Multivariate Data Analysis for Embedded Sensor Networks Within the Perishable Goods Supply Chain

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ABSTRACT

This study was aimed at exploring data analysis techniques for generating accurate estimates of the loss in quality of fresh fruits, vegetables and cut flowers in chilled supply chains based on data from advanced sensors. It was motivated by the recent interest in the application of advanced sensors, by emerging concepts in quality controlled logistics, and by the desire to minimise quality losses during transport and storage of the produce. Cut roses were used in this work although the findings will also be applicable to other produce. The literature has reported that whilst temperature was considered to be the most critical post-harvest factor, others such as growing conditions could also be important in the senescence of cut roses. Kinetic modelling was the most commonly used modelling approach for shelf life predictions of foods and perishable produce, but not for estimating vase life (VL) of cut flowers, and so this was explored in this work along with multiple linear regression (MLR) and partial least squares (PLS).

As the senescence of cut roses is not fully understood, kinetic modelling could not be implemented directly. Consequently, a novel technique, called Kinetic Linear System (KLS), was developed based on kinetic modelling principles. Simulation studies of shelf life predictions for tomatoes, mushrooms, seasoned soybean sprouts, cooked shrimps and other seafood products showed that the KLS models could effectively replace the kinetic ones.

With respect to VL predictions KLS, PLS and MLR were investigated for data analysis from an in-house experiment with cut roses from Cookes Rose Farm (Jersey). The analysis concluded that when the initial and final VLs were available for model calibration, effective estimates of the post-harvest loss in VL of cut roses could be obtained using the post-harvest temperature. Otherwise, when the initial VLs were not available, such effective estimates could not be obtained. Moreover, pre-harvest conditions were shown to correlate with the VL loss but the correlation was too weak to produce or improve an effective estimate of the loss. The results showed that KLS performance was the best while PLS one could be acceptable; but MLR performance was not adequate.

In another experiment, boxes of cut roses were transported from a Kenyan farm to a UK distribution centre. Using KLS and PLS techniques, the analysis showed that the growing temperature could be used to obtain effective estimates of the VLs at the farm, at the distribution centre and also the in-transit loss. Further, using post-harvest temperature would lead to a smaller error for the VL at the distribution centre and the VL loss. Nevertheless, the estimates of the VL loss may not be useful practically due to the excessive relative prediction error. Overall, although PLS had a slightly smaller prediction error, KLS worked effectively in many cases where PLS failed, it could handle constraints while PLS could not.

In conclusion, KLS and PLS can be used to generate effective estimates of the post-harvest VL loss of cut roses based on post-harvest temperature stresses recorded by advanced sensors. However, the estimates may not be useful practically due to significant relative errors. Alternatively, pre-harvest temperature could be used although it may lead to slightly higher errors. Although PLS had slightly smaller errors KLS was more robust and flexible. Further work is recommended in the objective evaluations of product quality, alternative non-linear techniques and dynamic decision support system.

DECLARATION

No portion of the work referred to in the thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.

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ABBREVIATIONS

ABA	Abscisic acid
APO	Asian Productivity Organization
DSS	Decision support system
EU	European Union
FAO	Food and Agriculture Organization of the United Nations
ISO	International Organization for Standardisation
KLS	Kinetic linear system
LV(s)	Latent variable(s)
MLR	Multiple linear regression
MS	Microbial spoilage
na	Not applicable
NS	Not significant
OLS	Ordinary least square
PC(s)	Principal component(s)
PCA	Principal component analysis
PCR	Principal component regression
PLS	Partial least squares
RFID	Radio frequency identification
RMSEP	Root mean squared errors of prediction
RRS	Relative rate of spoilage
SSO	Specific spoilage organism
SSSP	Seafood safety and shelf life prediction
TTI	Time-temperature indicator
UK	United Kingdom
US	United States of America
VL(s)	(Remaining) vase life or vase lives

UNITS

d	Day
h	Hour
min	Minute
N	Newton
J	Joule
K	Degree Kelvin
^{o}C	Degree Celsius
cfu	Colony-forming unit
g	Gram
L	Littre
mL	Millilitre

1 INTRODUCTION

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This chapter describes the major motivations behind the study, which include the potential of RFID technology, the issue of quality loss in the perishable produce supply chain, and the emerging concept of quality-controlled logistics. It also establishes the research hypothesis that the loss in quality of perishable produce can be estimated based on the data collected by an embedded sensor network; and the research objective which is to develop data analysis technique(s) and identify the existing ones for the estimation. In terms of scope, cut roses are used as an exemplar for horticulture produce while RFID tags and data loggers were used for data collection purpose. Previous studies that appear to have similar objectives are briefly reviewed. The research challenges are identified and discussed.

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1.1 RFID TECHNOLOGY

1.1.1 HISTORY OF RFID TECHNOLOGY

Radio Frequency IDentification (RFID) is not a new technology. Its application can be dated back as early as the 1950s in "identification, friend or foe" systems for military aircraft or in electronic article surveillance for anti-counterfeiting (Landt 2001; Landt 2005). Despite such a long history, its implementation within the supply chain industry has only been relatively recent (Hardgrave and Miller 2006). The RFID adoption strategy in 2003 by Wal-Mart, the largest US retailer, was probably the first. The retailer mandated that by the end of 2006 its top 100 suppliers must be RFID compliant (Bansal 2003). In the same year, the US Department of Defence initiated a similar policy for adopting RFID technology. It required all equipment to be supplied with passive RFID tags by January 2005 (US Department of Defence 2003). These two concerted initiatives have since brought RFID technology into industry's focus. As a consequence, a number of companies have started pilot studies to investigate the feasibility of adopting the technology. A survey by AMR Research in 2005 found that 69% of the 500 companies that were involved in the survey, planned to study the feasibility of RFID adoption at various scales, ranging from evaluation phase to pilot, and even full implementation of the technology (Rashid 2005). Large retailers such as Wal-Mart, Target, Metro and multi-national companies including Airbus, Boeing and Procter & Gamble were among those at the forefront of the trend (Airbus 2003; Metro 2003; Griffin 2005; Procter & Gamble 2005; Rashid 2005).

1.1.2 WHAT IS IN AN RFID SYSTEM

Traditionally, an RFID system always consists of two essential components: interrogators (or readers) and transponders, commonly referred to as "tags". The readers send and receive radio frequency data to and from the tags via antennas. An RFID tag is the device which stores the data that identifies the object it is attached to. Such data contain a unique ID number for the object and other details such as its manufacturing date, origin and chemical composition for food products. Depending on their capability to read and write data, RFID

tags can be classified into five classes. For class 0 and class 1 tags, the data can be written once only either at manufacturing sites or at the users' sites. In contrast, the RFID tags in the later classes 2-4 can perform an unlimited number of "read" or "write" operations. Class 3 and class 4 tags are integrated with on-board sensors, which enable data such as temperature, pressure and motion to be recorded at pre-programmed intervals. The most advanced RFID tags, which belong to class 4, can interact with each other and form a wireless sensor network without the presence of a reader. Furthermore, RFID tags can also be classified based on how they are powered. Passive RFID tags depend on their readers for the power source while the active tags are battery-powered. (The semi-passive class refers to the tags that have built-in batteries but still depend on their readers for data communication) (Laran RFID 2004).

The integration of sensors into an RFID tag is a recent development in RFID technology. Adding sensors that can measure the conditions that the products are exposed to such as temperature, vibration, chemicals and gases can provide much more valuable information about their current and historical conditions. While few sensor-integrated RFID systems are commercially available, it is expected that this new generation of RFID systems would lead to a whole new world of imaginable applications in the food supply chain, homeland defence, military operations, manufacturing, animal health, medical operations and other applications (Cain and Lee 2008).

1.1.3 RFID TECHNOLOGY – WHY NOW?

The principal causes of the recent interest in RFID technology can be attributed to both its technological potential and business-related factors.

RFID is capable of realising traceability and eventually real-time visibility along the supply chains, which could have huge implications across many industry sectors, including the horticultural produce supply chain. By definition, traceability is "the ability to follow the movement of a feed or food through specified stage(s) of production, processing and distribution" (ISO 2007). An effective food traceability system can provide a complete history of a product at

various stages and operations from primary production to consumption. The demand for traceability has come not only from consumers but also from distributors and regulatory bodies. For the latter, traceability can facilitate timely root-cause identification and cost effective product recalls if necessary, an issue that has been problematic without effective traceability. For example, in the hepatitis A outbreak in Pennsylvania, US in November 2003 it took the government over three weeks to establish the potential link between the illness and farms outside US, by which point most of the damage had been done (Labuza and Myers 2004). Consequently, there is a growing focus on traceability for all foods as exhibited by a number of US and EU laws and regulations (Labuza and Myers 2004). For the consumers, increased health awareness (e.g. preference for organic products) and major food scares such as Bovine Spongiform Encephalopathy (BSE), *Escherichia coli*, *Salmonella* species and dioxin residues have made them become increasingly critical when purchasing food (FAO 2001). Traceability can provide information on production and processing aspects of the products, and thereby help the customers in making their buying decision.

In addition, strategic RFID policies adopted by a few large (multi-)national organisations seem to contribute to the recent interest in the technology, possibly irrespective of its maturity. An AMR research report indicated that large business entities such as Wal-Mart and the US Department of Defence represented the principal drive in RFID adoption. The report found that many companies would cite customer mandates as the primary reason of their interest in the technology (Rashid 2005). Given its market disruptive potential, other larger companies could not afford to let their business competitors get too far ahead and hence they believed waiting for a more mature RFID technology is unrealistic (Goth 2005).

1.1.4 THE VERDICTS

Three years after Wal-Mart's initiative, different industry sectors started to look back and evaluated the success of their RFID adoption programmes. In 2006, Wal-Mart reported, as a result of its RFID initiative, a 16% reduction in the

number of times it experienced out-of-stock situations and a 60% improvement in efficiency of replenishing the shelves with products from its backroom stores (Cecera and Suleski 2007). Procter & Gamble, one of Wal-Mart's top providers of consumer goods, praised the initiative saying its multi-million RFID investment had been recovered (Songini 2007). However, results from other RFID adopters were less impressive. Plans to expand RFID deployment at Target and the US Department of Defence were postponed; an RFID pilot study at Albertson, another U.S. giant retailer, was discontinued (Cecera and Suleski 2007). Even Wal-Mart itself was reportedly to re-assess its RFID strategy (Weier 2007).

Nowadays, the general industry view of RFID technology has become more cautiously positive: its potential is enormous but there exist challenges that need to be addressed. Cost, lack of practical knowledge about the technology, difficulty of demonstrating Return-on-Investment (ROI), practical issues (e.g. difficulty of attaching tags) and technological issues (integration, reliability, lack of standards) were reportedly among the barriers to RFID adoption (Riedel *et al.* 2008). One major challenge that has been pointed out in numerous publications lies in the management of the data captured by RFID (Han *et al.* 2006; Lin *et al.* 2006; Attaran 2007; Sabbaghi and Vaidyanathan 2008; Kapoor *et al.* 2009). Specifically, the question for interested companies is how they are going to handle and interpret the enormous volume of RFID data to achieve competitive advantages in their business. Companies have become increasingly aware that adopting RFID solely for compliance purpose may not be economically justified. They realise that in order to achieve a return on investment in RFID technology, valuable information must be mined from the captured RFID data, interpreted and shared within the companies as well as with external partners to solve a specific business problem (Goth 2005; Faber 2007; Fred *et al.* 2007; Murphy 2007). This view effectively emphasises the essential role of data analysis in the successful deployment of RFID technologies.

1.2 LOSS IN QUALITY OF FRESH HORTICULTURAL PRODUCE

1.2.1 FRESH HORTICULTURAL PRODUCE

Amongst all the agricultural sectors, horticulture focuses on cultivating plants that are used by people for food, for medicinal purposes and for aesthetic gratification. Its products generally include fruits, vegetables, ornamentals, nuts and medicinal plants. Of those, fruits, vegetables and flowers are often marketed soon after harvest without significant processing, leading to such terminologies as fresh produce and fresh cut flowers.

Fresh fruits, vegetables and cut flowers are important agricultural products for their nutrition, pleasure and hence economic values. In 2008, fresh fruits and vegetables alone accounted for £8.34bn in the UK retail market (KeyNote 2009). A significant proportion of fresh produce (89.5% and 42.2%, respectively) is imported for UK domestic consumption with the main sources of supply being South Africa, France, the Netherlands, New Zealand Chile, Spain, Turkey and the US (KeyNote 2009). The UK retail market for cut flowers is smaller and was worth £1.84bn in 2008, of which approximately £700m was accounted by imports from countries including Kenya and the Netherlands (MINTel 2008). The value of world export in fresh fruits, vegetables and cut flowers was estimated at £63bn in 2003 (Pinckaers 2005).

1.2.2 THE SUPPLY CHAIN

Beside the farms and the consumers, there are 3 major stakeholders in the supply chain of horticultural produce, including the cooperative agents, the wholesalers and the retailers. Figure 1.1 outlines the roles that these stakeholders play in the supply chain. The cooperative agents are primarily the first outlet for the products after leaving the farms. Traditionally, the produce would be brought to a wholesale market where the bulk shipment is sold to a wholesaler. Nowadays auction markets are the more popular destination. For example, FloraHolland, the world largest auction of floricultural products, reported an annual sale of €3.8 billion in flowers and plants for 2009. The auction imports flowers from 60 countries while its products are exported to

almost 140 different ones (FloraHolland 2010). This has made the FloraHolland auction and the likes become international centres for the supply and demand of floricultural products (van Dantzig and Boonstra 2005). However, the auction system may be heading toward more challenging times as a number of growers have started to move away from auction and chose to deal with wholesalers and distributors directly (Yanik 2010), particularly for fresh fruits and vegetables (Pinckaers 2005).

The wholesalers, the second major stakeholders, are normally a multi-national distributor but could be any combination of exporters, importers and distributors. They are responsible for transporting the produce from the auction houses and wholesale markets to their distribution centres, which are often closer to the retailers. Two of the biggest UK-based distributors of cut flowers are World Flowers, which delivers over 1.5 billion cut flower stems a year to its customers around the world, and Flamingo Holdings, supplying 600 million flower stems each year to the UK market (MINTel 2008).

The retailers, the outlets that directly sell cut flowers to consumers, are supermarkets, florists, street markets and garden centres. Among these, supermarkets have the largest share of cut flower markets, accounting for 65% of the total UK market in 2007 while the other three altogether captured some 26% (MINTel 2008). For their advantages of strong buying power and in-store capacity to offer a wider choice of flowers, supermarkets such as Marks & Spencer are believed to continue to dominate the market although mail order and online sales are increasingly popular (MINTel 2008).

Logistically, from the farm to their retail outlets, fresh vegetables, fruits and cut flowers often go through a combination of transport modes. Trucks and trailers are by far the primary transportation means. For long distance delivery, air shipments or sea freight may also be involved. Of those two, although temperature abuse is a concern in air freight (Pearce 2003; Staby and Reid 2007), it is often the preferred mode solely due to the shorter delivery time (Anonymous 2005).

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                    │  The producers (i.e. farms) │
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        ┊              │  • Wholesale market       │
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                    │  • Distributors           │
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                    │  • Supermarkets           │
                    │  • Florists               │
                    │  • Street markets         │
                    │  • Garden centres         │
                    │  • Mail order/ online     │
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                    │  The consumers            │
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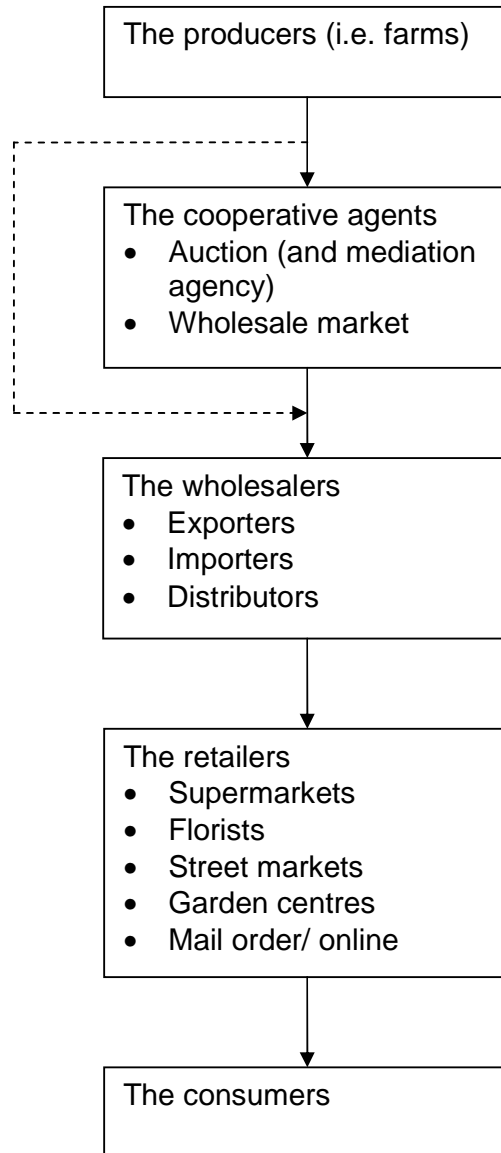
Figure 1.1: Major stakeholders in supply chain of horticultural produce

1.2.3 QUALITY CONCEPT AND REMAINING SHELF LIFE DEFINITION

In general, the quality of a product is a combination of its characteristics that enable it to meet consumer expectations and needs (FAO 2008). For foods, including fresh horticultural produce, the concept of quality becomes increasingly complex as the consumers' needs and expectations have evolved over the years. In the past, most children probably grew up being told by their parents to eat whatever that was given to them. Most of the attention then was whether the food was edible; little interest was paid to how such food got to their

dining table in the first place. Nowadays, consumers, particularly those from developed countries, are likely to expect more than just "food as fuels" (Promar International 2006). They want exotic products to be affordable and available all year round (KeyNote 2010). They would assess the product quality using sensory attributes such as taste, texture and appearance, nutritional attributes such as energy, protein, carbohydrate and fat, and safety attributes e.g. allergy-related information. Other factors that also attract increasing consumer interest include product origin, environmental consideration, worker's welfare, and sustainable agriculture (FAO 2008). Therefore, those attributes and factors, being considered as a whole and relative to each other, although rather subjective, together determine the quality of fresh horticultural produce as perceived by a consumer.

For wholesalers and producers of fresh fruits, vegetables and cut flowers, the product quality involves additional considerations. The wholesalers would be concerned with issues such as the supply security, the ease of packaging and labelling, and the stability of the product during transport and storage. For the producers, a product that requires less input but can be sold at higher price is the one that has higher quality.

As information regarding the quality of horticultural produce (and other food products) is not readily reflected or accessible on its label, some measures are used as an indirect indication of its quality. "*Remaining shelf life*" (or vase life for cut flowers) is one such measure. A universally accepted definition for the term does not seem to exist (Fu and Labuza 1993) possibly because consumers, retailers and other stakeholders have different preferences over the attributes of produce quality. Examples of its definition are:

- "*the time period for the product to become unacceptable from sensory, nutritional or safety perspectives*" (Fu and Labuza 1993).
- "*the time during which the food product will remain safe, be certain to retain desired sensory, chemical, physical and microbiological characteristics, comply with any label declaration of nutritional data when*

stored under the recommended conditions" (Institute of Food Science and Technology 1993).

- "*the period during which the product maintains its microbiological safety and sensory qualities at a specific storage temperature*"(Chilled Food Association 2006).

Perhaps due to the lack of a universal definition, the shelf life period that is shown on some food products could be quite arbitrary and in some cases not supported by scientific studies (Panagou 2004).

This study adopts the definition by Chilled Food Association. However, for cut roses, the requirement of microbiological safety is irrelevant as the flowers are inherently safe.

1.2.4 THE POST-HARVEST LOSSES IN QUALITY

Due to their perishable nature, the quality of fresh fruits, vegetables and cut flowers deteriorate with time after harvest. A number of factors can speed up or slow down such post-harvest senescence but none can stop it. Eventually, the product quality will become so poor that it will not be suitable for human consumption. This happens to a significant proportion of horticultural produce in chilled supply chains even before reaching their prospective consumers, which is a major issue that is recognised by the industry. It was reported at the 2006 world cut flower congress that approximately 20 - 30% of fresh produce was lost during transport (Gregory 2006). For developed countries, Kader and Rolle (2004) estimated that 12% of fresh fruits and vegetables were lost between production and consumption sites. For developing countries, the loss was likely at a greater scale, with estimates as high as 40% (APO and FAO 2006) or 50% (Brown *et al.* 2005). To make matters worse, quality loss does not always result in a product being discarded but it does lead to loss in profitability. Losses in quality during transport and storage could transform high quality premium products into acceptable economy class ones. This loss, which was not quantified, was believed to be even more significant (Brown *et al.* 2005). Consequently, given the size of the industry, the post-harvest loss poses a significant economic burden.

1.2.5 THE CAUSES OF THE POST-HARVEST LOSSES

There are many factors that lead to post-harvest loss in quality of horticultural produce. The most obvious one lies in post-harvest management of the products. Experts have pointed to providing optimal ranges of temperature and humidity as the most important practice to minimise quality loss after harvest (Kader 2003; Kader and Rolle 2004; Brown *et al.* 2005; Gregory 2006). However, industrial experience indicates that this is far from being achieved; a typical shipment of cut roses would be at 10 - 20 ^{o}C, much higher than the ideal temperature of less than 5 ^{o}C, for most part of their journey from the farms to the retailers (Pearce 2003; Staby and Reid 2007; Klümpen 2010); temperature abuse was reported in 15 - 30% of the trips, according to an industrial survey (White 2007). In addition, produce genotype, pre-harvest conditions and other post-harvest factors (such as mechanical stress) are believed to contribute to the post-harvest loss in quality (Brown *et al.* 2005). The effects of all of these factors are discussed more fully in Section 2.3.

1.3 QUALITY-CONTROLLED LOGISTICS

In the food industry, the increases in business competition and in the complexity of the supply chain networks have driven companies to continue optimising their supply chain management. Recently, a new inventory management concept called "quality-controlled logistics" has emerged. Conceptually, it is based on the idea of directing product flows according to product quality and customers' quality demands (van Der Vorst *et al.* 2005). For horticultural produce, indirect measure of quality such as shelf life, "sell-by date", and "expiry date" could be used in place of the product quality. For that reason, quality-controlled logistics have lead to policies such as "first expire first out" or "last expire first out", which are all related to the quality of the produce, as opposed to the traditional "first in first out" (Emond and Nicometo 2006).

The benefits of quality-controlled logistics are already recognised; it could improve food safety and customer service (Roberti 2005), reduce unnecessary

buffers in inventory (Jedermann *et al.* 2008), and ultimately reduce distribution costs and cycle times (Hingley *et al.* 2007).

A critical requirement for an effective quality-controlled logistics system is that the produce quality must be known. In order to implement such policies as "first expire first out", this knowledge must always be timely accessible throughout the supply chain. Clearly, this rules out laboratory testing for quality measurements as it would not be practical, and hence necessitates quality modelling and prediction for horticultural produce.

1.4 RESEARCH MOTIVATION AND SCOPE

The work in this thesis is motivated by these major factors: the potential of RFID technology (Section 1.1), the issue of quality loss in the supply chain of fresh horticultural produce (Section 1.2), and the recent trend in logistics management (Section 1.3). While RFID technology can potentially offer great benefits, a major challenge to its adoption is how to identify and realise a competitive advantage using the technology. Data analysis is one of the keys to overcoming this challenge. In addition, quality prediction is required for the horticultural produce industry to manage and reduce the significant post-harvest losses encountered in the supply chain, and to move toward quality-controlled logistics. As a result, this thesis investigates the development of data analysis techniques to estimate the quality of horticultural produce from the data captured by RFID sensors.

In terms of scope, the study focuses on cut roses as an exemplar for horticultural produce and the data analysis techniques that it develops will be equally applicable to other produce. The reason for selecting cut roses is because they are reportedly the leading cut flower crop (Pinckaers 2005), and are considered to be a high-valued product. In addition, cut roses are reportedly one of the horticultural produce that are most susceptible to the transport condition (particularly temperature). The supply chain for cut roses is not very long (about 72 h). Furthermore, remaining vase life (VL) has been used as a measure of the quality of cut roses throughout this study.

In addition, data loggers are used throughout this study for data collection while temperature-sensor-integrated RFID tags are used occasionally for demonstration purpose. This is solely due to the unavailability of the RFID tags. Nevertheless, it is expected that the data analysis will be the same regardless of whether data loggers or RFID tags are used.

1.5   RESEARCH HYPOTHESES AND OBJECTIVES

This study investigates the hypothesis that whether or not using multivariate data analysis techniques the loss in quality of the perishable produce can be estimated based on the data collected by embedded sensor networks. Specifically, it examines the possibility of estimating the loss in remaining VLs of cut roses using post-harvest temperature recorded by data loggers or RFID tags. The study aims at developing novel data analysis technique(s) as well as identifying existing ones for the quality estimation.

1.6   PREVIOUS STUDIES

A number of studies have been identified as having some similarity with this work. One of them was publicised in 2009 by Ambient Systems and Information Highway Group (IHG). During their demonstration study, RFID tags were placed in strawberry pallets which were subsequently transported from a farm in Spain to a distribution centre in Germany. During the transport, temperature was measured and remaining shelf life of strawberries in each pallet were estimated and transmitted through a wireless network with general packet radio service (GPRS) connection. Both the temperature and the remaining shelf life were available upon the produce's arrival at the distribution centre (Ambient Systems and Information Highway Group 2009). Details of how the remaining shelf life was estimated from the temperature measurements are not available and no patent for the algorithm has been identified. The study demonstrated the emerging interest from perishable goods supply chain industry in using RFID technology.

Another study was carried out to investigate the microbiological impact of transport temperature on fresh-cut endive (Rediers *et al.* 2009). Data loggers were placed in crates of fresh-cut endive that were transported from the farm to the processor and from the processor to different restaurants. Endive samples were taken for microbiological analyses at three different points along the supply chain. The study observed that higher levels of indicator microorganisms were associated with temperature fluctuation during transport (Rediers *et al.* 2009). The result implied that transport temperature was an important factor that could influence the microbiological quality of the produce. However, the study used the data collected by data loggers for observation purpose only i.e., it did not perform any quantitative analysis with the data, which is the main focus of this work.

1.7 RESEARCH CHALLENGES

Estimating the quality of horticultural produce based on RFID collected data has two major challenges. The first one lies in the characteristics of the data itself. The data consists of different variables of the perishable produce system, which may be broadly classified as pre-harvest, at-harvest and post-harvest variables. From a system engineering point of view, the first two classes of variables, i.e. pre-harvest and at-harvest, can be seen as the initial conditions of the produce system; the post-harvest variables represent its system dynamics during the supply chain. Post-harvest variables including temperature, and possibly humidity, are recorded along the supply chain by RFID tags or data loggers, resulting in series of measurements of the variables. These could be considered as nonlinear time series because the variables, e.g. temperature, are not properly controlled. The number of measurements per time series is usually quite limited, e.g. less than 100 temperature measurements for a typical supply chain of cut roses, due to the limited memory capacity of RFID tags or data loggers, while a normal time series would often exceed 1000 samples. Consequently, any existing time series data analysis techniques may not be readily applied to the current data. In short, the post-harvest data is similar to a nonlinear multivariable time series but existing techniques may not be used for its analysis.

The second major challenge of the study is due to the complex biology associated with the perishable produce. It is believed that the understanding of the underlying biological system (i.e. the produce) and its associated processes (e.g. senescence) can greatly improve the performance of any data analysis technique. However, as the underlying biological system of horticultural produce is inherently complex, its associated processes are not completely understood. As a result, little *a priori* information exists linking the collected data with the produce quality. The challenge is therefore how to develop a data analysis technique that could describe the link between the post-harvest data collected by RFID tags and the quality of the produce with little *a priori* knowledge of the senescence process.

In short, the challenges involved in this thesis are the multivariate, nonlinear, time series nature of the variables and the lack of knowledge of the senescence process that links the collected data to the quality of the produce.

1.8 ORIGINAL CONTRIBUTION

There are a number of original contributions that the work reported in this thesis makes to scientific understanding. These are briefly summarised below:

1. A novel technique termed Kinetic Linear System (KLS) was developed for modelling the effect of temperature on the remaining shelf life of perishable products. The technique is based on kinetic principles and hence is applicable to perishable products the shelf life of which is governed by chemical, biochemical, microbial and physical processes. It is data-driven and so can be applied to products which do not normally have a traditional kinetic model.

2. Using cut roses as an exemplar, this work demonstrates that multivariate data analysis techniques can be used to generate effective estimates of the post-harvest loss in quality of perishable produce based on real supply chain data collected by advanced sensors. The prediction capabilities of KLS, PLS and MLR were investigated for the analysis of

real supply chain data in various contexts such as with or without an *a priori* constraint, using pre-harvest data, using post-harvest data or both.

3. In terms of the physiological understanding of cut roses, this work confirmed an expert opinion that temperature is the most critical post-harvest environmental factor that affects the post-harvest vase life of cut roses. While it agrees with the opinion, this work also shows that other factors such as pre-harvest growing temperature could be equally important.

4. This work also delivers two original data sets that were collected in large scale experiments with international supply chains of cut roses. These two data sets are extensive as they contain measurements collected during pre-harvest, at-harvest and post-harvest periods, and the results of the vase life tests.

1.9 ORGANISATION OF THE THESIS

This thesis consists of eight chapters. Chapter 1 establishes the context of the study with research motivations, scope of the study, research hypothesis, objectives and challenges. Chapter 2 reviews current literature in the senescence of cut flowers, particular roses, and the techniques that can be used to estimate the quality of perishable produce. Subsequently, Chapter 3 describes the technical issues involved in implementing the data analysis techniques identified in Chapter 2 (i.e. PLS and MLR), and subsequently outlines the solutions that are adopted in this study. The procedure for performance assessment of the data analysis techniques is also established in this chapter.

Chapter 4 describes the mathematical development of a novel data analysis technique (KLS) for estimating the quality loss of perishable produce. Different aspects of implementing the technique are discussed, including the possible mathematical scenarios, the assumptions and the implementation procedure. Chapter 5 demonstrates the validity of the newly developed technique by comparing its performance with the simulated outputs from a number of kinetic simulation models. Chapter 6 reports the performance of KLS, PLS, and MLR

techniques in an in-house experiment with Cookes Rose Farm. Similarly, Chapter 7 reports the implementation of the three techniques in a study of a chilled supply chain of cut roses. The thesis conclusion is presented in Chapter 8, together with a discussion on potential future work.

2 LITERATURE REVIEW

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This chapter reviews existing literature in post-harvest studies of cut flowers, particularly roses. Two major areas are addressed: the current understanding of post-harvest senescence of cut roses; and the existing techniques to determine the post-harvest loss in terms of remaining VL. More specifically, the chapter provides general information on the production of cut roses and then describes the phenomena that are commonly associated with cut flower senescence. The understanding of those phenomena provides the foundation for the discussion, of the effects of various genetic, pre-harvest, and post-harvest factors on the longevity of cut roses. Existing techniques to determine the losses in VL of cut roses can be classified into evaluation techniques and estimation techniques. Both of these classes of techniques are reviewed in this chapter.

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2.1 Cut rose production

For commercial cultivation, roses are grown mainly in a protected, i.e. greenhouse, environment. This facilitates advanced control over the growing conditions: temperature, carbon dioxide, light, humidity, irrigation, nutrient delivery, etc., of the crop and thereby extends its availability during the year as well as increases production. The total worldwide greenhouse area devoted to cut rose production was estimated to be approximately 8500 ha; close to half of that area was from the top three countries including Ecuador, Colombia and Kenya. Over the past decade, individual production facilities have become larger (over 10 ha) to optimise their marketing and logistic operations as well as to reduce labour cost (Blom *et al.* 2003).

As greenhouse roses can be produced year-round, their cultivation and harvest have been scheduled to target special occasions such as Valentine's Day and Mother's Day. To facilitate such crop timing, detailed planting and harvesting are generally required. During winter-to-spring seasons, roses are grafted on rootstock, a plant with an established, healthy root system, and are allowed to sprout. Subsequently, the growers could harvest or pinch the shoot to force the development of more new shoots from the bud(s) at the node below the harvest cut or pinch. The average time from pinching to the next harvest is approximately 6 to 10 weeks. This duration varies significantly with flower varieties and the time of a year (Reid 2008).

Roses possess a wide variety of colour. Red has been the traditional and predominant colour; however, yellow, pink and white cut roses are widely available. Recently, Suntory Ltd announced its commercialisation of the genetically modified blue-violet roses in Japan (Suntory Ltd. 2009). New varieties are constantly being developed.

Rose prices depend on a number of quality attributes, of which the two most common are bud size and stem length. In terms of bud size, roses are classified as hybrid tea, sweethearts or miniatures, where the hybrid tea class usually has

a higher price. For stem length, a general rule is that the taller the stems, the higher the price. Cut roses are commonly graded on stem length in 10 cm intervals, e.g. 20-30 cm, 30-40 cm, 40-50 cm and 50-60 cm (Blom *et al.* 2003).

2.2 SENESCENCE OF CUT ROSES

While floral senescence may not yet be completely understood (van Doorn 2004; Rogers 2006; van Doorn and Woltering 2008), previous studies generally agreed that for cut flowers it is always accompanied by most, if not all, of the following physical phenomena: a reduction in xylem hydraulic conductance due to vascular occlusion, lower stomatal conductance, decrease in phloem transport and sugar starvation.

2.2.1 VASCULAR OCCLUSION

After harvest, cut flowers are deprived of their natural supplies of water and nutrients, which were previously provided by their root system. Although these resources can be artificially supplied by placing cut flowers in vases filled with nutrient solution, the translocation of water and nutrients through the stem is progressively diminished. The most important cause is that the translocation ability is significantly impaired by xylem occlusion. A number of factors leading to the occlusion of the xylem include air aspiration, cavitation formation, bacteria-induced blockage and the metabolic response of the stem to cutting.

Cavitation formation and air aspiration

Cavitation, the formation of vapour bubbles inside flowing liquid, is a routine phenomenon in all transpiring plants including intact or cut flowers. A popular hypothesis for the formation of cavitation inside xylem conduits is the 'air seeding' hypothesis first advanced by Zimmermann (1983). The hypothesis suggests that due to a critical pressure difference across the pit membranes, the radius of the air-water menisci is reduced until the entering of air seeds, which nucleates cavitation. In addition to cavitation, air aspiration also leads to embolisms in the xylem of cut flowers. Immediately after harvest, the xylem of cut flowers is exposed to air, which enters its conduits through the cutting surface. The presence of aspired air in the xylem conduits contributes to xylem

occlusion and a decrease in subsequent water uptake (van Meeteren *et al.* 2006).

Microorganism-induced blockage

Studies have shown that microorganisms are partly responsible for xylem occlusion. For example, washed microbial cells of *Bacillus*, *Enterobacter*, *Kluyveromyces* and *Pseudomonas* spp. upon being added to vase water were able to infiltrate into the cut xylem vessels of roses; microbial polysaccharides (mol. wt. > 10 000) in the vase water led to total occlusion of xylem transport, subsequently resulting in "bent-neck" in cut roses (Put and Rombouts 1989). In addition, aerobic pectolytic microorganisms are believed to play a major role in disturbing the water uptake in plants (Put and Rombouts 1989). This is because they produce enzymes that are capable of degrading pectin, the major cell-wall constituent of herbaceous plants. Overall, the number of exogenous bacteria in vase water is negatively related to the longevity of cut flowers by upsetting the water uptake (Put and Jansen 1989; van Doorn *et al.* 1995). In addition, by preventing microorganisms from occluding the xylem, antimicrobial chemicals such as 8-hydroxyquinoline sulphate (HQS) are capable of alleviating the reduction in the hydraulic conductance, and thereby prolonging the VL of cut roses (Ichimura *et al.* 1999).

Metabolic response to wounding

Plants possess metabolic mechanisms to prevent the entry of micro-organisms into their opened tissues at wounded sites. Although many aspects of such mechanisms are not yet clear (Loubaud and van Doorn 2004), it is known that wounding results in occlusion of the xylem conduits, due to diverse processes such as gum deposition, formation of tyloses and balloon-shaped outgrowths of cells adjacent to a conduit (van Doorn and Cruz 2000).

Chemicals that inhibit the plants' wound healing appear capable of extending remaining VL of cut flowers. This was demonstrated when applying *S-carvone*, a putative antibacterial and anti-wound healing chemical, on Maiden's Blush (*Baeckea frutescens*; Myrtaceae) and Geraldton waxflower (*Chamelaucium uncinatum*; Myrtaceae) (Damunupola *et al.* 2010).

2.2.2 A REDUCED XYLEM HYDRAULIC CONDUCTANCE

There are a number of hypotheses as to how stomata respond to a reduction in xylem hydraulic conductance. One common hypothesis is that there exists a simple feedback system between stomata conductance and leaf water potential, which is influenced by xylem occlusions. For that feedback system, low leaf water potential would lower stomata opening so as to reduce water loss by transpiration. In turn, low water status at the leaf would be caused by a decrease in xylem hydraulic conductance, a consequence of xylem occlusions (Saliendra *et al.* 1995; Hubbard *et al.* 2001). However, there were conditions in which stomatal response appeared independent of leaf water status; but rather it seemed to be directly dependent on the variables influencing the leaf water potential (Saliendra *et al.* 1995) such as xylem hydraulic conductance.

Regardless of what the mechanism of stomatal response was involved, it is generally agreed that a reduction in the xylem hydraulic conductivity would result in lower stomata opening. This observation, that the two factors were positively correlated, was supported by a number of studies (Sperry *et al.* 1993; Sperry and Pockman 1993; Saliendra *et al.* 1995; Hubbard *et al.* 2001; Tuzet *et al.* 2003). For example, evidence from Sperry and Pockman's study of *Betula occidentalis* showed that a reduced xylem hydraulic conductance, by injecting air into the xylem, induced a decrease in stomatal conductance (Sperry and Pockman 1993); in a similar study for ponderosa pine under controlled stead-state conditions, Hubbard and colleagues (2001) also found that the stomatal conductance and the plant assimilation were directly proportional to the xylem hydraulic conductance.

2.2.3 DECREASING PHLOEM SUGAR TRANSPORT

Photosynthetic products and other nutrients are transported via phloem from plant sources to plant sinks. At the sources e.g. mature leaves, the photosynthetic assimilate is produced in excess and hence is available for re-distributing to other parts of the plant. At the sinks e.g. flowers and young leaves, the photosynthesis production does not satisfy the local demand and hence assimilate import is necessary. As stomatal conductance is reduced,

photosynthesis is affected and consequently the concentration of sucrose, the main photosynthetic product, in the leaves decreases. In turn, research showed that this sucrose concentration is linearly correlated with the net carbon export rate into the sieve tube sap (Fader and Koller 1983; Grodzinski *et al.* 1998). As a result, it is likely that a reduction in stomatal conductance would lead to a decrease in sucrose availability from photosynthesis.

2.2.4 SUGAR STARVATION

Intuitively, a reduction in photosynthetic sugar would eventually lead to sugar starvation, provided that no sugar remobilization by the plant itself or exogenous compensation was attempted. In cut flowers, sugar starvation is most likely to occur at the petals themselves as they certainly represent major sugar-sinks. It is therefore tempting to conclude that insufficient (sugar) energy for maintenance would be the cause of petals' and eventually flowers' senescence. This hypothesis was first proposed in (Thimann *et al.* 1977) for leaf senescence. Since then, seemingly supporting as well as contradicting evidences have been observed. van Doorn (2004) presented a review of arguments both in favour of the hypothesis, that sugar deprivation causes senescence, and against it, that an excessive sugar level causes senescence. The review found that there was not good evidence in cut flowers to invalidate the hypothesis, while considerable evidence existed in substantiation of it. For example, Ichimura *et al.* added sucrose to the vase solution in which cut roses (*Rosa hybrida L.* cv. Sonia) were displayed, and observed an increase in soluble carbohydrates in the petals of the flowers, leading to an extended VL. It was therefore concluded that a positive correlation existed between sugar level in petals and the VL of cut roses (Ichimura *et al.* 1999; Ichimura *et al.* 2003). Similar conclusion for other cut flowers has also been observed (Chanasut *et al.* 2003).

In summary, a much simplified picture of senescence in cut flowers would begin with a reduction in xylem hydraulic conductance due to vascular occlusion. The reduction in turn leads to a decrease in stomatal conductance. As a result, photosynthesis is affected and less sugar is available for export to major sinks

such as flower petals. This eventually results in sugar starvation, which was believed to initiate flower senescence.

2.3 FACTORS AFFECTING THE SENESCENCE OF CUT ROSES

2.3.1 GENOTYPE – THE GENE THAT IS INHERITED

Genotype is undoubtedly the most critical factor in the growth, development and senescence of plants. It carries structural information according to which plant machinery is built. For example, plants of different genotypes have structural differences in their xylem networks, which influence air embolism removal and xylem hydraulic conductance recovery during their subsequent post-harvest life (van Ieperen *et al.* 2002; van Meeteren *et al.* 2006). This would partly explain the observation that water stress tolerance varies with cut flower cultivars as van Doorn and Vojinovic (1996) observed in cut Frisco roses and cut Sonia roses. Furthermore, flowers of different genetic origins were shown to have different abscisic acid (ABA) level in petals, different endogenous ethylene production (Mayak *et al.* 1972), different sensitivity to exogenous ethylene (Müller *et al.* 2001; Macnish *et al.* 2004), all of which directly correlates with flower longevity. In fact, by modifying the genotype, genetic engineering can create new cultivars of flowers with better longevity, as well as other desirable attributes such as novel colour, scent, and better resistance to abiotic and biotic stress (Zuker *et al.* 1998; Bovy *et al.* 1999; Rout *et al.* 1999; Onozaki *et al.* 2001; Suntory Ltd. 2009).

