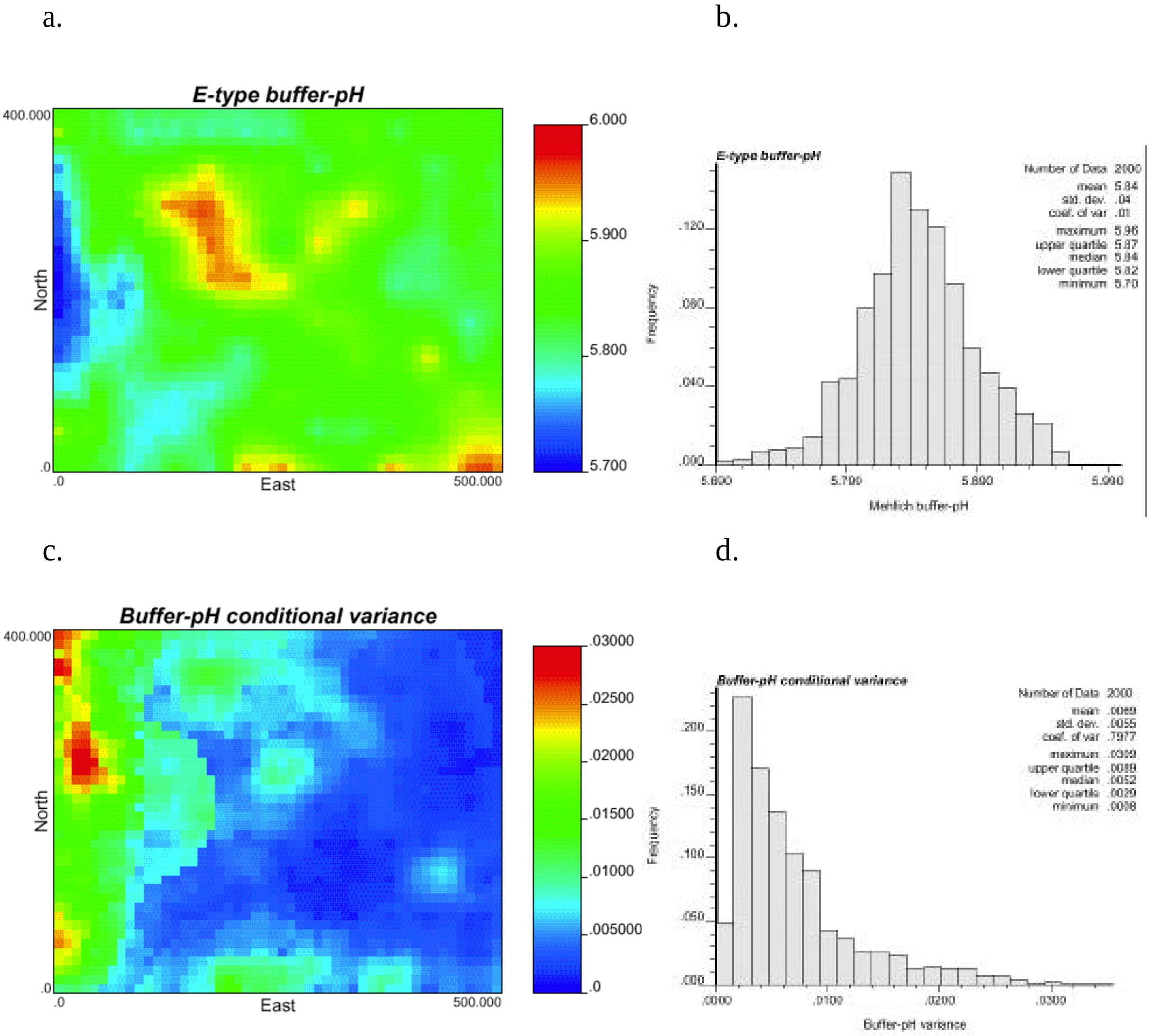


Figure 10.2 Flowchart of the assessment and propagation of uncertainty using indicator kriging (IK) and Latin Hypercube Sampling (LHS) of probability distributions

10.4 RESULTS AND DISCUSSION

Unlike kriging estimates, optimal mean (E-type) estimates derived form conditional *cdfs*, are dependent on data values. Their advantage lies in the provision of a model of uncertainty that is much more practical than the kriging variance (Chapter II). The major problem with the kriging variance is that it exhibits homoscedasticity *i.e.* it depends only on data configuration and not actual data values (Chapter II). The error variance provided by kriging algorithms is hence poorly correlated with actual estimates of error, and on its own does not provide a measure of local uncertainty (Goovaerts, 1997). A more appropriate measure of uncertainty is the conditional estimation variance, which is specific to data values. Figure 10.3 shows the E-type estimate and variance of the conditional *cdfs* of Mehlich $\text{pH}_{\text{buffer}}$ derived using IK.



a. b.

c. d.

Figure 10.3 Maps of (a.) the E-type estimates of $\text{pH}_{\text{buffer}}$ and (c.) its conditional variance and their respective distributions. Histograms and summary statistics of their distributions are shown in (b.) and (d.) respectively

pH_{buffer} values are not very variable, values range from 5.7 to 5.96 and the coefficient of variation (CV) is smaller than 0.01 (Figures 10.3a and 10.3b). Consistent with previous findings (Chapter VIII), the lowest values occurred on the westernmost part of the field. Figure 10.3c shows that the uncertainty about pH_{buffer} estimates, as measured by the *ccdf* variance, is smallest in the central and eastern parts of the field.

The regression functions (Equations 10.9 and 10.10) used to derive target pH_{CaCl_2} and wheat yield respectively are displayed in Figure 10.4.

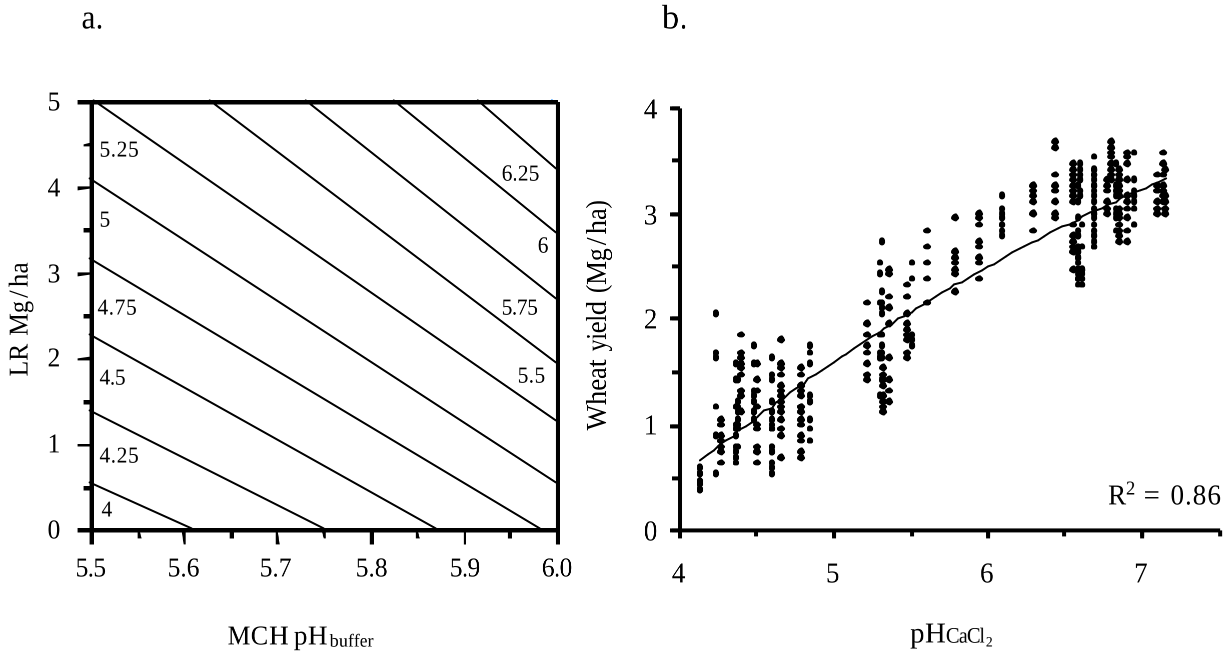


Figure 10.4 (a.) response-surface of pH_{CaCl_2} as a function of pH_{buffer} and lime requirement: Equation (10.9) and (b.) wheat yield as a function of soil pH_{CaCl_2}: Equation (10.10)