2.3.2 PRE-HARVEST GROWING CONDITIONS

Flower genotype interacts with environmental conditions and subsequently results in different phenotypes of flowers with varying characteristics. Consequently, pre-harvest factors such as water stress, air humidity and light play significant roles in the development of flower plants and eventually the senescence of their flowers. Research found that water availability during pre-harvest periods could influence the xylem anatomy of a plant. The abiotic stress leads to smaller diameter xylem conduits in grapevine plants (Lovisolo and Schubert 1998) and in an *Olea europaea* L. cultivar (Verdeal Transmontana)

(Bacelar *et al.* 2007). Subsequently, plants with smaller xylem vessels are less susceptible to cavitation than those with larger xylems (Tyree and Dixon 1986). Moreover, cut flowers with a smaller xylem diameter had a better capability to recover from xylem occlusion due to air aspiration following subsequent placement in water (Yang and M. T. Tyree 1992; van Ieperen *et al.* 2002), and hence would have longer VL. This phenomenon was observed in sugar maple (*Acer saccharum*) (Sperry *et al.* 1988) and cut chrysanthemum flowers (*Dendranthema x grandiflorum* Tzvelev) (van Meeteren *et al.* 2006).

Relative air humidity during the growing period is also capable of affecting the post-harvest VL of cut flowers. Research showed that plants grown in humid conditions developed highly conductive stomatal systems that would be less capable of controlling water loss during the post-harvest stage (Nejad and Meeteren 2005; In *et al.* 2007a). The water balance in the cut stems of these plants is more susceptible to being upset, which ultimately leads to shorter post-harvest life. This conclusion was verified for 14 rose cultivars when Mortensen and Gislerød (1999; 2005) observed that high humidity levels during growing periods had negative effects on the subsequent VL of the roses.

Light, a critical yet variable environmental factor to plants, also plays an important role in the post-harvest life of cut flowers. Lighting period during pre-harvest was shown to have negative effects on the subsequent VL of cut roses (Mortensen and Gislerød 1999). In addition, research showed that light quality (red to far-red wavelength) also had a complex effect on the accumulation of ABA in flower petals. It was observed that red light resulted in higher level of ABA in rose petals compared to far-red (Loveys 1979; Garello *et al.* 1995). Conversely, Tucker (1976) and Tillberg (1992) showed the opposite when studying Scots pine seed and tomato. As higher ABA levels are associated with longer VLs in cut flowers (Mayak *et al.* 1972), light conditions during the growing period could have significant impact on the longevity of cut flowers.

Urban *et al.* studied the effect of pre-harvest CO_2 level on water balance and senescence of cut roses. They found that cut roses grown in an elevated CO_2

atmosphere were able to maintain their water balance longer and hence their VL was extended (Urban *et al.* 2007).

2.3.3 POST-HARVEST TEMPERATURE

It is generally agreed that temperature is probably the most critical post-harvest environmental factor affecting the VL of cut flowers. The higher the storage temperature, the shorter the VL of cut flowers is, particularly cut roses (Faragher *et al.* 1986; Ichimura *et al.* 1999; Pompodakis *et al.* 2005). Being intrinsic, temperature influences the rate of all metabolic reactions that occur in cut flowers from harvest to the end of their VL. However, the extent of such kinetic influence has not been quantified because the metabolism in plants and specifically in flowers is not yet fully understood. For cut roses, the dramatic effect of temperature on the VL of the flowers is believed due to its kinetic role in the respiration process. A study showed that respiration in cut roses increased exponentially with temperature and could reach up to 6-fold for a $10^{o}C$ increase in temperature (Reid and Andrew 2003). A similar result was also observed in Narcissus flowers (Cevallos and Reid 2000).

In addition to its kinetic effect, post-harvest temperature was found to play a significant role in different stages that lead to senescence of cut flowers. For xylem functioning, Ichimura *et al.* (1999) found that higher temperature resulted in a more rapid decrease in hydraulic conductance of cut roses, and thereby shortened their VL. Moreover, when cut roses were held in colder water, higher water uptake rate was observed (In *et al.* 2007b), which may be attributed to an inhibitive effect of low temperature to xylem occlusion. A study on excised wheat shoots revealed that the transpiration through the stem under the same transpiration tension from the ear varies significantly with temperature (Kuppelwieser and Feller 1991). Other research in the temperature effects on xylem transport is mostly for intact plants and focuses more on freezing conditions (Cavender-Bares *et al.* 2005; Qu *et al.* 2007). Nevertheless, these studies also found temperature to be a significant factor on the functioning of xylem.

In addition, post-harvest temperature was also shown to influence stomata functioning. Research showed that temperature was the crucial physiological factor stimulating the opening and closing of tulip petals (Azad *et al.* 2004). During such petal movements, the proportion of open and closed stomata on the inside and outside of the same petals were redistributed, which could influence turgor pressure and other physiological functions, including water balance (Azad *et al.* 2007).

Moreover, temperature was also capable of inducing inhibitions to phloem translocation. This inhibition was believed to be the consequence of physical blockages of the sieve plates (Minchin *et al.* 1983). A further study by Minchin and Thorpe (1983) on Common Morning Glory *Ipomoea purpurea* revealed that the inhibition of phloem transport was dependent on the rate of cooling rather than the temperature *per se*. More recently, Peuke *et al.* (2006) in a study of *Ricinus communis* observed a decrease in the solute (sucrose) concentration in the phloem sap, which was believed to be due to the effect of low temperature on the retrieval of sugar into the phloem. One common conclusion from these studies was that the temperature effect on phloem translocation is temporary and the phloem blockages are fully reversible. However, it is noted that these studies were carried out on intact plants. Whether or not cut flowers could recover from such inhibitions needs further investigation.

Post-harvest temperature may also have an important impact in cultivating diseases in cut flowers. Research showed that cut roses that were exposed to cooling and slow re-warming were more susceptible to fungal infection from *Botrytis cinerea* (van der Sman *et al.* 1996). As cooling is often employed to remove field heat from cut flowers, subsequent temperature control is important to avoid re-warming, and thereby reduce *Botrytis* infection.

2.3.4 POST-HARVEST HUMIDITY

Humidity is one of the post-harvest factors that affects stomata functioning (Tuzet *et al.* 2003). The underlying mechanism of such influence is complex and not yet fully understood (Buckley 2005; Bunce 2007). However, it seems that in

general stomatal response would counteract the effects of the changes that occur to the plant possibly to maximize its maintenance and hence longevity. For example, stomata closure was observed after a decrease in atmospheric humidity (Saliendra *et al.* 1995). This may be explained by the fact that a lower atmospheric humidity results in a larger humidity gradient which leads to a reduction in stomata apertures in plants to restrict water loss.

In practice, compared to temperature, post-harvest humidity appears to have less direct impact on the VL of cut flowers. Faragher *et al.* (1986) stored cut roses at 65% and 95% relative humidity, and found that the latter treatment slightly extended the VL of the flowers (4.6 d at 95% relative humidity compared to 3.9 d at 65% relative humidity). Consequently, the researchers concluded that humidity levels during cold storage were found to have little effect on the VL of cut roses (Faragher *et al.* 1986).

However, the most significant problem associated with relative humidity is its promoting effects of diseases. For example, *Botrytis* infection, one of the most common post-harvest diseases in cut flowers, is particularly promoted at high relative humidity (Salunkhe *et al.* 1990; Droby and Lichter 2004). These diseases contribute further to losses in quality and subsequently quantity of perishable produce. Visually, *Botrytis* blight reduces the ornamental value of cut roses. Metabolically, it produces additional ethylene, ABA and other plant hormones (Salunkhe *et al.* 1990; Sharon *et al.* 2004), which initiate senescence symptoms such as petal necrosis and petal abscission (Droby and Lichter 2004). Various treatments to overcome *Botrytis* infection have been developed and the use of anti-*Botrytis* products cost US$ 15-25 million a year (Elad *et al.* 2004), which highlights the scale of the *Botrytis* problem.

2.3.5 ETHYLENE AND OTHER HORMONES

Ethylene is one of the most studied plant growth regulators. It plays a key role in promoting senescence of most flowers, especially those that are climacteric, showing an abrupt increase in respiration rate during senescence (Gan 2004). Prior to such respiratory increase, a burst of endogenously synthesised

ethylene was observed, which was believed to initiate the senescence process in flowers (Reid and Wu 1992). When cut flowers are exposed to exogenous ethylene, senescence symptoms including petal abscission, petal wilting, flower abscission and flower wilting could occur (Mayak and Halevy 1972). It was concluded that petal abscission in eudicotyledon flowers, including roses, is generally sensitive to ethylene while petal wilting may or may not be (Woltering and Van Doorn 1988; van Doorn 2001). In addition, flower abscission was shown to be highly sensitive to ethylene in most plants (Van Doorn 2002). The effects of ethylene in promoting senescence are further supported by the response of cut flowers to ethylene inhibitors. The VL of cut flowers was extended when silver cation (Ag$^+$), an effective and specific inhibitor of ethylene action, was applied (Reid and Wu 1992).

Ethylene also correlates with the susceptibility of cut flowers to *Botrytis* infection. It was shown that the disease incidence increased significantly when exogenous ethylene was applied while it was reduced by treatment of silver thiosulphate, an ethylene inhibitor (Elad 1988).

In addition to ethylene, ABA is another plant growth hormone that shows a significant role in the senescence of cut flowers. Exactly how ABA affects cut flower senescence still remains unclear (Trivellini *et al.* 2007) although research has led to strong evidence that ABA has a key part in regulating plant stomata to minimize water loss (Wilkinson and Davies 2002). However, ABA level was also found to correlate well with the water deficit in rose petals even though they have no stomata (Borohov *et al.* 1976). Regardless of its mechanism, endogenous ABA has a direct relationship with cut flower longevity (Mayak *et al.* 1972). For example, late in their senescence, petals of cut roses experience a sharp increase in the level of ABA activity (Le Page-Degivry *et al.* 1991; Kumar *et al.* 2008). Because the abrupt increase in ABA occurs after the climacteric jump in endogenous ethylene production, it was suggested that one of the actions of ethylene in the senescence process is to induce the increase in ABA activity (Mayak and Halevy 1972). The endogenous ABA level in stock leaves and petals of other cut flowers also increases as their senescence progresses (Aneja *et al.* 1999; Ferrante *et al.* 2004). Treatment of exogenous

ABA not only promotes senescence but also increases botrytis disease incidence in cut flowers (Shaul *et al.* 1995).

2.3.6 DISCUSSION

Senescence of cut flowers is complex and not fully understood. However, basic ideas on a macro level have been generally agreed. It is known that xylem occlusion occurs due to a number of various factors such as mechanical wounding, the presence of microorganisms and cavitations. The occlusion reduces the availability of water, and hence possibly results in lower stomatal openings. In turn, this closure of stomata would affect photosynthesis in cut flowers and subsequently decrease the production of carbohydrates, which are vital to the maintenance, the growth and the development of the flowers. Research seems to point to sugar starvation as the cause of senescence in cut flowers.

The factors that affect the remaining VL of cut flowers can be classified into genotype, pre-harvest conditions, post-harvest factors and plant growth regulators. Temperature has been shown to be the most critical post-harvest factor in the senescence of cut flowers. It affects not only the kinetic rates of all metabolic reactions in the flowers, but also the occurrence of xylem occlusion, stomata regulation and sugar transport in phloem networks. Consequently, post-harvest temperature should be used in any effort to estimate the post-harvest loss in the VL of cut flowers. However, the effects of other factors including genotype, pre-harvest and other post-harvest conditions, and the actions of plant growth regulators should not be discounted. The extent to which post-harvest temperature alone can provide the basis of a useful VL prediction remains unclear, and this matter forms a central component of the research investigations presented in this thesis.

2.4 TECHNIQUES FOR EVALUATING VL

Techniques for evaluating the VL of cut flowers provide a means to determine accurately the VL. Two different approaches to evaluating the VL of cut flowers were identified. One is the vase life test approach, which is commonly applied in

industry; the other relies on analytical techniques, which are normally performed in a laboratory.

2.4.1 THE VASE LIFE TEST APPROACH

The vase life test is carried out in laboratory studies, whether for academic or business purposes. The basic principle of the test is to simulate the conditions that the cut flowers would normally experience during their transport, sale and home display. As a result, the conditions during the vase life test depend on specific studies and their objectives. However, for comparison purpose, recommended testing conditions are 20 ^{o}C, 60% relative humidity, 12 hours of light (1000 lux) and 12 hours of darkness (Floral Solutions 2006). The VL of cut flowers is determined as the time duration, commonly in days, under the specified conditions between the start of the test and the end of the VL of the flowers. In order to identify the end of the flower VL, a number of write-off criteria must be used. These criteria can be objective or subjective. An example of objective criteria is the occurrence of petal or flower abscission (Chanasut *et al.* 2003). Subjective criteria are based on the perceived extents of phenomena such as flower wilting, petal discolouration (Faragher *et al.* 1984; Faragher *et al.* 1986; Put and Jansen 1989; Pompodakis *et al.* 2005) and bent neck (Put and Jansen 1989; Ichimura *et al.* 1999; Mortensen and Gislerød 1999). For these criteria, a scale from 1 to 5 is normally used to rate the phenomena.

While the vase life test is simple and easy to perform, it must be carried out in a laboratory where specific conditions can be stimulated and controlled. More importantly, the test offers little value in quality control of in-transit cut flowers because its result, the remaining VL of the flowers, would only become available after the flowers have reached their customers. Therefore, the technique is mostly used for verification purposes.

2.4.2 ANALYTICAL TECHNIQUES

Analytical techniques to evaluate the VL of cut flowers are not common, regardless of which write-off criteria are used. The primary reason is that the underlying biological processes that are responsible for such phenomena as

flower wilting, flower abscission, petal discolouration and stem bend are not completely understood. However, progress, especially in the area of genetic analysis, has been made in developing such a technique. The link between the expression profiles of certain genes and the quality of horticultural produce is well established. For example, single genes and families of genes are likely to be involved in key metabolic pathways related to the colour, texture, respiration, carbohydrate composition and the flavour of strawberries (Manning 1994; Manning 1998).

For ethylene-insensitive cut flowers, progress in developing an analytical instrument to estimate their quality is underway. In a research project supported by the Department for Environment, Food and Rural Affairs (DEFRA), UK, researchers carried out an extensive survey of gene expression in *Alstroemeria*, and identified five genes that seem indicative of the potential floral quality and VL. These genes could be the basis of diagnostic tools which can measure not only the potential VL of cut flowers but also the accumulative adverse effects of post-harvest treatments (DEFRA 2004).

More recently, a spin-off company from Wageningen University called NSure in 2006 has marketed a technology to determine accurately the quality of horticultural products, including cut flowers (NSure Co. Ltd.). The procedure to obtain an estimate using NSure technology is that the user must prepare a test sample from the product tissues, and transfer it onto a test card provided by the company. Then, the card must be sent back to the company for analysis. At the company, a set of indicator genes are selected based on the gene expression analysis of the sample and expert knowledge of distribution chain logistics. The combined expression of these genes, which are believed to reflect the history and actual conditions of the product, provides an indication of its quality (van Wordragen *et al.* 2008). News releases indicated that the technology was tested on many products such as cut roses (NSure Co. Ltd. 2006), pears (NSure Co. Ltd. 2007b) and potatoes (NSure Co ltd 2008).

Both of these attempts represent progress in the analytical approach to estimating quality of cut flowers. While they might be at various stages of

development, the technologies could potentially replace the traditional vase life test. However, the major shortcoming is that these technologies can only be performed in a laboratory. It may be a long time before such diagnostic tools become readily applied in an industrial context where real-time quality monitoring is desired.

2.4.3 DISCUSSION

At the present, the most practical way to determine the VL of cut flowers is to carry out what is known as the vase life test. While it is sufficiently accurate for the purposes of the cut flower industry, the vase life test offers little value in planning and management of cut flowers in the chilled supply chain. Research in genetic technology may offer alternative solutions, where diagnostic tools can be developed to estimate accurately the remaining VL of cut flowers. However, such technologies must be used in a laboratory, which may not be suitable for practical real-time quality monitoring.

2.5 MODELLING TECHNIQUES FOR ESTIMATING VL

In general, modelling techniques can be classified based on the amount of first-principle knowledge they require. Model-based techniques need extensive knowledge and understanding of the biochemical processes occurring in the produce. On the other hand, data-driven techniques use only observed measurements to obtain a model. Kinetic modelling may be considered as somewhere in between the two extremes: some first-principle knowledge of the products is usually required but empirical understanding could be used in substitution.

2.5.1 THE KINETIC MODELLING TECHNIQUE

General principle
The kinetic modelling technique is probably the most widely applied technique in modelling the quality of perishable products. The reason that makes it so popular is probably that it is based on kinetic principles, which can be used to model changes in chemical, biochemical, microbial and physical processes occurring in any food product (van Boekel 2008). Therefore, a kinetic model

could describe accurately the behaviour, for example quality changes, of a food product, if the kinetics of the underlying processes is captured. Even when such knowledge is not fully available, an empirical kinetic model may also be built and perform effectively (van Boekel 2008).

Reliance on mathematical descriptions of measureable quality attributes

For perishable products such as cut flowers, fruits, vegetables, seafood and meat, quality is defined as a combination of various quality attributes (see Section 1.2.3). In such applications, measureable quality attributes that are critical to the product quality are normally selected and subsequently modelled. The quality attributes are selected usually based on consumer's preference e.g., colour in mushroom (Lukasse and Polderdijk 2003), or based on physiological properties of the product itself e.g., growth of spoilage bacteria in chilled fish (Taoukis *et al.* 1999).

A key requirement of kinetic modelling is the measurement of quality attributes that are critical to the overall quality of the product (Labuza 1984). This immediately presents a significant challenge in applying kinetic modelling to products of which the important quality attributes are not measurable. For example, attributes such as flower wilting or fruit crunchiness are not directly modelled by kinetic modelling possibly because they are not easy to measure. In addition, since it may not be possible to know in advance which quality attribute would be the limiting one, multiple quality attributes are often desired for a product (Nunes *et al.* 2007). In such case, multiple kinetic models may be required as kinetic modelling must identify and model each attribute independently.

Another key requirement of kinetic modelling is the use of mathematical models to describe the quality deterioration in the product. The identification of such mathematical description depends on the first-principle knowledge of the products as well as the available empirical reasoning. For each kinetic model, the specific mathematical description of the quality attribute is ideally derived from the complete knowledge of the chemical, biochemical, microbial and physical processes affecting the attributes themselves. However, due to the

complexity of those processes, such knowledge may not always be available (Labuza 1984). Consequently, empirical reasoning is often used in substitution to formulate the kinetic description. For example, Lukasse and Polderdijk (2003) studied the post-harvest dynamic quality evolution of mushrooms and derived kinetic models using knowledge of mushroom physiology. Three mushroom quality attributes were modelled, including colour, stipe length and hat opening. The physical basis of the model for mushroom colour evolution was based on two chemical reactions which described the conversion of polyphenol oxidase (PPO) precursor into PPO and subsequently into chinons. However, by arguing that any quality model must be irreversible, the researchers introduced an empirical term k_{loss} which represented the PPO that was lost without being converted into chinons (Lukasse and Polderdijk 2003). While such modification led to an irreversible model, the validity of the introduction of k_{loss} was not discussed. Moreover, the same model structure was implemented for modelling stipe length and hat opening without describing the physical basis for these two attributes. Therefore, these models seem to be based more on empirical reasoning than on the first-principle knowledge.

Differences in empirical reasoning may lead to different models and interpretations. In a kinetic model, the function of quality attributes often has a low-order polynomial form although more complicated ones are also common (Tijskens and Polderdijk 1996). For example, the tomato firmness model from Schouten *et al.* (2007a) is different from the firmness model used by van Dijk *et al.* (2006b). Schouten *et al.* (2007a) argued that tomato firmness can be either enhanced or diminished during the pre-harvest period but it can only deteriorate during the post-harvest period. Consequently, the researchers formulated two kinetic equations corresponding to pre-harvest and post-harvest variation in tomato firmness (Schouten *et al.* 2007a). On the other hand, van Dijk *et al.* were interested in the effect of chilling injury and hence introduced an additional term for it in their tomato firmness model (van Dijk *et al.* 2006b). For their differences, both models, which were validated reasonably well against experimental data, provide different interpretations concerning tomato firmness.

Various mathematical descriptions of the environmental effects

A kinetic model must include a description of the effects of environmental conditions, which often play a critical role in the degradation of the product quality. Temperature is probably the most common environmental factor in kinetic modelling studies. For each model of a quality attribute, the kinetic modelling technique must select a temperature dependence, the most common form of which is the Arrhenius relation (see (Delignette-Muller *et al.* 1995)). Other expressions for the temperature dependence include the square root relation, the linear relation and the exponential relation, which were reviewed in (McMeekin *et al.* 1992; Fu and Labuza 1993). Although they are used less commonly, a few applications of these kinetic expressions have been reported; for example, linear temperature dependence for shelf life predictions of mushrooms (Lukasse and Polderdijk 2003), a square root model for the temperature dependence in seasoned soybean sprouts (Lee *et al.* 2007), and a square root model in the study of shelf life control of chilled fish (Taoukis *et al.* 1999). Opinions may vary as to which models to use (Delignette-Muller *et al.* 1995).

Expressions for other environmental factors such as humidity are less common compared to temperature. One example is the modification of the Arrhenius expression to account for the effect of humidity on bacteria growth, which was proposed by Davey (1989).

Implications of a dynamic environment

Provided that the mathematical descriptions for the quality attributes and for the temperature dependence are identified, at constant temperature the kinetic equation can be integrated and the quality (attribute) evolution may be obtained. However, environmental conditions during the product storage in practical applications may vary significantly. In such dynamic conditions, solving the kinetic equation could pose an additional challenge. Varying temperature leads to solving ordinary differential equations in the kinetic modelling, which may be mathematically challenging (Schouten *et al.* 2007b). A numerical approach is usually taken, where the basic principle is the integration on time sub-intervals over which the temperature can be assumed constant (Fu and Labuza 1993).

The approach is not popular possibly because the historical record of past temperature is not usually accessible at a reasonable cost, especially when food item levels are considered (Fu and Labuza 1993). However, significant improvements in sensor technology and in particular RFID tags, which could dramatically reduce the cost of automatically measuring and recording temperature and humidity, may revitalise this approach in the near future.

Applications in studies of cut flowers and other perishable produce

Not many applications of kinetic modelling can be found in studies of cut or intact flowers. One application of kinetic modelling in potted plants was reported by Tijskens *et al.* (1996). In their study, quality was described in terms of "acceptability", the probability that one plant in the batch becomes unacceptable. Based on previous research (Sterling and Molenaar 1986) and population dynamics, the researchers argued that a logistic function would be a good model of the quality of potted plants. The temperature dependence of the kinetic rate was expressed as a sum of two Arrhenius expressions. Each of the expressions represented the decaying rate of the plant's acceptability due to chilling injury and due to high temperature deterioration, both of which were particularly active at different ranges of temperature. Although simulation results at constant temperatures compared reasonably with observed measurements, the dynamic performance at varying temperatures was not assessed. Other issues that may need to be explored include the validity of summing two kinetic rates for an overall rate of decrease in the acceptability, and the credibility of applying population dynamics (i.e. logistic curve) when the sample size, 12 samples, was quite limited (Tijskens *et al.* 1996).

Currently applications of kinetic modelling were more common in fruits and vegetables than in cut flowers. Tijskens and Polderdijk developed a model for keeping quality of vegetable produce during post-harvest storage and distribution (Tijskens and Polderdijk 1996). In their model, most common issues in kinetic modelling were addressed, including model kinetics (zero order, first order and logistic kinetics), temperature dependence, effects of initial quality and quality limits, multiple limiting quality attributes and dynamic modelling. Validation at constant temperatures for lettuce and tomato showed good

agreement although some deviation was observed in Brussels sprouts. However, the proposed dynamic formulation was complicated, especially for variable initial quality and quality limits, and its dynamic performance was not validated. Other applications were also reported in mushrooms (Lukasse and Polderdijk 2003), tomatoes (van Dijk *et al.* 2006b; van Dijk *et al.* 2006a; Schouten *et al.* 2007a, 2007b) and seasoned soybean sprouts (Lee *et al.* 2007).

Kinetic modelling also plays a fundamental role in applications of time-temperature indicator (TTI) in perishable produce. TTI is a measuring device which embeds a system that enables direct and quantitative measurement of the cumulative effect of temperature acting on the product. For a chemical or biological TTI to work, its embedded system and the quality decaying process in the perishable product must have similar kinetics, such as reaction order, activation energy and reference rate constants (Wells and Singh 1988; Bobelyn *et al.* 2006). This requirement highlights the major limitations of TTI which are the product(s) must be kinetically characterized, and a biological or chemical system with similar kinetics must exist. In addition, the use of TTI in shelf life prediction of perishable products seems to assume that all products would have the same initial quality state. This assumption may not hold in cases where the effects of genotype and pre-harvest conditions on post-harvest quality are not negligible. Despite these limitations, TTI has become increasingly popular in dairy products (Sherlock and Labuza 1992), chilled fish (Taoukis *et al.* 1999; Tsironi *et al.* 2008), meat (Vaikousi *et al.* 2009) and vegetables (Giannakourou and Taoukis 2002, 2003; Bobelyn *et al.* 2006).

Discussion

Kinetic modelling is the most widely used in estimating post-harvest quality loss in perishable produce. It requires three essential elements: a measurable quality attribute, its mathematical description and an expression describing the temperature dependence. Without any of those three elements, kinetic modelling can not be carried out, which may explain why no applications in the post-harvest modelling of cut flowers have been identified in the literature. In addition, dynamic environments, where temperature is changing, could present a computational problem to kinetic modelling.

2.5.2 DATA-DRIVEN TECHNIQUES

For estimating the VL of cut flowers, data-driven techniques may be a better choice than their model-based counter-part. The main reason is that measurements concerning the storage conditions of cut flowers such as in-transit temperature and humidity will be more readily available than the understanding of how cut flowers behave. The availability of such measurements without sufficient knowledge of the embedded biochemical system would naturally facilitate more data-driven studies than first-principle modelling techniques.

Thermal integration technique

The thermal integration technique, also known as the "heat unit approach" or "degree-days approach", is based on the idea that the summation of temperatures that a plant is exposed to characterises its maturity stage. Implicitly, the thermal integration approach assumes that plant developmental rate varies linearly with the temperature sum and hence with temperature over a restricted range. Clearly, many other genetic and environmental factors are known to affect the plant developmental rate. However, as Johnson and Thornley noted the temperature summation technique worked well in many cases because temperature, the most important environmental variable, was captured effectively (Johnson and Thornley 1985).

The thermal integration technique has been used widely in plant development studies for its simplicity and effectiveness. Most of the studies were carried out on growing crops and vegetables such as maize (Ruiz *et al.* 1998), chickpeas (Bello *et al.* 2005), olives (Orlandi *et al.* 2005), rice (Chopra and Chopra 2004) and soybeans (Voldeng *et al.* 2003). A few other studies were performed on intact flowers (mostly roses). For example, Pasian and Lieth (1994) studied a number of developmental events in rose shoots, such as the occurrence of new shoot, unfolding of a new leaf and visible flower bud. The researchers used thermal units, calculated from average air temperature to predict these developmental events. For validation, the predicted day of event was compared with corresponding observation, showing that the technique worked

satisfactorily. However, considerable variability was observed, particularly in estimating the thermal units required in each developmental stage (Pasian and Lieth 1994). In addition, it should be noted that the plants used in the study were of the same age (4 year old plants), from the same cultivar (*Rosa hybrida* 'Cara Mia'), and were grown under the same water and nutrient conditions. The purpose was obviously to keep all factors except temperature constant. Doing so enabled the examination of the effect of temperature. However, the model that was obtained may not be practical because in practice the growing conditions are constantly changing. Moreover, the validation data was collected on plants grown inside a glass greenhouse under constant temperature. Consequently, the performance under changing temperature remains to be validated. Other more recent studies in flower development include November cactus (Larsen *et al.* 1998), rose (Steininger *et al.* 2002; Mattson and Lieth 2006) and *Ambrosia* (commonly known as ragweed) (Laaidi *et al.* 2003).

Despite its popularity in plant development research, no application of this technique in cut flowers has been found. This could be explained by the limitations of the thermal integration technique which have also been well documented. An obvious limitation of the technique was that it assumed a linear relationship between plant development and temperature. While this assumption seemed reasonable in many reported studies, it remains an empirical observation, which can only be applied on a case-by-case basis. Another shortcoming of the heat integration technique is that it does not account for other genetic and environmental variables that would also have significant effects on plant development (Wang 1960). The inclusion of such variables as day length and radiation integral, using similar expression as for temperature was shown to improve the technique's performance (Johnson and Thornley 1985). A similar conclusion was obtained when cultivar-specific temperature thresholds were used (Pasian and Lieth 1996). A more subtle disadvantage of the heat sum method is that it does not capture the time sequence of temperature records. As a result, two different temperature regimes that could lead to different plant developments may correspond to the same heat sum. This limitation, illustrated and discussed in (Wang 1960), remains to be addressed.

Multiple linear regression (MLR) and partial least squares (PLS)

In regression studies, an MLR model involves more than one independent variable. The coefficients of those variables are evaluated from experimental data using estimation techniques. The most common estimation technique is ordinary least squares (OLS).

The principal idea of OLS is to minimise the sum of squares of the residual; i.e., the difference between the observed and predicted values of the dependent variable for each observed sample. Its applications can be found in virtually any fields such as economics, agriculture, environment and food processing, and its implementation is built in many data analysis software packages including SAS/STAT, SPSS, and Matlab. However, OLS can not be applied to multi-collinear data sets, in which a linear relation exists among the observed variables. Multi-collinearity leads to a singular correlation matrix, which does not have an inverse that is in turn required by OLS. Although pseudo-OLS can be used instead, this alternative could lead to multiple solutions, as opposed to a unique solution by OLS. Consequently many statistical derivations for the OLS estimator may no longer hold. For example, when multi-collinearity exists, the OLS estimator is no longer the Best Linear Unbiased Estimator (BLUE), as it would be otherwise. Due to measurement noise, exact multi-collinearity is relatively rare compared to near multi-collinearity. It was suggested that OLS should be avoided in analyzing data with near multi-collinearity because the precision in the estimate obtained would be significantly deteriorated (Sundberg 2000).

PLS is among the most widely used regression techniques, especially in chemometrics and analytical chemistry. Its mathematical derivations are described in many textbooks and articles such as (Martens and Naes 1989; Frank and Friedman 1993). A major motivation for its preference over the conventional OLS is from its capability in handling (near) multi-collinearity. The PLS regression technique is based on using latent variables (LVs) which maximise the covariance between the independent and dependent variables.

By eliminating some LVs that are deemed insignificant from the regression, the PLS model performance may be improved compared to an OLS model, especially when the data at hand suffers from near multi-collinearity; the same improvement is also seen compared to principal components regression where the LVs, more commonly known as principal components (PCs) in principal component analysis, maximise variance on the independent variables only (Martens and Naes 1989). It should be noted that the trade-off in overcoming (near) multi-collinearity using PLS is the presence of bias in the estimated regression coefficient. How much bias would be present depends on the number of LVs used in the regression. This was discussed in (Frank and Friedman 1993) where similarities and differences between OLS and PLS were highlighted.

Despite being used widely in many fields, very few applications of linear regression techniques, including OLS and PLS, for estimating the VL of cut flowers were found in literature. One of them was reported by In *et al.* studying the relation between various pre-harvest and post-harvest factors and the VL of cut 'Asami Red' roses (In *et al.* 2007a). The researchers used linear regression analysis to obtain a model of the VL of cut roses in terms of the minimum pre-harvest humidity and a few other morphological and physiological factors. As In *et al.* concluded, this model was not good enough for practical application (In *et al.* 2007a). Its coefficient of determination was rather low, which indicated that a significant amount of variance in the VL data was not captured. The major reason was probably that the independent variables were selected with an objective of avoiding multi-collinearity. Consequently, important factors such as pre-harvest growing temperature were prematurely eliminated from the regression analysis. Clearly, a better variable selection strategy could lead to a different set of independent variables, where the potential multi-collinearity can be overcome using such techniques as PLS. In addition, another potential shortcoming of the reported model was the use of the average value of pre-harvest factors over 15 days. It was not clear how the duration of 15 days was selected as In *et al.* (2007a) neither explained their decision in detail nor provided any supporting references.

Another application of regression analysis in predicting the VL of cut flowers was the work by Hansen *et al.* (1991). Both linear and nonlinear regression models of total damage rating in terms of post-harvest time were reported for various cut flowers and foliage. As the data that were used in the modelling had been obtained at constant temperature (25 ^{o}C) and humidity conditions (50%), those models would have little applicability in a dynamic environment such as in chilled supply chains, where temperature and humidity are variable.

In contrast to cut flowers, applications of linear regression techniques for other perishable products were found more readily. The most common ones are perhaps in analysing near infra-red spectra data. The combination of near infra-red spectroscopy with linear regression analysis provides the framework for many non-invasive techniques for measuring the quality attributes of various perishable produce such as kiwifruits (McGlone and Kawano 1998), apples (McGlone *et al.* 2005), mango, banana and peach (Subedi and Walsh 2009)). Nicolai *et al.* published a detailed review of these techniques including their principles, instrumentation and the linear regression involved (Nicolaï *et al.* 2007). Applications for other analytical data were also reported. For example, Brockhoff *et al.* (1993) and subsequently Sundberg (2000) examined different linear regression techniques in predicting the flavour of *Jonagold* apples using gas chromatographic measurements. Another example was found in a study of spoilage in meat products, where the spoilage was correlated with microbiological and physicochemical measurements using PLS (Mataragas *et al.* 2007). However, while the combination of linear regression with analytical measurements found many useful applications, a major limitation still remains: these measurements may only be available in a laboratory, which is likely to prevent the research findings from being implemented in an industrial context.

Linear regression analysis of readily available measurements for estimating the quality of perishable products was far less common. For example we (Doan *et al.* 2008) have compared the performance of three linear regression techniques including OLS, Principal Component Regression (PCR) and Latent Root Regression (LRR) in predicting changes in the shelf life of chilled seafood. The study demonstrated that using the measurements of the environmental

conditions, which can be recorded along the chilled supply chain by data loggers, changes in the quality can be estimated. Nevertheless, further validation work on real data is still required.

Discussion

Linear data-driven techniques that could potentially be used in predicting the VL of cut roses have been reviewed. These include the thermal integration technique and linear regression approaches, including OLS and PLS. The thermal integration technique enjoys many applications in plant development studies, but at the same time exhibits many significant limitations; these include assuming a linear relationship between temperature and plant development, not accounting for effects of other environmental variables, and being unable to capture the correlation in serial measurements of temperature. It was probably those shortcomings that have so far prevented the technique from being applied to cut roses.

For linear regression techniques, the two issues that are common to all were reviewed: variable selection and missing data. OLS is probably the most common technique in linear regression. However, it can not work effectively with multi-collinear data. PLS was selected to overcome this problem of multi-collinearity. The application of linear regression techniques to spectra data form the basis of non-invasive techniques for measuring the quality attributes of perishable products such as fruits, fishes and meat. However, few applications of OLS or PLS in estimating the quality changes of cut roses currently appear in literature.

2.5.3 MODEL-BASED TECHNIQUES

Few first-principle models that predict the VL of cut flowers have been identified. The reason for this is that senescence as a biological process in cut flowers has not been completely understood (van Doorn 2004; Rogers 2006; van Doorn and Woltering 2008). The FLORES model, proposed in 1991 by van Doorn and Tijskens (1991) was one of the earlier attempts in building a first-principle model for the VL of cut flowers. However, it was not a truly first-principle model, even though important processes were described within it. Specifically, the

researchers identified a number of important physiological effects such as time and temperature, dry storage or transport, infection by fungi, bacteria in the vase solution, suboptimal temperatures, exogenous ethylene, and absence of flower preservative in the vase solution. Each of the identified effects was subsequently modelled based on empirical and experimental knowledge. The response of those sub-models was expressed in terms of the percentage reduction of the maximum VL of the cut flower, which had also been determined empirically. This model by van Doorn and Tijskens (1991) represented a reasonable attempt in modelling for VL of cut flowers. Its key contribution was probably the inclusion of the important physiological stresses. However, van Doorn and Tijskens' model is not truly a mechanistic model. Empirical modelling of the identified physiological stresses effectively meant that the underlying biological processes that drive the stress response of the cut flowers were not captured. In addition, those processes could be highly coordinated in a complex biological system, which would question the validity of a key assumption made by van Doorn and Tijskens: the responses of the physiological stresses were additive and hence summed to form the overall response (van Doorn and Tijskens 1991).

Another attempt was from the work of Reid and co-workers (1996). The researchers built a complex model of the water balance in cut roses. Although its validation results were not published, the model illustrated the importance of maintaining a proper water balance in cut rose stems. Nevertheless, a potential extension for this model would be the description of how the water balance affects the VL of cut roses. As Reid *et al.* noted, a negative water balance, where more water is lost than taken up, was the cause of flower wilting (Reid *et al.* 1996). This could also be the controlling signal to stomata functioning (Sperry *et al.* 1993; Sperry and Pockman 1993; Saliendra *et al.* 1995; Hubbard *et al.* 2001; Tuzet *et al.* 2003) and may therefore affect the photosynthesis, where chemical energy is produced to maintain cut flowers.

Other existing models of flowers concern the growth of intact flowers or the production of cut flowers in a greenhouse. For example, Lieth and Pasian developed a model for the growth and development of intact rose shoots (Lieth

and Pasian 1991). These researchers considered the carbon balance in the rose shoot, and empirically modelled important biological processes including photosynthesis, carbon translocation and respiration. The validation results were mixed: only one out of two shoots showing good agreement with experimental measurements (Lieth and Pasian 1991). This might be explained by the fact that the modelling was rather empirical, and perhaps more importantly that the water balance and critical environmental factors such as humidity were not considered.

2.5.4 DISCUSSION

In this section, modelling techniques for estimating the VL of cut roses were reviewed. These techniques were classified into kinetic modelling, data-driven and model-based techniques. Kinetic modelling has been popular in modelling the shelf life of perishable produce and food products, but no application in cut flower has been reported. This could be due to the difficulty in identifying a measurable quality attribute, its function in the kinetic equation and a mathematical description of temperature dependence. Linear regression techniques including OLS and PLS have been used to analyse spectra data for evaluating the quality of perishable produce but few attempts in modelling the VL of cut flowers were reported. Mechanistic models of the VL of cut flowers have not been available. The primary reason is that the biological processes embedded within the cut flowers are complex and not fully understood.

2.6 CHAPTER CONCLUSION

Senescence of cut flowers in general and specifically of cut roses is a complex biological phenomenon that has not been completely understood. However, it is generally agreed that genetic, pre-harvest and post-harvest factors and the action of plant growth regulators, ethylene in particular, all affect how cut roses senesce. Temperature is considered the most important post-harvest factor and hence must be used to estimate the post-harvest loss in VL of cut roses. However, it must be kept in mind that the precision of such an estimate may depend a lot on the other factors including genetic, pre-harvest and other post-harvest conditions and the presence of plant growth regulators.

Due to the complexity of their senescence, there are not many techniques to determine the post-harvest loss in the VL of cut roses. Techniques for evaluating the VL, including the vase life test approach and other genetic-based techniques, are limited to a laboratory context. On the other hand, modelling techniques for estimating the post-harvest loss can be further classified into kinetic modelling, data-driven and model-based techniques. In modelling perishable produce, kinetic modelling is the most popular whilst data-driven techniques including OLS and PLS are also used in analysing spectral data from the products. Model-based techniques were rarely used due to the incomplete first-principle knowledge.

This review has identified the lack of application of kinetic modelling and linear regression techniques in modelling the VL of cut roses using post-harvest measurements. What needs to be understood better is the suitability of these data-driven techniques given the biological characteristics of cut flowers or other produce. The literature review indicates that this is a new area of research where little previous work exists. This thesis aims to contribute new knowledge to this area. Consequently, this area will be further investigated in this thesis for studying the post-harvest loss in cut roses, as an exemplar for the perishable goods supply chain. Specifically, kinetic modelling, OLS and PLS will be used to estimate based on post-harvest temperature measurements and the post-harvest loss in VL of cut roses, while acknowledging the potential effects of other factors including genetic, pre-harvest conditions.

3 METHOD

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This chapter has three main objectives. First, it describes relevant technical issues that are encountered in implementing MLR and PLS modelling techniques. These issues such as selection of variables and selection of the number of the latent variables are widely recognised, but their solutions are often problem-dependent. The respective solutions that were implemented in this thesis are subsequently explained. The second objective is to establish the framework for assessment and comparison of model performance. This framework consists of the statistics that are required in evaluating the performance, the approach used to evaluate them, and any performance limits that could be established. Finally, this chapter also discusses the relevance and implementations of the a priori *knowledge which states that the higher storage temperature results in the greater loss in remaining VL.*

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3.1 TECHNICAL ISSUES IN MLR AND PLS MODELLING TECHNIQUES

Three implementation issues were identified in MLR and PLS modelling techniques; these include the requirement of a uniform number of measurements (i.e. independent variables) in MLR and PLS, variable selection in MLR, and the selection of the number of the latent variables to use in PLS. These issues and their solutions are described below.

3.1.1 UNIFORM NUMBER OF MEASUREMENTS IN INPUT SAMPLES

Both MLR and PLS require their input samples to have the same number of measurements. This means that it must be possible to arrange all the input samples into a 2-D data matrix. However, this requirement is not often satisfied in monitoring storage temperature of in-transit perishable produce. Due to uncertainty in transport processes, every shipment may take a different duration of time, resulting in temperature profiles with different number of temperature measurements. Consequently, the temperature profiles must be adjusted to have the same number of measurements before MLR and PLS techniques can be applied.

The issue of having to adjust the "length", the number of measurements, of a temperature profile prior to MLR and PLS modelling is known as the "unequal batch length" problem in online monitoring of chemical batch processes (Nomikos and MacGregor 1995; Undey and Cinar 2002). A trivial solution is to only consider the profiles up to a uniform length and ignore the additional measurements in the input profiles. However, this would require a proper adjustment of the corresponding dependent variable, which might not be possible. For example, consider an input profile of 25 temperature measurements (sampling time at 1 measurement per h) that corresponds to a loss of 48 h in remaining VL of a cut rose stem. If only the first 20 measurements of this input profile were considered, the corresponding loss in the remaining VL would not always be known. Consequently, ignoring the extra measurements in input profiles is not applicable.

Undey and Cinar (2002) discussed several techniques to overcome this issue in batch process monitoring, including indicator variable technique, dynamic time warping and curve registration. These techniques were designed specifically to align data profiles collected from a batch process according to their common features or landmarks. However, similar landmarks may not be defined in data samples from the supply chain of perishable produce as the transport process is subject to external events such as changes in transport routes. Therefore, these techniques are not suitable for this study.

Techniques developed to overcome missing data in linear regression can also be applied to overcome this issue. For example, the first two approaches that Nomikos and MacGregor proposed for filling in the unknown independent variables (Nomikos and MacGregor 1995) were essentially the single imputation technique with different imputed values. Instead of ignoring the extra measurements, input profiles could be appended with "dummy" measurements so as to make the profiles equal in length. This is the strategy that was implemented in this work, with the "dummy" measurement being the reference temperature at which the remaining VL of cut flowers was defined. The reference temperature was used because it would allow the remaining VL to be adjusted. Figure 3.1 illustrates the strategy with an example. Initially, the required length, the desired number of measurements in each input profile, is evaluated. In the example, suppose that each profile must have 11 temperature measurements but the original input profile only has 8 (represented by black dots). For profiles that have fewer than the required number of measurements, the reference temperature is appended to the profiles until they have the required number of measurements. In the example shown in Figure 3.1, three reference temperature measurements are appended to the original profile, resulting in the adjusted input profile having a total of 11 measurements. Subsequently, the remaining VL must be adjusted as well. Appending one reference temperature measurement to the original temperature profile would resemble the scenario that upon exiting the supply chain, the product is stored at the reference temperature for an additional duration of one sampling period. Therefore, the remaining VL at the end of such additional storage is one unit less than the remaining VL at the end of the supply chain. So, for every

appended measurement, one unit of VL is subtracted from the corresponding remaining VL. Consequently, the adjusted remaining VL in Figure 3.1 is 9, which is obtained from the original remaining VL of 12. This procedure was performed in the case studies for Cookes Rose and World Flowers.
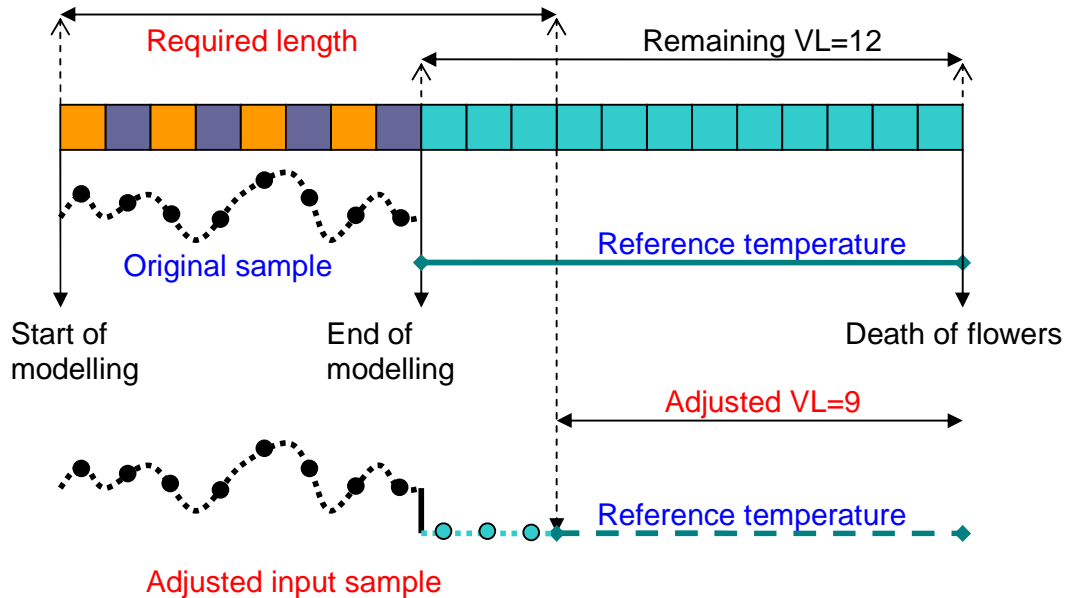
Figure 3.1: Strategy for modifying temperature profiles to achieve uniform length

3.1.2 VARIABLE SELECTION IN MLR

Variable selection is a task of significant importance in MLR. This is the problem of selecting the "best" subset of available independent variables for building a regression model. A major motivation for the task is to avoid over-fitting. The Occam's Razor, the principle of parsimony, suggests that models containing only necessary variables should be preferred (Hawkins 2004). When that principle is not followed, over-fitting often occurs, where the models may capture statistical features that are present in the current data but are not representative of the population (Babyak 2004). The coefficients corresponding to the extra independent variables add random variation to subsequent predictions, the precision of which is consequently reduced (Hawkins 2004). As a result, prediction performance of over-fitting models is likely to be affected. In addition, another danger of over-fitting is that such models may be overlooked

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and falsely accepted as good models; this is because they often have high coefficient of determination R^2 values. In fact, it was illustrated that sufficient independent variables, regardless of whether they are true predictors of the dependent variable, always lead to a linear model with R^2 close to unity (Babyak 2004). It was the high R^2 value that usually leads to a false confidence in an over-fitting model. Consequently, variable selection must be performed carefully so as to avoid over-fitting in MLR modelling.

For the variable selection task, two items must be decided upon: a set of evaluation criteria, and a strategy to identify tentative sets of independent variables from the ones that are available. For evaluation criteria, a statistical test based on the F distribution can be carried out for a null hypothesis of eliminating a subset of explanatory variables. Alternatively, an adjusted coefficient of determination can be utilised (Rao *et al.* 2007). Other criteria that have been proposed and used frequently are the predicted residual sum of squares (PRESS), the C_p statistic, the Akaike Information Criterion (AIC) (Akaike 1973), and the Bayesian Information Criterion (BIC) (Schwarz 1978). As prediction performance was the main objective, this work selected root mean squared error in prediction (*RMSEP*) as the criterion. Its definition and mathematical formula are described in more detail in Section 3.2.1.

For selection strategy, forward or backward stepwise selection is commonly used to select the subset of variables. It is based on correlation between each independent variable and the dependent one, and only variables that have significant correlation are selected. However, this strategy may not completely eliminate the risk of over-fitting because variables may behave differently in isolation compared to simultaneous interactions with others (Babyak 2004). Alternatively, a combination of forward and backward selection such as proposed in (Walmsley 1997) could also be used. Nevertheless, if all independent variables (e.g. temperature readings from a temperature profile) have the same potential to affect the dependent variable (e.g. the loss in remaining VL), it is unreasonable to exclude any independent variable completely from the subsequent modelling. Consequently, stepwise selection was not suitable for the present study.

As described in detail in the subsequent chapters, the data sets of temperature profiles from the Cookes Rose experiment and from the World Flowers experiment typically have 60-70 profiles each of which has more than 100 temperature readings (collected at 0.5 h per reading). If all temperature readings from a temperature profile are used as independent variables, over-fitting is likely to occur. Consequently, this study used the average of consecutive temperature readings as independent variables. Figure 3.2 illustrates the strategy using an input profile with 11 readings and an averaging window of $k=3$ readings. The new input data x has only four independent variables.

Input profile with 11 temperature readings
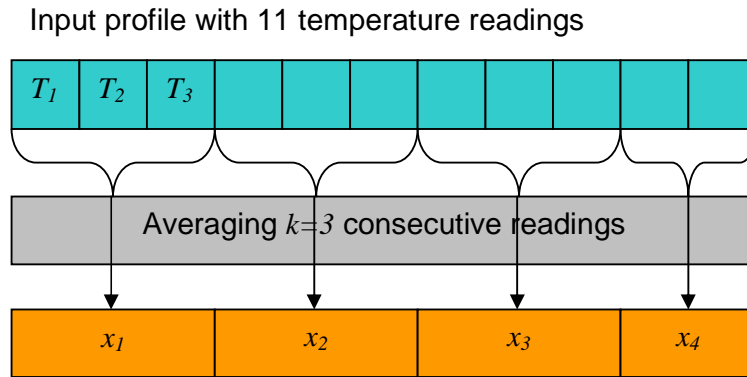
Figure 3.2: Averaging temperature readings for variable selection

The size of the averaging window k is an important parameter. It can vary from one reading to the whole length of the original input sample. As mentioned previously, when $k=1$, the number of profiles is smaller than the number of independent variables, leading to over-fitting. On the other hand, if k is equal to the total number of readings, then only the average temperature over the studied period would be used as the sole independent variable in model calibration. The optimal k is identified based on the evaluation criterion $RMSEP$; i.e., the "best" k is the one that produces the lowest $RMSEP$.

3.1.3 SELECTION OF THE NUMBER OF LATENT VARIABLES IN PLS

PLS is among the most widely used regression techniques. PLS regression only retains the first few latent variables (LVs) to maximise the covariance between

the independent and dependent variables. By excluding some LVs that are deemed insignificant, PLS prediction performance may be improved compared to MLR, especially when the data at hand is close to multi-collinearity.

The issue of which LVs to retain is a challenging task and a lot of research has been done to address this problem. In one way, it may be viewed as a variable selection task, and hence as discussed in Section 3.1.2, strategies and criteria must be established. Owing to the fact that the eigenvalues are a measure of the covariance (in PLS) or variance (in PCA) captured in the corresponding LVs (in PLS) or PCs (in PCA), the most common strategy is to retain only the LVs (or PCs) that have the corresponding eigenvalues exceeding a certain threshold, and thereby eliminate the LVs (or PCs) with small variances. This strategy is likely to overcome the (near) multi-collinearity problem. However, since it is done solely on the variance of independent variables in PCA, PCs having significant correlation with the dependent variable(s) may be erroneously deleted (Sutter *et al.* 1992; Jolliffe 2002).

This work implemented a stepwise strategy for LV selection. Initially, all the LVs were ranked in the order of decreasing eigenvalues. Then, models retaining increasing number of LVs were built and *RMSEP* of each model was evaluated. The optimal model was selected based on the prediction performance that gave the lowest *RMSEP*. This strategy is illustrated in Figure 3.3.

3.2 PERFORMANCE EVALUATION APPROACH

In order to assess the prediction performance of the modelling techniques, a number of statistics are normally used. Consequently, the selection of those statistics is important and so is the way those statistics are to be evaluated. Furthermore, if the lower and upper thresholds of those statistics could be evaluated, they can provide indications of how good the techniques are, and how much they can be improved.

3.2.1 PERFORMANCE STATISTICS

A number of statistical indices were used to assess prediction performance of the modelling techniques being investigated. These statistics included *RMSEP*, R^2, slope and intercept of the best fit line of predicted *versus* observed loss in remaining VL. *RMSEP* represents the average error in prediction while R^2, the square of the Pearson's product-moment correlation coefficient, measures how well the linear relationship between the predicted loss in VL and the observed one.
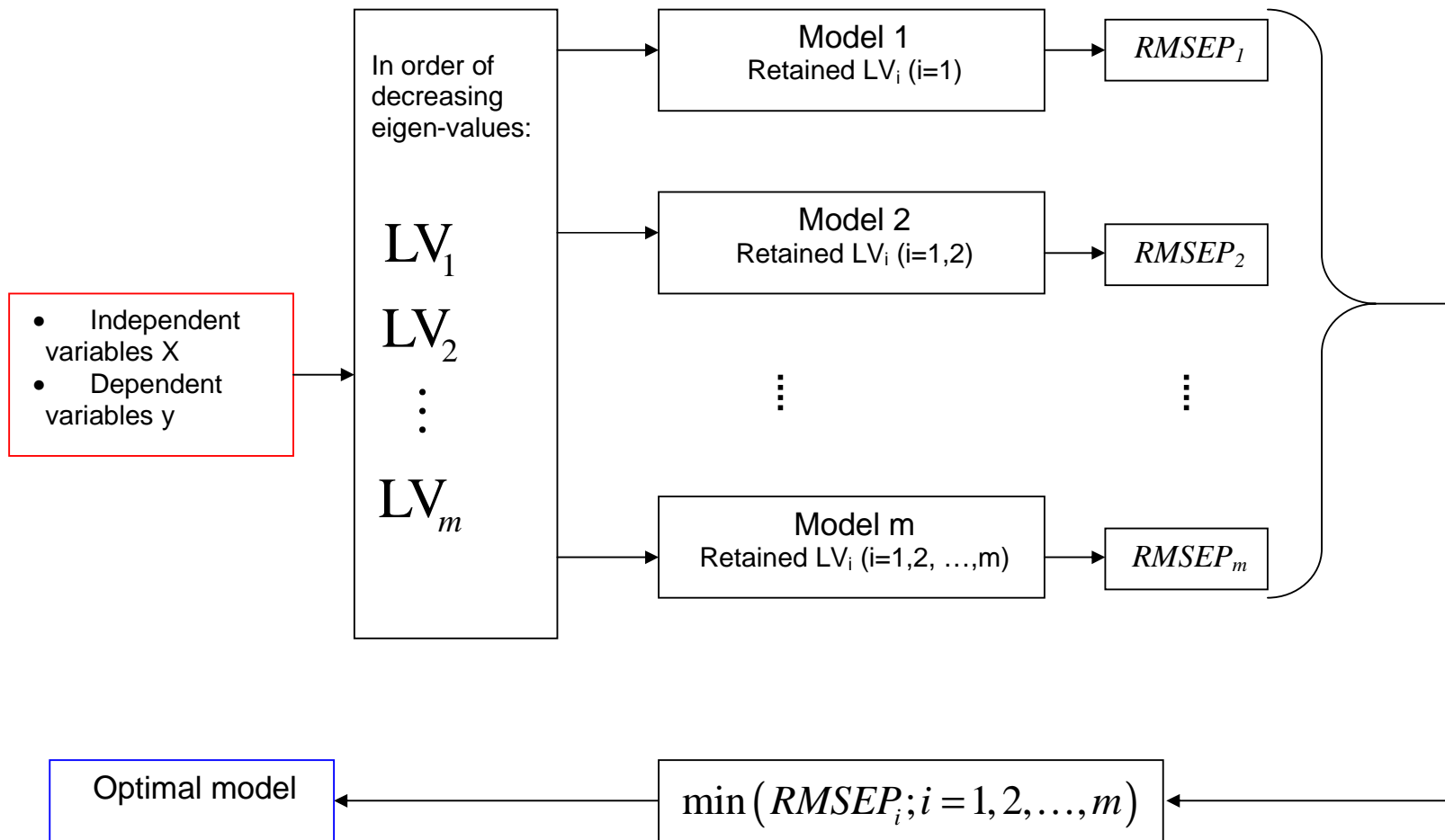
Figure 3.3: LV selection strategy in PLS modelling

In an ideal situation, the best fit line should coincide with the equality line $y = x$ and therefore its slope and intercept should approach 1 and 0 respectively. The formula for the statistics used are summarised below.

Let the prediction error e be defined as

$$e_i = y_{pred,i} - y_{obs,i}$$

Where $y_{pred,i}$ is the predicted loss in remaining VL for the cut rose i^{th} $(i = 1, 2, \ldots, m)$;

$y_{obs,i}$ is the observed VL for that cut rose sample.

RMSEP statistic is defined as

$$RMSEP = \sqrt{\frac{1}{m} \sum_{i=1}^{m} e_i^2} \tag{3.1}$$

In addition, R^2, which measures the goodness of the linear relationship between $y_{pred,i}$ and $y_{obs,i}$, was also used in the performance assessment.

$$R^2 = \frac{\left[\sum_{i=1}^{m} \left\{ \left(y_{pred,i} - \overline{y_{pred}} \right)\left(y_{obs,i} - \overline{y_{obs}} \right) \right\} \right]^2}{\left[\sum_{i=1}^{m} \left(y_{pred,i} - \overline{y_{pred}} \right)^2 \right]\left[\sum_{i=1}^{m} \left(y_{obs,i} - \overline{y_{obs}} \right)^2 \right]} \tag{3.2}$$

Where $\overline{y_{obs}}$ is the mean of all $y_{obs,i}$, $(i = 1, 2, \ldots, m)$.

$\overline{y_{pred}}$ is the mean of all $y_{obs,i}$, $(i = 1, 2, \ldots, m)$.

The best fit line of the predicted *versus* the observed loss in the remaining VL is given by

$$y_{pred} = a \cdot y_{obs} + b \tag{3.3}$$

The slope a and intercept b of the best fit line were evaluated as

$$a = \frac{\sum_{i=1}^{m} \left(y_{pred,i} - \overline{y_{pred}} \right)\left(y_{obs,i} - \overline{y_{obs}} \right)}{\sum_{i=1}^{m} \left(y_{obs,i} - \overline{y_{obs}} \right)^2} \tag{3.4}$$

$$b = \overline{y_{pred}} - a \cdot \overline{y_{obs}}$$

3.2.2 CROSS VALIDATION STRATEGY

Cross validation is commonly implemented in performance assessment of predictive models. It offers a better use of the data, especially when their availability is limited. Although many variants of cross validation exist, they share the same principle: the division of the available data into two subsets, one of which is used for model calibration, while the other is for performance assessment. The variation between different cross validation techniques comes from how the division is implemented. A widely used cross validation is the leave-one-out (LOO) strategy where one data sample is left out for performance assessment; the rest of the data is used for model calibration and the procedure is repeated until each sample is left out once. Alternatively, leave-two-out or leave-multiple-out cross validations are also used.

In a similar fashion to performance assessment, cross validation is also implemented in the calibration of predictive models; especially when model calibration involves optimization for predictive performance i.e. selection of an optimal model from a number of alternatives. Such alternatives could arise from variable selection in MLR models (Anderssen *et al.* 2006) or from LV selection in PLS models (Westerhuis *et al.* 2008; Filzmoser *et al.* 2009).

When cross validation is used in both performance assessment and model calibration, it is referred to as cross model validation (Westerhuis *et al.* 2008) or repeated double cross validation (Filzmoser *et al.* 2009). This strategy, which was adopted from Filzmoser *et al.* (2009), is illustrated in Figures 3.4 – 3.6. As shown in these figures, the whole procedure consists of two cross validation loops. Initially, the original data set is randomly divided into a number of sub-sets of preferably equal size (Figure 3.4). These sub-sets are the inputs to the outer cross validation loop, which then produces the predicted values for the dependent variable in every data sample. Based on the predicted and experimental values, performance indices including $RMSEP$, R^2, slope and intercept of best fit line can be evaluated (Figure 3.4). Further, it should be noted that there are many ways in which the original data set can be divided into sub-sets. If the procedure is repeated for a large number of times, each

time with a different set of sub-sets, statistical distributions of the performance indices can be obtained.

The outer cross validation starts with selecting one of the N_{test} sub-sets as the test set while the others form the calibration set (Figure 3.5). This outer loop is repeated N_{test} times, until each of the sub-sets has been selected once. Within this outer loop, the calibration set is used to develop and optimise a predictive model. Initially, it is sub-divided into N_{val} smaller sub-sets, which are inputs to the inner cross validation loop. This inner loop results in N_{model} predicted values for every data sample in the calibration set, where N_{model} is the total number of alternative models being considered. Based on these predicted and observed values of the dependent variable, the loss in remaining VL, N_{model} values of the *RMSEP* index are evaluated. Consequently, the model with the minimum *RMSEP* is identified and then it is re-calibrated using the whole calibration data set. The test data set is subsequently applied to the optimised model which produces predicted values for data in the test set (Figure 3.5).

The inner cross validation loop (Figure 3.6) begins where one of the N_{val} sub-sets is used as the validation set while the others form the training data set. The inner cross validation loop is repeated until each of the N_{val} sub-sets is used as the validation set once. Based on the training data set, N_{model} alternative models are developed. Subsequently, the validation data are applied to the N_{model} models, leading to N_{model} predicted values for each data sample in the validation data set.
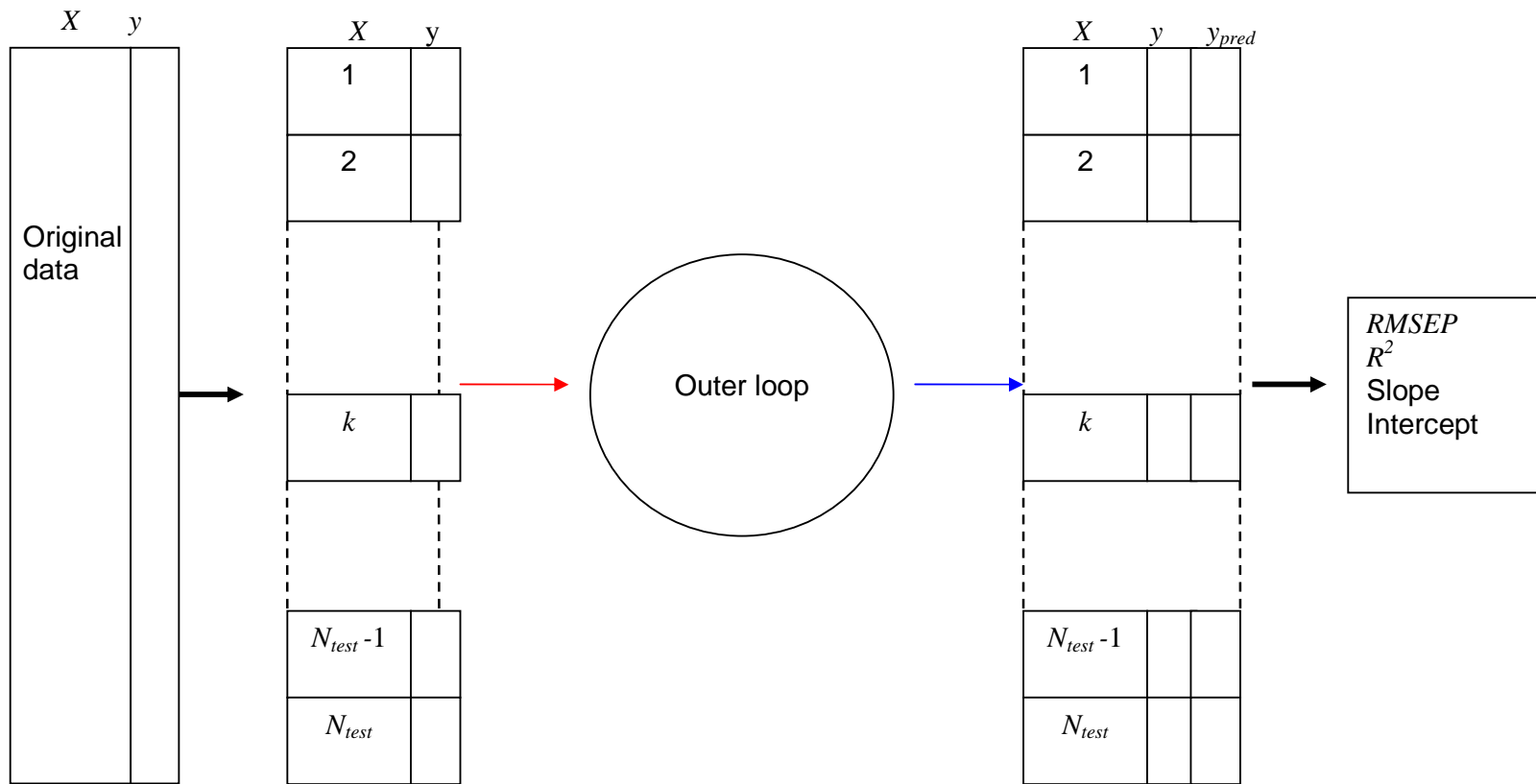
Figure 3.4: Double cross validation strategy
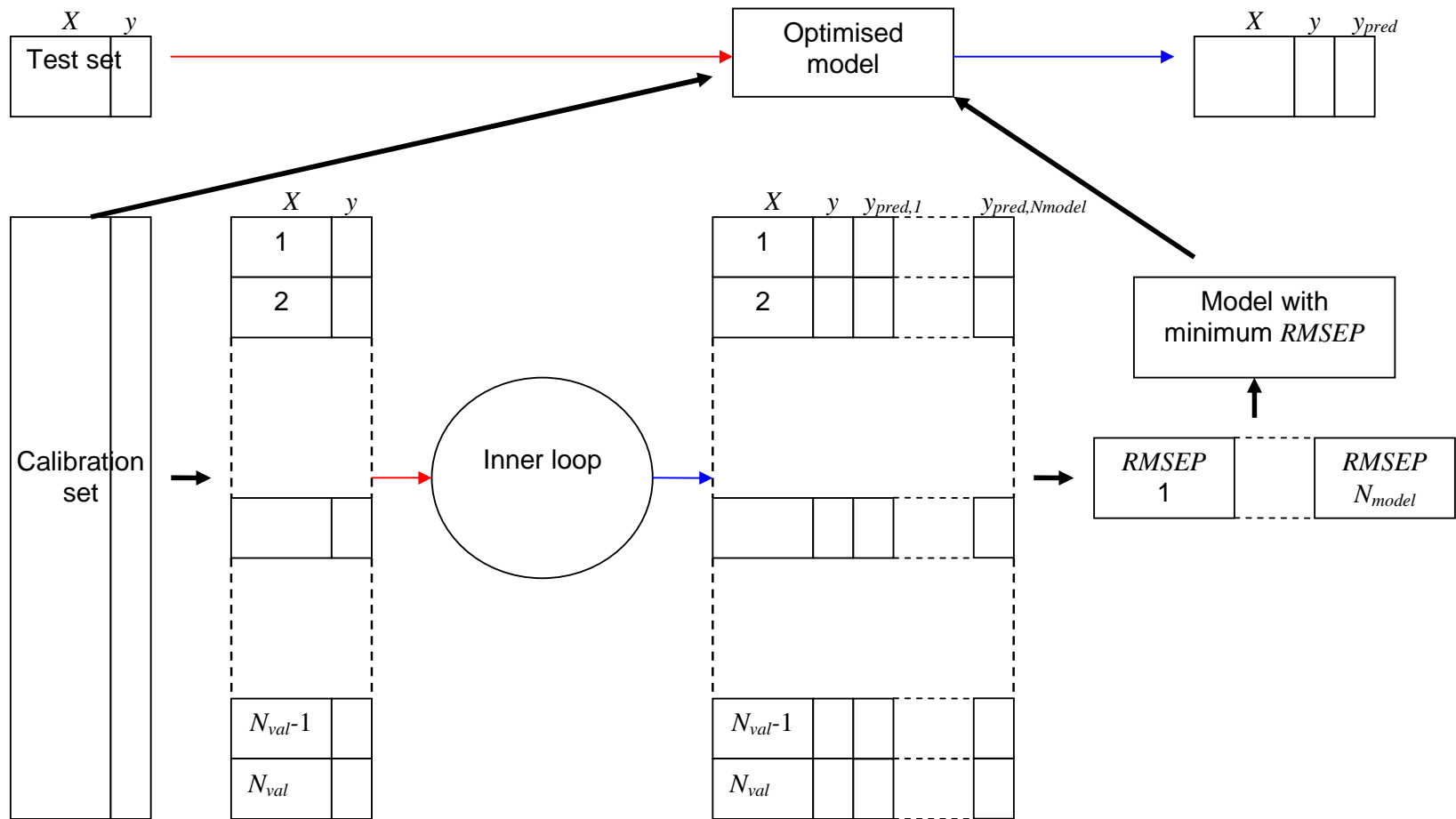
Figure 3.5: Outer cross validation loop
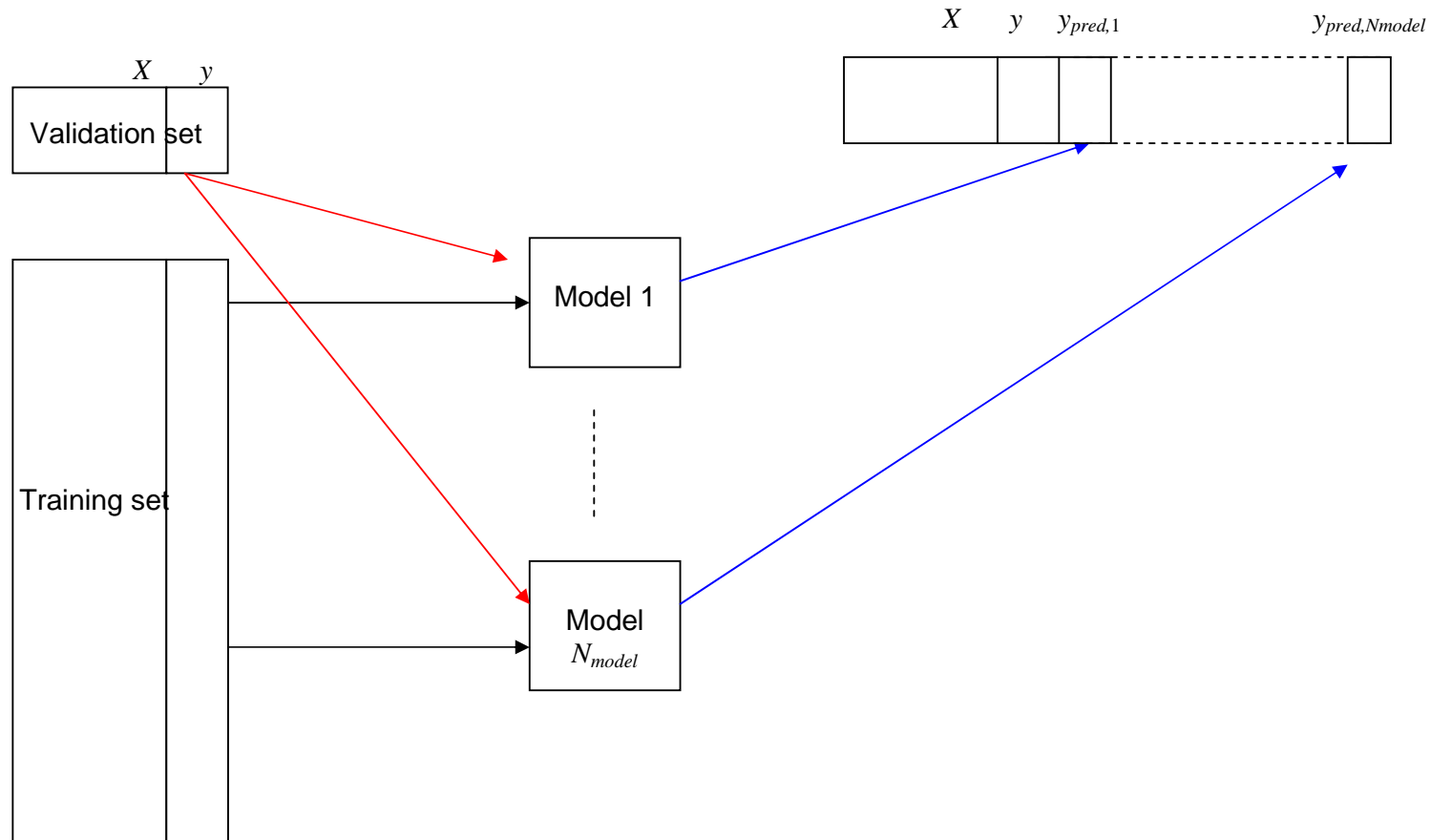
Figure 3.6: Inner cross validation loop

3.2.3 PERMUTATION TESTING

Permutation testing is a statistical technique that has an origin in statistical hypothesis testing. It has been applied in many areas such as canonical analysis of multivariate data (Anderson and Legendre 1999), and statistical classification (Golland *et al.* 2005; Westerhuis *et al.* 2008). It belongs to the non-parametric class of techniques, which means no assumption on statistical distribution is required. This is a major advantage of permutation testing technique, particularly for small data sets where insufficient data prevent such an assumption from being made and verified. The most significant limitation of permutation testing is its computational requirement. Nevertheless, with the increasing power of today's computers, this shortcoming has become less significant (Potvin and Roff 1993).

The essential idea of permutation testing is to assess the statistical significance of some observation based on the probability of it occurring purely by chance. Two key steps in permutation testing are selecting a statistic and evaluating its nonsense (i.e., randomised) distribution. For example, in a pattern classification context, the statistic is usually the cross-validation error, or the test error. The nonsense distribution is obtained by permutating the class labels while fixing the data sample, and then evaluating the statistic (Golland *et al.* 2005). The permutations need not be exhaustive; i.e., not all possible permutations need to be considered. Instead, it was suggested that generally 5000 permutations are sufficient (Potvin and Roff 1993).

Permutation testing was applied in this work to evaluate the statistical significance of the predictive performance of the modelling techniques used. The procedure of implementing permutation testing is shown in Figure 3.7. Initially, the selected modelling technique is applied to the original data, and performance statistics including *RMSEP*, R^2, slope and intercept of the best fit line are evaluated using the cross validation approach (see Section 3.2.2). Subsequently, the observed dependent variable, but not the independent ones, in the original data set is permutated i.e. shuffled randomly. Then, the same

modelling technique is applied to the permutated data set and $RMSEP$, R^2, slope and intercept of the best fit line are evaluated. These observed values belong to the nonsense distributions of the performance statistics. Consequently, the loop consisting of data permutation, modelling, and evaluation is repeated a large number of times (typically 10000 times). As a result, the nonsense distributions of $RMSEP$, R^2, slope and intercept of the best fit line are obtained. Permutation testing is completed by evaluating the probability of the performance statistics of the original data under the nonsense distributions.

3.2.4 STATISTICAL PERFORMANCE ASSESSMENT

A statistical assessment of an estimate or prediction of (the loss in) VL of cut roses is based on the comparison between the actual and nonsense distributions of $RMSEP$ statistics. The three following criteria are considered:

1. The statistical significance of the hypothesis that the mean of the actual $RMSEP$ distribution is smaller than that of the nonsense distribution. The selected significant level was 0.05. This criterion is to ensure that on average, the estimate based on the actual data has a smaller error than the one based on the randomised data. When this criterion is not satisfied, the estimation is labelled "not significant" or NS.

2. The p-value (type I error) of the lower 5 percentile of the nonsense distribution. This p-value is the proportion of the actual distribution that exceeds the lower 5% percentile of the nonsense distribution (Figure 3.8). The smaller this p-value is the smaller the probability that the actual $RMSEP$ would appear as if it belonged to the nonsense distribution.

3. The q-value (type II error) of the upper 5 percentile of the actual distribution. This q-value is the proportion of the nonsense distribution that is exceeded by the upper 5 percentile of the actual distribution (Figure 3.9). The smaller this q-value is the smaller the proportion of the nonsense distribution that appears as if it belonged to the actual distribution.

The estimation is effective when its actual $RMSEP$ distribution has smaller mean than the nonsense distribution and its p-value and q-value are both smaller than 10%.
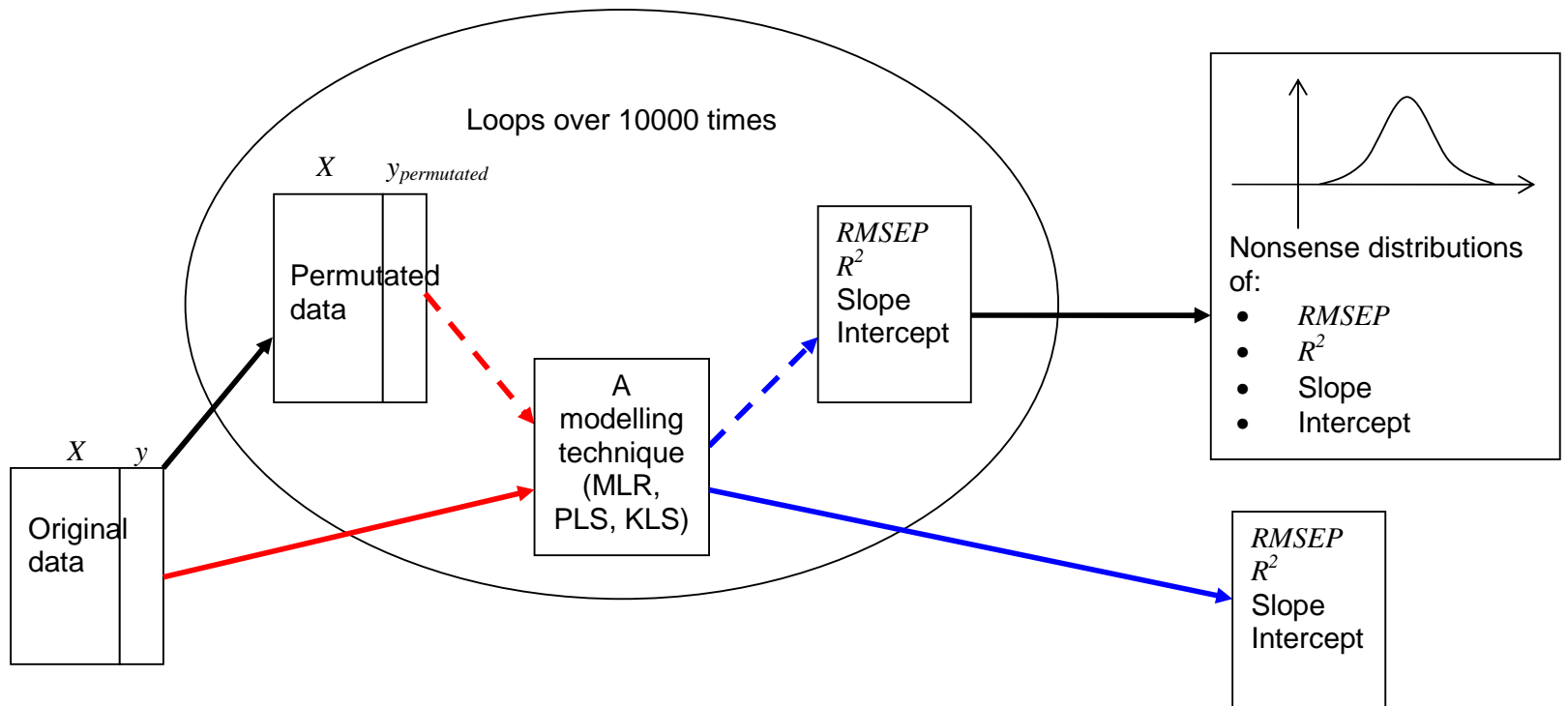
Figure 3.7: Permutation testing strategy
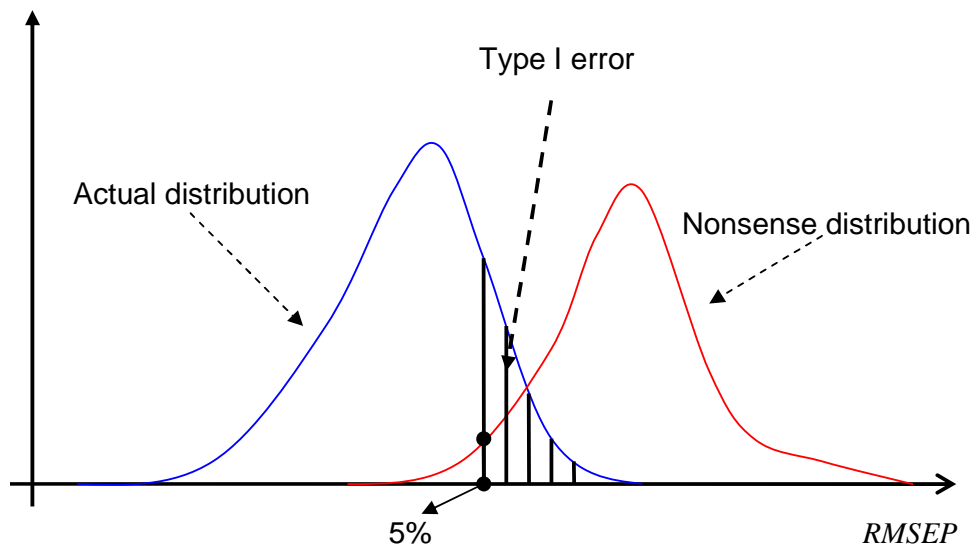
Figure 3.8: *p*-value (type I error) for comparison between the actual and nonsense *RMSEP* distributions
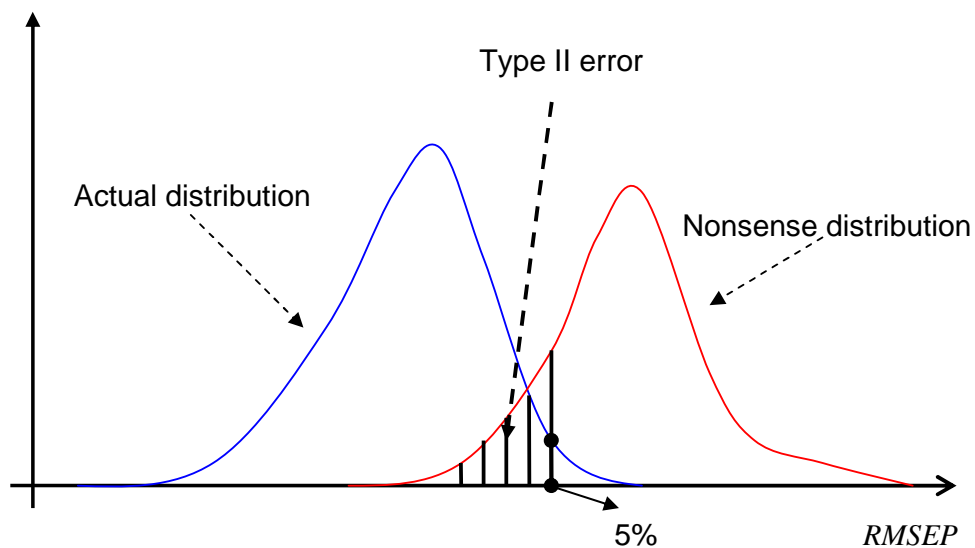
Figure 3.9: *q*-value (type II error) for comparison between the actual and nonsense *RMSEP* distributions

3.3 *A PRIORI* CONSTRAINT

There is some evidence to suggest that the higher the storage temperature of cut roses, the shorter their remaining VL. A few studies on cut roses (Faragher *et al.* 1986; Ichimura *et al.* 1999; Pompodakis *et al.* 2005) and other flowers such as Narcissus flower (Cevallos and Reid 2000) seemed to support this

observation. It could be argued that those studies were carried out at different constant storage temperatures and hence the conclusion would only be limited to such isothermal conditions. Nevertheless, the counter-argument would be that storage at dynamic temperature may be considered as a sequence of storages at constant temperatures. Consequently, unless substantial evidence is established against it, this work accepts the hypothesis, meaning that a higher storage temperature leads to a bigger loss in VL of cut roses.