The combined uncertainties about pH_{buffer}, the range of lime requirements (0 to 5 Mg/ha) and regression parameters of the two models (Figure 10.4a, b) were propagated through to the output data for each management scenario. The three management alternatives will now be examined.

10.4.1 NO-LIME APPLICATION SCENARIO

This scenario may be thought of as a base case, where no management was considered to ameliorate the soil acidity problem of the field. The simulation of pH_{CaCl_2} values was accomplished using zero lime application in Equation 10.9. The arithmetical average of the sets of simulated values is mapped in Figure 10.5a, and their distribution shown in Figure 10.5b. The simulation of wheat yield estimates used these pH_{CaCl_2} values in the

regression function given by Equation (10.10). The average of the sets of simulated values is illustrated in Figure 10.5c, and their distribution shown in Figure 10.5d.

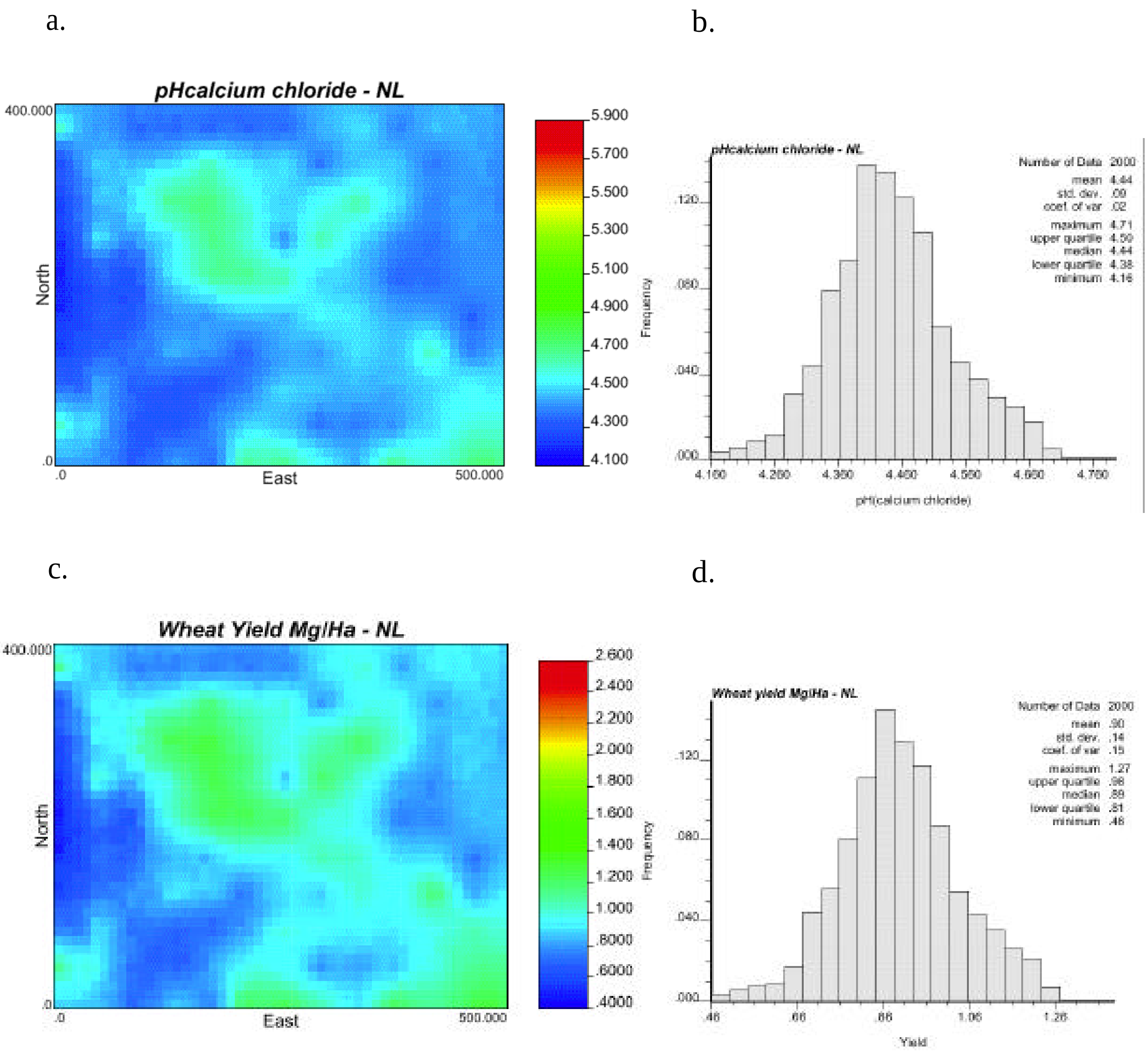


Figure 10.5 (a.) Map of pH$_{CaCl_2}$ estimates, (b.) histogram and descriptive statistics, (c.) map of wheat yield estimates, and (d.) histogram and descriptive statistics, for the no lime (NL) scenario

The average pH$_{CaCl_2}$ of the field was 4.44, it ranged from 4.16 to 4.71 units (Figure 10.5b). Wheat yield was low throughout the field (Figure 10.5c). The yield map displays the expected restrictions on yield imposed by acidic soil condition where Al and Mn toxicities are the likely causes of poor plant growth (Chapters VI and IX), particularly in the very acidic western portion of the field. The average yield was 0.9 Mg/ha, it ranging from 0.46 Mg/ha to 1.27 Mg/ha (Figure 10.5d).

10.4.2 SINGLE-RATE LIME APPLICATION SCENARIO

Single-rate application of input resources to the production process is the conventional method of agricultural management (Chapters I, II, IV). It is not unusual for the decision on how much lime to apply to be based on only a few averaged soil test results, farmer intuition and the cost of lime and application (Chapters VI and VIII). As such lime is commonly applied at low single-rates of one or two Mg/ha. To manage the soil acidity of the field, and to regain some of the diminished production, an application of 3.5 Mg/ha of lime was considered to be realistic. This amount also corresponds to the average lime requirement of the field. Figure 10.6a shows the simulated pH_{CaCl_2} map and Figure 10.6b respective statistics. Figures 10.6c and 10.6d display the resulting wheat yield map and ensuing statistics, respectively.

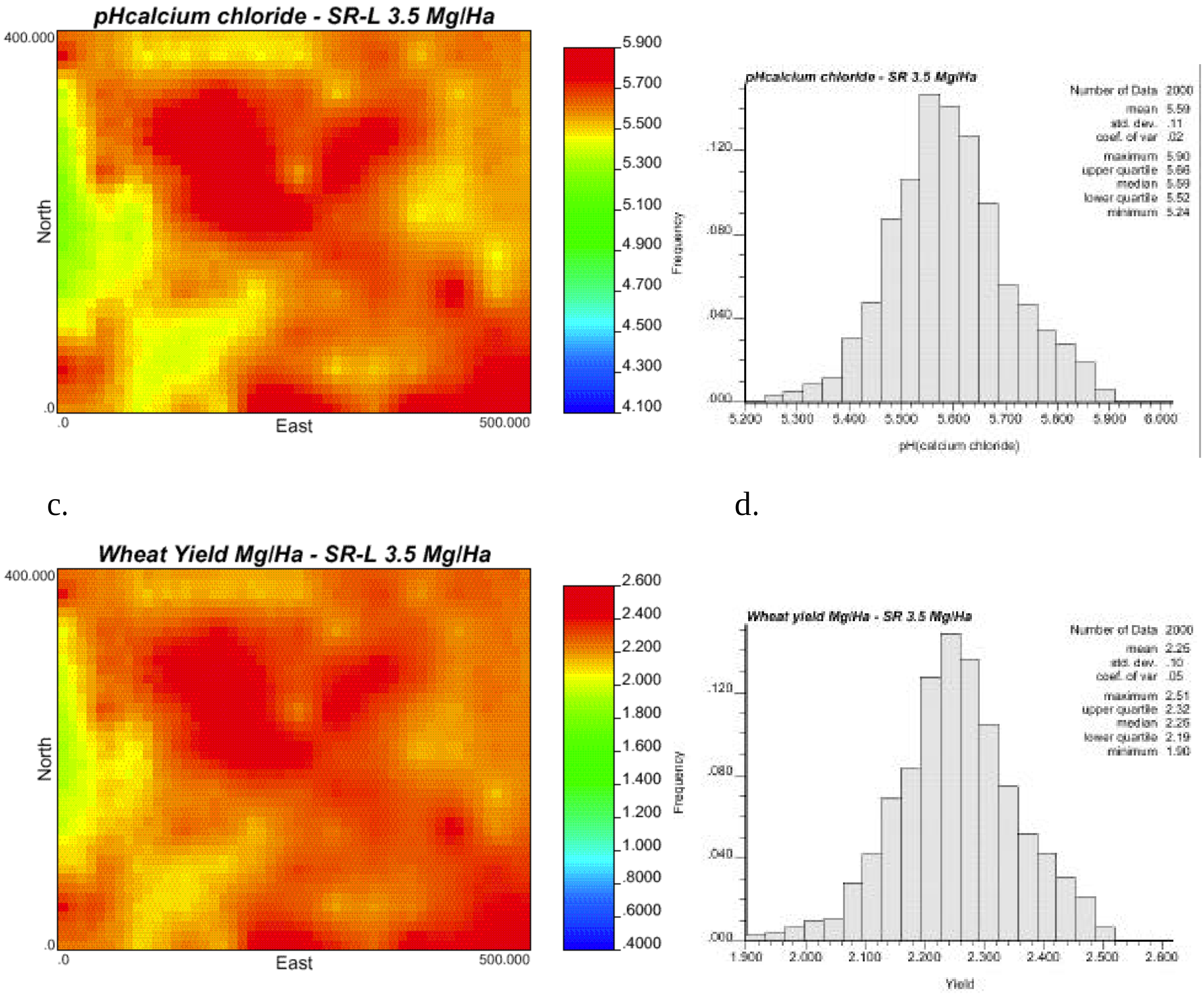

a. b. c. d.

Figure 10.6 (a.) Map of pH_{CaCl_2} estimates, (b.) histogram and descriptive statistics, (c.) map of wheat yield estimates, and (d.) histogram and descriptive statistics for the single-rate liming (SRL) scenario

The single-rate lime application of 3.5 Mg/ha induced an increase in the average pH_{CaCl_2} of the soil from 4.44 (NL scenario, Figure 10.5b) to 5.59 units (Figure 10.6b). The western part of the field exhibited the lowest pH_{CaCl_2} values (Figure 10.6a). The minimum pH_{CaCl_2} increased from 4.16 to 5.24 units. This increase eliminated the risk of elemental toxicities and their adverse repercussions on crop production. Consequently, the average yield roughly doubled that observed when lime was not applied (compare Figures 10.6c with 10.5c).

10.4.3 SITE-SPECIFIC LIMING SCENARIO – OPTIMISING NET PROFIT

Site-specific liming is based on more accurately matching applications of lime to the acid soil's lime requirement (Chapter VIII) and crop requirements as these vary within the management unit. Theoretically, this type of management minimises under-applications that may lead to less than optimal crops yield and gross margins, and over-applications that are expensive and hinder production by inhibiting the availability of micronutrients (Chapter IX). Precision agriculture has been proposed as an economically and agronomically sensible management option (Chapters I, II, VI).

A variable-rate application map was produced by optimising lime application in terms of NP (Equation 10.11). That is, the lime requirement that resulted in the largest expected NP was selected at each node. The resulting map is shown in Figure 10.7a.

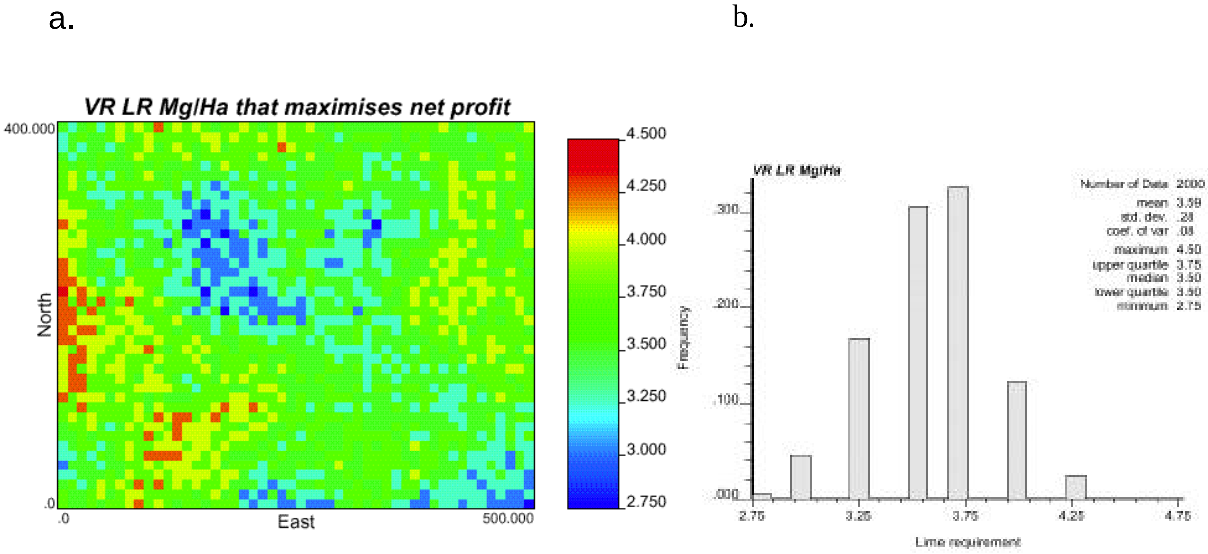


Figure 10.7 (a.) Map of optimal variable-rate lime requirement (VRL)and (b.) histogram showing descriptive statistics

The economically optimum lime requirement ranged from 2.75 Mg/ha to 4.5 Mg/ha (Figure 10.7b). The lime requirement map has a 10 m block resolution (Figure 10.7a), which may be suitable for site-specific management using variable-rate technology (Clark & McGuckin, 1996; Anderson & Humburg, 1997; Chapter II). As for previous scenarios, resulting pH$_{\text{CaCl}_2}$ and wheat yield maps were produced (Figures 10.8a and 10.8c).