However, it should be noted that such *a priori* knowledge was derived from and hence only correct for two identical samples of cut flower; i.e., the samples must have the same genotype and the same history of growth and development e.g. same pre-harvest conditions. (These conditions would more often than not be satisfied in laboratory studies only). As a result, the implication of the *a priori* knowledge depends on whether or not other non-thermal factors are included in the modelling. In other words, if the modelling does not account for other non-thermal factors such as the pre-harvest conditions and cultivar-specific information, then the *a priori* knowledge may not necessarily be met. On the other hand, if those factors of the flowers are also modelled, a constraint representing the *a priori* knowledge would have to be imposed. This thesis investigates two classes of scenarios: Scenarios A – only post-harvest temperature is modelled without the *a priori* constraint, and Scenarios B – post-harvest temperature is modelled with the *a priori* constraint.

3.3.1 *A PRIORI* CONSTRAINT IN MLR MODELLING

Consider a MLR model for the loss in remaining VL in terms of temperature,

$$\Delta t_{rs} = t_s - t_{rs} = \beta_1 T_1 + \beta_2 T_2 + \ldots + \beta_n T_n + \beta_{n+1} \tag{3.5}$$

Where β_i: the ith regression coefficient ($i = 1, 2, \ldots, n+1$).

T_i: the ith temperature readings ($i = 1, 2, \ldots, n$).

n: the number of temperature readings.

t_s: the initial VL of the roses (evaluated at reference temperature) before being exposed to temperature profile $T_1, \quad T_2, \quad \ldots \quad T_n$.

t_{rs}: the remaining VL of the roses (evaluated at reference temperature) after being exposed to temperature T_1, T_2, … T_n.

Δt_{rs}: the loss in VL of the roses due to temperature T_i.

The role of β_{n+1} is important. In a "regression" sense, it is the free coefficient i.e. independent from the explanatory variables. β_{n+1} is a constant when the model (3.5) is used to explain the effect of temperature without any regard to other non-thermal effects (such as humidity, or pre-harvest conditions) on remaining VL of cut flowers. In such cases, the *a priori* constraint is not necessarily satisfied, and hence was not imposed. On the other hand, if the model (3.5) is meant to capture both thermal and non-thermal effects, and assuming that those effects are additive, β_{n+1} is not a constant, but rather a variable representing the non-thermal components in the remaining VL. The *a priori* constraint must be imposed, which implies the higher the storage temperature, the bigger the reduction in VL over the same duration of storage. By taking the derivative of (3.5), the constraint was

$$\frac{\partial\left(\Delta t_{rs}\right)}{\partial T_i} = \beta_i > 0 \qquad (i = \overline{1,n}) \tag{3.6}$$

In summary, there are two scenarios as follows:

1. Scenario A: modelling effects of temperature only

$$\begin{cases} \Delta t_{rs} = t_s - t_{rs} = \beta_1 T_1 + \beta_2 T_2 + \ldots + \beta_n T_n + \beta_{n+1} \\ \beta_{n+1} \text{ is the free (constant) coefficient} \end{cases} \tag{3.7}$$

2. Scenario B: modelling thermal and non-thermal effects

$$\begin{cases} \Delta t_{rs} = t_s - t_{rs} = \beta_1 T_1 + \beta_2 T_2 + \ldots + \beta_n T_n + \beta_{n+1} \\ \beta_{n+1} \text{ is the non-thermal (variable) component} \\ \beta_i > 0 \ \left(i = \overline{1,n}\right) \end{cases} \tag{3.8}$$

3.3.2 *A PRIORI* CONSTRAINT IN **PLS** MODELLING

Using the notation from (de Jong 1993) the overall regression coefficients obtained by PLS is

$$\boldsymbol{\beta}_{PLS} = \mathbf{W}(\mathbf{P}^T\mathbf{W})^{-1} diag(\mathbf{b})\mathbf{Q}^T \tag{3.9}$$

Where $\boldsymbol{\beta}_{PLS}$: the overall regression coefficients;

$\mathbf{W}$: the weight matrix of input data;

$\mathbf{P}$: loading matrix of input data;

$\mathbf{b}$: inner regression coefficient;

$\mathbf{Q}$: loading matrix of output data;

As with MLR modelling, PLS modelling also has two scenarios as follows:

1. Scenario A: modelling effects of temperature only. No constraints were required nor imposed

$$\begin{cases} \Delta t_{rs} = t_s - t_{rs} = \boldsymbol{\beta}_{PLS}(1)T_1 + \boldsymbol{\beta}_{PLS}(2)T_2 + \ldots + \boldsymbol{\beta}_{PLS}(n)T_n + \beta_{n+1} \\ \beta_{n+1} = \overline{\Delta t_{rs}} \end{cases} \qquad (3.10)$$

2. Scenario B: modelling thermal and non-thermal effects. The constraints were

$$\begin{cases} \Delta t_{rs} = t_s - t_{rs} = \boldsymbol{\beta}_{PLS}(1)T_1 + \boldsymbol{\beta}_{PLS}(2)T_2 + \ldots + \boldsymbol{\beta}_{PLS}(n)T_n + \beta_{n+1} \\ \beta_{n+1} = \overline{\Delta t_{rs}} \\ \boldsymbol{\beta}_{PLS} > 0 \end{cases} \qquad (3.11)$$

3.4 CHAPTER CONCLUSION

In implementing MLR and PLS techniques, the selection of variables, the selection of the number of LVs to use, and the requirement of a uniform number of input measurements per sample are often encountered. This chapter explained the strategy that was adopted to overcome those two issues. In addition, it also described the performance assessment framework, which includes the performance statistics and the evaluation procedure. This framework will be applied in the subsequent chapters to compare and assess the prediction performance of different analysis techniques in estimating the vase life loss of cut roses. Finally, the chapter discussed the relevance of the *a priori* knowledge which states that the higher storage temperature leads to a greater loss in quality, as measured by the remaining VL, and its implementation in MLR and PLS techniques was outlined.

4 MATHEMATICAL DEVELOPMENT OF KINETIC LINEAR SYSTEM (KLS) TECHNIQUE

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This chapter describes the mathematical development of a new technique, developed as part of the work reported in this thesis, called Kinetic Linear System (KLS) for modelling the post-harvest loss in the remaining shelf life of perishable produce (such as fresh fruit, vegetables and cut flowers) resulting from temperature stresses. KLS is based on kinetic principles so that it can be applied to any perishable produce where senescence is governed by biochemical processes. In addition, KLS is also data-driven so that it does not suffer from the disadvantage of the kinetic modelling technique, where model parameters have to be specified.

The chapter is organised as follows. Section 4.1 explains the motivation for developing KLS. Section 4.2 describes the mathematical development of KLS including derivation, model calibration, shelf life prediction, and assumptions. Section 4.3 discusses various issues that may be encountered when using the KLS technique. These issues include the different mathematical scenarios that may occur in KLS model calibration, the requirement for an initial shelf life and the different parameters involved in KLS modelling. Section 4.4 demonstrates KLS model calibration and prediction using an example.

_____

4.1 **MOTIVATION**

A major challenge for the perishable produce industry is to deliver consistently high quality, long-lasting fruits, vegetables and cut flowers to its customers. Product quality and particularly shelf life are important because the perception of these is one of the key criteria that consumers use when considering which produce to purchase.

Perishable produce is transported from farms to wholesalers and distribution centres through supply chains at low temperature (e.g., 0-10°C depending upon the specific produce). Previous studies have established that temperature in such chilled supply chains is not optimal (Grieve and Waltham 2008). As sub-optimal temperature accelerates deterioration of the produce, their quality at delivery locations is reduced. The loss in quality of perishable produce is potentially significant, depending on the specific produce (Section 1.2.4). Consequently, this presents an economic incentive to monitor the in-transit temperature, and subsequently to address temperature-based quality problems.

Two capabilities are required for quality control: temperature monitoring and linking the temperature stresses to the loss in quality (Verdijck and van Straten 2002). The first is possible through the use of data loggers, sensor-integrated RFID tags, or wireless sensor networks (Carullo *et al.* 2009). The second, linking the temperature stresses to loss of quality, is the topic of this chapter.

Generally, modelling techniques can be classified based on the amount of first-principle knowledge they require. At one extreme, there are techniques that are based on first principles. Such model-based techniques are rarely used as the biological systems and processes embedded in the produce are complex. At the other extreme, there are data-driven techniques that use only observed measurements to obtain a model. In the area of quality modelling of fresh perishable produce, as the literature review shows, these techniques have hardly been applied.

The literature review (Chapter 2) has revealed that kinetic modelling is the most commonly used technique in modelling the effect of temperature on the quality of perishable produce. Kinetic modelling is the preferred approach in this field of study because it is based on kinetic principles which govern all biochemical processes. However, building a kinetic model is complicated and time consuming. As illustrated in Figure 4.1, kinetic modelling must identify and model each quality attribute independently. Multiple quality attributes and hence multiple models may be required (Nunes *et al.* 2007).

In addition, for each quality attribute model based on the kinetic modelling technique it is necessary to select a temperature dependence (e.g., Arrhenius or Ratkowsky) and a function of the attribute (e.g., Monod or Gompertz for modelling microbial growth in meats and fishes) (McDonald and Sun 1999; Shimoni and Labuza 2000; Isabelle and André 2006). Opinions often vary on which types of functions should be used. Expert reasoning are often combined with parameter estimation to obtain an empirical kinetic model. However, different reasoning may lead to different models and interpretation. For example, the tomato firmness model from Schouten *et al.* (Schouten *et al.* 2007a) is different from the model from Van Dijk *et al.* (van Dijk *et al.* 2006b). Which model to use may not be straightforward.

Most reported studies have been for constant temperatures. Dynamic temperature leads to solving ordinary differential equation in kinetic modelling, which may be mathematically complicated (Schouten *et al.* 2007a).

Consequently, a technique is desired that it is based on the kinetic principle, but which does not suffer from the above disadvantages of current kinetic modelling techniques. This is the motivation for the development of KLS.

$\Delta Q = $ **???**

Attribute Q_1 (e.g. firmness)

- Model: $-\dfrac{dQ_1}{dt} = f_1(T)\,g_1(Q_1)$
- Must specify: f_1, g_1
- Calibrating data: $(T,\ Q_1)$

Q_1

Attribute Q_2 (e.g. colour)

- Model: $-\dfrac{dQ_2}{dt} = f_2(T)\,g_2(Q_2)$
- Must specify: f_2, g_2
- Calibrating data: $(T,\ Q_2)$

Q_2

Attribute Q_n (e.g. taste)

- Model: $-\dfrac{dQ_n}{dt} = f_n(T)\,g_n(Q_n)$
- Must specify: f_n, g_n
- Calibrating data: $(T,\ Q_n)$

Q_n
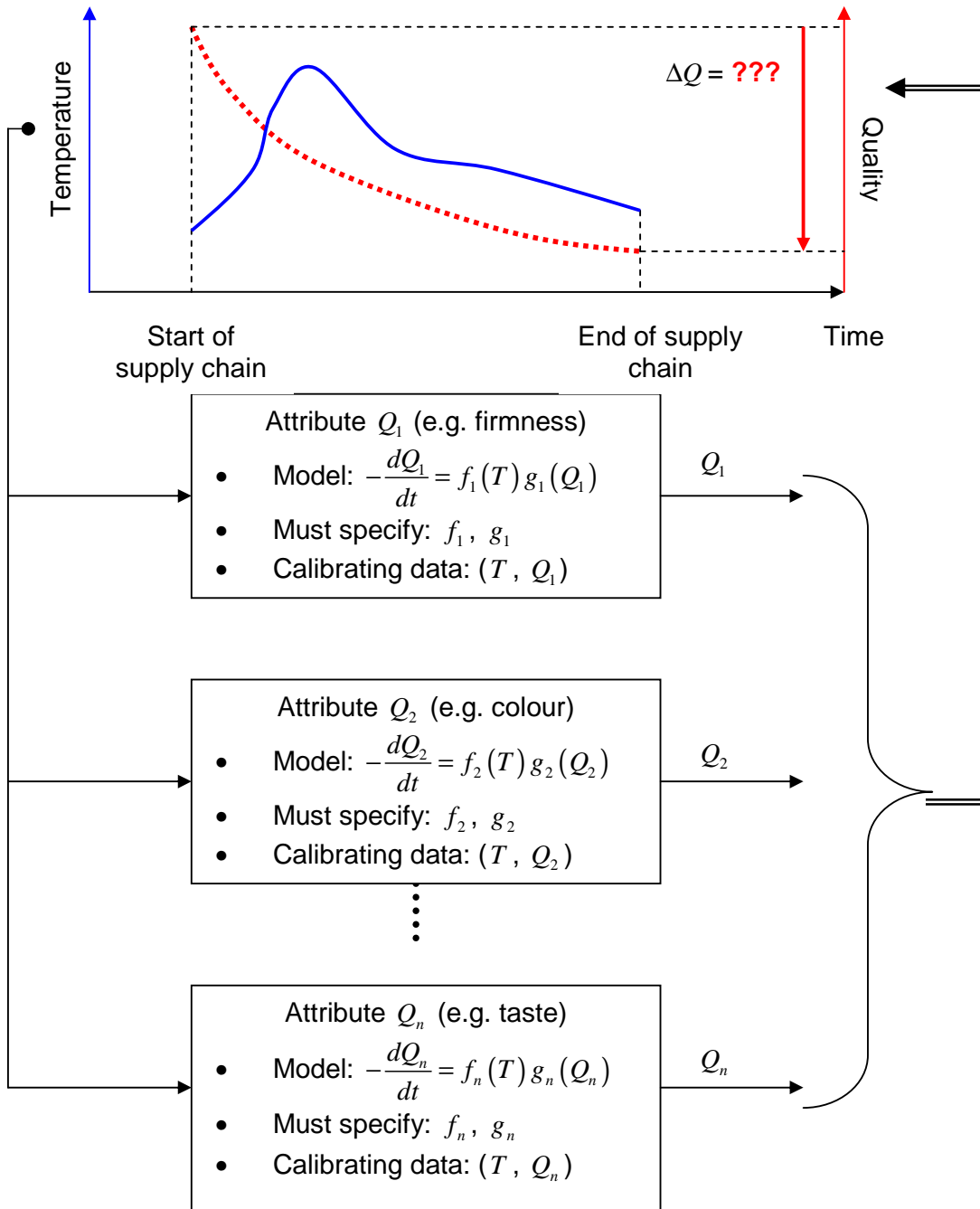
Figure 4.1: Multiple kinetic models corresponding to different quality attributes are required to evaluate shelf life.

4.2 KLS MATHEMATICAL DERIVATION

4.2.1 DERIVATION

For any perishable produce item, the quality attribute Q that solely determines its shelf-life is expressed as:

$$-\frac{dQ}{dt} = f(T) \cdot g(Q) \tag{4.1}$$

Where $f(T)$ represents the temperature effects on the quality attribute Q and $g(Q)$ is a function of Q. Referring to Figure 4.2, the following definitions apply:

t_{dist} is the time the item is transported from a producer (farm) i.e. the start of the supply chain, to a distribution centre considered here as the end of the supply chain.

T is the temperature of the perishable item.

Q_{init} is the initial quality of the perishable item at the producer's location.

Q_{rem} is the quality remaining when the product item is received at the distribution centre.

Q_{end} is the lower limit on quality which indicates the end of the shelf life of the produce. When this limit is reached, the product is no longer acceptable for consumption, nor does it have any economic value.

t_{rem} is the time associated with the remaining quality of the produce Q_{rem}. It is the time duration that the product would take to deteriorate at reference temperature T_{ref} from Q_{rem} to Q_{end}. t_{rem} is an unknown parameter that, if it can be modelled or predicted, would provide the basis for determining an expiry date (often called a *best before* date) for the produce; this would be an expiry date related to actual temperature stresses experienced in the supply chain.

t_{init} is the initial shelf-life associated with the initial quality Q_{init}. It is the time duration that the product would take to deteriorate at reference temperature T_{ref} from Q_{init} to Q_{end}.
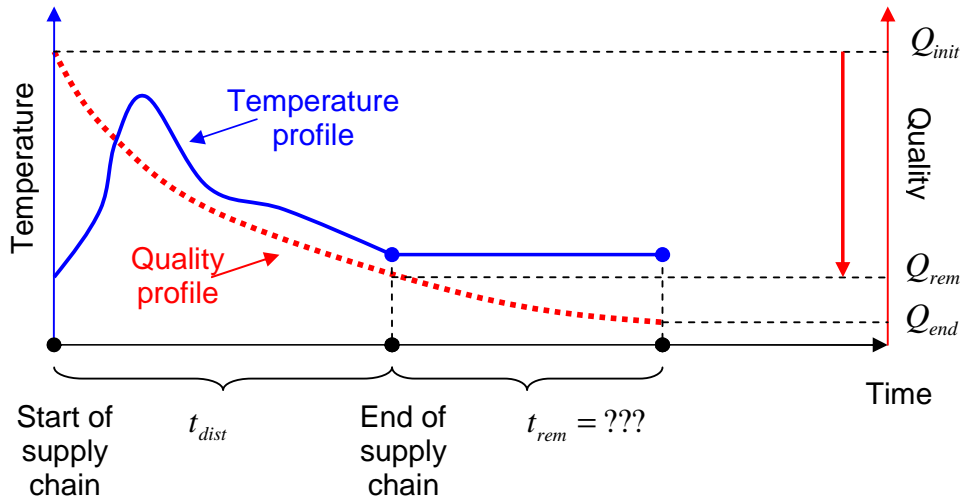
Figure 4.2: Definition of notations of variables used in KLS development

In practice the quality measurements $Q_{init}, Q_{rem}, Q_{end}$ are not normally available. Instead, a temperature profile T for the distribution period and consequently t_{dist} are recorded using data loggers or RFID tags. The objective of the KLS method is to estimate the remaining shelf life t_{rem} of the product after the distribution period, given the temperature profile T, distribution time t_{dist}, and the initial shelf life t_{init} i.e. without any knowledge of quality measurements $Q_{init}, Q_{rem}, Q_{end}$.

Divide Equation (4.1) by $g(Q)$ and then integrate

$$\int_{Q_{init}}^{Q} \frac{-dQ}{g(Q)} = \int_{0}^{t} f(T)dt \tag{4.2}$$

The time period of interest is the shelf life t_{init}, thus integration of Equation (4.2) is over the interval 0 to t_{init}, which corresponds to the quality change Q_{init} to Q_{end}. Consequently, for any item that is kept under a constant reference temperature T_{ref} (which might apply if the produce were not transported and just held in constant storage conditions until Q_{end} was reached), and using these integration intervals, Equation (4.2) leads to

$$\int_{Q_{init}}^{Q_{end}} \frac{-dQ}{g(Q)} = \int_{0}^{t_{init}} f\left(T_{ref}\right)dt = t_{init} \cdot f\left(T_{ref}\right)$$ (4.3)

On the other hand, if the same produce item was kept at T_{ref} after going through a transportation period during which storage temperature varied, Equation (4.2) is equivalent to:

$$
\begin{aligned}
\int_{Q_{init}}^{Q_{end}} \frac{-dQ}{g(Q)} &= \int_{0}^{t_{dist}+t_{rem}} f(T)dt \\
&= \int_{0}^{t_{dist}} f(T)dt + \int_{t_{dist}}^{t_{dist}+t_{rem}} f\left(T_{ref}\right)dt \\
&= \int_{0}^{t_{dist}} f(T)dt + t_{rem} \cdot f\left(T_{ref}\right)
\end{aligned}
$$ (4.4)

Equations (4.3) and (4.4) both have the same left-hand sides, thus it follows, after rearranging, that

$$\int_{0}^{t_{dist}} f(T)dt = f\left(T_{ref}\right) \cdot \left(t_{init} - t_{rem}\right)$$ (4.5)

Note that T is a series of k measurements $\left\{T_{t=t_i}\right\}_{i=\overline{0,k}}$. Thus, the left-hand side of Equation (4.5) becomes the integral expression:

$$\int_{o}^{t_{dist}} f(T)dt = \sum_{i=1}^{k} \int_{t_{i-1}}^{t_i} f(T)dt \qquad where \ \ t_0 = 0 \ and \ t_k = t_{dist}$$ (4.6)

Assume that both T and $f(T)$ are linear in terms of time over one sampling interval, and using the Trapezoidal Rule, the integral term in the right –hand side of Equation (4.6) becomes:

$$\int_{t_{i-1}}^{t_i} f(T)dt = \frac{1}{2}\left(t_i - t_{i-1}\right)\left[f\left(T_{t=t_i}\right) + f\left(T_{t=t_{i-1}}\right)\right]$$ (4.7)

Substituting Equation (4.7) into Equation (4.6) and assuming that the time sampling is one unit, gives:

$$\int_{o}^{t_{dist}} f(T)dt = \frac{1}{2}\left[f\left(T_{t=t_0}\right) + f\left(T_{t=t_k}\right)\right] + \sum_{i=1}^{k-1} f\left(T_{t=t_i}\right)$$ (4.8)

Let us now examine the function over the temperature range $[T_{min} \quad T_{max}]$. Owing to the finite resolution of temperature measuring devices (e.g. data loggers), the temperature T can only take on a finite number of values in the range $[T_{min} \quad T_{max}]$. Let $\left\{ T_{min} = T_1 \;\; < \;\; T_2 \;\; < \;\; \ldots \;\; < \;\; T_j \;\; \ldots \;\; < \;\; T_n = T_{max} \right\}_{j=\overline{1,n}}$ denote these temperature values. As a result, the function $f(T)$ can only take on values in the set $f_j = \left\{ f(T_j) \right\}_{j=\overline{1,n}}$. In other words, the set $f_j = \left\{ f(T_j) \right\}_{j=\overline{1,n}}$ contains all values of the function of interest.

Example

Let us suppose that there was a data logger that had a minimum resolution of 1 °C and that the logger was used to record the temperature of a produce item that had the minimum and maximum temperatures of $T_{min} = 12 \; {}^{o}C$ and $T_{max} = 15 \; {}^{o}C$, respectively. Consequently, any reading from the logger will be one of the following temperatures $\left\{ T_{min} = 12, \;\; 13, \;\; 14, \;\; T_{max} = 15 \right\} \; {}^{o}C$. As a result, any function of the temperature measurement $f(T)$ can only assume the values in the set $\left\{ f\left(T_{min} = 12 \; {}^{o}C \right), \;\; f\left(13 \; {}^{o}C \right), \;\; f\left(14 \; {}^{o}C \right), \;\; f\left(T_{max} = 15 \; {}^{o}C \right) \right\}$.

Rewriting the set $f_j = \left\{ f(T_j) \right\}_{j=\overline{1,n}}$ in vector form i.e. $\mathbf{f_v} = \left[f(T_1) \quad f(T_2) \quad \ldots \quad f(T_j) \quad \ldots \quad f(T_n) \right]^{T}$. Equation (4.8) leads to

$$\int_{o}^{t_{dist}} f(T) dt = \mathbf{\alpha}^{T} \cdot \mathbf{f_v} \tag{4.9}$$

Where: $\mathbf{\alpha}$ is the coefficient vector which is related to the statistical distribution of temperature measurements over the range being considered. Equation (4.9) numerically approximates the left hand side integral by a linear combination of the function values at discretised states.

Example (cont.)

Let us continue with the above example and assume that the following temperature profile was recorded.

$$T_{profile,1} = \{15 \quad 12 \quad 14 \quad 14 \quad 13 \quad 15 \quad 14 \quad 13\}$$

Equation (4.8) becomes

$$
\begin{aligned}
\int_{o}^{t_{dist}} f(T)dt &= \frac{1}{2}\Big[f(15\,{}^{o}C) + f(13\,{}^{o}C)\Big] + f(12\,{}^{o}C) \\
&\quad + f(14\,{}^{o}C) + f(14\,{}^{o}C) + f(13\,{}^{o}C) \\
&\quad + f(15\,{}^{o}C) + f(14\,{}^{o}C) \\
&= f(12\,{}^{o}C) + 1.5f(13\,{}^{o}C) + 3f(14\,{}^{o}C) + 1.5f(15\,{}^{o}C)
\end{aligned}
$$

Consequently, $\qquad \boldsymbol{\alpha}_1 = (1 \quad 1.5 \quad 3 \quad 1.5)^T \qquad$ and

$$\mathbf{f_v} = \{f(12\,{}^{o}C), \quad f(13\,{}^{o}C), \quad f(14\,{}^{o}C), \quad f(15\,{}^{o}C)\}^T .$$

Substituting Equation (4.9) into Equation (4.5) yields the expression.

$$\boldsymbol{\alpha}^T \cdot \mathbf{f_v} = f(T_{ref}) \cdot (t_{init} - t_{rem}) \tag{4.10}$$

This equation can be used to predict t_{rem} (remaining shelf life) given knowledge of the other parameters, thus providing the basis of a numerical or data-driven means of shelf life prediction using kinetic principles.

4.2.2 MODEL CALIBRATION

Let us consider only temperature profiles of m produce items for which the remaining shelf-life $t_{rem,m}$ after the distribution period $t_{dist,m}$ is available. The coefficients vectors $\boldsymbol{\alpha}_m$ (Equation (4.9)) together form a matrix $\mathbf{A}$ of size $m \times n$ where n is the number of temperature states in the range $[T_{min} \quad T_{max}]$.

$$\mathbf{A} = [\boldsymbol{\alpha}_1 \quad \boldsymbol{\alpha}_2 \quad \ldots \quad \boldsymbol{\alpha}_m]^T \tag{4.11}$$

Hence, Equation (4.10) leads to

$$
\begin{aligned}
\mathbf{A} \cdot \mathbf{f_{aug}} &= \Big[t_{init,1} - t_{rem,1} \quad t_{init,2} - t_{rem,2} \quad \cdots \quad t_{init,m} - t_{rem,m}\Big]^T \\
&\quad where \ \mathbf{f_{aug}} = \frac{1}{f(T_{ref})} \mathbf{f_v}
\end{aligned}
\tag{4.12}
$$

Example (cont.)

Let us continue with the example and assume that the loss in shelf life of the produce item 1 (corresponding to $T_{profile,1}$) is $t_{init,1} - t_{rem,1} = 12.5$. Further, let us assume that there is another produce with the following data

$$T_{profile,2} = \{12 \quad 12 \quad 13 \quad 14 \quad 15 \quad 14 \quad 15 \quad 15 \quad 15 \quad 14\}$$

$$t_{init,2} - t_{rem,2} = 22.5$$

By repeating the previous step for the produce item 2, we obtain $\boldsymbol{\alpha}_2 = \begin{pmatrix} 1.5 & 1 & 2.5 & 4 \end{pmatrix}^T$. Consequently, Equation (4.12) becomes

$$\begin{pmatrix} 1 & 1.5 & 3 & 1.5 \\ 1.5 & 1 & 2.5 & 4 \end{pmatrix} \cdot \mathbf{f}_{aug} = \begin{pmatrix} 12.5 \\ 22.5 \end{pmatrix}$$

$$\text{where } \mathbf{f}_{aug} = \left\{ \frac{f(13\,^oC)}{f(T_{ref})}, \quad \frac{f(13\,^oC)}{f(T_{ref})}, \quad \frac{f(14\,^oC)}{f(T_{ref})}, \quad \frac{f(15\,^oC)}{f(T_{ref})} \right\}^T$$

Note that the linear system described by Equation (4.12) represents the training information that is available. Solving the linear system for $\mathbf{f}_{aug}$ gives a KLS model of the reduction in the produce shelf life owing to temperature stresses. This KLS model is therefore obtained from the temperature profile T, the remaining shelf life t_{rem}, and the initial shelf life t_{init}; i.e., without quality measurements Q_{init}, Q_{rem}, Q_{end} or any knowledge of the functions for Q or f.

4.2.3 SHELF LIFE PREDICTION

Given a KLS model, now consider the produce item p that has the temperature profile T_p, while being transported from the farm to a distribution centre. Its remaining shelf-life $t_{rem,p}$ (upon being delivered at the distribution centre) is **unknown** and **to be estimated**. Applying similar derivation, Equation (4.10) leads to

$$\boldsymbol{\alpha}_p^T \cdot \mathbf{f}_{aug} = \left(t_{init,p} - t_{rem,p} \right) \tag{4.13}$$

Let us suppose that some vector $\mathbf{f_{aug}}$ exists that satisfies Equation (4.12), then

$$t_{rem,p} = t_{init,p} - \boldsymbol{\alpha}_p^T \cdot \mathbf{f_{aug}} \tag{4.14}$$

Equation (4.14) shows that the remaining shelf-life of the new product item $t_{rem,p}$ can be evaluated using the initial shelf life of the product $t_{init,p}$, the temperature profile T_p (which determines $\boldsymbol{\alpha}_p$) and the KLS model $\mathbf{f_{aug}}$.

4.2.4 ASSUMPTIONS

There are a number of assumptions made during the derivation of the KLS method. The most important one is that the KLS method assumes that all produce items have the same model KLS, $\mathbf{f_{aug}}$. This is critical so that the KLS model can be applied to new produce items that were not used in model calibration. Mathematically, $\mathbf{f_{aug}}$ is a vector representing the effect of temperature $f(T)$ at each temperature state $\left\{ T_{\min} = T_1 \; < \; T_2 \; < \; \ldots \; < \; T_j \; \ldots \; < \; T_n = T_{\max} \right\}_{j=\overline{1,n}}$ compared to the corresponding effect at reference temperature $f\left(T_{ref}\right)$. Therefore, the assumption effectively implies that all items were assumed to respond to temperature stresses in the same way and that temperature is the single determinant of changes in shelf life. While making this assumption is necessary, caution must be taken because there are circumstances where it may not hold. The literature review in Chapter 2 has revealed that post-harvest temperature is not the only factor that could significantly affect the remaining shelf life of fresh perishable produce. The review pointed out that factors including genotype, pre-harvest conditions and other post-harvest factors such as humidity can all play important roles in the deterioration of perishable produce and thereby shorten their shelf life. As a result, designing experiments specifically aimed at minimising variation in those factors may result in data sets which could potentially improve the performance of the KLS method. Nevertheless, such improvement may not be practical because variation in some factors such as growing conditions and post-harvest humidity is likely to exist in real contexts.

Another assumption is that the effect of temperature $f(T)$ and the behaviour of quality (attribute) $g(Q)$, are decoupled in the kinetic equation (Equation (4.1)). This assumption appears reasonable in most cases where only a single biochemical process affects quality Q. In fact, in such simple cases the assumption was usually made implicitly without any explanation (e.g. (Yan *et al.* 2008)). However, the situation becomes more complicated when multiple biochemical processes are involved. For example, the kinetics of mushroom colour is believed to involve at least two chemical reactions: the first is to form polyphenol oxidase (PPO) and the second is to convert PPO into chinons, the precursor of the brown colouring agents in mushroom (Lukasse and Polderdijk 2003). As a result, the corresponding kinetic model is a non-separable system of three differential equations, which does not seem to be reducible into a general form as in Equation (3.1). This suggests that the kinetic model in (Lukasse and Polderdijk 2003) may not have a mathematically equivalent KLS model. However, whether the assumption of decoupling $f(T)$ and $g(Q)$ is valid or not in modelling mushroom colour is still inconclusive.

Another assumption in KLS development is that both temperature T and its effect $f(T)$ are linear in terms of time over a sampling interval. This assumption is necessary in order to approximate numerically the integral in Equation (4.7). The assumption is reasonable when the sampling interval is sufficiently small.

4.3   DISCUSSIONS

4.3.1   MATHEMATICAL SCENARIOS IN MODEL CALIBRATION

In calibrating a KLS model (Equation (4.12)), there are a number of possible mathematical scenarios. In the following, recall that m is the number of perishable produce items, from which the data used in training the KLS model was obtained, and n is the number of temperature states in the range $\begin{bmatrix} T_{\min} & T_{\max} \end{bmatrix}$.

<u>Case a</u>: over-determined system ($m > n$)

In this case, the linear system is over-determined and no analytical solution can be obtained. The reason is that the true behaviour of each produce sample (as expressed by $\mathbf{f_{aug}}$) is likely to be different from one another. Consequently, no single $\mathbf{f_{aug}}$ can satisfy the linear system (Equation (4.12)). However, KLS assumes that such a difference is negligible and hence all $\mathbf{f_{aug}}$ for all samples should converge to some "average" solution, which is often the least square solution.

<u>Case b</u>: under-determined system ($m < n$)

The linear system in Equation (4.12) is under-determined when there are fewer samples (for calibration) than the temperature states; i.e., $m < n$. For such systems, there would be an infinite number of solutions $\mathbf{f_{aug}}$ which do not normally converge. Clearly, additional information is required to identify the solution which best describes the true behaviour of the produce being modelled. Effectively, the mathematical inequality means that given available data (m), there is an upper limit on how much details of the produce's behaviour can be deduced.

To deal with under-determined system, a trivial way is to collect more data samples, and hence increase m. Alternatively, reducing the temperature resolution i.e. increasing the temperature step and thereby reducing the number of temperature states n could also help, although the prediction accuracy could be affected. In addition, *a priori* information may also help as well. For example, $\mathbf{f_{aug}}\left(T = T_{ref}\right) = 1$ can be used as an additional constraint if T_{ref} is within the temperature range $\begin{bmatrix} T_{min} & T_{max} \end{bmatrix}$ being considered.

<u>Case c</u>: well-defined system ($m = n$)

A well-defined system is relatively rare and a unique solution can be obtained from the linear system.

4.3.2 MODELLING PARAMETERS

KLS modelling involves a number of parameters including a reference temperature T_{ref}, upper and lower temperature thresholds T_{max} and T_{min}, and temperature steps $\Delta T = T_{j+1} - T_j$ $(j = 1, 2, ..., n-1)$. T_{ref} is the temperature at which the remaining shelf life of perishable produce is evaluated in a shelf life test. For cut roses, an industry standard (Floral Solutions 2006) suggests that T_{ref} should be set at 20 ^{o}C to resemble conditions under which the flowers would commonly be displayed in customers' environments. The other three parameters, $T_{max}, T_{min}, \Delta T$, are design parameters, which are problem-dependent. The values for these parameters are normally selected such that they capture the temperature range of interest. However, as discussed earlier, when insufficient data are available for model calibration, leading to an under-determined system of linear equations, the design parameters could be modified to deal with the ill-defined mathematical system.

4.3.3 USING KLS AS A REGRESSION TECHNIQUE

As illustrated in (Figure 4.2), a KLS model expresses the change from initial shelf life to the final shelf life of perishable produce under the effect of temperature. In other words, the temperature that the produce is exposed to during such a change in shelf life is analysed. However, there are scenarios where it is desired to investigate the effect of temperature on the subsequent changes in shelf life of the produce i.e. the changes in shelf life occur after the produce is exposed to the temperature. An example is investigating the effect of temperature during growing period on the post-harvest changes in shelf life of a certain produce. The mathematical development of the KLS technique (Section 4.2) is not applicable in such scenarios. However, procedurally a KLS model could still be obtained as before although the mathematical foundation, which is based on kinetic principle (Equation (4.1)), may no longer hold; rather, the model is a regression of the coefficient vector $\boldsymbol{\alpha}$.

4.3.4 ACCOUNTING FOR NON-THERMAL EFFECTS IN KLS MODELLING

As detailed in the literature review (Section 2.3), post-harvest temperature is not the only factor that could affect the remaining shelf life of perishable products. Other factors such as genotype, pre-harvest (i.e. growing) conditions, and post-harvest humidity may also play important roles in their post-harvest deterioration. When the effects of such non-thermal factors are not negligible, those factors must be accounted for in the modelling. KLS technique facilitates this by introducing slack variables.

Let us define the slack variables $\mathbf{f}_{slack}$ as a vector $(m \times 1)$ where $\mathbf{f}_{slack,i}$ represents the loss in shelf life of the ith perishable product item $(i = \overline{1,m})$ that is due to the effects of the non-thermal factors. To account for the non-thermal factors, Equation (4.12) is modified as follows

$$\mathbf{A} \cdot \mathbf{f}_{aug} + \mathbf{f}_{slack} = \left[t_{init,1} - t_{rem,1} \quad t_{init,2} - t_{rem,2} \quad \cdots \quad t_{init,m} - t_{rem,m} \right]^{T} \qquad (4.15)$$

Let us define

$$\mathbf{x}_{cal} = \begin{pmatrix} \mathbf{f}_{aug} \\ \mathbf{f}_{slack} \end{pmatrix} \qquad (4.16)$$

$$\mathbf{y}_{cal} = \left[t_{init,1} - t_{rem,1} \quad t_{init,2} - t_{rem,2} \quad \cdots \quad t_{init,m} - t_{rem,m} \right]^{T}$$

Then, Equation (4.15) becomes

$$\left[\mathbf{A} \quad \mathbf{I}_{m} \right] \cdot \mathbf{x}_{cal} = \mathbf{y}_{cal} \qquad (4.17)$$

Where $\mathbf{I}_{m}$ is the unity matrix of size m.

Clearly, the linear system described in Equation (4.17) is under-determined (i.e., has more unknowns than equations), and hence would lead to an infinite number of solutions. Additional information is required to identify an optimal solution. In a general case, it is reasonable to select the solution that minimises the variance of the slack variables $\mathbf{f}_{slack}$. There are two reasons for that. The first reason is that although the non-thermal factors are not negligible, the post-harvest temperature is considered to be the dominant factor affecting the loss in shelf life of the perishable products. As a result, it is unlikely that the slack variables would vary significantly. The second reason is that the different product items could have shared some common non-thermal factors. For

example, many could come from the same farm, or same batch of harvest. These common factors reduce the variance in the slack variables.

In order to obtain a solution of Equation (4.17) that minimises the variance of $\mathbf{f}_{\text{slack}}$, let us define a matrix $\mathbf{H}$ where

$$\mathbf{H} = \begin{bmatrix} \mathbf{0}_{m,n} & \left(m\mathbf{I}_m - \mathbf{1}_{m,m} \right) \end{bmatrix} \tag{4.18}$$

Where

$\mathbf{0}_{m,n}$ is the matrix of zeros with m rows and n columns;

$\mathbf{1}_{m,m}$ is the matrix of ones with m rows and m columns.

Consequently,

$$\begin{aligned} \mathbf{H} \cdot \mathbf{x}_{\text{cal}} &= \begin{bmatrix} \mathbf{0}_{m,n} & \left(m\mathbf{I}_m - \mathbf{1}_{m,m} \right) \end{bmatrix} \begin{pmatrix} \mathbf{f}_{\text{aug}} \\ \mathbf{f}_{\text{slack}} \end{pmatrix} \\ &= \left(m\mathbf{I}_m - \mathbf{1}_{m,m} \right) \cdot \mathbf{f}_{\text{slack}} \\ &= m \left(\mathbf{f}_{\text{slack}} - \overline{\mathbf{f}_{\text{slack}}} \right) \end{aligned} \tag{4.19}$$

Where $\overline{\mathbf{f}_{\text{slack}}} = \dfrac{1}{m} \sum_{i=1}^{m} \mathbf{f}_{\text{slack},i}$.