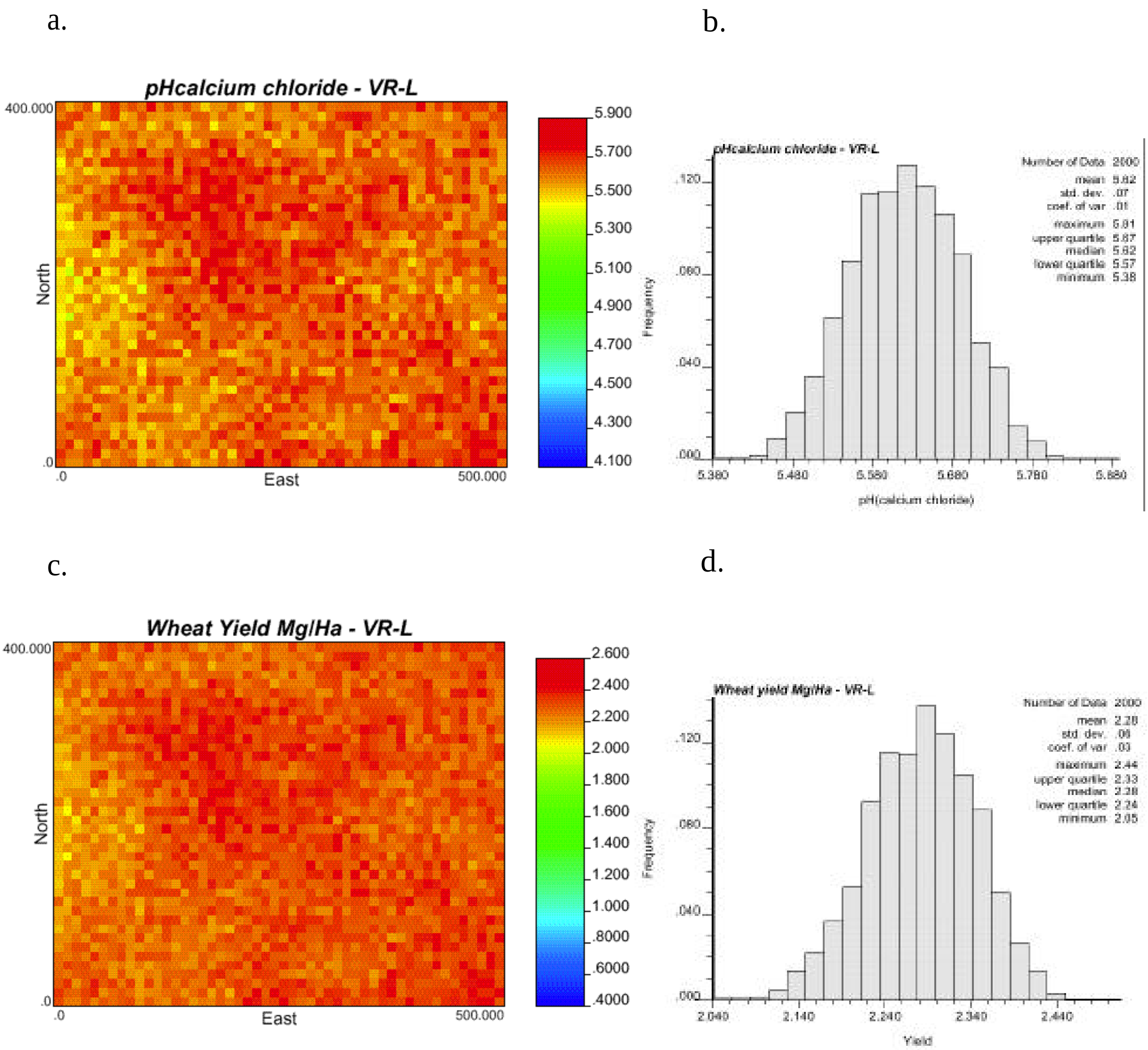


Figure 10.8 (a.) Map of pH$_{\text{CaCl}_2}$ estimates, (b.) histogram and descriptive statistics, (c.) map of wheat yield estimates, and (d.) histogram and descriptive statistics for the variable-rate liming (VRL) scenario, optimising net profit

Both single-rate and variable-rate liming produced similar field-average pH$_{\text{CaCl}_2}$ values (pH$_{\text{CaCl}_2}$ 5.59 (Figure 10.6b) versus 5.62 (Figure 10.8b) respectively). This results was to be expected since the field-average lime requirement was 3.6 Mg/ha, a value close to the single-rate application of 3.5 Mg/ha. However, variable-rate liming reduced the spatial

heterogeneity of pH_{CaCl_2}. The narrower range of the pH_{CaCl_2} statistics (Figure 10.8b) reflects this homogenisation. The yield map also appeared less variable (Figure 10.8c). Wheat yield from site-specific liming showed little improvement to yield that resulted from single-rate liming (field average 2.25 Mg/ha (Figure 10.6d) versus 2.28 Mg/ha (Figure 10.8d) respectively).

10.4.4 ECONOMIC COMPARISON OF SCENARIOS

An economic comparison of the three liming management opportunities was performed to establish the best practice for the field. Maps of NP (*i.e.* where the price of wheat exceeds the cost of liming), and corresponding NP probability maps for no-liming, single-rate and site-specific lime applications are shown in Figure 10.9. The NP map corresponding to the no-lime scenario, where the average NP was A$180/ha is shown in Figure 10.9a. The probability of making a profit for this scenario ranged from 73 % to 96 % (Figure 10.9b). The benefits of liming acid soil are clearly illustrated by the maps on Figure 10.8c to 10.8f. A 3.5 Mg/ha single-rate application of lime over the entire field caused the average NP of the field (Figure 10.8c) to increase by almost A$80/ha. Likewise the range of probabilities of making a profit increased to almost 100 % for all but the western portions of the field (Figure 10.8d). In these areas, pH_{CaCl_2} values were lowest (Figure 10.3a).

Optimal variable-rate liming produced maps of expected NP and probability of positive NP (Figures 10.9e and 10.9f), that are very similar to single-rate maps(Figures 10.9c and 10.9d). In this instance site-specific lime applications are not economically warranted since almost optimal profits may be obtained by applying the average 3.5 Mg/ha of lime across the entire field. These results seem consistent with the fact that optimal application rates (Figure 10.7) vary around the average optimal lime requirement value of 3.6 Mg/ha.

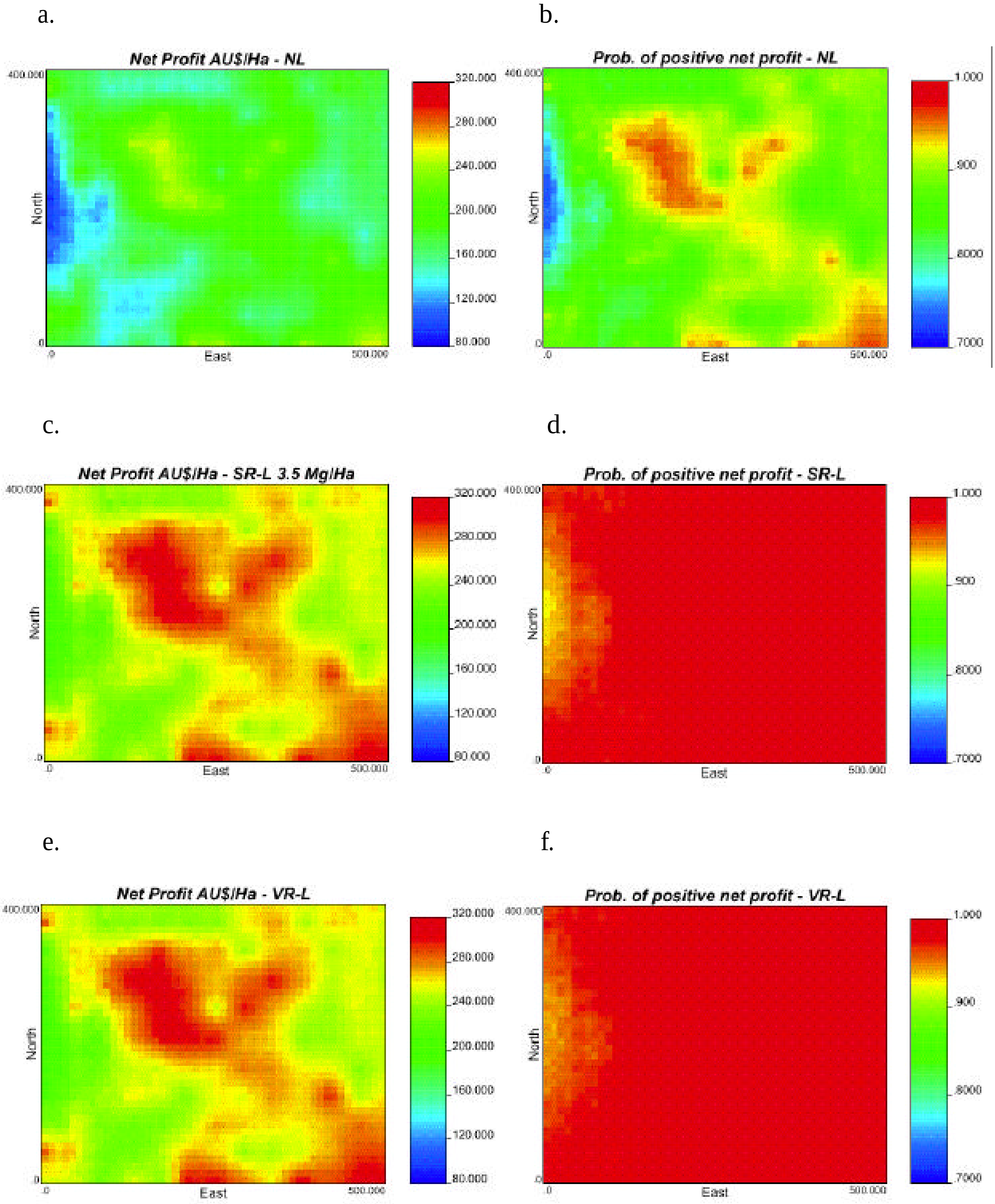


Figure 10.9 Maps of expected net profit (NP) and probability of making a profit respectively, for (a.) & (b.) no-lime application (NL); (c.) & (d.) single-rate liming (SRL); and (e.) & (f.) variable-rate liming (VRL)

10.4.5 OPTIMISING TO ENSURE 100 % PROBABILITY OF MAKING A PROFIT

Lime requirement was also optimised to guarantee a 100 % probability of making a profit under minimum application costs. Figure 10.10 shows the variable-rate map and Figure 10.10b shows the descriptive statistics of the data.

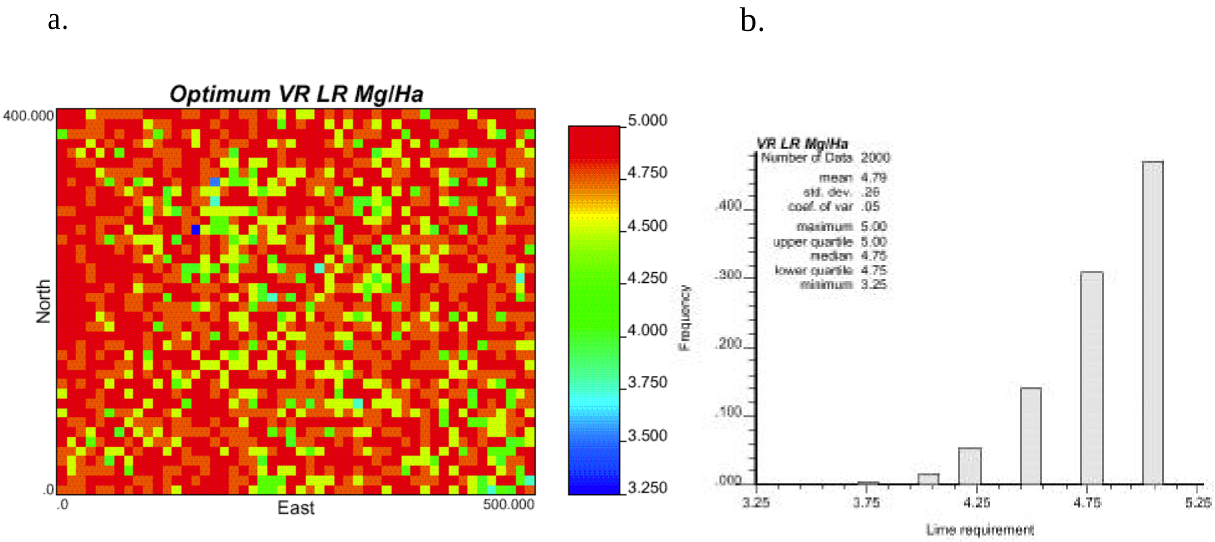


Figure 10.10 (a.) Map of expected optimal variable-rate lime requirement (VRL), and (b.) histogram with statistics

Optimisation to ensure a 100 % probability of making a profit resulted in a higher average field lime requirement of 4.79 Mg/ha (Figure 10.10b) than that optimised in terms of net profit (Figure 10.7a). The resulting pH_{CaCl_2} and wheat yields are shown in Figures 10.11a to 10.11d. Consistent with Figure 10.4a, increasing the amount of lime added to the acid soil (within the 0 – 5 Mg/ha range), resulted in higher pH_{CaCl_2} values across the field. These ranged from pH_{CaCl_2} 5.62 to 6.38 (Figure 10.11b). Wheat yields were also higher (Figure 10.11c). The field-average wheat yield was 2.57 Mg/ha (Figure 10.11d), 0.29 Mg/ha higher than when lime requirement was optimised based on solely NP (Figure 10.8c), and 0.32 Mg/ha higher than that from single-rate liming (Figure 10.6c).