Therefore, the variance of the slack variables can be expressed as follows

$$\begin{aligned} \text{var}(\mathbf{f}_{\text{slack}}) &= \left(\mathbf{f}_{\text{slack}} - \overline{\mathbf{f}_{\text{slack}}} \right)^T \cdot \left(\mathbf{f}_{\text{slack}} - \overline{\mathbf{f}_{\text{slack}}} \right) \\ &= \frac{1}{m^2} \left(\mathbf{H} \cdot \mathbf{x}_{\text{cal}} \right)^T \cdot \left(\mathbf{H} \cdot \mathbf{x}_{\text{cal}} \right) \\ &= \frac{1}{m^2} \mathbf{x}_{\text{cal}}^T \cdot \left(\mathbf{H}^T \cdot \mathbf{H} \right) \cdot \mathbf{x}_{\text{cal}} \end{aligned} \tag{4.20}$$

Consequently, the mathematical problem of solving Equation (4.17) for a solution that minimises the variance of the slack variables is transformed into an optimisation problem

$$\min_{\mathbf{x}_{\text{cal}}} \left(\frac{1}{m^2} \mathbf{x}_{\text{cal}}^T \cdot \left(\mathbf{H}^T \cdot \mathbf{H} \right) \cdot \mathbf{x}_{\text{cal}} \right)$$

$$\textit{subjected to}:$$

$$\begin{bmatrix} \mathbf{A} & \mathbf{I}_m \end{bmatrix} \cdot \mathbf{x}_{\text{cal}} = \mathbf{y}_{\text{cal}} \tag{4.21}$$

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The above optimisation problem (Equation (4.21)) can be solved using mathematical software packages such as Matlab which has a built-in *quadprog* function that is specifically designed for quadratic programming.

For estimating the remaining shelf life of a product item, the unknown contribution of the non-thermal factors is approximated by the average of the slack variables $\overline{\mathbf{f}_{\mathbf{slack}}}$. Consequently, Equation (4.14) becomes

$$t_{rem,p} = t_{init,p} - \boldsymbol{\alpha}_p^T \cdot \mathbf{f}_{\mathbf{aug}} - \overline{\mathbf{f}_{\mathbf{slack}}} \tag{4.22}$$

In short, when the non-thermal factors must be accounted for, Equation (4.21) is used for model calibration while Equation (4.22) is for estimating the remaining shelf life.

4.3.5 REQUIREMENT OF INITIAL SHELF LIFE

It should be noted that a KLS model (Equation (4.12)) describes the effect of temperature on the *changes* in shelf life and not the shelf life itself. Consequently, in order to evaluate the remaining shelf life of a perishable product after a storage (or transport) period, its initial shelf life at the beginning of that period must be available.

There are scenarios where the initial shelf life of the produce was not available e.g. as in the case study with Cookes Rose Farm. Two approaches could be used to overcome the requirement of the initial shelf life. The first is to make some assumption about it. The assumption could be that all the produce samples have the same initial shelf life; or that their initial shelf lives vary but the variation is minimised (see Section 4.3.4 for a similar mathematical derivation). The second approach, that could be employed when the initial shelf life was not available, was to use the final remaining shelf life in place of the changes in shelf life. However, it should be noted that the mathematical development of the KLS technique (Section 4.2) does not support the substitution of the changes in shelf life by the final remaining shelf life; the model that is obtained is a regression model of the coefficient vector $\boldsymbol{\alpha}$ (see Section 4.3.3).

4.3.6 *A PRIORI* CONSTRAINT IN A **KLS** IMPLEMENTATION

Frequently, *a priori* knowledge about perishable produce exists and should be captured in their models. For example, studies in the physiology of cut flowers seemed to suggest that the higher the temperature at which cut roses are stored, the shorter their remaining VL (Section 3.3). In such cases, mathematical constraints must be implemented to express the *a priori* knowledge. For example, the following constraints impose the above *a priori* knowledge for cut flowers.

$$f(T_1) < f(T_2) < \ldots < f(T_n) \tag{4.23}$$

This could be expressed in a matrix form as follows:

$$\begin{pmatrix} 1 & -1 & 0 & \ldots & 0 \\ 0 & 1 & -1 & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & \ldots & \ldots & 1 & -1 \end{pmatrix} \cdot \mathbf{f_{aug}} < \mathbf{0} \tag{4.24}$$

The linear system (Equation (4.12)) and the *a priori* constraint (Equation (4.24)) might be solved using most numerical software such as Matlab.

In a similar fashion, other *a priori* knowledge such as chilling injury at some temperature, or the smoothness of the function $f(T)$ could also be implemented.

4.4 PROCEDURE FOR A **KLS** IMPLEMENTATION

4.4.1 MODEL CALIBRATION PROCEDURE

Figure 4.3 outlines the procedure to obtain a KLS model. It starts with temperature profiles for model calibration and ends when $\mathbf{f_{aug}}$ is completely identified. Essentially, three steps are involved including parameter specification, evaluation of $\boldsymbol{\alpha}_i \left(i = \overline{1,m} \right)$ and forming and solving the linear system (Equation (4.12)).
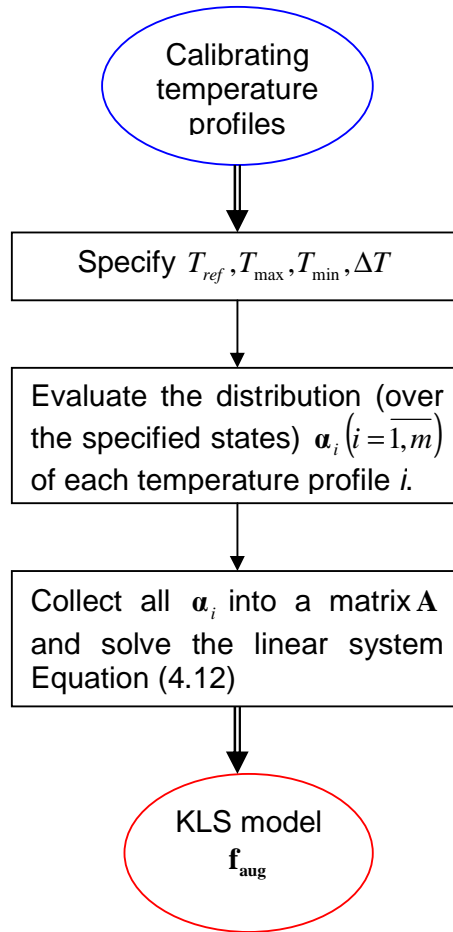
Figure 4.3: Model calibration procedure

Example

For illustration purpose, let us revisit and expand on the example that was considered in Section 4.2.

$$T_{profile,1} = \{15 \quad 12 \quad 14 \quad 14 \quad 13 \quad 15 \quad 14 \quad 13\}; t_{init,1} - t_{rem,1} = 12.5$$

$$T_{profile,2} = \{12 \quad 12 \quad 13 \quad 14 \quad 15 \quad 14 \quad 15 \quad 15 \quad 15 \quad 14\}; t_{init,2} - t_{rem,2} = 22.5$$

Step 1: parameter specification

The parameters are selected as following:

$$T_{ref} = 14\,^{o}C$$

$$T_{max} = 15\,^{o}C$$

$$T_{min} = 12\,^{o}C$$

$$\Delta T = 1\,^{o}C$$

Step 2: Evaluation of $\alpha_i \left(i = \overline{1,m} \right)$

From specification of parameters in Step 1, the temperature states are $\{12 \quad 13 \quad 14 \quad 15\}\,^0C$. Consequently, the vector of variables in Equation (4.12) is

$$\mathbf{f}_{aug} = \frac{1}{f\left(T = T_{ref} = 14^0 C\right)} \left[f\left(T = 12^0 C\right) \quad f\left(T = 13^0 C\right) \quad f\left(T = 14^0 C\right) \quad f\left(T = 15^0 C\right) \right]^T$$

Or equivalently

$$\mathbf{f}_{aug} = \left[\mathbf{f}_{aug}(1) \quad \mathbf{f}_{aug}(2) \quad \mathbf{f}_{aug}(3) \quad \mathbf{f}_{aug}(4) \right]^T$$

$$= \left[\frac{f\left(T = 12^0 C\right)}{f\left(T = 14^0 C\right)} \quad \frac{f\left(T = 13^0 C\right)}{f\left(T = 14^0 C\right)} \quad 1 \quad \frac{f\left(T = 15^0 C\right)}{f\left(T = 14^0 C\right)} \right]^T$$

Where $f(T)$ is the effect of temperature $T\ ^0C$ on the shelf life of the produce sample.

From the previous examples, $\alpha_1 = \begin{bmatrix} 1 & 1.5 & 3 & 1.5 \end{bmatrix}^T$ and $\alpha_2 = \begin{bmatrix} 1.5 & 1 & 2.5 & 4 \end{bmatrix}^T$.

Step 3: forming and solving the linear system (Equation (4.12))

Given temperature profiles $T_{profile,1}, T_{profile,2}$ and parameters as in Step 1, the matrix $\mathbf{A}$ which collects all vector $\alpha_i \left(i = \overline{1,2} \right)$ is

$\mathbf{A} = \begin{pmatrix} 1 & 1.5 & 3 & 1.5 \\ 1.5 & 1 & 2.5 & 4 \end{pmatrix}$. Consequently, the linear system in Equation

(4.12) can be explicitly expressed as

$$\mathbf{A} \cdot \mathbf{f}_{aug} = \begin{pmatrix} t_{init,1} - t_{rem,1} \\ t_{init,2} - t_{rem,2} \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} 1 & 1.5 & 3 & 1.5 \\ 1.5 & 1 & 2.5 & 4 \end{pmatrix} \cdot \mathbf{f}_{aug} = \begin{pmatrix} 12.5 \\ 22.5 \end{pmatrix} \tag{4.25}$$

Substituting $\mathbf{f}_{aug} = \left[\mathbf{f}_{aug}(1) \quad \mathbf{f}_{aug}(2) \quad \mathbf{f}_{aug}(3) \quad \mathbf{f}_{aug}(4) \right]^T$, the linear system becomes

$$\begin{pmatrix} 1 & 1.5 & 3 & 1.5 \\ 1.5 & 1 & 2.5 & 4 \end{pmatrix} \cdot \begin{pmatrix} \mathbf{f}_{aug}(1) \\ \mathbf{f}_{aug}(2) \\ 1 \\ \mathbf{f}_{aug}(4) \end{pmatrix} = \begin{pmatrix} 12.5 \\ 22.5 \end{pmatrix} \tag{4.26}$$

Or equivalently,

$$\begin{pmatrix} 1 & 1.5 & 1.5 \\ 1.5 & 1 & 4 \end{pmatrix} \cdot \begin{pmatrix} \mathbf{f}_{aug}(1) \\ \mathbf{f}_{aug}(2) \\ \mathbf{f}_{aug}(4) \end{pmatrix} = \begin{pmatrix} 9.5 \\ 20 \end{pmatrix} \tag{4.27}$$

Clearly, the above system has more variables ($n=3$) than equations $m=2$ and as discussed previously this situation would lead to infinite number of solutions for $\mathbf{f}_{aug}$. Therefore, more information or data would be required to solve this system.

Let suppose data from another sample is collected additionally where

$$T_{profile,3} = \{12 \quad 12 \quad 13 \quad 14 \quad 13 \quad 15 \quad 14 \quad 13 \quad 15\}; t_{init,3} - t_{rem,3} = 14$$

Incorporating the new data, the linear system becomes

$$\begin{pmatrix} 1 & 1.5 & 1.5 \\ 1.5 & 1 & 4 \\ 1.5 & 3 & 1.5 \end{pmatrix} \cdot \begin{pmatrix} \mathbf{f}_{aug}(1) \\ \mathbf{f}_{aug}(2) \\ \mathbf{f}_{aug}(4) \end{pmatrix} = \begin{pmatrix} 9.5 \\ 20 \\ 12 \end{pmatrix} \tag{4.28}$$

Consequently, the unique solution is

$$\begin{aligned} \mathbf{f}_{aug} &= \begin{bmatrix} \mathbf{f}_{aug}(1) & \mathbf{f}_{aug}(2) & \mathbf{f}_{aug}(3) & \mathbf{f}_{aug}(4) \end{bmatrix}^T \\ &= \begin{bmatrix} 2 & 1 & 1 & 4 \end{bmatrix}^T \end{aligned} \tag{4.29}$$

4.4.2 PROCEDURE TO ESTIMATE THE LOSS IN SHELF LIFE

The procedure to perform estimation of the loss in the remaining shelf life using a KLS model is depicted in Figure 4.4.
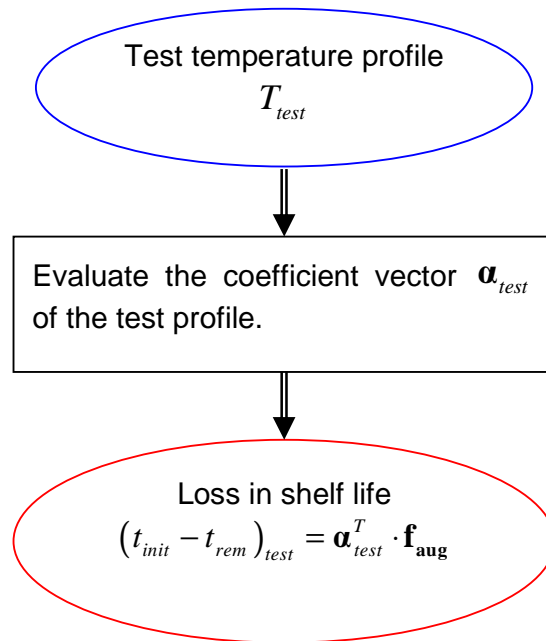
Figure 4.4: Using KLS model to evaluate the loss in shelf life due to a test temperature profile.

Example (cont.)

Let us continue with the above example and assume that a test data sample is $T_{profile,test} = \{13 \quad 13 \quad 12 \quad 14 \quad 14 \quad 15 \quad 13\}$

The corresponding vector of coefficients is $\alpha_{test} = \begin{bmatrix} 1 & 2 & 2 & 1 \end{bmatrix}^{T}$.

Consequently, the estimated loss in shelf life is

$$\left(t_{init,test} - t_{rem,test} \right)_{estimated} = \left(\alpha_{test} \right)^{T} \cdot \mathbf{f_{aug}}$$

$$= \begin{pmatrix} 1 & 2 & 2 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \\ 1 \\ 4 \end{pmatrix} = 10 \qquad (4.30)$$

4.5 CHAPTER CONCLUSION

This chapter described the mathematical development of the new KLS technique for modelling the temperature-related loss in shelf life of perishable fresh produce. KLS is based on the kinetic principle and is data-driven. As a result, it can be applied in studies of products such as cut flowers, where the understanding of the product is incomplete and hence its first-principle model is not available. The procedure for KLS implementation (i.e., model calibration and shelf life prediction) was outlined and illustrated with an example.

5 KLS SIMULATION CASE STUDIES

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This chapter reports the performance of the KLS technique in a number of simulated perishable products. These products include fresh produce (tomato and mushroom), processed food (seasoned soybean sprout), and seafood products (fresh seafood from temperate waters and from tropical waters, and cold-smoked salmon). Their simulated remaining shelf life is determined by the kinetic models which are implemented either in Matlab R2009a or in seafood safety and shelf life prediction (SSSP) v2.0, a software package that is available on Internet. A set of 116 temperature profiles typical of conditions during chilled supply chain were used as input to the simulations. KLS models are calibrated based on the temperature profiles and the simulated shelf life. Model performance was assessed by comparing the remaining shelf life obtained from the kinetic simulations and that obtained from the KLS models.

The performance assessment typically showed that R^2=1.00, prediction errors were small, and best fit lines were close to the equality line $y=x$. This demonstrates that KLS technique, being data-driven, could effectively replace the kinetic ones.

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5.1 INTRODUCTION

In Chapter 4, the new KLS technique was mathematically developed from kinetic principles. Based on its theoretical development, the most important advantage of KLS is that it is a data-driven technique and hence it does not require any first-principle knowledge to develop a model for estimating the loss in quality of perishable products due to temperature stress. In addition, while the traditional kinetic modelling would need as many models as the number of the quality attributes involved in determining the shelf life, only one KLS model is required.

This chapter aims to demonstrate these advantages of the KLS modelling technique and its capability in replacing traditional kinetic models. The motivation is that being data-driven KLS could be used in applications where kinetic principles would apply but traditional kinetic models are not available or not easy to implement. Such applications can be found readily in perishable products such as cut flowers.

The chapter is organised as follows. Section 5.2 explains the overall methodology that is used in this simulation study. It also outlines the strategies in KLS model calibration and validation. Section 5.3 describes the data and information available for the simulation study. All simulations in this chapter use the same set of temperature data, which is described in Section 5.3.1. A brief description of the simulation models is provided in Section 5.3.2 while more details are available in subsequent Sections 5.4 and 5.5. These later two sections explain the details and the results of the simulation studies of perishable produce (Section 5.4) and of food products (Section 5.5). Discussion of simulation results is presented in Section 5.6, which is followed by a chapter conclusion Section 5.7.

5.2 METHODOLOGY

In order to investigate the capability of KLS in substituting kinetic models, two consecutive stages are involved. In the first stage, a KLS model must be calibrated from the input and output data of a selected kinetic model. This is normally known as "training" or "calibrating" and during this process the KLS model "learns" the performance of the kinetic model. The second stage is model validation where new inputs are applied to the kinetic model as well as to the newly calibrated KLS model and the corresponding outputs are compared. Details of the two stages are explained below.

5.2.1 KLS MODEL CALIBRATION
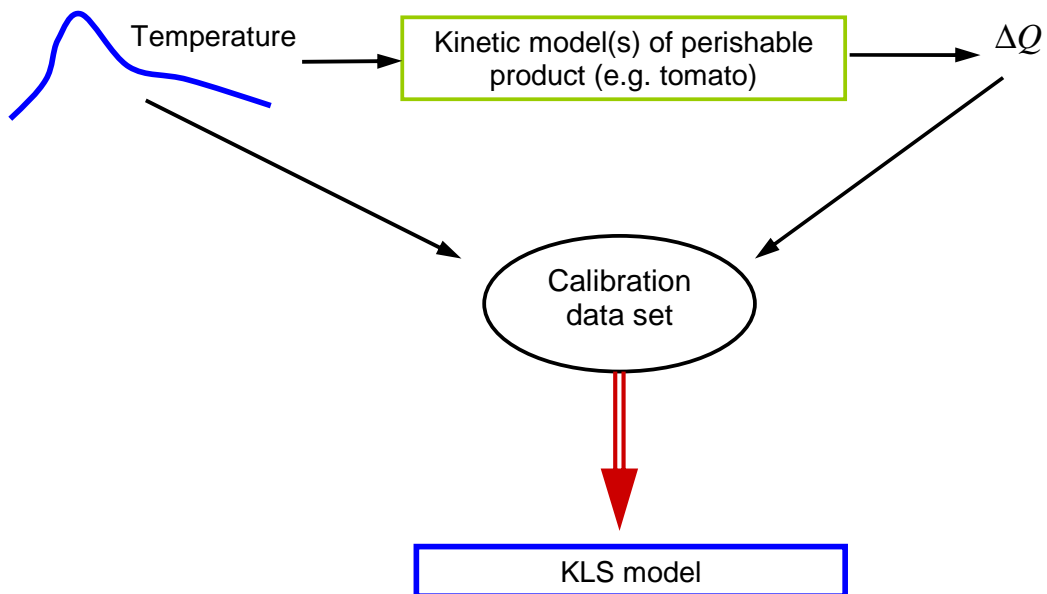
Figure 5.1: KLS calibration strategy

Figure 5.1 outlines the strategy used in calibrating a KLS model. Initially, a set of temperature profiles are input into the simulation of a perishable product to generate a set of corresponding changes in quality ΔQ. Subsequently, the sets of the temperature profiles and the corresponding ΔQ together form the calibration data set that is used to generate the KLS model for the simulated product. (Chapter 4 details the procedure to derive a KLS model from a calibration data set).

5.2.2 KLS MODEL VALIDATION

Figure 5.2 shows the strategy used for validation of a KLS model of simulated perishable products. Basically, a test temperature profile that was not used during calibration is input into the KLS model. The output, ΔQ_{KLS} is compared with the corresponding output $\Delta Q_{simulated}$ of the simulated model that was used during the calibration stage.
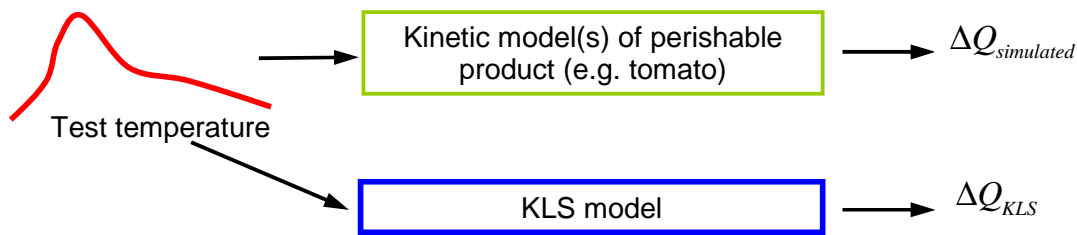
Figure 5.2: Validation strategy

In addition, leave-one-out cross validation and statistical indices including $RMSEP$, R^2, slope and intercept of the best fit line were implemented in assessing the performance of KLS models. Details of the strategy as well as definitions of the indices were described in Chapter 3.

5.3 TEMPERATURE DATA AND SIMULATIONS

5.3.1 TEMPERATURE DATA

Temperature profiles gathered from field trials in an international supply chain of an unspecified perishable produce were made available for use. Whilst neither the remaining shelf life nor the kinetic model of the produce was available for subsequent analysis; the use of the temperature profiles would closely simulate the temperature conditions that may be expected in a perishable produce supply chain. In total, there were 116 temperature profiles, each contained 22-23 temperature readings collected by data loggers. This set of data was divided into two subsets: one was used for KLS model calibration while the other was for model validation.

Figure 5.3 shows typical temperature profiles used in this simulation study. The maximum and minimum temperatures in the data set were 21.5 $^{\circ}$C and 2.5 $^{\circ}$C, respectively. The temperature readings in the data set varied about a mean of 10.4 $^{\circ}$C, and by a standard deviation of 3.4 $^{\circ}$C.
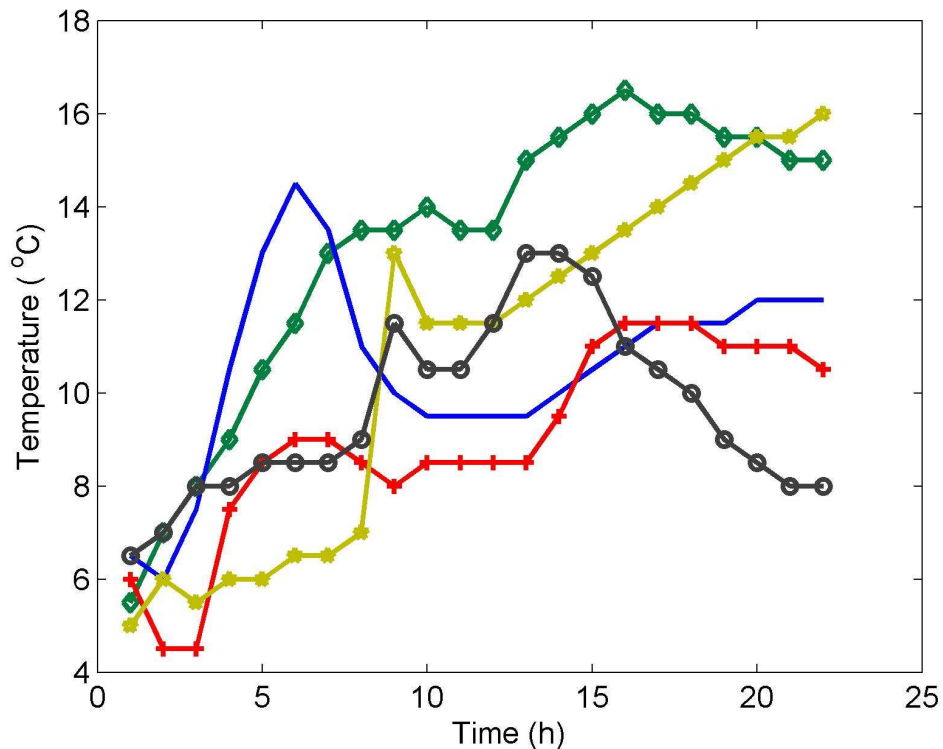
Figure 5.3 Examples of the temperature profiles used in simulation studies

5.3.2 KINETIC SIMULATION OF PERISHABLE PRODUCTS

In order to investigate the capability of KLS in reproducing the performance of kinetic models, a number of published kinetic models of perishable products were selected for simulation studies. These products and their kinetic models were studied in two sections.

- Section 5.4 focused on perishable produce including tomatoes and mushrooms. Their kinetic models involved sensory quality attributes such as firmness and colour.

- Section 5.5 focused on food products including seasoned soybean sprout and seafood. The models of these food products contained kinetic descriptions of microbial bacteria growth in the food systems.

All of the kinetic models are described in details in their respective sections.

5.4 PERISHABLE PRODUCE SIMULATION CASE STUDIES

5.4.1 KINETIC MODELLING OF TOMATOES

Tomato is an important agricultural produce. It is most commonly consumed fresh as in salads, or cooked such as in Italian dishes, or in making juice. In 2008 the world produced more than 136 million tons of tomatoes, of which Europe and the United States together accounted for 34 million tons or approximately 25% (FAOSTAT 2010). Therefore, research in many aspects of tomato including its shelf life after harvest has attracted significant interest over the years.

Numerous kinetic models exist for linking tomato quality attributes such as firmness, colour and taste to the various stresses that tomatoes may endure after harvest. Many of these models are first order kinetic and were developed at constant temperature. For example, in an investigation of the kinetic approach to food quality prediction Wells and Singh (Wells and Singh 1988) stored mature green tomatoes at various temperature conditions and examined their quality attributes including firmness, sourness and flavour. The researchers found significant differences in tomato firmness between storage temperature conditions but not in the other two attributes: sourness and flavour. Subsequently, they proposed a first-order kinetic model for tomato firmness and evaluated the activation energy and the reference rate constant from the Arrhenius plot of reaction rate *vs*. temperature using regression analysis (Wells and Singh 1988). Their approach is common in kinetic modelling and is used to identify the quality attribute of importance, select a kinetic model and then estimate the model parameters by regression analysis. The key decisions of which quality attributes and/or which kinetic models to use may not always be as apparent.

A variant of first order kinetics considers firmness of tomatoes (and other fruits and vegetables) as consisting of two parts: a variable part of the firmness, which is modelled by first order mechanism, and a constant part that is due to fixed factors such as cellulose or structure-based firmness. Lana *et al.* (Lana *et al.* 2005) used that rather empirical approach to study firmness of fresh-cut tomatoes under the effects of storage temperature and at-harvest ripening stage. Later, the researchers also reported a similar study modelling the colour of fresh-cut tomatoes (Lana *et al.* 2006). While firmness and subsequently colour were selected for studying, Lana *et al.* (Lana *et al.* 2005) observed that the limiting quality attribute, which determines the shelf life of fresh-cut tomatoes, was not known. From a shelf life prediction perspective, the question is again which attribute and hence model to use. If the shelf life of fresh-cut tomatoes was limited by multiple quality attributes, e.g. both firmness and colour, modelling each quality attributes independently as in (Lana *et al.* 2005; Lana *et al.* 2006) may not be very useful for practical applications in shelf life prediction.

A more complicated model of tomato firmness was reported by van Dijk *et al.* (van Dijk *et al.* 2006b) and van Dijk *et al.* (van Dijk *et al.* 2006a). The researchers reasoned that chilling injury and enzymatic degradation were the two major processes responsible for firmness decay. The enzymes that were considered include polygalacturonases, pectin methyl esterase and β-galactosidases. The researchers noted that their integrated model of tomato firmness was a set of differential equations which had "cumbersome" solutions. Without such analytical solutions, the firmness of tomatoes that were exposed to variable temperature stresses (e.g., during supply chain) may require repeated integration of the set of differential equations. Yet, the enzymes that were studied may not be the only ones; there could be other enzymes that were responsible for cell wall degradation and hence firmness decay in tomatoes but were not modelled (van Dijk *et al.* 2006a). Incorporating any additional enzymes into modelling could introduce significant complexity to the already complicated model.

In short, all of these previous studies used kinetic modelling principles to model tomato behaviour. The studies had to identify a specific quality attribute and a kinetic model using some (usually incomplete) first-principle knowledge of tomato senescence.

5.4.2 SELECTED KINETIC MODELS OF TOMATO

This study selected the kinetic models reported in (Schouten *et al.* 2007a) to simulate the behaviours (i.e., firmness and colour) of tomato under variable temperature stresses.

Firmness model

Based on previous work (Lana *et al.* 2005; Lana *et al.* 2006; van Dijk *et al.* 2006b), Schouten and colleagues (2007a) defined firmness as the maximum force required for a 1 mm compression of a tomato at speed of 40 mm/min. They reasoned that tomato firmness consists of a variable part which can be modelled by first-order kinetics and a fixed invariable part due to its biophysical structure. In addition, the researchers also adopted the viewpoint which stated in Tijkens *et al.* (2002) that firmness can be generated and diminished prior to harvest but it can only be decayed post harvest. Based on those two concepts, Schouten and colleagues (2007a) derived the following kinetic model for tomato firmness:

$$\begin{cases} F(t) = \left(F_0 - F_{fix}\right)e^{-k_{Fpost}\cdot t} + F_{fix} \\ F_0 = \left(F_{ref} - F_{fix}\right)e^{-k_{Fpre}\cdot \Delta t_F} + F_{fix} \end{cases} \tag{5.1}$$

Where

k_{Fpre} and k_{Fpost} the reaction rate constants (d^{-1}) for the firmness breakdown before and after harvest respectively;

F_0 and $F(t)$ the firmness (N) at harvest and at time t (d);

F_{fix} the invariable firmness (N) at infinite time;

F_{ref} an arbitrary reference firmness;

Δt_F the (firmness) biological age, which is defined as the time needed for the firmness to change from

F_{ref} to F_0.

Arrhenius' law was used to describe the temperature dependence of all kinetic reaction rates constants

$$k = k_{ref} e^{-\frac{E_a}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)}$$

(5.2)

Where

E_a	activation energy (J.mol^{-1});
T_{ref}	reference temperature (K);
k_{ref}	the reaction rate constants (d^{-1}) at reference temperature;
R	gas constant (8.314 J.mol^{-1}.K^{-1}).

As KLS method requires the initial quality of all samples, it was assumed for simplicity that the samples start their post-harvest periods with the same initial quality content. In this case, the assumption effectively means that F_0 is constant and as a result, the model from (Schouten *et al.* 2007a) was modified as followed:

$$\begin{cases} \dfrac{dF_{var}(t)}{dt} = -k_{Fpost} \cdot F_{var}(t) \\ F(t) = F_{var}(t) + F_{fix} \end{cases}$$

(5.3)

With $F_{var}(t)$: the variable contribution of tomato firmness (N) at time t (d).

This kinetic model of tomato firmness was implemented in Matlab R2009a with an initial firmness of 10 N, which was arbitrarily selected in the range of the initial firmnesses shown in Figure 4 in Schouten *et al.* (2007a). Other parameter values that the model required were taken from Schouten *et al.* (2007a) and are reproduced in Table 5.1 below.

Table 5.1 Kinetic parameter for tomato firmness modelling

Parameters	Unit	Values
$k_{Fpost,ref}$	d^{-1}	0.0509
E_{Fpost}	$J.mol^{-1}$	22320
F_{fix}	N	0.816
T_{ref}	K	285.15

Colour model

Schouten *et al.* (2007a) studied colour evolution in tomato by focusing on the synthesis of the red components in the tomato skin. The researchers reasoned that a colourless precursor is converted into the red (mainly lycopene) components by an enzyme system according to the following reaction:

$$prec \quad + \quad E \quad \xrightarrow{k_{Rpost}} \quad 2E \quad + \quad Red \quad (5.4)$$
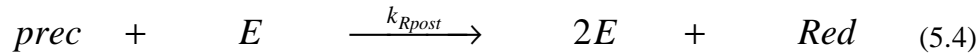
Where

$prec$ is a colourless precursor;

E is the enzyme;

Red is the red components;

k_{Rpost} is the reaction rate constants (d^{-1}) during post-harvest period.

From Equation (5.4), the changes in colour of tomatoes can be summarised in the following differential equations.

$$\frac{\partial Red}{\partial t} = -\frac{\partial prec}{\partial t} = \frac{\partial E}{\partial t} = k_{Rpost} \cdot E \cdot prec \quad (5.5)$$

In terms of the red components, Equation (5.5) is mathematically converted into

$$\frac{\partial Red}{\partial t} = k_{Rpost} \cdot Red \cdot (c - Red)$$

$$c = Red_{max} - Red_{min} \quad (5.6)$$

Where Red_{max} and Red_{min} are the asymptotic colour value at plus and minus infinite time (1000/G).

Other parameter values that the model required were taken from Schouten *et al.* (2007a) and are reproduced in Table 5.2 below.

Table 5.2 Kinetic parameter for tomato colour modelling

Parameters	Unit	Values
$k_{Fpost,ref}$	$(prec\,.\text{d})^{-1}$	0.02355
E_R	J.mol^{-1}	40553
Red_{min}	1000/G	4.086
Red_{max}	1000/G	17.308
T_{ref}	K	285.15

5.4.3 REMAINING SHELF LIFE EVALUATION

In this study, it is assumed that a tomato reaches its end of useful life when its firmness is equal to or less than a threshold firmness value of 3 N. For tomato colour, the lower threshold is 13.22 for the red colour component. The remaining shelf life of a tomato is defined as the time duration (in days) that it would take to reach its end of useful life under the reference storage condition $T_{ref} = 10$ °C.

5.4.4 SIMULATION RESULTS

5.4.4.1 VALIDATION OF THE IMPLEMENTATION OF THE KINETIC MODELS
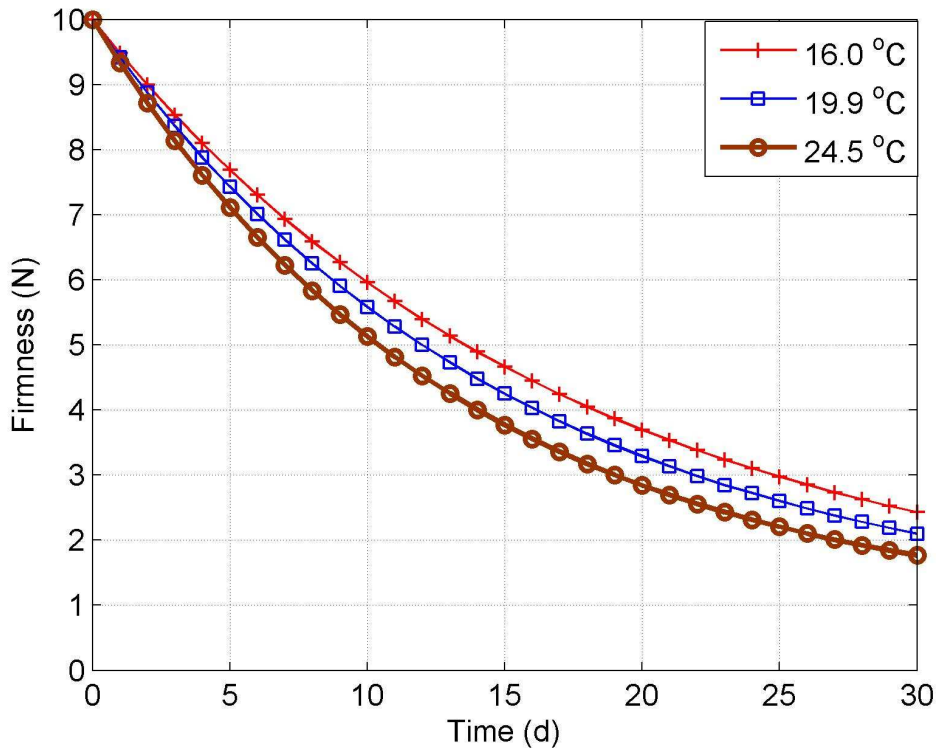
Figure 5.4: Simulated tomato firmness during storage at different isothermal temperatures

Initially, the tomato simulation was run at three isothermal temperatures, including 16 $^{\circ}$C, 19.9 $^{\circ}$C and 24.5 $^{\circ}$C, for comparison with results shown in (Schouten *et al.* 2007a). As Figure 5.4 shows, the results were in qualitative agreement with the results in (Schouten *et al.* 2007a). In general, the tomato firmness decreases monotonically from an initial value of 10 N to approximately 3 N after 20 days. Note that the monotonic decrease was due to the modelling view that tomato firmness can only be diminished post harvest, as described earlier. A notable difference between Figure 5.4 and Figure 4 in (Schouten *et al.* 2007a) is that the initial tomato firmness took different values in Schouten and colleagues study. In addition, the position of tomato in the truss, which was examined in the previous paper, was not within the scope of the present study.

Figure 5.5 shows the simulated remaining shelf life of tomatoes as determined by firmness. The tomatoes started with the same initial firmness of 10 N. After being subjected to each of the 116 temperature profiles (Section 5.3.1), their remaining shelf life varies about a mean of 8.3 d with a standard deviation of 1.5 d. The maximum and minimum remaining vase lives are respectively 11.2 d and 4.0 d.
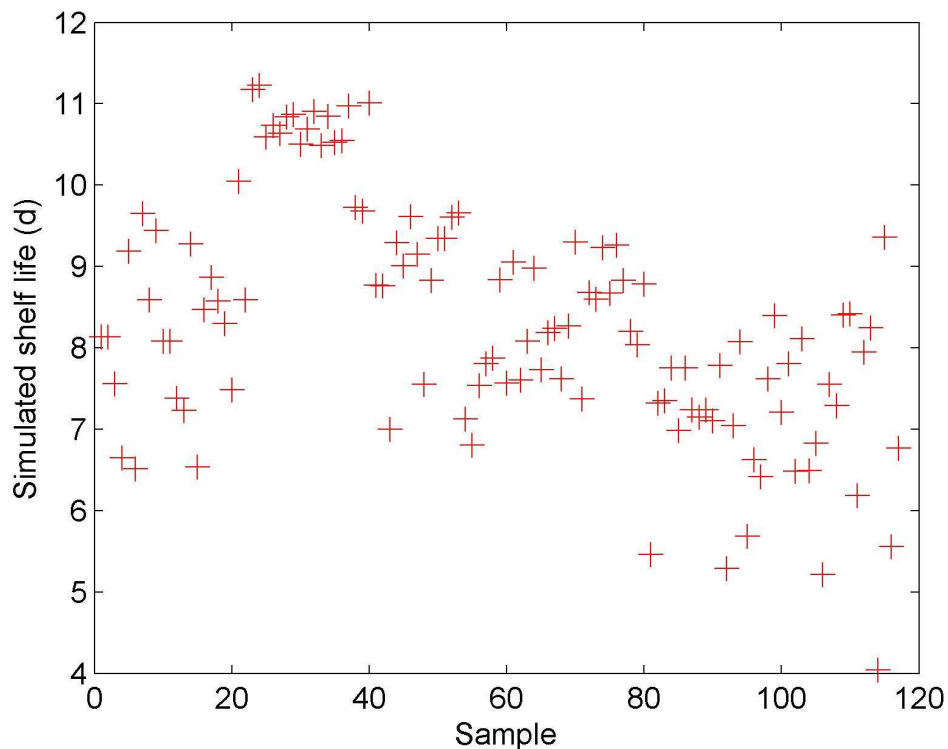
Figure 5.5: Simulated remaining shelf life of tomato by firmness

Figure 5.6 shows the simulated remaining shelf life of tomatoes as determined either by firmness, or by firmness and (red) colour. As shown, the remaining shelf life by firmness and by firmness and colour often coincides. This implies that the firmness attribute is more likely to be the limiting factor in determining the shelf life of tomatoes. However, there are many occasions where the shelf life by firmness is greater than the shelf life by firmness and colour. This suggests that the colour attribute is the limiting factor in those cases. As a result, Figure 5.6 illustrates that the remaining shelf life of tomato could be

determined by different quality attributes and hence multiple attributes (e.g. firmness and colour) are usually required.
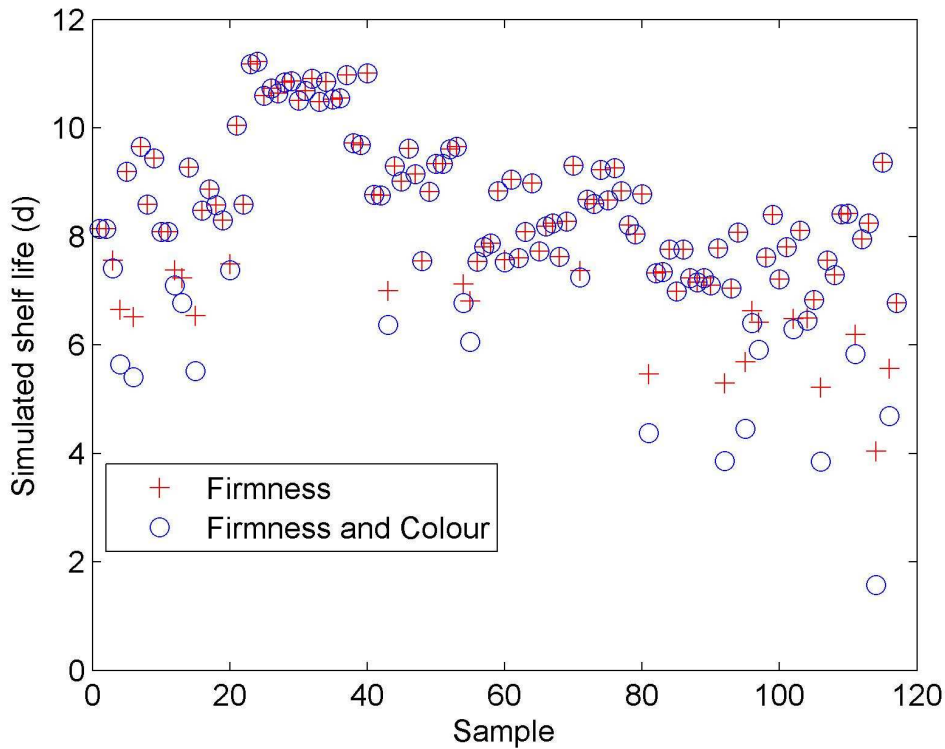
Figure 5.6: Simulated remaining shelf life of tomato by firmness, and by firmness and colour

5.4.4.3 KLS MODEL CALIBRATION

The reference temperature for KLS method was set at $T_{ref} = 10^{o}C$. Minimum and maximum temperatures in the temperature data set were 2.5 ^{o}C and 17.5 ^{o}C. The temperature resolution was chosen to be 0.5 ^{o}C.