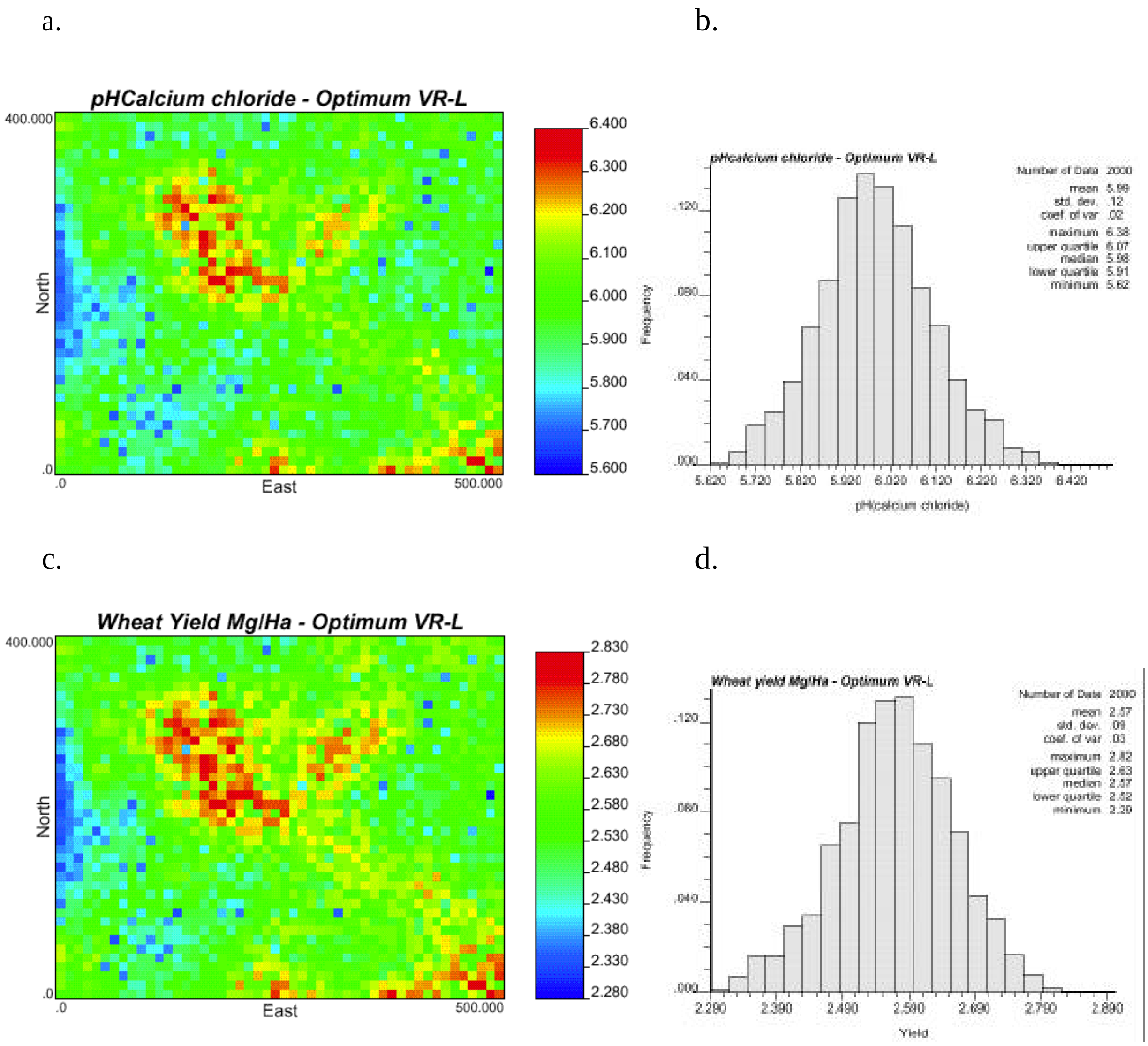


Figure 10.11 (a.) Map of pH_{CaCl_2} estimates, (b.) histogram and descriptive statistics, (c.) map of wheat yield estimates, and (d.) histogram and descriptive statistics for the variable-rate liming (VR-L) scenario, optimising to ensure 100 % of making a profit

The increases in pH_{CaCl_2} and yield were not economically justified by the greater applications of lime. Figure 10.12 shows the resultant NP map when lime requirement is optimised subject to 100 % probability of making a profit. The average NP was A$250/ha, it ranged from A$189/ha to A$305/ha. The average NP is approximately A$8/ha less than the average NP obtained from the economically optimised lime requirement and the 3.5 Mg/ha single application rate (Figures 10.9).

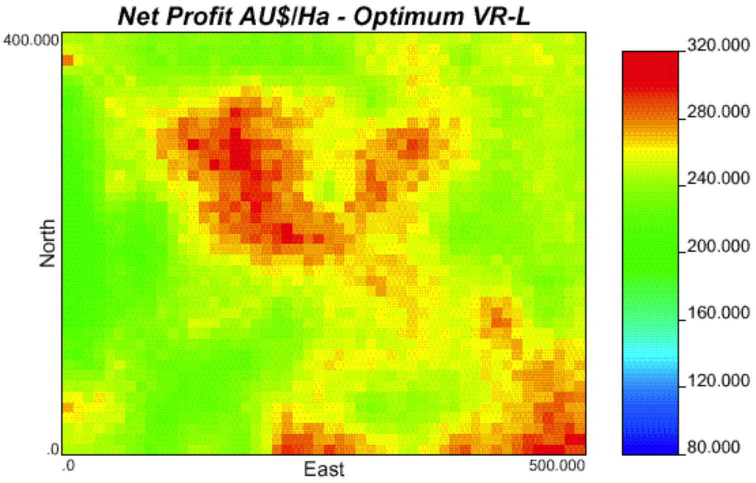


Figure 10.12 Map of expected net profit for variable-rate liming (VRL), optimisation subject to 100 % probability of making a profit.

10.4.6 SENSITIVITY ANALYSIS

The decision to implement PA management will depend mainly on two basic factors: their production objectives and their perceived consequences of alternative operations. Both of these factors will vary amongst farmers, but one can speculate that their decision to adopt will be influenced by how much the implementation of technology will increase yields (hence NP) and lower their production risk (or uncertainty).

The results presented in this chapter suggest that site-specific liming in the experimental field may not be economically justified under the cost / price conditions of the analysis, *i.e.*, A$200 for the price of wheat and A$55 for liming. Because NP (and hence the decision of whether to adopt a site-specific liming practice) depends on the ratio of cost of lime to price of wheat, a number of different scenarios were compared (Table 10.1). In Table 10.1, the italicised values represent the combinations of cost and price where the average NP resulting from site-specific lime applications is higher than the NP obtained from single-rate liming, A$258/ha. The italicised-bold value of A$259/ha represents the critical NP value above which adoption of site-specific liming is profitable and below which adoption is not economically justified.

Table 10.1 Sensitivity analysis for the adoption of site-specific liming.

Average net profit A$/ha		Combined cost of lime and application A$/Mg/ha					
		35	40	45	50	55	60
Farm-gate wheat price A$/Mg	210	*354*	*336*	*318*	*300*	*282*	*264*
	200	*331*	*313*	*295*	*277*	***259***	241
	190	*308*	*290*	*272*	254	234	218
	180	*285*	*267*	249	231	213	195
	170	*262*	244	226	208	190	172

The inferences of these cost / price scenarios are illustrated in Figure 10.13.

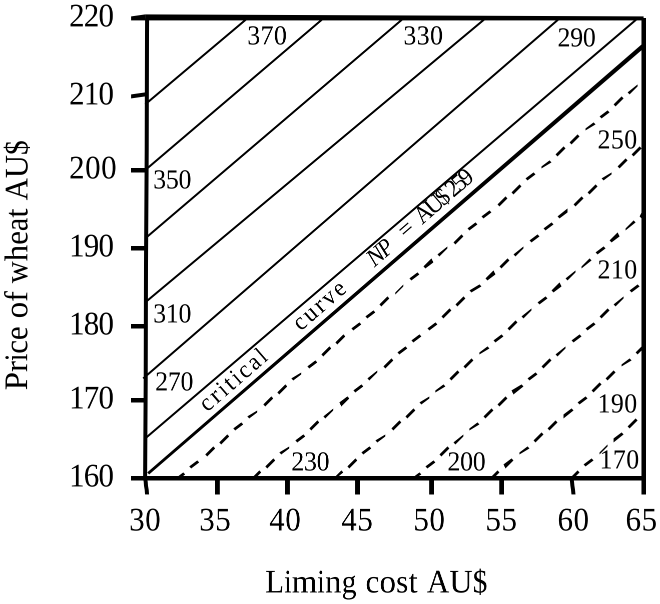


Figure 10.13 Sensitivity analysis for the adoption of site-specific liming in the experimental field at Kelso, NSW. Above the critical net profit (NP) curve site-specific liming is economically justified, while below the critical curve a single-rate application of 3.5 Mg/ha is more profitable resulting in a NP of A$ 258/ha.

For example, if the cost of liming drops to A$47/Mg/ha and the price of wheat remains at A$200/Mg, then site-specific liming will produce a NP of A$290/ha, which is A$32/ha higher than the single-rate NP. Net profits below the critical curve (Figure 10.13 broken lines) do not warrant site-specific liming since the profit obtained from a single-rate application across the field is A$258/ha. Conversely, cost/price combinations above the critical curve (Figure 10.13 solid lines) produce profits that are higher than that resulting from a single-rate application of lime, hence under such economic conditions site-specific liming may be justified.

Note that the costs of equipment hire (i.e. spreader, variable-rate lime controllers and applicators, etc.) and consultancy for variable-rate lime applications were not considered in the analysis. The sensitivity analysis aims only to provide a basic insight into the current economic effects of site-specific liming. The inclusion of more complex economic scenarios (and arguably more realistic) is warranted to thoroughly examine the consequences of site-specific liming.

10.5 CONCLUDING REMARKS

Experimental modelling to date has shown that the level of uncertainty about crop yield data remains difficult to assess in a reliable manner. This final chapter presented a methodology for modelling crop yields in the presence of uncertainty. The local uncertainty about soil properties and the uncertainty about model parameters were accounted for by using an indicator kriging and the Latin Hypercube sampling approach for the propagation of uncertainties through two regression functions. The first resolved soil pH_{CaCl_2} after lime applications, while the second was a pH_{CaCl_2} dependent production function for wheat. The methodology was used to determine the best liming practice in an agricultural field with acid soil.

The consequences of not liming acid soil were compared to two management practices, namely single-rate liming over the entire field, and variable-rate liming on 10 m blocks. In the latter case, liming was optimised in terms of both profit and the probability of making a 100 % profit. The comparisons were based on biological production and net profit calculations that considered the farm-gate price of wheat and the cost of liming. Under the constraints of the analysis, single-rate liming was determined to be the best management option. The implications of these results on the null hypothesis of precision agriculture are that where variability is low and knowledge-based uncertainty high, the optimal risk aversion strategy is uniform management.

A simple economic sensitivity analysis was presented only to provide an indication of when site-specific liming may be economically feasible in the experimental field.

The methodology presented may be used to help decide which type of management to implement for maximum profit. As such, this research is not specific to this particular scenario but may be generally applied to assess the risk associated with the adoption of site-specific soil and crop management techniques.

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General Conclusions and Future Work

GENERAL CONCLUSIONS AND FUTURE WORK

Management using PA will eventually be conducted continuously and in real-time, so that data acquisition, decision-support and management are carried out in a single pass over the field as the agricultural vehicle traverses the field. The primary objective of this work was to conduct research towards the development of an ‘on-the-go’ proximal soil pH and lime requirement sensing system for real-time continuous management of acid soil. However, each of the ten chapters had specific aims. Their general conclusions and where appropriate suggestions for future work are described below.

Chapter I documented the most significant global and historical factors that converged into the development of precision agriculture. Most pertinently it discussed global population, food security, the decline in arable land area, land degradation, the need for increased environmental awareness and the current global economy. It also described recent advances in science, information and communications technologies, and the increasing consumer demand for more stringent quality control in agriculture as contributing factors towards the foundation of precision agriculture. The theme of the chapter suggested that through scientific research in agriculture, and the consequent adoption of innovative sustainable systems, it might be possible to avoid potential global environmental and social disasters.

Chapter II presented a literature review on topics that are relevant to the concept of precision agriculture and techniques used for the quantification of soil spatial variability and the acquisition of soil data. It reviewed classic statistical and geostatistical methods used to quantify soil spatial variability. Descriptions of each method were supported with corresponding reviews pertaining to the quantification of the spatial variability in soil pH. The chapter then focused on precision agriculture. Particular emphasis was given to the methods used to collect data on the spatial variability of soil, especially those that attempt a complete enumeration of field soil variables, namely remote and proximal sensing. The chapter closed with a review of developing options for the characterisation of fine-scale soil variability using proximal soil sensing systems, and emphasises that for further evolution and adoption of precision agriculture, their development is imperative.

Chapter III provided a general description of the environment and the farming systems in the region surrounding the farm and experimental field. In more detail, it gave quantitative descriptions of the field site, topography, soil condition at the time of sampling and the spatial variability of surface soil chemical properties that are relevant to the management of acid soil. It also described the methods of sampling and laboratory analyses. Future work may encompass modelling of the landscape at Kelso, NSW using the digital elevation model and derived terrain attributes. These may be used as auxiliary variables for the prediction of soil properties *e.g.* to help predictions of soil pH (refer to Chapter V).

The main conclusion from Chapter IV was that for the evolution of precision agriculture, the development of techniques to characterise soil spatial variability timely, rapidly, economically and accurately is imperative. Current sampling and analysis techniques are time-consuming, costly, labour intensive, and in some instances, inaccurate and imprecise. The development of 'on-the-go' proximal soil sensing systems and scanners with equivalent or improved accuracy is essential for the adoption and implementation of precision agriculture. Their development is also important for the evolution of precision agriculture into a real-time continuous management system. While sensing systems are being developed to overcome these problems, the solution to the sampling and analysis dilemma is being addressed. In doing so, it should be clear that the sampling procedure and the way in which samples are handled after collection ultimately determine the accuracy of analytical results. Sensing systems should be developed for soil properties like pH, organic matter, N, P, K and cation exchange capacity. These properties are good indicators of soil quality and should form the basis for routine soil chemical analysis in precision agriculture. Use of the VERIS 3100 mobile sensing system was used to characterise the soil electrical conductivity in the experimental field. It's use demonstrated the advantages of using an 'on-the-go' proximal soil sensing system.

As well as correct, unbiased soil sampling and laboratory analyses, the choice of spatial modelling and mapping techniques is important for reliable results and accurate representations of field soil variability. There are various good examples in the literature that compare spatial modelling and mapping techniques. Chapter V constrained itself to comparing some of the methods that may be used to model and map sparsely sampled soil that exhibits spatial drift. Intrinsic random funcitions of order *k* produced the most accurate and parsimonious predictions of all of the methods tested. This was anticipated since the technique was originally developed to 'filter out' the drift component of the random function and to overcome the problems associated with universal kriging.