Note that the coefficient vector $\boldsymbol{\alpha}$ of each temperature profile in the calibration data set can be derived from its histogram over the interval [2.5 ^{o}C, 17.5 ^{o}C] (Chapter 4). The set of these coefficient vectors constitutes the matrix $\mathbf{A}$ as shown in Equation (4.11). The calibration of the KLS model completes with the evaluation of $\mathbf{f_{aug}}$ according to Equation (4.12).
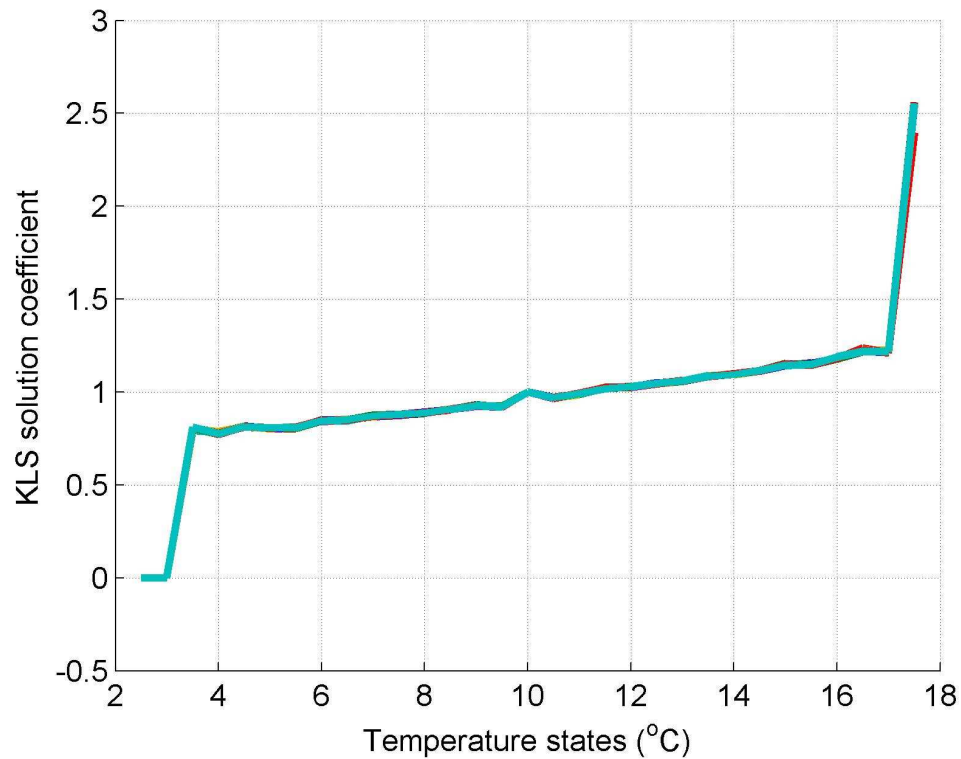
Figure 5.7: $\mathbf{f}_{aug}$ as evaluated in tomato firmness simulation. Using leave-one-out strategy, 116 $\mathbf{f}_{aug}$ were obtained and converged.

The solution vector $\mathbf{f}_{aug}$ that expresses the KLS model was evaluated and shown in Figure 5.7. As leave-one-out strategy was implemented, there were a total of 116 $\mathbf{f}_{aug}$ vectors, one for each of the temperature profiles. As can be seen in Figure 5.7, these solution vectors converged to a single vector, which characterised the simulated tomato firmness model. In addition, there were abrupt changes at both ends of the temperature states i.e. at 2.5-3 ^{o}C and at 17.5 ^{o}C. It is believed that the firmness decay at low temperature would be negligible. Consequently, the effect of low temperature on firmness decay and hence the KLS solution vector at such temperature would be very small.

On the other hand, the jump in the KLS solution vector going from 17 ^{o}C to 17.5 ^{o}C was because the value at 17.5 ^{o}C actually accounted for all temperatures equal to or greater than 17.5 ^{o}C. As stated earlier, the maximum temperature was 21.5 ^{o}C and so the KLS solution vector at 17.5 ^{o}C would be an average of the effect of temperature between 17.5 ^{o}C and 21.5 ^{o}C on firmness decay.

Setting the maximum temperature state at 17.5 ^{o}C was a design decision, so as to prevent the coefficient matrix **A** from being ill-conditioned.

5.4.4.4 KLS MODEL VALIDATION

The performance of the KLS models, shown in Figure 5.7, in predicting remaining shelf life of tomatoes was assessed using leave-one-out strategy and statistical indices including *RMSEP*, R^2, slope and intercept of the best fit line (Section 3.2).

Shelf life by firmness

R^2 =1.00

RMSEP =0.10

best fit y = 1.00 x + 0.03
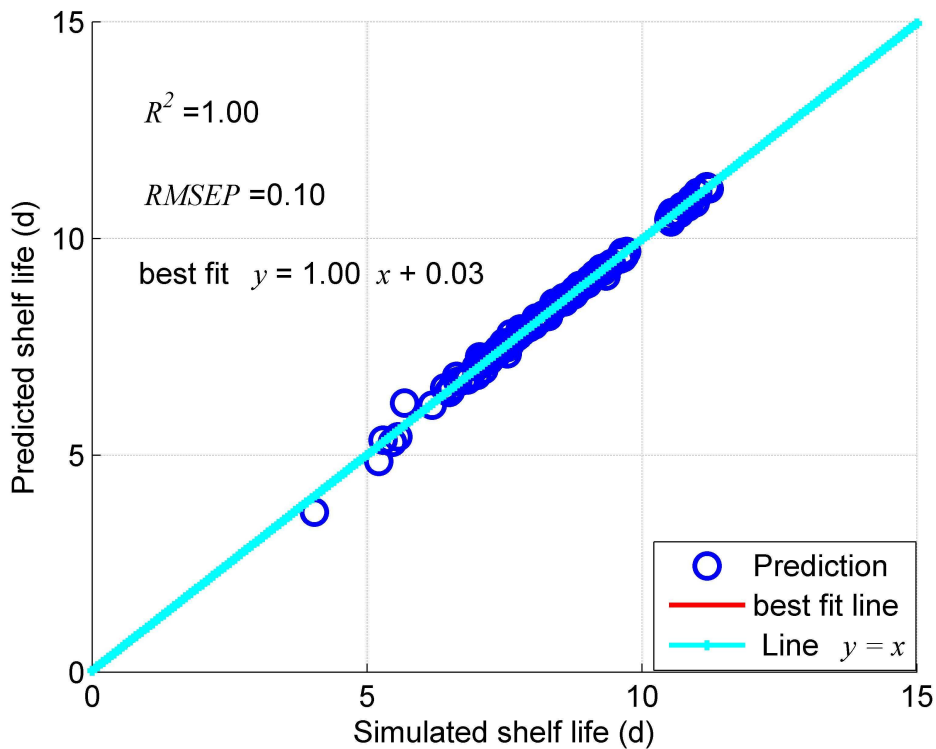
Figure 5.8: Comparison between simulated shelf life of tomato (by firmness) and the corresponding KLS prediction. The best fit line coincides with the line $y = 1.00x$.

Figure 5.8 shows the comparison between the simulated shelf life of tomatoes and its corresponding KLS prediction. The simulated shelf life of tomatoes was determined based on firmness level. The KLS predicted shelf life was evaluated using the KLS solution vector (shown in Figure 5.7) as in Equation (4.14). Performance assessment was carried out as described in Section 3.2. The

values of the performance indices are shown in Figure 5.8, together with the best fit line and the equality line $y = 1.00x$. As the figure indicates, the predictions by the KLS model agree well with the simulated shelf life of tomatoes. The coefficient of determination $R^2 = 1.00$ suggests that the KLS model captured all variation in the simulated data. Moreover, average prediction error *RMSEP* was only 0.1 d, which represents only 1.2% error for an average shelf life of 8.3 d. From the figure, the best fit line and the equality line $y = x$ are not visually differentiated. Indeed, the mathematical equation for the best fit line is $y = 1.00x + 0.03$, which only differs from the line $y = 1.00x$ by a small intercept of 0.03. In short, the KLS predicted shelf life matched closely with the simulated shelf life of tomatoes (by firmness). In other words, the KLS model is capable of reproducing the simulated shelf life of tomatoes by the kinetic firmness model.

Shelf life by firmness and colour
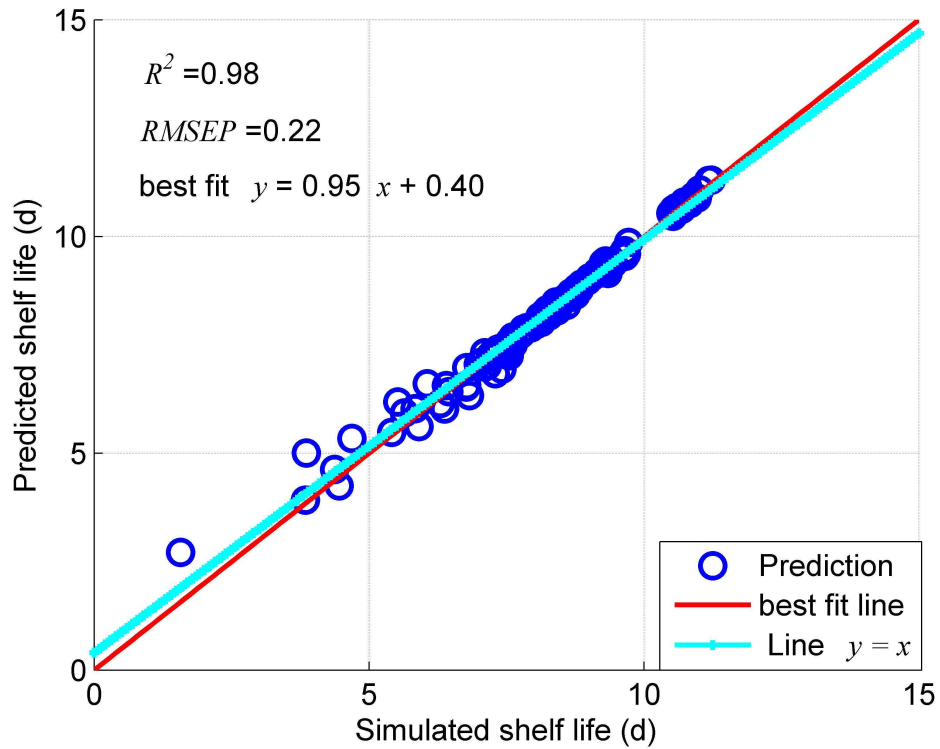
Figure 5.9: Comparison between simulated shelf life of tomato (by firmness and colour) and corresponding KLS prediction

When both firmness and colour were considered, another KLS model was calibrated. Performance assessment was carried out based on the same statistics as previously. Figure 5.9 shows that although it is not quite as good as in the case of one kinetic model (Figure 5.8), using one KLS model to reproduce the simulated shelf life of tomato from two kinetic models still has good performance. All variation in simulated data was captured ($R^2 = 0.98$); average prediction error was small ($RMSEP$=0.22 d); the best fit line only deviated slightly from the equality line $y = 1.00x$. Therefore, the performance statistics suggest that KLS model is capable of "learning" the output of two kinetic models of tomato firmness and (red) colour.

Additional results from mushroom colour simulation studies

A similar approach to the tomato simulation studies was also carried out for mushroom colour simulation studies. The kinetic models for colour evolution in mushroom were taken from (Bobelyn *et al.* 2006), including a first order kinetic model and a sigmoid kinetic model. The performance of the KLS technique in reproducing those mushroom models is summarised in Table 5.3 below. Similar conclusion can be made: the KLS technique was capable of "learning" the output of the mushroom kinetic models.

Table 5.3: Results from mushroom colour simulation studies

Kinetics	1st order kinetic	Sigmoid kinetic
Source	(Bobelyn *et al.* 2006)	
Coefficient of determination R^2	0.99	0.92
RMSEP (d)	0.33	0.72
Slope of best fit	1.00	0.94
Intercept of best fit	0.04	-0.10

5.5 Food product simulation case studies

5.5.1 Background

Food quality changes with time and storage conditions. Therefore, it is necessary to model the chemical, biochemical, microbial and physical processes that occur in food systems to monitor, predict and control their quality changes. The most common approach so far has been based on kinetic modelling principles. The kinetic models used in food quality modelling can be broadly classified into first-principle kinetic models and empirical kinetic models. First-principle kinetic models of food systems are derived based on fundamental understanding of the mechanisms of the processes that occur in the systems. They are available in elementary processes that only exist in simple, usually dilute, ideal systems. However, real foods are neither dilute nor ideal systems and so the quality changes are due to many interacting and complex reaction mechanisms rather than a single elementary step. This is why simplified empirical models are needed. The use of empirical models in studying real food systems suffers from a limitation that the understanding about the system is not captured (van Boekel 2008).

Microbiological decay is an important aspect in food deterioration, especially for fresh or minimally processed refrigerated products. Microorganisms may play a significant part in food spoilage. Predictive microbiology refers to studies which are to predict the shelf life of refrigerated foods based on microbial growth. These studies usually involve a number of steps. First, an appropriate growth curve model (e.g. Gompertz model) is selected and experimental data are gathered to estimate the model parameters (such as specific growth rate and lag time). Subsequently, the effects of compositional and environmental factors on the microbial growth are investigated using another model such as the square root model. The combination of the two steps enables the prediction of the microbial level and thereby can be used to estimate the shelf-life of

perishable foods under commercial distribution conditions (Fu and Labuza 1993).

5.5.2 KINETIC MODELS

Food systems including seasoned soybean sprouts and seafood products were selected for the simulation study. The kinetic model of seasoned soybean sprouts was taken from (Lee *et al.* 2007) while models of seafood products were previously developed and implemented in the Seafood spoilage and safety predictor software (SSSP) (Dalgaard 1999; Dalgaard *et al.* 2002).

5.5.2.1 KINETIC MODEL OF SEASONED SOYBEAN SPROUTS

Lee and colleagues (2007) modelled the growth of aerobic bacteria on Korean seasoned soybean sprouts to estimate microbial spoilage and shelf life of the food product at varying temperatures. These researchers believed that while studies of specific strains of spoilage bacteria were common, practical shelf life evaluation often used the total aerobic bacterial growth as a criterion (Lee *et al.* 2007). For a description of the microbial growth, Lee and colleagues (2007) adopted the following model, that was published in (Baranyi and Roberts 1994).

$$
\begin{cases}
\dfrac{dq}{dt} = \mu_{\max} q \\[2ex]
\dfrac{dN}{dt} = \mu_{\max} \left(\dfrac{q}{1+q} \right) \left(1 - \dfrac{N}{N_{\max}} \right) N
\end{cases}
\tag{5.7}
$$

Where

q : the normalized concentration of an unknown substance that is believed critical to cell growth in soybean sprout;

$\mu_{\max}$: the maximum specific growth rate (h^{-1});

N : the microbial count ($cfu.g^{-1}$);

$N_{\max}$: the maximum cell density ($cfu.g^{-1}$).

Lee *et al.* (2007) fitted Equation (5.7) with experimental data at many fixed temperatures to obtain corresponding sets of values for parameters including $\mu_{\max}$, $N_{\max}$, q_o and N_o, where the latter two parameters represent the initial

values of q and N respectively at initial temperature T_o. The sets of parameter values were then regressed against temperatures to obtain the following temperature dependence:

$$\begin{cases} \mu_{max} = \dfrac{1}{24}\left[0.0541(T+28.85)\right]^2 \\ \log N_{max} = 0.1726T + 7.7985 \\ \log q_o = 0.1152T_o^2 - 0.2554T_o - 3.7468 \\ N_o = 10^{4.2} \end{cases} \quad (5.8)$$

Equations (5.7) and (5.8) were implemented in Matlab R2009a to estimate the simulated total aerobic bacterial counts in seasoned soybean sprout at dynamic temperatures and thereby the remaining shelf life of the product.

5.5.2.2 KINETIC MODELS IN SSSP V2.0 SOFTWARE

Seafood spoilage and safety predictor (SSSP) v2.0 software was developed by Dalgaard and colleagues (2002) at The Danish Institute for Fisheries Research. It was originated from the Seafood spoilage predictor (SSP) software and has been freely available online at http://www.dfu.min.dk/micro/ssp/ since February 1999. The software predicts shelf life and growth of bacteria in a number of fresh and lightly preserved seafood products under dynamic storage conditions (e.g., temperature, CO_2 concentration, water activity). There are basically two classes of models in SSSP v2.0 software: relative rate of spoilage (RRS) models and microbial spoilage (MS) models. For fresh seafood, RRS models are purely empirical, meaning they are developed using shelf life data obtained at different storage temperatures and that they do not take into account the underlying biochemical mechanism responsible for the spoilage. As a result, RRS models tend to be simpler, yet effective albeit over a limited range of temperature. On the other hand, MS models are based on the concepts of specific spoilage organism (SSO) and the spoilage domain. While SSO is referred to as the part of the total micro-flora that participates in the spoilage process, its spoilage domain is defined as the range of conditions (pH, temperature, water activity, and atmosphere) under which a SSO can grow and produce spoilage metabolites (Gram and Dalgaard 2002).

SSO models often involve environmental factors other than temperature such as CO_2 concentration and water activity; these are out of the scope of the present study. Consequently, only seafood products that are described by an RRS model in SSSP v2.0 software were selected for simulation. These products include fresh seafood from temperate and tropical waters, cold-smoked salmon and cooked-and-brined shrimps. Two types of RRS models including exponential and square-root are implemented in SSSP v2.0. Their empirical relations are described in the following equations

$$\text{Exponential: } \ln(RS) = k_1 + a \cdot T$$
$$\text{Square root: } \sqrt{RS} = k_2 \left(T - T_{min}\right)$$

(5.9)

Where

RS : rate of spoilage (d^{-1});

k_1 and k_2 : the rate constants;

T_{min} and a : model parameter.

By definition, RRS is the ratio of RS at temperature T (^{o}C) to RS at T_{ref}, which is usually set at 0 ^{o}C. As a result,

$$\text{Exponential: shelf life at } T\,^{o}C = \frac{\text{shelf life at } T_{ref}}{\exp\left[a \cdot \left(T - T_{ref}\right)\right]}$$

$$\text{Square root: shelf life at } T\,^{o}C = \frac{\text{shelf life at } T_{ref}}{\left(\dfrac{T - T_{min}}{T_{ref} - T_{min}}\right)^{2}}$$

(5.10)

The simulation of seafood products was carried out by applying the temperature data (Section 5.3.1) to the corresponding models available in SSSP v2.0 at default parameter settings.

5.5.3 REMAINING SHELF LIFE EVALUATION

For seasoned soybean sprout simulation, it is assumed that the product reaches its end of useful life when its total aerobic bacterial count is equal to or greater than a threshold value of 10^8 (cfu.g^{-1}). The remaining shelf life is defined

as the time duration that it would take to reach its end of useful life under standard storage condition $T_{ref} = 10 \; {}^{o}C$.

For seafood simulation, RRS models in SSSP v2.0 were used to evaluate the simulated remaining shelf life of various seafood products after being exposed to a dynamic temperature profile. The default parameter settings were employed (the initial remaining shelf life of 14 d at 0 ^{o}C). The final remaining shelf life (i.e., after being exposed to the temperature profile) was produced by SSSP v2.0.

5.5.4 SIMULATION RESULTS

5.5.4.1 VALIDATION OF THE IMPLEMENTATION OF THE KINETIC MODELS

Seasoned soybean sprout
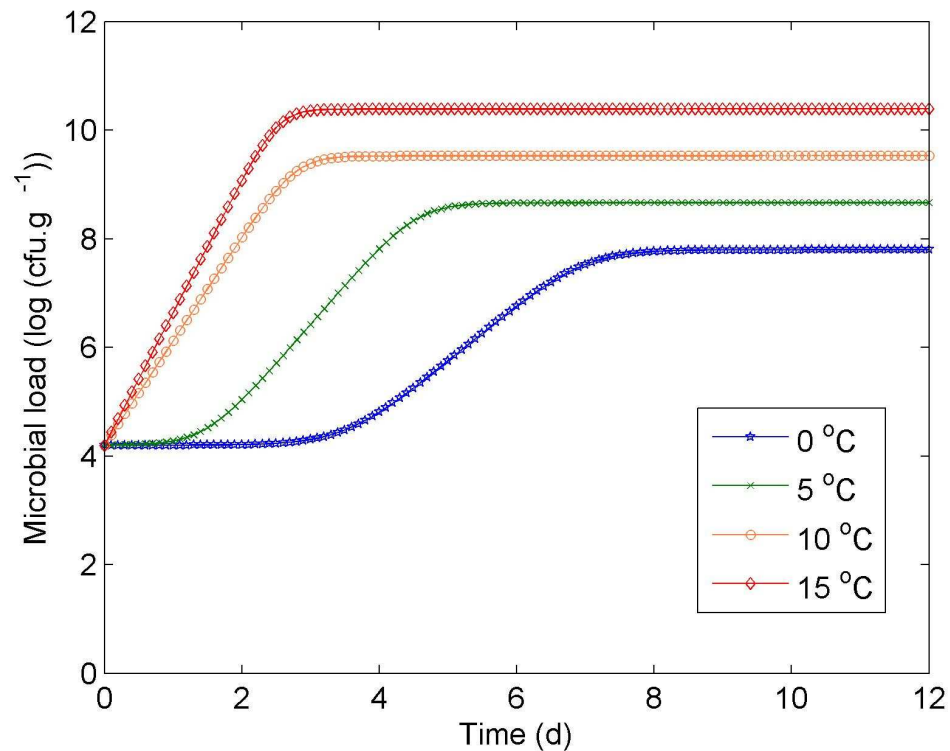
Figure 5.10: Total aerobic bacterial counts in seasoned soybean sprouts simulated at different temperatures

Equations (5.7) and (5.8) were programmed for simulating the microbial growth in seasoned soy bean sprout. The simulations were run at temperatures of 0, 5, 10 and 15 ^{o}C, and the results were plotted in Figure 5.10. Visual comparison of Figure 5.10 with Figure 2 in Lee *et al.* (2007) indicated that the results in the two figures agreed well with each other. This comparison confirmed that the kinetic model for microbial growth in seasoned soy bean sprout was implemented correctly.

Seafood products

Kinetic models for seafood products were already implemented in SSSP v2.0, which was used directly without any modification or validation.

5.5.4.2 EVALUATION OF SIMULATED REMAINING SHELF LIFE
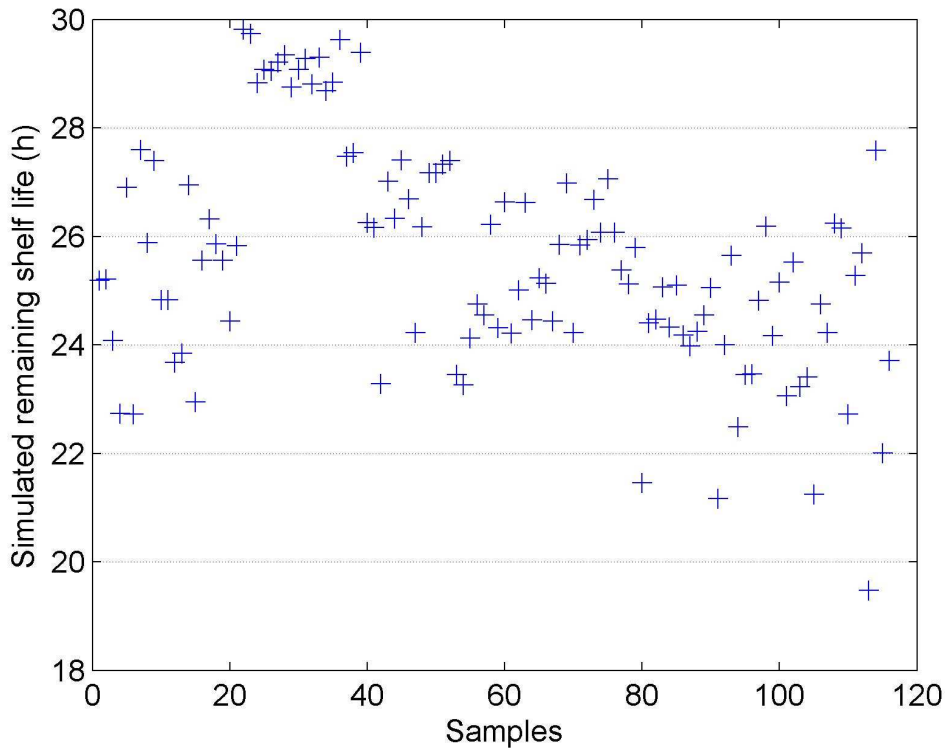
Figure 5.11: Simulated shelf life (as determined by the level of total aerobic bacteria) of seasoned soybean sprout after exposing to the simulation temperature data

Figure 5.11 shows the simulated remaining shelf life as determined by the level of total aerobic bacteria in seasoned soybean sprout. The simulated food product starts with an initial level of total bacterial count at $10^{4.2}$ (cfu.g^{-1}). After being exposed to one of the 116 temperature profiles available for simulation

studies (Section 5.3.1), their remaining shelf life, the time the total aerobic bacteria count of the products would take to reach 10^8 (cfu.g^{-1}) at 10 ^{o}C, varies about a mean of 25.6 h with a standard deviation of 2.08 h. The maximum and minimum remaining shelf lives are respectively 29.8 and 19.5 h.

Similar observations were obtained in the simulation of seafood products using SSSP v2.0.

5.5.4.3 KLS MODEL CALIBRATION

The same set of model parameters were used for calibrating the KLS model of simulated food products including seasoned soybean sprouts and seafood products. The reference temperature was set at $T_{ref} = 10\,^o C$ which is equivalent to the reference temperature used in remaining shelf life evaluation. Minimum and maximum temperatures in the temperature data set were 2.5 ^{o}C and 17.5 ^{o}C. The temperature resolution was chosen at 0.5 ^{o}C.

Similarly to the simulation study for perishable produce (Section 5.4), the solution vector $\mathbf{f}_{aug}$ that expresses the KLS model for the simulated seasoned soybean sprout was evaluated. As leave-one-out strategy was implemented, there were a total of 116 $\mathbf{f}_{aug}$ vectors, one for each of the temperature profiles. These solution vectors converged to a single vector, which characterised the simulated level of total aerobic bacteria count in seasoned soybean sprout.

5.5.4.4 KLS MODEL VALIDATION

Seasoned soybean sprout

Figure 5.12 shows the comparison between the simulated shelf life of seasoned soybean sprout and its corresponding KLS prediction. The simulated shelf life was determined based on the level of the total aerobic bacterial organism. The predicted shelf life was obtained using the KLS solution vector, as in Equation (4.14). The values of the performance indices were also shown in Figure 5.12, together with the best fit line and the equality line $y = 1.00x$.
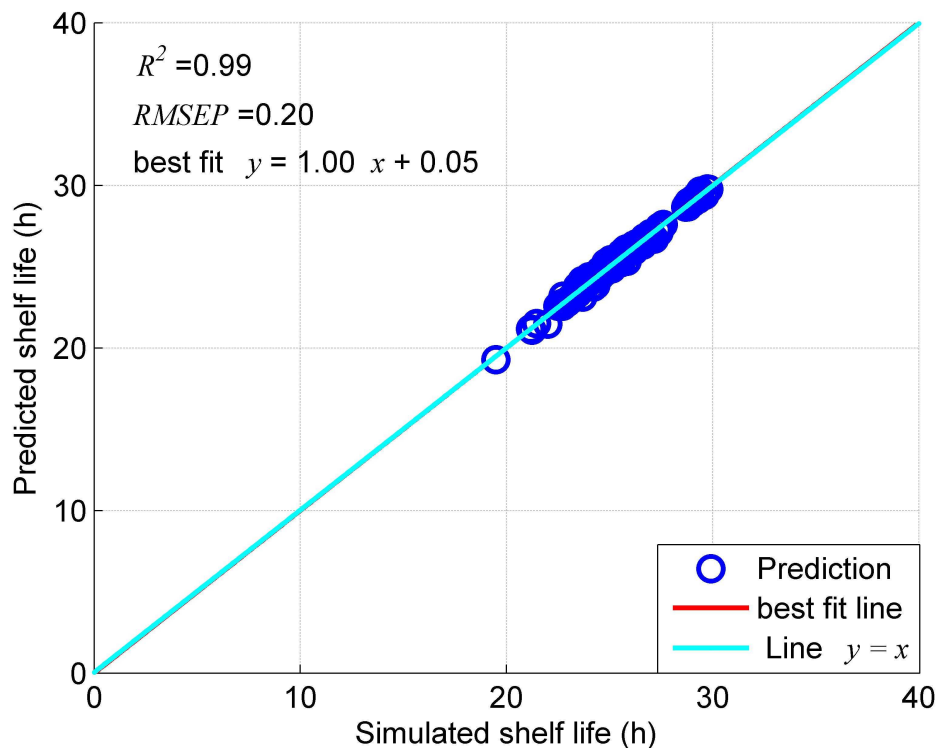
Figure 5.12: Comparison between the simulated shelf life of seasoned soybean sprout (by bacterial load) and the corresponding KLS prediction.

As Figure 5.12 indicates, the predictions by KLS model agree well with the simulated shelf life. The coefficient of determination $R^2 = 0.99$ suggests that the KLS model captured virtually all the variation in the simulated data. Moreover, the average prediction error *RMSEP* was only 0.2 h, which represents less than 1% error for an average shelf life of 25.6 h. From the figure, the best fit line and the equality line $y = 1.00x$ are not visually differentiated. Indeed, the mathematical equation for the best fit line is $y = 1.00x + 0.05$, which only differs from the line $y = 1.00x$ by a small intercept of 0.05. In short, the KLS shelf life predictions matched closely with the simulated shelf life of seasoned soybean sprout. In other words, the KLS model is capable of reproducing the simulated remaining shelf life of seasoned soybean sprout by the kinetic model in Lee *et al*. (2007).

Seafood products
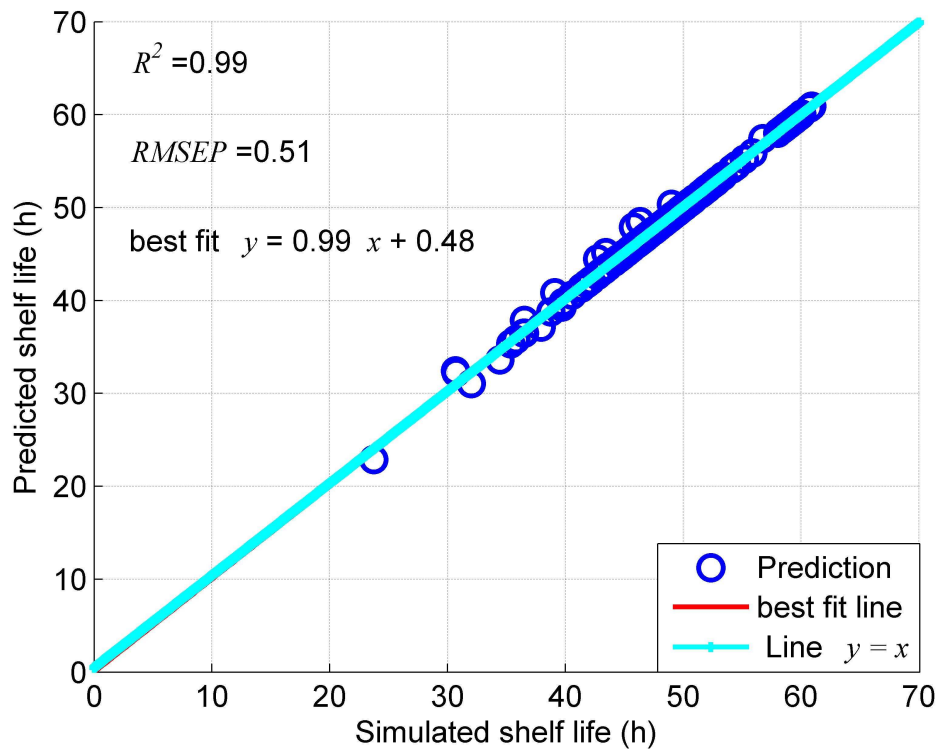
Figure 5.13: Comparison between simulated shelf life of cooked and brined shrimps and corresponding KLS prediction.

Figure 5.13 shows the comparison between simulated shelf life of cooked and brined shrimps and its corresponding KLS prediction. The simulated shelf life was determined using SSSP v2.0 based on empirical RRS models (Section 5.5.2.2). The predicted remaining shelf life was obtained using the KLS model. The values of the performance indices are shown in Figure 5.13, together with the best fit line and the equality line $y = x$. As the figure indicates, the predictions by the KLS model agree well with the simulated shelf life. The coefficient of determination $R^2 = 0.99$ suggests that the KLS model captured almost all the variation in the simulated data. Moreover, average prediction error *RMSEP* was only 0.51 h and the best fit line $y = 0.99x + 0.48$, which only slightly deviates from the line $y = 1.00x$. In short, the KLS prediction of remaining shelf life of cooked and brined shrimps matched closely with their simulated shelf life.

Results from the simulation studies of other seafood products are tabulated in Table 5.4. From this table, a similar conclusion can be made: KLS predictions agreed well with the simulated remaining shelf life. The worst KLS performance was obtained in simulation of fresh seafood from temperate waters, where the intercept of the best fit line was much greater than zero, its ideal value. It was noted that a square root RRS model was implemented in SSSP v2.0 for this fresh seafood from temperate waters while exponential models were used for other seafood products. Therefore, it seemed that KLS performed better with exponential RRS model than with square root ones.

Table 5.4: Results from similar SSSP v2.0 simulation studies

Statistics	Fresh seafood from temperate waters	Fresh seafood from tropical waters	Cold-smoked salmon
Model information	Square root RRS	Exponential RRS	Exponential RRS
Source	SSSP v2.0		
Coefficient of determination R^2	0.91	1.00	1.00
$RMSEP$ (h)	0.85	0.31	0.20
Slope of the best fit line	0.90	1.00	1.00
Intercept of the best fit line	6.29	0.42	0.27

5.6 DISCUSSION

The ability of KLS for modelling was investigated, as a first step, using simulation studies for perishable produce (including tomato and mushroom) and food products (including seasoned soybean sprout and seafood products). The results demonstrated that KLS can reproduce the remaining shelf life from the various simulation models with very low error. More importantly, it does so with the advantage of being simpler and data-driven. The simulation studies showed

that KLS model calibration only requires knowledge of the temperature data set and the remaining shelf life data. It does not require any models or measurements for any quality attributes.

The data-driven feature of the KLS technique is particularly important for perishable products where multiple quality attributes (e.g., firmness and colour in tomatoes) are considered in evaluating remaining shelf life. Collecting measurements and developing a kinetic model for each of the quality attributes concerned would be time consuming at least and may even be impossible if the fundamental understanding of the product is too complex or not available. For example, predicting VL of cut roses and other flowers in general has been studied for decades and yet little information was found about models of quality attributes (such as wilting, colour) for cut flowers (Chapter 2). As understanding about flower senescence is still being gathered, it is unlikely at the present that a kinetic model could be developed to predict remaining VL for cut flowers. Consequently, this is where KLS can be used in place of a kinetic model.

Moreover, the performance of the KLS technique in simulation studies of the various kinetic models emphasises its flexibility. It should be noted that the original mathematical development for KLS started with a single differential equation (Equation (4.1)). However, only the kinetic model of tomato firmness fitted this description while the other simulated models involved multiple (coupled) differential equations. Yet, KLS was shown to perform well in predicting the output of all those models.

A KLS model is expressed by the solution vector $\mathbf{f}_{aug}$ which represents the effect of temperature at each temperature state (relative to the reference temperature) on the loss in remaining shelf life. For example, Figure 5.7 suggested that tomato firmness would deteriorate approximately twice as fast at temperature of 17 ^{o}C compared to 4 ^{o}C. The solution vector at reference temperature ($T_{ref} = 10$ ^{o}C) is always equal to 1, which was used as a constraint in solving for $\mathbf{f}_{aug}$. This highlights another potential advantage of the KLS technique: additional *a priori* knowledge of the underlying biochemical system may be implemented by

constraining the solution $\mathbf{f_{aug}}$. For example, if it is established that certain products would lose their shelf life faster at higher temperature, the solution vector $\mathbf{f_{aug}}$ can be constrained to be (strictly) increasing. This KLS capability of incorporating *a priori* knowledge was discussed in Section 4.3.6 and is explored further in subsequent chapters.

An assumption that was made in the simulation studies was that the simulated products started and ended their shelf life with the same values of quality attribute Q. In other words, all perishable products started their shelf life with the same Q_{start} value and ended their shelf life with the same Q_{end} value. For example, all simulated tomatoes had the same firmness at harvest and at the end of their shelf life. This assumption was made to simplify the task of running simulations and generating simulated data. As described in Equation (4.13), the KLS technique can work with varying initial shelf life values, and hence varying initial conditions. Consequently, it is believed that the assumption did not artificially enhance KLS performance in the simulation studies. In other words, the assumption would not have any effect on KLS performance.

5.7 CHAPTER CONCLUSION

This chapter demonstrated that KLS modelling technique can be used as an alternative to the traditional kinetic modelling in predicting the remaining shelf life of perishable products. As KLS is data-driven, it has potential applications in products where kinetic models would be complicated to implement or simply not available. Examples of such applications are in cut flowers, and hence, as the next step, the method is then applied to cut roses, using real-world data collected from actual supply chains. Results relating to this work are presented in the next two chapters.

6 A NON-CHILLED SUPPLY CHAIN CASE STUDY

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This chapter analyses the data collected from an in-house experiment with cut roses from Cookes Rose Farm (Jersey). Cut roses were delivered via postal service from the farm to the University of Manchester, where vase life tests were carried out. The temperature during the tests, and during the flower display in an ambient office environment, was recorded by data loggers. The logged temperature data were analysed by the kinetic linear system (KLS) technique, multiple linear regression (MLR), and partial least square (PLS) regression.

The analysis showed that post-harvest temperature stress can be used to estimate changes in the remaining VL of cut roses. In addition, it also showed that pre-harvest meteorological temperature may have some correlation with the post-harvest loss in the VL of cut roses, although such correlation was too weak for an effective estimation. The best prediction performance was obtained from KLS modelling, which is fundamentally different from MLR and PLS. KLS is developed from kinetic modelling; it does not assume a linear relationship between temperature and the vase life loss (as MLR and PLS do), and it had a better capability in data reduction.

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6.1 BACKGROUND

Cookes Rose Farm is located in Jersey (Channel Islands). The farm grows roses, and delivers them to local florists. Deliveries are also made via postal service to continental consumers in the UK. Boxes of cut flowers are flown to the UK once a day by the Post Office, where they are then sent through the UK postal system to customers. Delivery time usually takes one or two days but occasionally could be up to 3 days. In the past, the farm has received quality-related complaints from customers in the North West region of the UK.

6.2 OBJECTIVES AND SCOPE OF THE STUDY

The literature review in Chapter 2 has concluded that post-harvest temperature plays a critical role in senescence of cut flowers and particularly cut roses. Therefore, the overall project has investigated the adequacy of using data-driven techniques to analyse post-harvest temperature for predicting the corresponding change in the remaining VL of cut roses. As part of the project, this chapter reports a study aimed at assessing the performance of the KLS technique, which was developed and described in Chapter 4, and comparing this technique to common linear regression techniques, including PLS and MLR. The data set to be analysed was collected during an experiment with Cookes Rose Farm. This involved Cookes Rose Farm sending cut roses from the farm to the University of Manchester where two types of tests were undertaken: one in a temperature controlled cabinet, and the other in an office subject to prevailing ambient conditions.

In terms of scope, the Cookes Rose Farm study primarily focuses on the effect of post-harvest temperature stress. The reason for this is that, although the effects of other environmental factors such as humidity and lighting are also significant, post-harvest temperature is widely considered to be a very important post-harvest factor influencing the remaining VL of cut roses. In addition to post-harvest temperature, a preliminary analysis of the effects of pre-

harvest factors including air temperature, humidity and rainfall levels during the growing period was also performed.

The study consisted of two stages: data collection and data analysis. In the data collection stage, cut roses in boxes of five stems were delivered to the University of Manchester, where tests were carried out to determine their VLs. Throughout this stage, various data such as temperature and observation photos were collected. Subsequently, the data were analysed in the second stage using a number of techniques including KLS, PLS and MLR. Details of the first stage are explained in Section 6.3 and Section 6.4, and the modelling techniques are described in Section 6.5. Results from the data analysis are presented and discussed in Sections 6.7 – 6.11, which is followed by conclusions in Section 6.12.

6.3 EXPERIMENTAL METHOD AND EQUIPMENT FOR DATA COLLECTION

6.3.1 OVERVIEW

The purpose of the experiment was to collect measurements on the temperature conditions that cut roses were exposed to during their transport from Cookes Rose Farm to the University of Manchester, and also the temperatures during the subsequent vase life testing period. In addition, the experiment also aimed at evaluating the remaining VL of cut roses, starting from the point of delivery, which was required for the subsequent predictive modelling exercise.
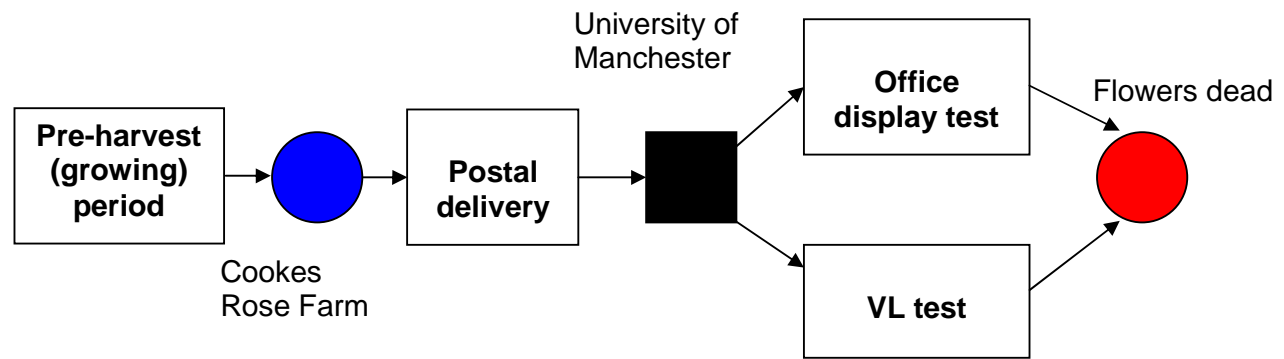
Figure 6.1: Different sub-stages during the Cookes Rose experiment

Figure 6.1 shows schematically the three different post-harvest sub-stages in the Cookes Rose experiment: postal delivery and two different testing regimes, including the office display test and the VL test. During the first sub-stage, boxes of five cut roses were delivered via UK postal service from Cookes Rose Farm to the University of Manchester. Two data loggers were placed in each box, one at each end, to record temperature. The delivery boxes had the following (external) dimensions: 56 cm long, 10.5 cm wide and 8 cm deep. Upon delivery, three out of five cut roses from each box went into the VL test, which was carried out at the controlled standard condition (i.e. 18 ^{o}C). The purpose of the VL test was to evaluate the remaining VL of the roses upon delivery. The two remaining stems went into the office display test where they were placed in a vase in an office environment, and were subjected to office ambient temperature conditions. The office display test, which ended when the cut roses died, was to record the series of office ambient temperature that led to the death of the flowers.

6.3.2 MATERIALS AND EQUIPMENT

Two boxes of cut roses (*cv Jacaranda*) were delivered to University of Manchester from Cookes Rose Farm every week for 15 weeks (25/06/2008 – 30/09/2008). Each box contained five cut rose stems of *ca*. 40 cm in length.

iButton data loggers (DS1921L-F52), products of Maxim Integrated Products Ltd (http://www.maxim-ic.com/), were used to record temperature measurements. The data loggers were programmed to record a temperature measurement every 30 min. These loggers were taken to Cookes Rose Farm and attached to the boxes (inside each box; one logger at each of its ends) prior to the start of the experiment. At the farm, the date and time when the roses were placed in the boxes was recorded and this information was sent to the University of Manchester.

The vase life tests were carried out in a LMS 300W temperature controlled cabinet (incubator). The operating temperature in the incubator was set to 18

^{o}C. Two fluorescent inspection lamps (230V-11W) were installed inside the incubator to provide adequate lighting condition for the vase life test. A weighing scale (a Kern & Sohn EMB220-I scale) was used to weigh the flowers. Photographs of the cut roses were taken using a digital camera (Canon SX100IS) during the vase life tests. An RS-1365 temperature and humidity meter, available from http://uk.rs-online.com, was used to measure temperature and humidity in the temperature controlled cabinet, and these measurements were used to validate the performance of the iButton data loggers that were also attached to the rose stems.

6.3.3 TESTING PROCEDURE

On the date of flower delivery, a test solution was prepared as following:

1. Measure 1 L clean water in a container.
2. Mix with 1 packet of Chrysal Clear Liquid Rosa – a liquid cut flower food that is especially made for roses by Pokon & Chrysal-Naarden-Holland.
3. Transfer 100 mL of the solution to a 100 mL measuring cylinder. Repeat for 4 other 100 mL measuring cylinders.
4. Label the cylinders with the date.

Upon the arrival of the cut roses at the University of Manchester, the following procedure was performed:

1. Record time, date of delivery and make initial observations on the status of the box.
2. Open the box, unpack the roses and cut the roses to 35 cm stem length (*on an angle)* using a sharp knife.
3. Weight and then place the roses in the labelled cylinders immediately after cutting.
4. Attach new activated data loggers to each rose stem.
5. Take photos of the roses (from approximately 1 m distance; against white background).
6. Transfer three cylinders (with cut roses) to the LMS incubator for the remaining vase life test; place the remaining two cylinders in an ambient office environment for the office display test.

7. Note the time of transference, and record any observation on condition of the roses (e.g., wilting, loss of petals, presence of botrytis, etc.).
8. Recover the data loggers from the box to retrieve the temperature profile data for the postal delivery stage.

All cut roses undergoing either the vase life test or the office display test were observed at least once a day. The following procedure was performed:

1. Record time and date of observation
2. (For roses in the incubator, take the cylinder with the rose out of the incubator). Take photos of the roses.
3. Record the liquid solution level in the cylinder
4. Note any observation e.g., is the flower developing? has the rose bud bent? are the petals wilted?
5. For any rose that has died, record its weight before discarding.

6.3.4 DETERMINING THE END OF CUT ROSE LIFE

In this study, "*remaining VL*" or "*VL*" (for short) is defined as the time period that a cut rose takes under a pre-specified standard condition (18 ^{o}C) to reach the end of its useful life (Section 1.2.3). As a result, the remaining VL of a cut rose undergoing the vase life test is given by the duration of the test. (This duration is likely to be different from the time it would take to die under non-standard conditions e.g., office ambient conditions). Therefore, it is important to determine when a cut rose has reached its end of useful life.

Subsequent to the vase life test, photos that were taken daily during the experiment were observed to determine when the life of the cut roses had ended. An example of the evaluation task is shown in Appendix B. Many criteria can be used to determine whether the flower has died. In this study, the criteria that were employed included the occurrence of darkening of the petal edge, flower wilting, bent neck, petal desiccating, petal discolouration, and petal abscission. If using these criteria did not allow a clear-cut decision on the VL of some samples, then the final judgement was based on whether such flowers still had visual appeal for home display. Clearly deciding when a flower is dead is a subjective decision and is a source of experimental variability because

different people might come to different decisions. Further, the photos were taken only once a day for each flower sample. Consequently, the vase life results were subject to a measurement resolution of 1 d.

6.4   DESCRIPTION OF EXPERIMENTAL DATA

Table 6.1 provides an overview of the data that were collected during the experiment. In total, 150 cut rose stems in 30 boxes were delivered to the University of Manchester over a 15 week period. For each stem, two temperature readings were taken (one at each end of the delivery box) every 0.5 h thus providing two delivery stage temperature profiles for each shipment. Consequently, there were 30 pairs of temperature profiles recorded during the postal delivery.

In addition, out of five stems in each box, two were placed in an office ambient environment for the office display test while the other three were placed in an incubator for the vase life test. During these tests, temperature readings were recorded every 0.5 h using data loggers attached to the flower stem.

Other measurements that were collected include the fresh weights and dry weights (as measured at the beginning and at the end of the tests respectively), daily readings of the liquid level in the cylinder, and a set of daily observation photos.

Table 6.1: Data collected during the Cookes Rose experiment

Data and quantity	Details
Time and date of dispatch of flowers from the farm and arrival at the University of Manchester. (30 pairs)	The time and date data were used to retrieve temperature recorded while the flowers were in the postal system.
Temperature profiles during postal delivery. (30 pairs)	Two data loggers were attached to each of the 30 boxes of cut roses to record temperature. A reading was taken every 0.5 h
Fresh weight (g) (150 readings)	Stems of cut roses were weighed after being re-cut to 35 cm in length.
Temperature profiles during the vase life tests and the office display tests. (150 temperature profiles)	Data loggers were attached to the flower stems to record temperature. A reading was taken every 0.5 h.
Liquid level (mL) (150 series of daily liquid level readings)	During the test, water was drawn up into the flower stems, and also loss owing to transpiration. The level of remaining liquid was recorded once a day.
Dry weight (g) (150 readings)	After the vase life test was completed, the dead flower was weighed.
Observation photos. (150 sets of photos taken every day for every cut rose)	Each time a rose was observed, two photos were taken. The first was to capture the overall outlook of the flower as well as its ID. The second provided a closer look of the flower petals.

In addition to post-harvest measurements, pre-harvest data in the form of daily meteorological measurements, including air temperature, sunshine duration and rainfall level for the farm region during the period 01/01/2008 – 31/10/2008, was kindly provided by Mr. A Pallot of the Jersey Meteorological Department. In the

absence of measurements directly obtained from greenhouses at the farm, the weather data were used in the preliminary analysis of the effects of pre-harvest conditions on subsequent remaining VL of cut roses.

6.5 MODELLING OVERVIEW

6.5.1 MODELLING OBJECTIVE

The modelling objective was to obtain a model that captures the effect of post-harvest temperature stress on subsequent changes in the VL of cut roses. For this objective, the study required temperatures recorded during a period where the initial and final VLs of cut roses were known. Therefore, a data set for modelling must include three essential components:

1. Initial VL data for cut roses before being exposed to the temperature stress.
2. Temperature (and possibly any other) data collected during the period the flowers are under temperature stress.
3. Final VL data for cut roses after being exposed to temperature stress.

When such a model is obtained, it can ideally be used to estimate one of the three components above given that the other two are known. For example, if initial VL and temperature stress are known, the model can be used to evaluate the final VL of the flowers. Similarly, if the initial VL is known, storage temperature can be controlled such that after a period of time the remaining VL of the flower still meets a specified lower threshold. In this study, the model is used to evaluate the VL (at 18 ^{o}C) of the cut roses that were delivered to the University.

6.5.2 MODELLING SCENARIOS

Figure 6.2 shows schematically the two modelling scenarios that were investigated. Scenario 1 corresponds with the office display test while Scenario 2 concerns the postal delivery period. The vase life test was not modelled in this study because the temperature during the test was set at constant 18 ^{o}C.

In Scenario 1, the temperature condition during the office display test was recorded by a data logger attached to each cut rose sample being displayed. The final VL was zero because the flowers were displayed until they were considered "dead". The initial VL was estimated by the average of the VLs of the three cut roses that were delivered in the same box but were used in the VL test. This estimation was possible by making the assumption that all five cut roses in the same box had the same VL upon delivery to the University of Manchester. (This assumption is discussed further in Section 6.5.3). Therefore, Scenario 1 has all three components necessary for modelling, as set out in the previous section.

In Scenario 2, temperatures during the postal delivery stage were recorded by data loggers placed inside each box of flowers. The final VL was also estimated by the average of the VLs of the three cut roses that were subsequently used for the VL test. However, the initial VL was unknown. Consequently, assumptions regarding the initial VL were made, so that Scenario 2 could be considered for modelling.

In addition, the hypothesis that higher storage temperature causes greater loss in VL was discussed in Section 3.3 and this was examined in each of the two scenarios. This led to further classification of the modelling scenarios where scenarios B and A correspond to modelling with and without the *a priori* constraint respectively (Section 3.3). Table 6.2 gives a summary of all modelling scenarios as well as the dependent and independent variables involved.
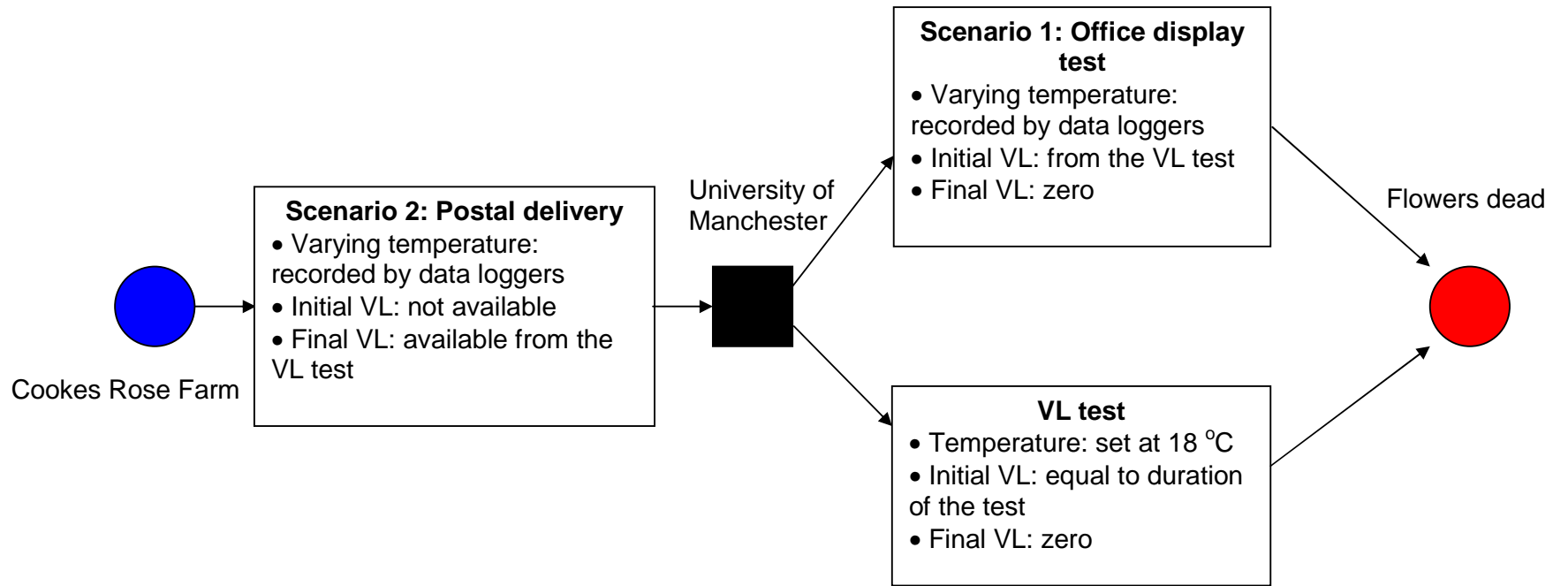
Figure 6.2: Modelling scenarios in the Cookes Rose study

Table 6.2: Dependent and independent variables in modelling scenarios. Scenarios B and A represent modelling with and without the *a priori* constraint, respectively.

Scenario		Based on data obtained from	Dependent variables	Independent variables
1	A	Flowers displayed in office environment	• Initial VL was the average duration of the VL test. • Final VL was zero.	• Temperature profiles logged during the office display tests of the roses.
	B			
2	A	Flowers in postal delivery system	• Initial VL was unknown. • Final VL was the average duration of the VL test.	• Temperature profiles logged during the postal delivery.

6.5.3 ASSUMPTIONS

An assumption that was made in establishing the modelling scenarios was that the cut roses in the same box had the same remaining VL upon delivery to the University. This assumption was necessary to derive the initial VL to Scenarios 1 (A and B) from the results of the vase life test. However, due to various pre-harvest factors including biological, environmental as well as experimental factors, the assumption is very unlikely to be satisfied. Cut roses from the same delivery box often had different vase lives. Such variation in VLs was illustrated by the varying durations of the vase life test that 3 out of 5 samples in every flower box went through. The variation represents the inherent uncertainty in estimating the VL and subsequently the loss in the remaining VL. As a result, any models that are derived based on the data for that vase life loss would not be able to eliminate such variation.

6.5.4 MODELLING TECHNIQUE

In this chapter, KLS, PLS and MLR techniques were used for each of the modelling scenarios (Table 6.2). Details of the mathematical formulations,

solution techniques and implementation issues involved were described in Chapter 4 for KLS and in Section 3.1 for PLS and MLR.

6.5.5 PERFORMANCE EVALUATION

The approach to performance evaluation that was used was described in detail in Section 3.2. Basically, performance evaluation involves the calculation of R^2, *RMSEP*, and the slope and intercept of the best fit line on the predictions, in a double cross validation strategy.

Permutation testing was performed to obtain the lower performance limits for R^2, *RMSEP*, and the slope and intercept of the best fit line. Details of permutation testing are described in Section 3.2.

6.6 RESULTS OF VERIFICATION ON DATA RELIABILITY

6.6.1 TEMPERATURE MEASUREMENT ACCURACY

To test the accuracy of the data loggers, 10 iButton data loggers (resolution: 0.5 ^{o}C; accuracy: ±1 ^{o}C) and an RS-1365 temperature meter (resolution: 0.1 ^{o}C; accuracy: ±0.8 ^{o}C) were placed together under an office ambient environment and subsequently inside a fridge. Temperature readings were taken every 15 min for 6 h. The difference between the data logger readings and the RS meter reading is plotted in a box and whisker diagram (Figure 6.3) and a histogram (Figure 6.4) below.
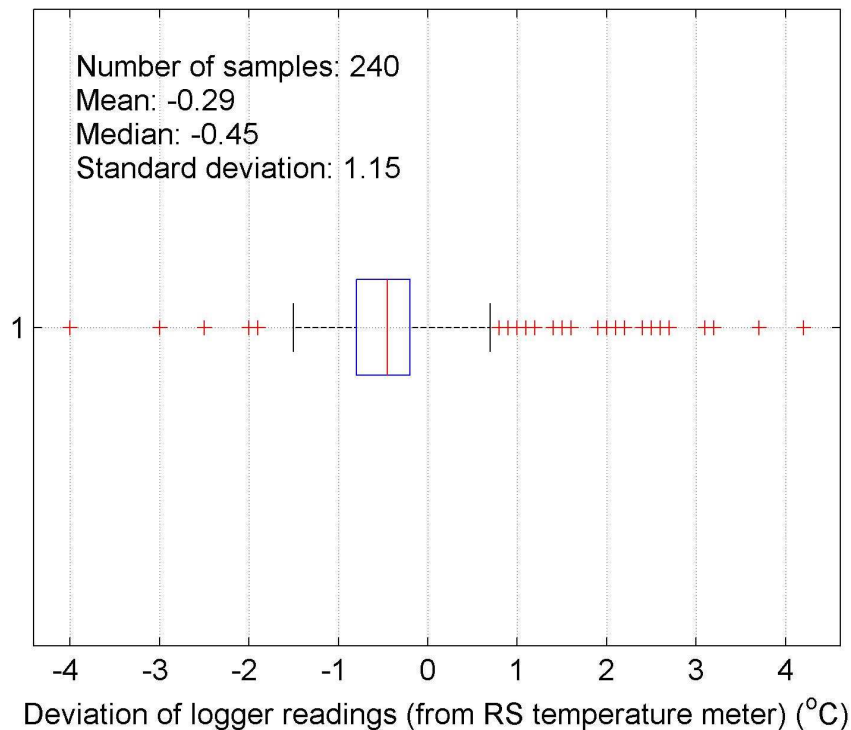
Figure 6.3: Box and whisker diagram for the temperature difference between data logger readings and the RS-1365 meter readings. The box has a line at the lower quartile, the median, and the upper quartile values. Extreme values (within 1.5 times the inter-quartile range) are marked with vertical lines (outside the box). Outliers shown by "+" symbols are the values that are either smaller or greater than those extreme values.

Figure 6.3 and Figure 6.4 plot the difference between a reading from the data loggers and the corresponding reading from the RS-1365 temperature meter. As can be seen, the readings from the data loggers were statistically different from those obtained from the RS-1365 meter. The fact that the mean and median of the difference were -0.29 and -0.45 respectively indicates that the data loggers would be likely to give a lower reading than the RS-1365 meter. Although the manufacturer's specification of data logger accuracy was $\pm 1\ ^oC$, only 179 out of 240 (74.6%) data logger readings were within 1 ^oC from the corresponding RS-1365 meter readings. The actual (217 out of 240) accuracy, based on 90% of readings, was $\pm 2\ ^oC$.
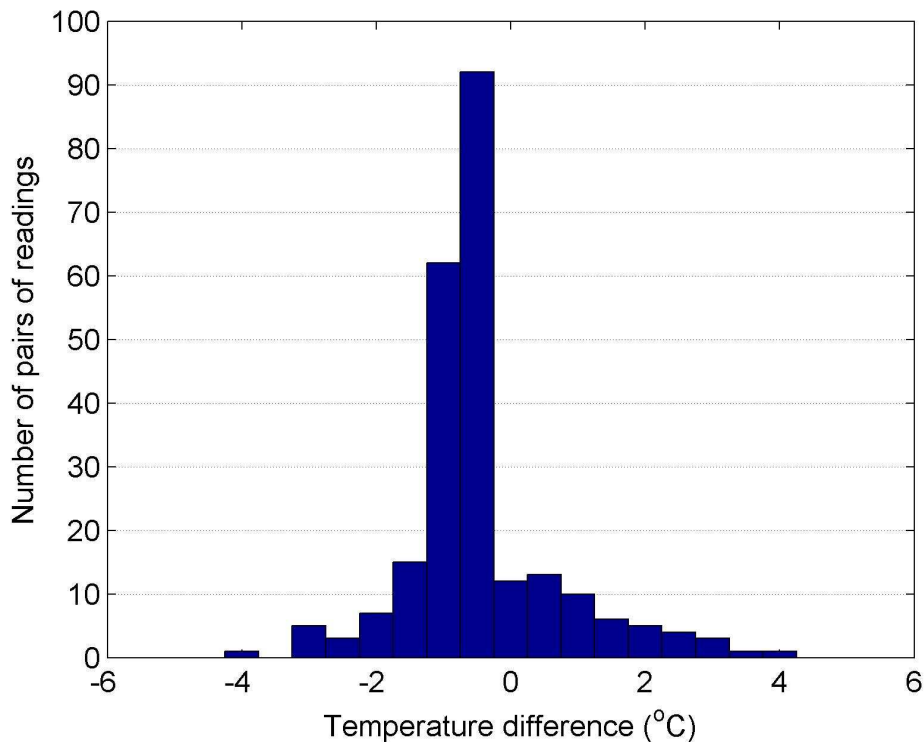
Figure 6.4: Frequency histogram showing the accuracy of data loggers. Y-axis shows the number of pairs of a data logger readings and a RS-1365 temperature meter's reading; x-axis indicates the temperature difference in the pair of reading.

Analysis of variance was carried out for the differences between readings from each of the ten data loggers and the readings from the RS-1365 temperature meter. The null hypothesis was that the differences were from the same distribution, which effectively implies that the readings from the different data loggers are consistent with each other. The results are shown in Table 6.3. As p=0.9999, the null hypothesis can not be rejected. In other words, it is accepted that the series of readings from the data loggers were consistent with each other.

Table 6.3: Analysis of variance (ANOVA) on difference between the readings from the 10 data loggers and from the RS meter

Source of variance	Sum of square	Degree of freedom	Mean Square	F statistic	Prob>F
Columns	31.1	10	3.1081	0.08	0.9999
Error	10249.5	253	40.5118		
Total	10280.6	263			

It can be concluded that the data loggers used in the Cookes Rose data collection experiment were consistent with each other, although their accuracy was ±2 ^{o}C.

6.6.2 EFFECTS OF DATA LOGGERS' POSITION

There were two data loggers in each of the 30 boxes of cut roses that were delivered to the University, each located at opposite ends of the boxes. As a result, every reading from a data logger had a corresponding reading from another data logger from the same box. The difference in the pair of readings is the difference in temperature at two ends of every box of flowers, which was plotted in a box-whisker diagram (Figure 6.5) and a histogram (Figure 6.6). Less than half of the readings (42.5%) were within 0.5 ^{o}C; most of the readings (75.1%) were within 1 ^{o}C while 90.8% of the temperature measurements were within 2°C difference. Given the loggers' accuracy of ±2 ^{o}C, this indicated that the difference in temperature at two ends of boxes of cut roses was negligible.
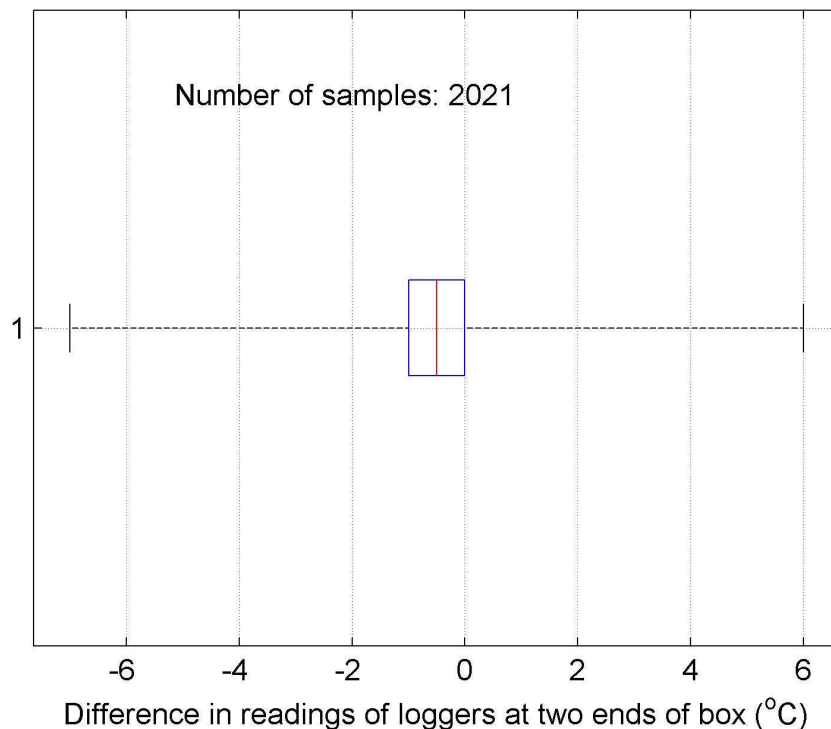
Figure 6.5: Temperature difference between one end of boxes (flower heads) and the other end of the same boxes (stem end)
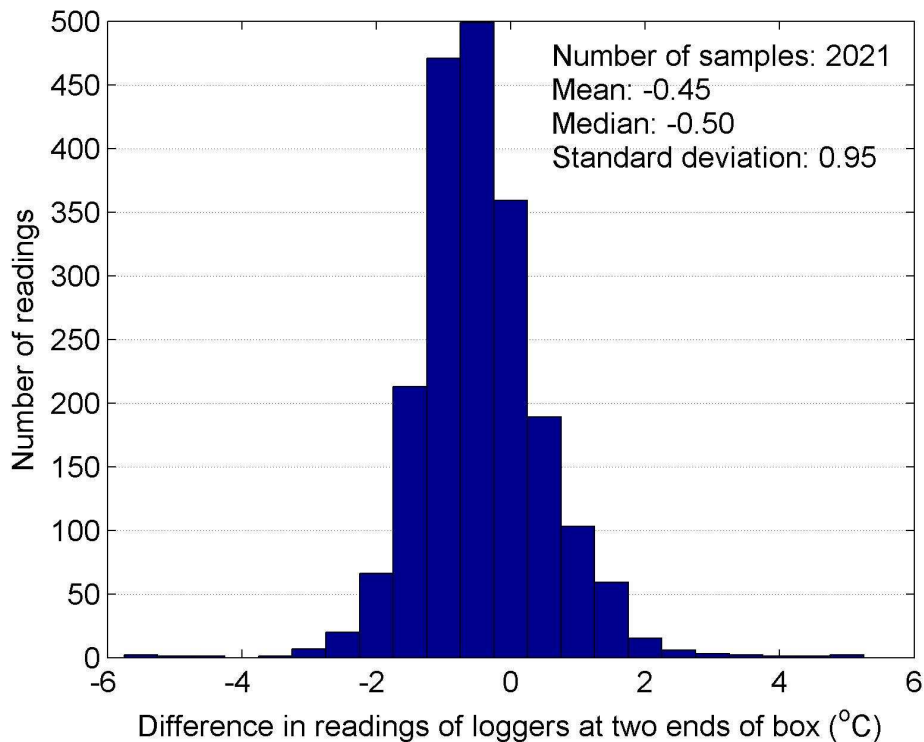
Figure 6.6: Frequency histogram showing the differences in temperature recorded at two ends of boxes

6.6.3 VARIABILITY IN VASE LIFE DATA

The variability in VL of cut roses that was not due to post-harvest temperature effect was studied. As described earlier, three of the five stems in each flower box were placed inside an incubator. These stems, therefore, had the same temperature profile during postal delivery (in the same box) and the same temperature during the vase life test. Yet, these stems often had different vase lives. Such variation in VL is depicted in Figure 6.7. Similarly, the other two stems from the box were subject to the office display tests in an office ambient environment, and hence were exposed to the same temperature stress yet they also died at different times. The variation in the duration of the office display test is plotted in Figure 6.8. As both variations arose from the stems that experienced the same post-harvest temperature, they were certainly not related to the effect of post-harvest temperature stress. Rather, as identified in the literature review (Section 2.3) other factors such as biology of the flowers and

variation in the environmental conditions during pre-harvest and at harvest could be the key driving forces that lead to the observed variations.
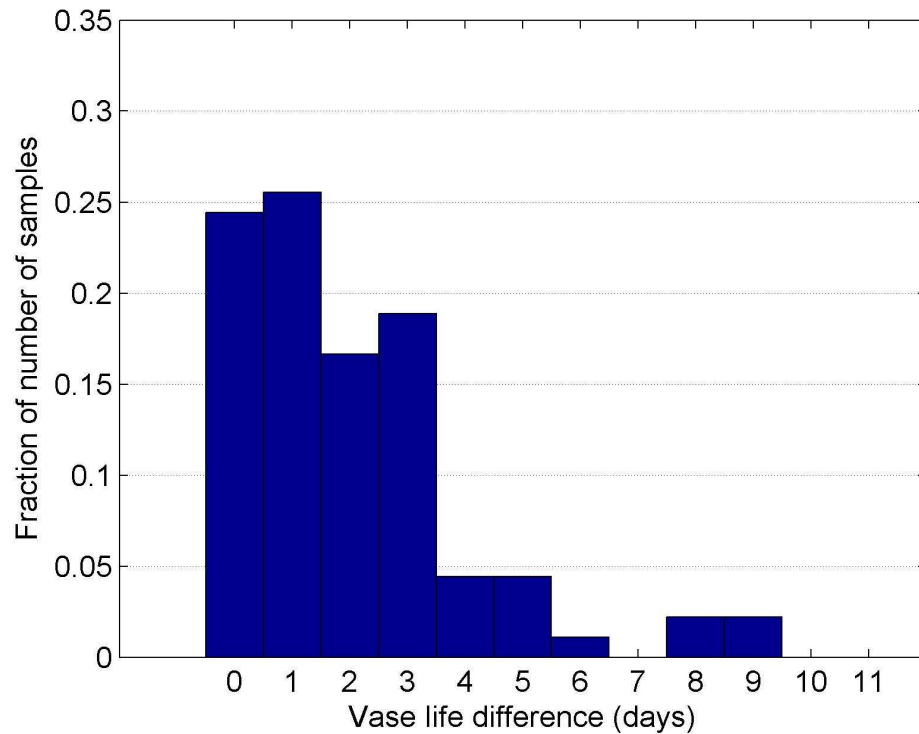
Figure 6.7: Histogram of variation in VL of cut roses at delivery as determined by the vase life test. X-axis shows the difference in VL of the cut roses that were exposed to the same temperature stress during postal delivery (i.e., in the same box) and subsequently placed in the incubator at standard condition (18 ^{o}C). Y-axis represents the fraction of samples that had the same vase life difference.
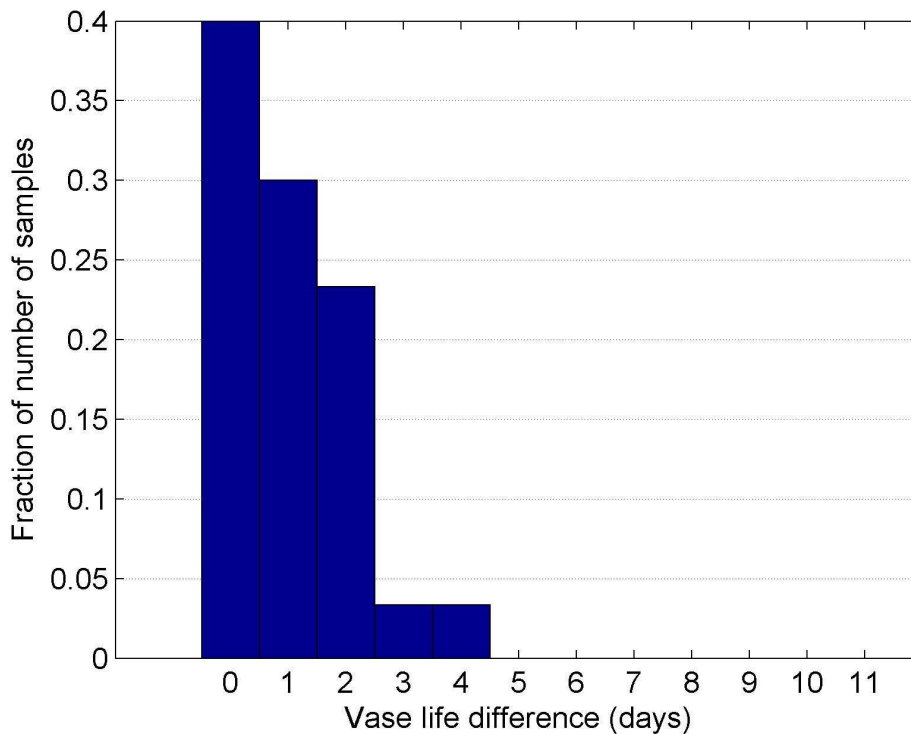
Figure 6.8: Histogram of variation in the duration of office display test. X-axis shows the difference in the durations of the office display tests for cut roses from the same delivery box. Y-axis represents the fraction of samples that had the same duration difference.

6.7 SCENARIO 1 – MODELLING THE OFFICE DISPLAY PERIOD

As described in Table 6.2, in Scenario 1 the display of cut roses in an ambient office environment was studied. The objective was to predict the VL loss during these office display tests. The data used for the modelling included the temperature readings recorded during the office display tests, and the initial and final VLs. The testing period ended when the roses died. Consequently, the final VL was zero. In addition, as two cut roses from each of the 30 boxes were displayed, 60 temperature series were collected. Further, the other three rose stems from the same delivery box were subjected to the vase life test in the LMS incubator. The average duration of the vase life tests for the three stems was used as the initial VL. The loss in VL, which was to be estimated, was the difference between the initial and final VL values, and hence was effectively equal to the initial VL. It should be noted that, as the temperature during the office display test varied, and was different from the reference temperature

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($T_{ref} = 18 \, ^oC$), the initial VL would be different from the duration of the office display test.

6.7.1 EXPLORATORY STUDY

Typical profiles of temperature during the office display tests, shown in Figure 6.9, reveal fluctuations in the office temperature. This was due to the fact that during the tests the flowers were displayed in an office where the environment (i.e. temperature, humidity) varied between night and day. Figure 6.9 also shows that the duration of the display tests and hence the number of temperature readings varied significantly. This would have implications on data pre-processing for MLR and PLS modelling.
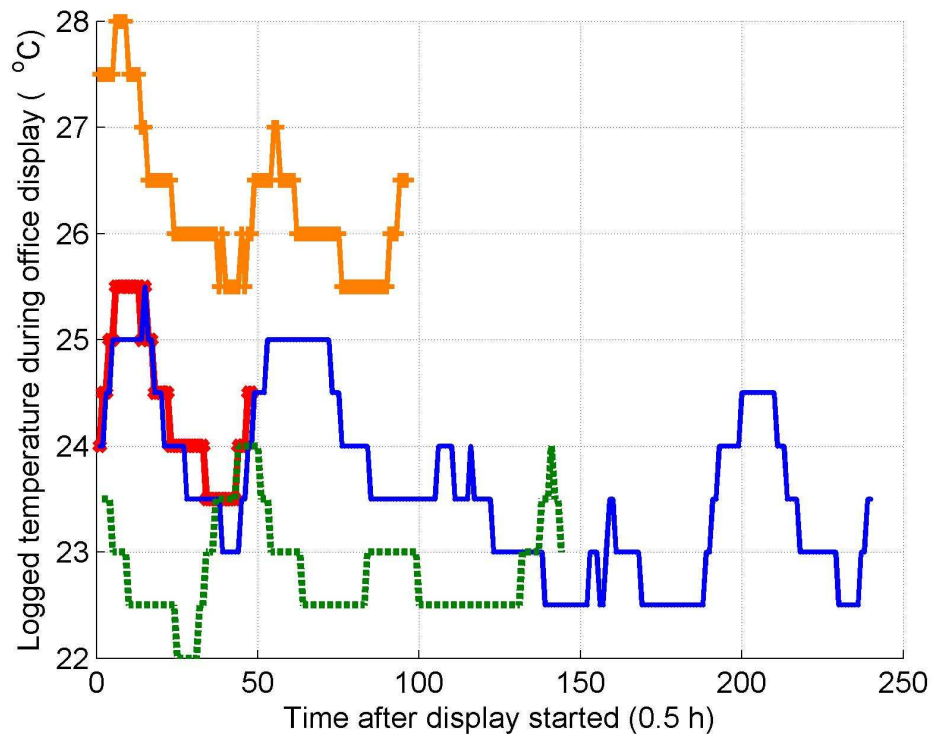
Figure 6.9: Typical temperature profiles logged during the office display tests of cut roses. The time (x-axis) was recorded in unit of 0.5 h from the start of the tests. The temperature was recorded by data loggers attached to the flowers.

After data pre-processing (see Section 3.1.1), PCA was performed on the data set. The analysis revealed that the first three PCs accounted for more than 80% of the data variance. The score plots for the first and second PCs are presented

in Figure 6.10 and Figure 6.11. (Figures for the third PC are similar and hence omitted). The observations were grouped according to the month of the delivery date of the rose samples in Figure 6.10 and according to the range of the vase life loss in Figure 6.11. As seen in Figure 6.10, most of the samples delivered in July had positive second PC scores (quarters 1 and 2). In addition, while the August deliveries seemed to have positive first PC scores (quarters 2 and 3) while 18 out of 22 samples delivered in September had negative first PC scores (quarters 4 and 1). Therefore, it seems that there was possibly a trend in the PCA observations with respect to the delivery date (month). This could be explained by the fact that during the office display test, the temperature in the office was not specifically controlled and hence closely correlated with the seasonal weather changes.
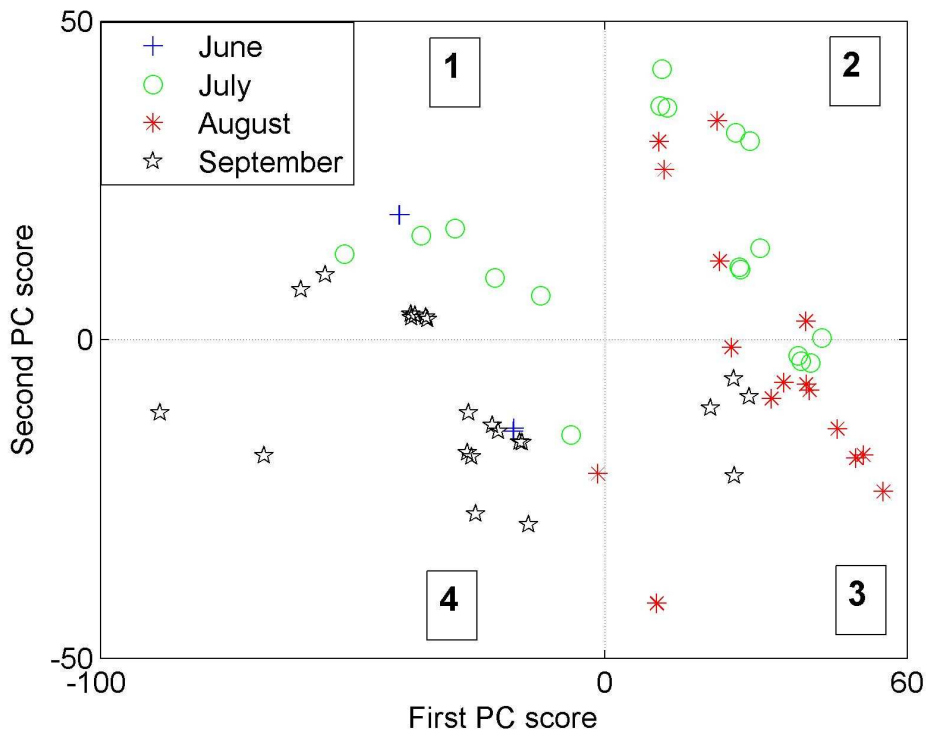
Figure 6.10: PCA scores plot for the first and second PCs, which together explain 72.2% of the total variance. Different symbols represent different delivery date (month).
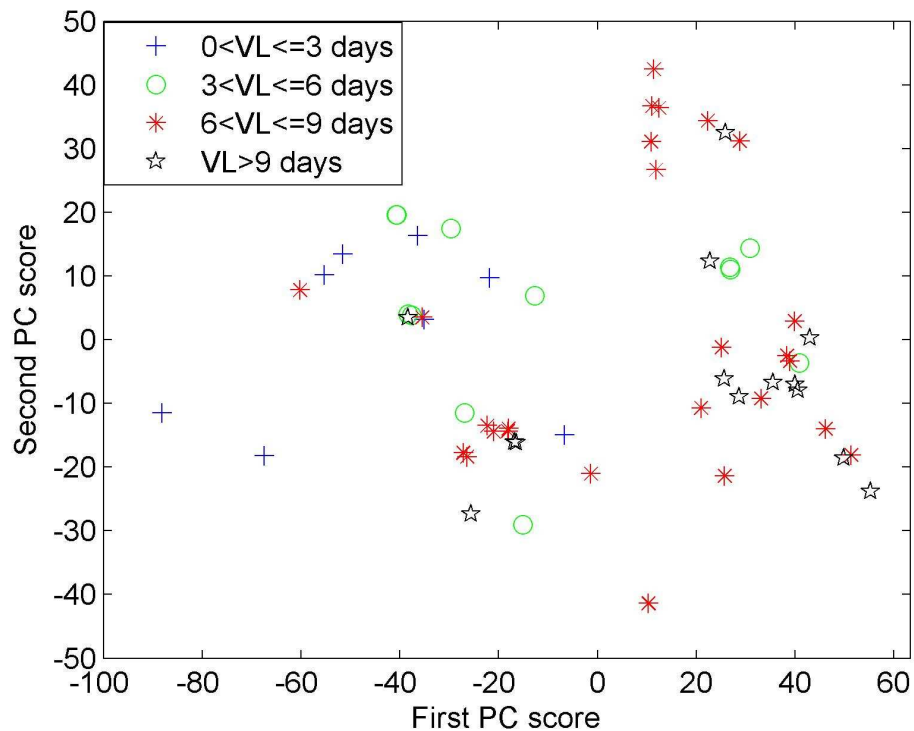
Figure 6.11: PCA scores plot for the first and second PCs, which together explain 72.2% of the total variance. Different symbols represent different range in VL loss.