Unexpectedly however regression residual-kriging, which aims to first define the global nature of the drift using a subjective trend model, performed poorly. The method was expected to produce similar results to, or better than, the intrinsic random function method, as it has done in other experimental studies. One reason for its poor performance was the little or no remaining semi-variogram structure in the regression residuals. Future work may encompass further investigation into the bias introduced in modelling the trend component of the random function. Furthermore, the validation method could be improved by conducting the analysis for a number of randomly selected independent jackknives and compute statistics from them.

Chapter VI reviewed soil acidity and acidification, their causes, consequences and their management. It looked at the global extent of the problem as well as its occurrence in Australia. It proposed that site-specific management of acid soil might prevent the adverse economic and environmental consequences of conventional management practices. The chapter also described a real-time continuous management system for the implementation of optimal and timely management using information collected ‘on-the-go’. Chapter VI suggested that the development of an ‘on-the-go’ proximal soil pH and lime requirement sensing systems and adequate spatial decision support for optimal predictions of lime requirement are imperative for the development of a real-time continuous management system for acid soil.

Chapter VII described the initial experimentation required for the development of an ‘on-the-go’ proximal soil pH and lime requirement sensing system to be used for the real-time continuous management of acid soil. An ion sensitive field-effect transistor (ISFET) has all the desirable characteristics required for ‘on-the-go’ proximal soil pH and lime requirement measurements. It is small, accurate and precise, responds rapidly to wide pH changes, is robust and may be used in an integrated sensor array containing ISFETs sensitive to various other ions important for plant growth. A design for the analytical component of the sensing system was proposed using principles derived from flow injection and sequential injection analyses systems. Two different models of operation were described. Also in chapter VII, kinetic experiments were conducted to characterise soil:0.01M $CaCl_2$ pH (pH_{CaCl_2})and soil:lime-requirement buffer pH (pH_{buffer}) reactions. The kinetics of soil:lime-requirement buffer reactions may be distinguished using different, though not incompatible, models. First, the reactions were characterised using two separate first-order reactions, each with a single rate coefficient. Second, using a continuous double-exponential function with two rate coefficients. Both models described the sequential, biphasic nature of the reactions. A statistical methodology was devised to predict equilibrium pH_{buffer} measurements at shorter time intervals than those suggested in the literature. Predictions of equilibrium pH_{buffer} using only initial soil:lime-requirement buffer reaction measurements at 0.5 s, 1 s, 2 s and 3s were made using the devised methodology. The accuracy of predictions was 0.1 pH_{buffer} units and the bias was low. The method may be used in the proposed sensing system to predict lime requirements 'on-the-go' using only initial pH_{buffer} measurements. The framework for the development of a prototype soil pH and lime requirement sensing system was presented and a creative design that describes the components of the 'on-the-go' proximal soil pH and lime requirement sensing system proposed. The design for an 'on-the-go' soil sampling mechanism and the data processing system were also described. Further work will encompass the construction of the analytical and sampling components of the sensing system as well as the development of the data processing algorithms and spatial decision-support system for real-time operation. The kinetics of soil:lime-requirement buffer reactions need to be investigated and the prediction method that was developed validated using a wider range of soil types.

A soil's lime requirement is influenced mainly by its buffering capacity and the amount of exchangeable acidity in the soil solution. The lime-requirement buffers are the most accurate rapid procedures for predictions of lime requirement. Single- and two-factor response surface models were developed for use with the buffer methods. The response surface models facilitate the choice of target pH without the need for excessive calibrations. These models were more accurate and more practical than more conventional techniques, and may be more suitably incorporated into the spatial decision-support system of the proposed real-time continuous system for the management of acid soil. Initially, the response surface methodology may be used to produce variable-rate lime-requirement maps to guide variable-rate lime applicators. In a real-time continuous system, the data collected by the 'on-the-go' proximal soil pH and lime requirement sensing system would be used in the response surface models to predict lime requirements for real-time applications of lime. The chapter noted that being empirical, the models would only make accurate predictions when they are applied to the range of soils that were used in their formulation. In this instance, the range of soils used was collected from across the southern wheat-belt of New South Wales. Hence the models may only be used for predictions of lime requirement in these regions. However the methodology may be widely and easily applied on a regional basis. Field lime requirements were predicted using the Woodruff and Mehlich buffers calibrated using the two-factor models. Spatial analysis of field pH_{buffer} values and respective lime requirements showed that both techniques are suitable for field predictions of lime requirement and for the production of variable-rate liming maps. The variable-rate maps to target pH 6.5 showed that lime requirements in the experimental field were high. Such high applications may be expected to occur only once, followed by lower rates of prophylactic liming in subsequent years. The response surface technique is, however, flexible and the farmer may choose lower target pH values depending on the crop grown and the economic outlook. The methodology also allows different areas of the field to be limed to different target pH values depending on the yield potentials of different areas in the field, thereby reducing the liming costs. A post-lime application map of (target) pH_{CaCl_2} for a single-rate liming scenario, together with quantification of the differences between single-rate and site-specific lime requirements demonstrated the inefficiency of using a mean, blanket application rate. Future work will involve widening the range of the calibration models for acid soils in the Australian wheat-belt.

The significance of Chapter IX lies in its authentication of the models derived in Chapter VIII so that they may be incorporated into the spatial decision-support system of the continuous system for the management of acid soil. The glasshouse experiment was conducted to study soil property interactions and soil-plant relationships in acid and ameliorated soil, to compare the effects of no lime applications, single-rate and variable-rate liming. The results accentuated the dynamics of soil interactions at low pH and the difficulty in deriving one specific cause for acid soil infertility. Relationships between soil properties (before and after liming) and crop yields were established by looking at yield response as functions of pH, aluminium, calcium and cation exchange capacity. The benefits of liming acid soil were clearly illustrated in all examples, as well as the significant advantages of variable-rate liming. Results from the yield comparison between the three treatments also provided the theoretical basis for VRL in the experimental field and verification for the developed response surface models. It was acknowledged that while glasshouse experiments are cheaper and more convenient than field trials, they are beset with some additional problems. Nevertheless glasshouse experiments are useful in an exploratory and theoretical sense. Future work will involve the confirmation of these results by designing and conducting spatially based field trials.

Experimental modelling to date has shown that the level of uncertainty about crop yield data remains difficult to assess in a reliable manner. Chapter X presented a methodology for modelling crop yields in the presence of uncertainty. The local uncertainty about soil properties and the uncertainty about model parameters were accounted for by using indicator kriging and Latin Hypercube Sampling for the propagation of uncertainties through two regression functions. The first resolved soil pH_{CaCl_2} after lime applications, while the second was a pH_{CaCl_2} dependent production function for wheat. This approach was used to determine the best liming practice in an agricultural field with acid soil. The comparisons were based on biological production and net profit calculations that considered the farm-gate price of wheat and the cost of liming. Under the constraints of the analysis, single-rate liming was found to be the best management option. The implications of these results on the null hypothesis of precision agriculture are that where variability is low and knowledge-based uncertainty high, the optimal risk aversion strategy is uniform management. A simple economic sensitivity analysis was presented only to provide an indication of when site-specific liming may be economically feasible in the experimental field. The methodology presented may be used to help decide which type of management to implement for maximum profit. The research is not specific to this particular scenario but may be generally applied to assess the risk associated with the adoption of site-specific soil and crop management techniques.

The inadequacies of conventional whole-field management systems arise from the fact that soil is an inherently variable medium. Real-time continuous management using precision agriculture and site-specific liming are offered as more efficient alternatives to uniform agronomic methods of acid soil management, particularly now that much of the technology is readily available to producers.