Figure 6.11 shows the PCA scatter plot (for the first and second PCs) with observations grouped according to ranges of the vase life loss. No clear trend between the groups of VL could be observed, which suggests that estimating the vase life loss using the display temperature would be challenging.

6.7.2 KLS PERFORMANCE

6.7.2.1 SETTING PARAMETERS

Figure 6.12 shows the histogram of the temperature of the cut roses during the office display tests in an ambient office environment. From this figure, the lower and upper bounds of temperature in Scenario 1 were set at 22 ^{o}C and 27 ^{o}C respectively. The temperature step was set at 1 ^{o}C as a result of the data loggers' accuracy (see Section 6.6.1).
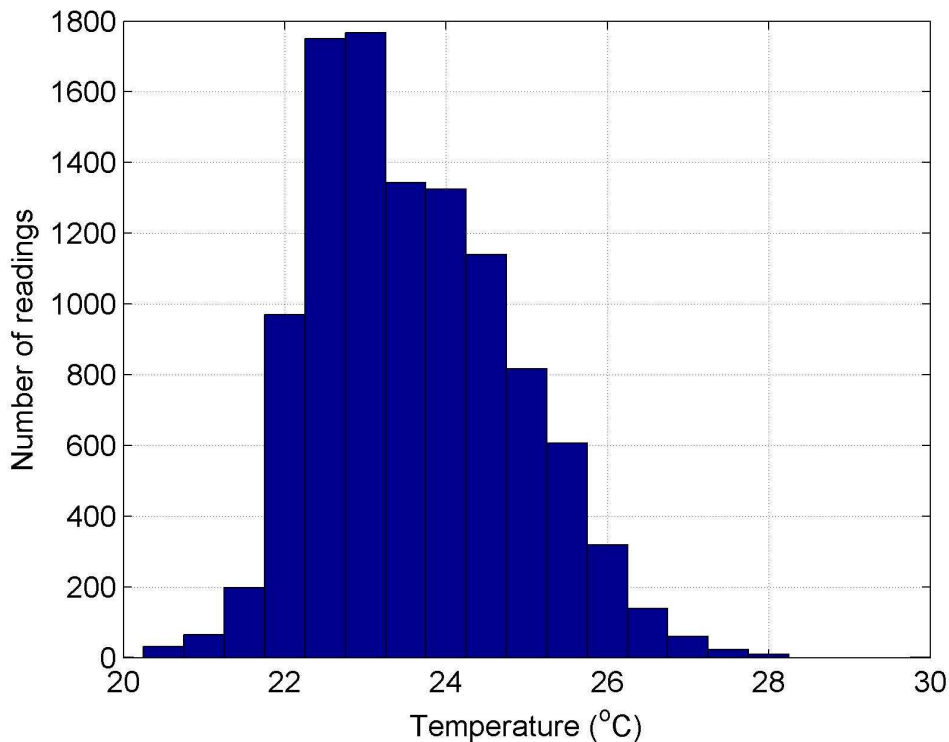
Figure 6.12: Scenario 1 – Variation in temperature logged during the office display tests of cut roses in an office environment.

6.7.2.2 SCENARIO 1A – WITHOUT THE *A PRIORI* CONSTRAINT

Figure 6.13 shows a typical performance of KLS model in Scenario 1A, modelling the office display period without the *a priori* constraint. A total of 60 samples, 2 from each of the 30 boxes, were designated for the office display test. However, two of the 60 stems died at the beginning of the test. Consequently, only 58 roses completed the office display test and these data were analysed in this scenario. The KLS predictions were obtained using cross validation strategy with $N_{test} = 10$ segments (Section 3.2.2).

As can be seen in the figure, there is a general agreement between the observed vase lives and their KLS predictions. Most of the blue circles, which represent the comparison between the observed VLs and their predictions, seem to follow the equality line quite well although the correlation between the observed and predicted VLs was small ($R^2 = 0.29$). The deviation between the

circles and the equality line is significant as reflected in the significance of the prediction error, *RMSEP* = 2.38 d.
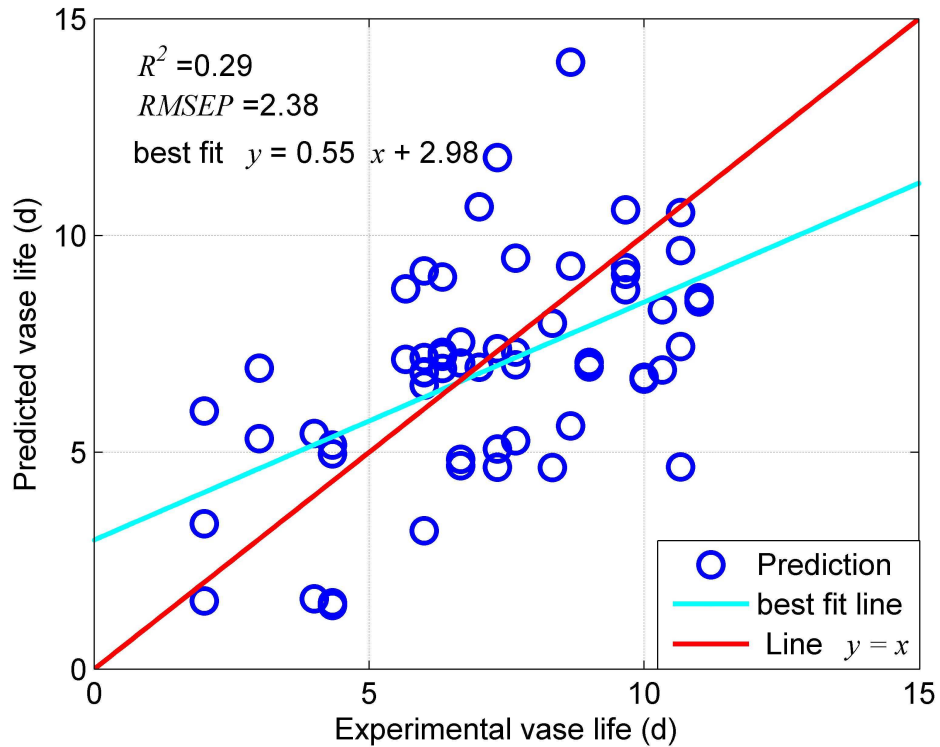
Figure 6.13: Scenario 1A – a typical KLS performance in modelling the office display test period <u>without</u> the *a priori* constraint. The best fit line and the equality line are also shown. X-axis represents the remaining VLs of the cut roses at the beginning of the office display test. Y-axis plots the corresponding KLS predictions.

The performance of KLS was evaluated for 10000 iterations, each with a different segmentation of the available data set used in cross validation. In addition, permutation testing (Section 3.2.3) was also performed.

Figure 6.14 plots the KLS solutions obtained during its performance evaluation. The numerical values of KLS solutions represent the vase life loss, measured in units of 0.5 h, per frequency at each temperature state. Across the selected temperature states, KLS solutions seem to converge quite well except at 27 °C. Significant variation as well as outliers were observed at $T = 27\,^{o}C$.
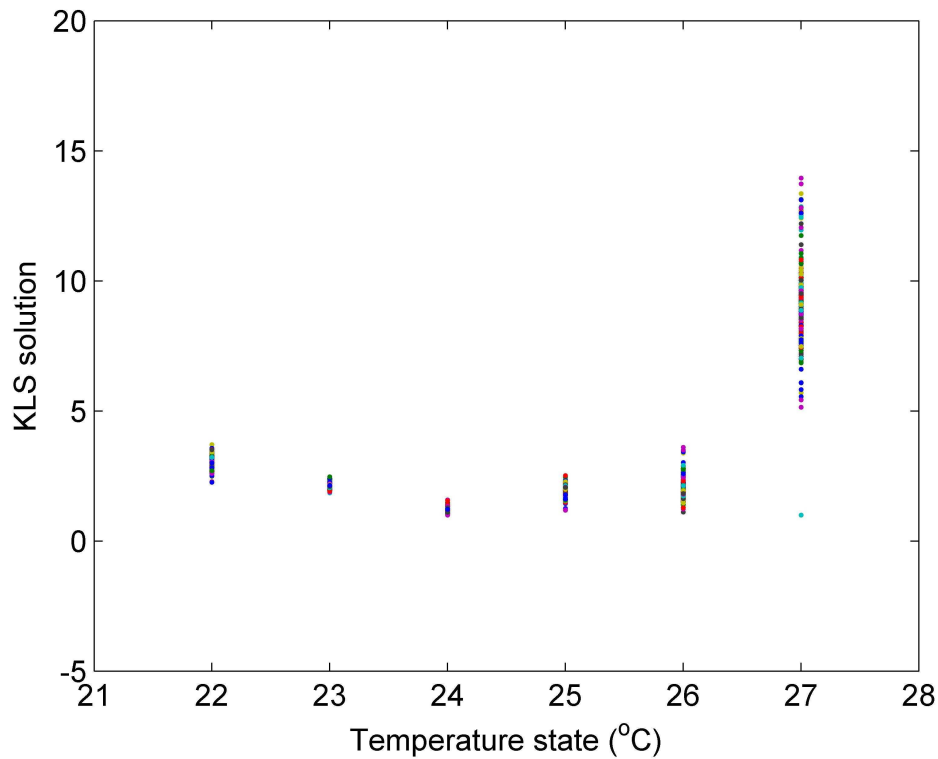
Figure 6.14: Scenario 1A – KLS models. X-axis represents the temperature states specified in KLS modelling. Y-axis shows the KLS solutions at each temperature state.

Figure 6.15 - Figure 6.18 shows the distributions of *RMSEP*, R^2, and the slope and intercept of the best fit lines, and their corresponding nonsense distributions from permutation testing. It should be noted that the nonsense distributions represent the lower performance limits. In all of the figures, the actual distributions of the performance statistics and their nonsense counter-parts are clearly far apart. This observation confirms that the estimation of the loss in VL, using the temperature data collected from the office display test, was effective (Section 3.2.4). Meaningful information embedded within the experimental data was captured by the KLS technique.
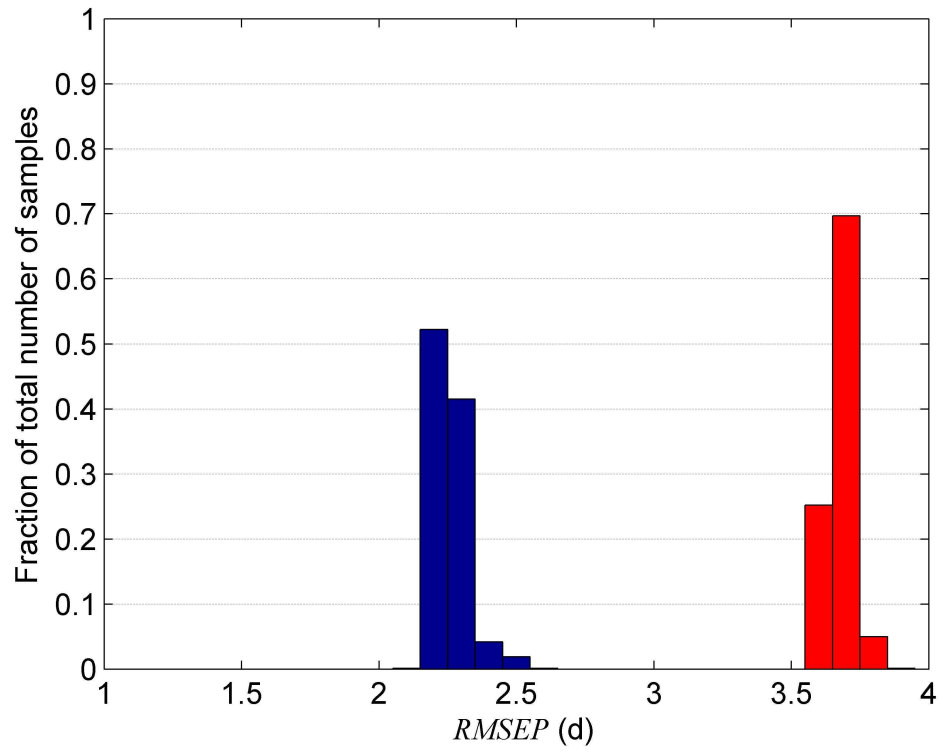
Figure 6.15: Scenario 1A – *RMSEP* distribution from KLS modelling. The blue distribution represents *RMSEP* from original data while the red one was from the permutated nonsense data.
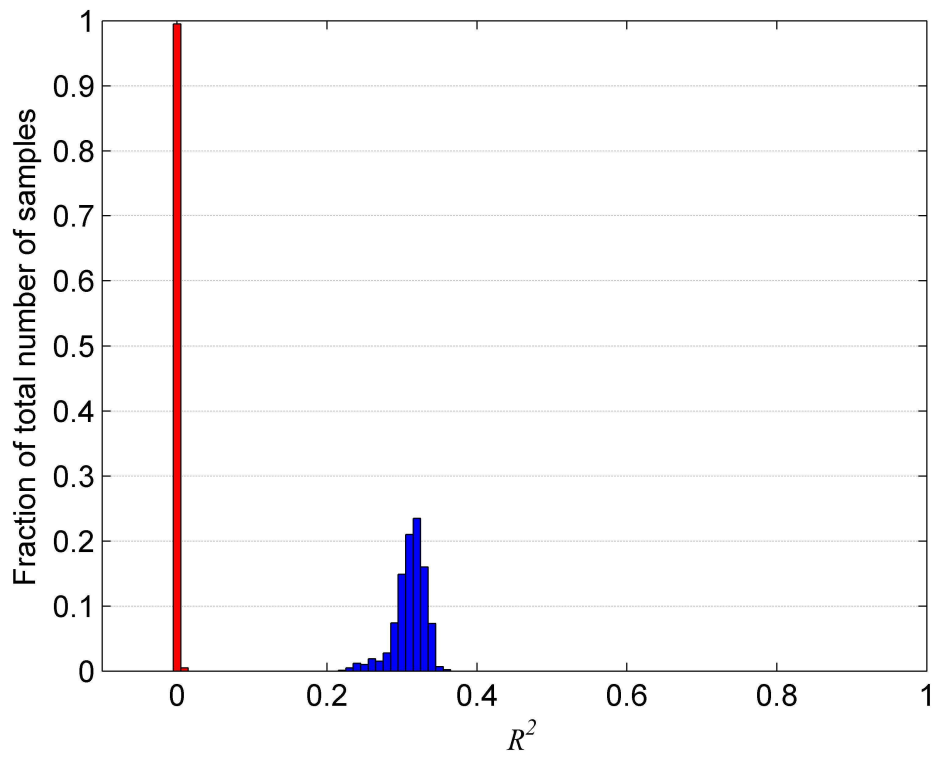
Figure 6.16: Scenario 1A – R^2 distribution from KLS modelling. The blue distribution represents R^2 from original data while the red one was from the permutated nonsense data.
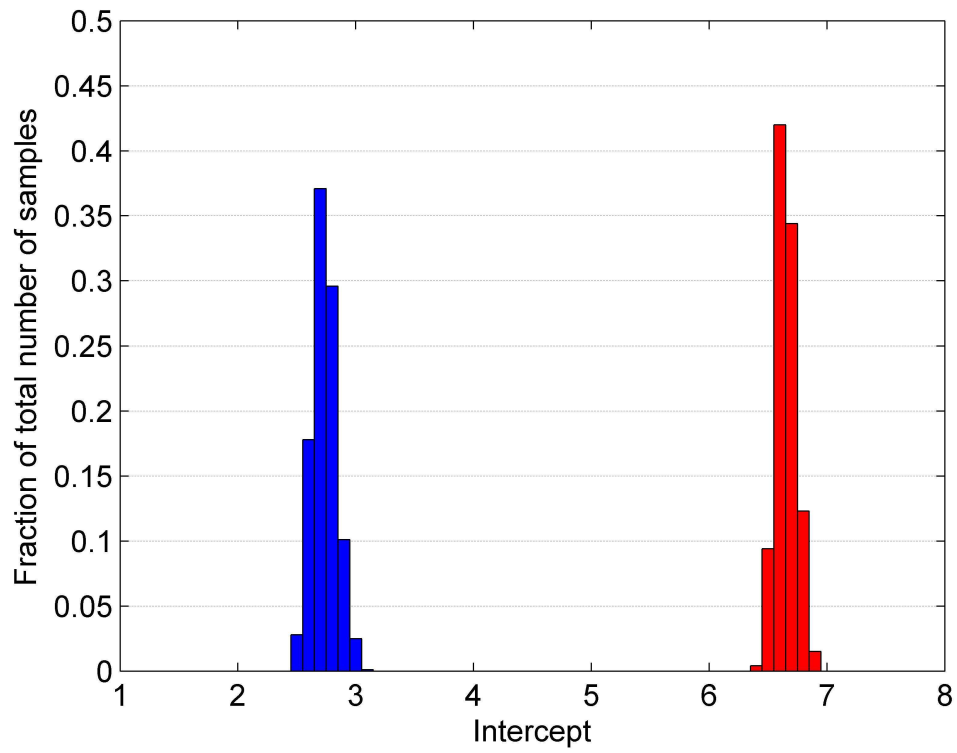
Figure 6.17: Scenario 1A – distribution of the intercepts of the best fit lines from KLS modelling. The blue distribution represents the intercepts from original data while the red one was from the permutated nonsense data.
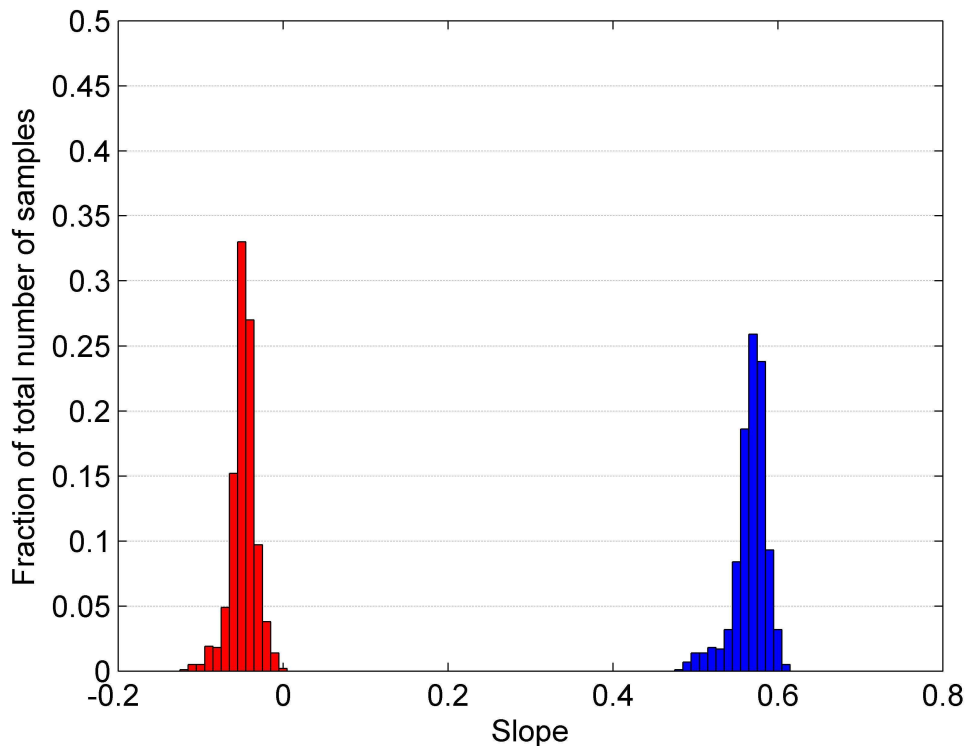
Figure 6.18: Scenario 1A – distribution of the slopes of the best fit lines from KLS modelling. The blue distribution represents the slopes from original data while the red one was from the permutated nonsense data.

6.7.2.3 SCENARIO 1B – WITH THE *A PRIORI* CONSTRAINT

The *a priori* constraint from studies of the physiology of cut flowers states that a higher storage temperature leads to a greater loss in the VL of cut flowers (see Section 3.3). In this scenario (1B), the constraint was implemented. However, inspection of the data from the office display tests revealed that there were more than 40 pairs of cut rose samples that had temperature profiles and corresponding losses in VL appear inconsistent with the constraint. An example of such pair is shown in Figure 6.19. Nevertheless, it should be emphasised that what was observed did not contradict the *a priori* knowledge derived from previous physiology studies. As explained in Section 3.3, such *a priori* knowledge only applies to two cut flower samples having identical history of stress (e.g., same pre-harvest conditions) and genotype (e.g., same variety). The pairs identified from the data set and exemplified in Figure 6.19 may have different pre-harvest conditions, and hence the *a priori* knowledge did not hold.
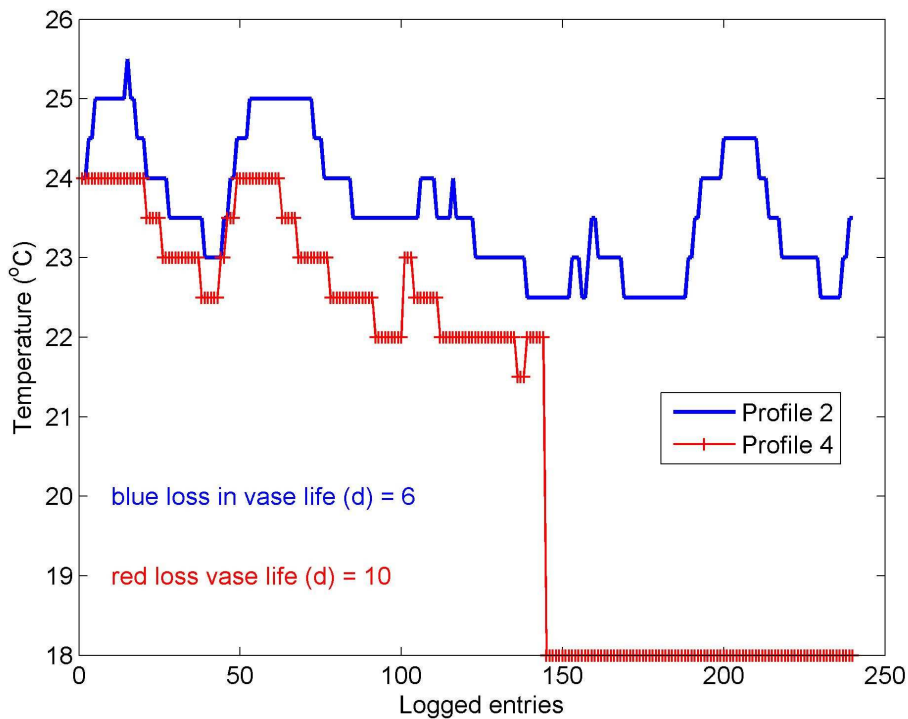
Figure 6.19: Pair of samples inconsistent with the *a priori* constraint: Sample 2 was displayed at higher temperature throughout but had lower loss in VL compared to Sample 4.

Clearly, implementing the *a priori* constraint requires non-thermal factors such as pre-harvest conditions, genetic variation and post-harvest humidity to be accounted for. Consequently, slack variables were introduced in order to account for the non-thermal factors other than the post-harvest temperature. Details of the modified KLS model were explained in Section 4.3.4. Quadratic programming optimisation was formulated with the objective of minimising the variance of the slack variables.

Figure 6.20 shows a typical KLS performance in Scenario 1B, modelling the office display test period with the *a priori* constraint. The KLS predictions were obtained using cross validation strategy (with $N_{test} = 10$ segments). As can be seen in the figure, most of the predictions are between 5-10 d and only 5 out of 58 are outside that range. In contrast, there is more variation in the experimental VL where 19 out of 58 samples have VL less than 5 d or more

than 10 d. This indicates that the KLS model with the *a priori* constraint does not sufficiently capture the variation in VL.

Figure 6.20: Scenario 1B – a typical KLS performance in modelling the office display period <u>with</u> the *a priori* constraint. The best fit line and the equality line are also shown. X-axis represents the remaining VLs of the cut roses at the beginning of the office display test. Y-axis plots the corresponding KLS predictions.

Similar to Scenario 1A, the performance of KLS was evaluated 10000 times, each time with a different segmentation of the available data set used in cross validation. In addition, permutation testing (see Section 3.2.3) was also performed. The two sets of results are presented in Table 6.4. The actual distributions of $RMSEP$ (d), R^2, slope and intercept of the best fit lines are clearly far apart from their corresponding nonsense counterparts; the p-values and q-values for the statistics are all zero.

Table 6.4: Scenario 1 – KLS performance with/without the *a priori* constraint. "Actual" results were obtained using original data while "nonsense" results were from permutation testing studies. 10000 repetitions of cross validation studies were performed. All statistics were presented as mean ± standard deviation.

Scenario 1		A (without *a priori* constraint)	B (with *a priori* constraint)
Predicted output		ΔVL (d) during office display (mean = 7.2; min = 2; max = 11)	
RMSEP	actual	2.3 ± 0.1	2.1 ± 0.0
	nonsense	3.7 ± 0.0	3.0 ± 0.0
	p-value	0.00	0.00
	q-value	0.00	0.00
R^2	actual	0.32 ± 0.02	0.24 ± 0.02
	nonsense	0.00 ± 0.00	0.00 ± 0.00
Slope	actual	0.57 ± 0.02	0.31 ± 0.01
	nonsense	0.04 ± 0.02	0.08 ± 0.01
Intercept	actual	2.79 ± 0.10	4.90 ± 0.09
	nonsense	6.26 ± 0.13	6.53 ± 0.11

A question is that whether 10000 iterations were sufficient for statistical assessment. Further inspection of the nonsense results suggests that they were. The nonsense R^2 distributes virtually at zero; the slope is very close to zero; and the intercept is closer to the mean of the observed VLs. These results indicate that there is no linear relationship between the nonsense predictions and the experimental VLs and that the best fit line is a horizontal line close to the mean of the observed VLs. These features are expected for the nonsense data and as 10000 iterations were able to reproduce the features, they were statistically sufficient for performance assessment in this case. In plain words, increasing the number of iterations would not significantly change the results shown in Table 6.4.

The above results in Scenario 1A and 1B for KLS were obtained under the assumption that for every box of cut roses, the two stems that were displayed had their initial VL equal to the average of the remaining VLs of the three stems that were subject to the vase life tests in the incubator. Alternative to this

assumption, each of the samples that were on display could have its initial VL equal to that of any of the three in the incubator. In this case, the results (not shown) were much worse than those in Table 6.4.

6.7.3 PLS PERFORMANCE

6.7.3.1 DATA PRE-PROCESSING

The same data set that was previously analysed by the KLS technique was studied using PLS. As 2 out of 60 cut rose samples died at the beginning of the display test, again data from only 58 samples were available.

PLS modelling technique requires a uniform number of measurements per input sample. To overcome this issue, the strategy, which was discussed in detail in Section 3.1.1, was essentially to use reference temperature $T_{ref} = 18 \ ^{o}C$ to make up for any data samples that had fewer than the required number of measurements.

In addition, two schemes of data scaling were also explored including:

1) The original data were scaled to zero mean and unit variance, i.e. auto-scaling.
2) The original data were scaled to zero mean only, i.e. zero-mean scaling.

6.7.3.2 SCENARIO 1A – WITHOUT THE A PRIORI CONSTRAINT

Double cross-validation, which was described in detail in Section 3.2.2, was implemented in evaluating PLS model performance. The optimal number of PLS factors, the PLS model dimension, was determined using the *RMSEP* statistic. The modelling data set, which contained 58 temperature series recorded during the office display test and 58 corresponding losses in the VL of the cut roses, was split into calibration and test subsets – the outer loop. Using the calibration subset, an inner cross validation study was performed and the *RMSEP* statistic was evaluated for all possible number of PLS factors. The optimal number of PLS factors, which produced the minimum *RMSEP*, was used to obtain an optimal PLS model based on the calibration data. Subsequently, the performance of the optimal PLS model was assessed using the test subset. The

whole procedure (from randomised splitting into calibration and test subsets to assessing prediction performance) was repeated 1000 times; in each time, the data set was divided into $N_{test} = 10$ sub-sets (Section 3.2.2), giving a total of 10000 PLS models that were generated. The results (where the original data were auto-scaled) are shown in Figure 6.21, Figure 6.22 and Table 6.5 below.
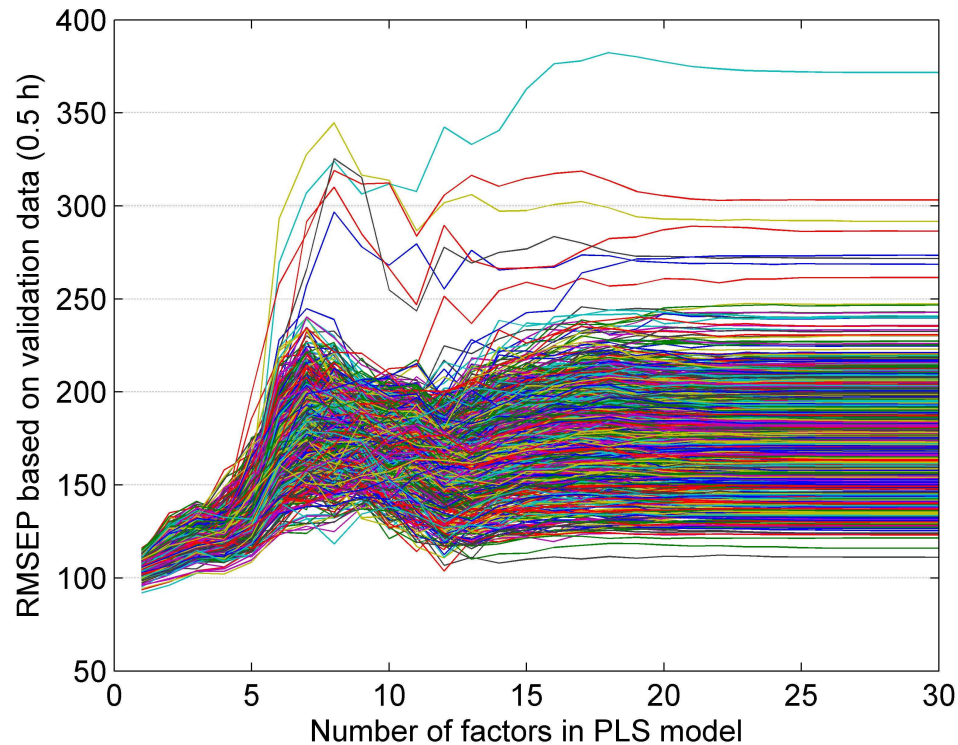
Figure 6.21: Scenario 1A – *RMSEP* of PLS models using validation subset (data were auto-scaled).

Figure 6.21 and Figure 6.22 suggest that to achieve minimum prediction error a PLS model was likely to retain only the first PLS factor. *RMSEP* based on validation subsets of data initially increases, fluctuates and subsequently levels off with the number of PLS factors retained. It was not clear as to why only one LV was optimal in terms of *RMSEP*. One possible reason is that no significant linear relationship between the temperature and the VL, as suggested in the exploratory PCA (Figure 6.11). Another reason could be due to the data pre-processing to have a uniform number of measurements. Inspection of the original temperature profiles revealed that few had 300-350 readings while most

of them had less than 200-250 readings. Consequently, the temperature profiles after data pre-processing were predominant by the reference temperature $T_{ref} = 18 \ ^oC$, which may lead to optimal PLS models with just one LV.
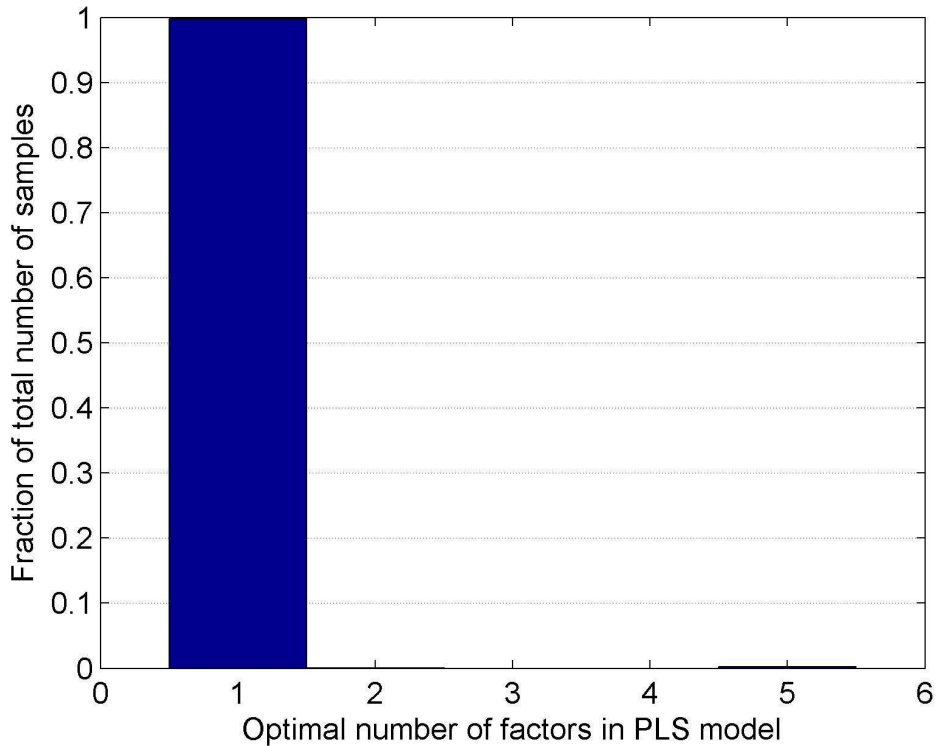
Figure 6.22: Scenario 1A – Distribution of optimal numbers of PLS factors (auto-scaling).

All of the statistics including *RMSEP*, R^2, and the slope and intercept of the best fit lines were evaluated using test data subsets in a double cross-validation strategy (Section 3.2.2). A typical PLS performance with auto-scaling is presented in Figure 6.23. A similar figure for the results using zeo-mean scaling can be found in Appendix B (Figure B. 1). Distributions of the performance statistics and their corresponding nonsense distributions from permutation testing are summarised in Table 6.5. The results showed that the zero-mean scaling strategy led to significant overlap between the actual distributions of the statistics and their nonsense ones; the *p*-values and *q*-values for *RMSEP* distributions were also greater than 0.10. Therefore, it can be concluded that using this scaling strategy, PLS failed to predict effectively the remaining VL. For auto-scaling, minimal overlaps occur at the tails of the distributions of

RMSEP, and hence small *p*-values and *q*-values; however, the common intersections of the two actual and nonsense distributions of the slope and intercept were considerably larger. As a result, the PLS performance in this case was effective (Section 3.2.4) based on *RMSEP* but could be improved, particularly in terms of the best fit line.
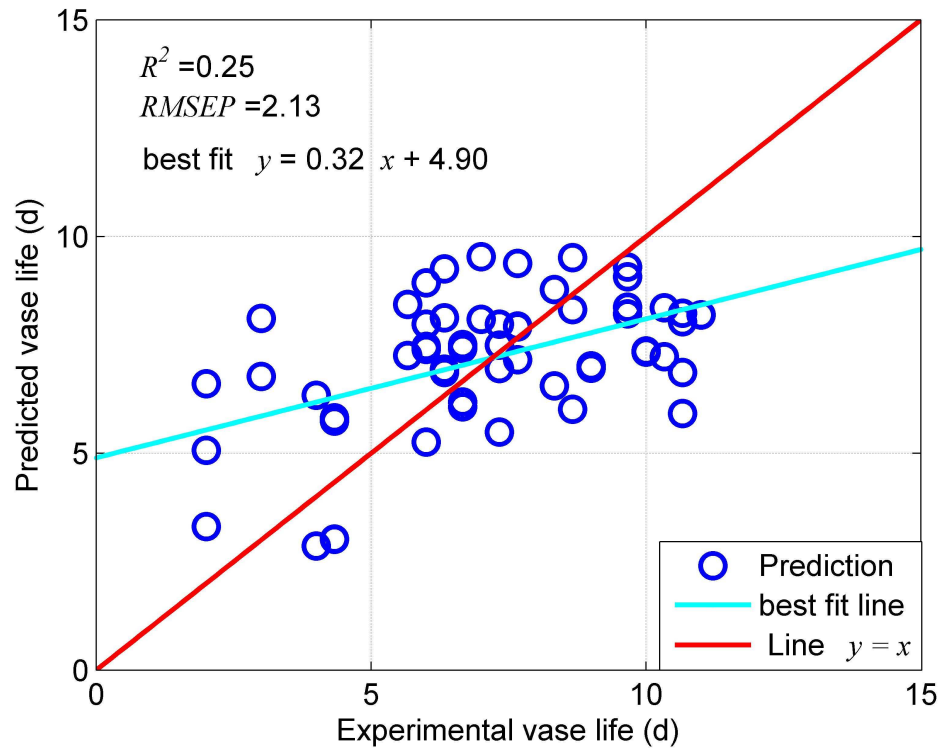
Figure 6.23: Scenario 1A – a typical PLS performance in modelling the office display period <u>without</u> the *a priori* constraint. (auto-scaling)

Table 6.5: Scenario 1A – PLS performance using different scaling strategies. "Actual" results were obtained using original data while "nonsense" results were from permutation studies. 1000 repetitions of double cross validation studies were performed. (10000 PLS models were generated.) All statistics are presented as mean ± standard deviation.

Scaling strategy		Zero-mean	Auto-scaling
Predicted output		ΔVL (d) during office display (mean = 7.2; min = 2; max = 11)	
Number of models (out of 10000) that used only one PLS factor		7832	9954
RMSEP	actual	2.2 ± 0.1	2.1 ± 0.1
	nonsense	2.4 ± 0.1	2.4 ± 0.1
	p-value	0.11	0.02
	q-value	0.26	0.02
R^2	actual	0.21 ± 0.03	0.24 ± 0.02
	nonsense	0.16 ± 0.03	0.15 ± 0.04
Slope	actual	0.30 ± 0.03	0.31 ± 0.02
	nonsense	0.26 ± 0.02	0.27 ± 0.03
Intercept	actual	5.02 ± 0.20	4.98 ± 0.15
	nonsense	5.31 ± 0.15	5.27 ± 0.27

In addition, results from the nonsense data suggested that 1000 repetitions were not statistically sufficient. Distributions of nonsense R^2 had a statistical mean around 0.15, which is significantly different from 0; the nonsense slopes and intercepts indicated that the nonsense best fit lines were not horizontal. These contradict with the characteristics of the nonsense predictions, which are not correlated with the observed VLs. The reason for the contradiction was that the nonsense data from the 1000 repetitions of the permutation testing were not representative of their statistical population, which is uncorrelated to the observed VLs. Consequently, increasing the number of the repetitions would eventually eliminate the contradiction and produce distributions of nonsense R^2 around zero, distributions of the best fit lines around a horizontal line.

6.7.3.3 SCENARIO 1B – WITH THE *A PRIORI* CONSTRAINT

No PLS algorithm has been identified to implement the *a priori* constraint. Consequently, PLS modelling is not available for this scenario.

6.7.4 MLR PERFORMANCE

6.7.4.1 DATA PRE-PROCESSING

Data pre-processing for MLR modelling was similar to that for PLS modelling (Section 3.1.1). In addition, as explained in Section 3.1.2, temperature readings in the original input profiles were averaged over a window of size k. The optimal parameter k was determined during the cross-validation exercise.

Moreover, two schemes of data scaling including auto-scaling and zero-mean scaling (Section 6.7.3.1) were also studied.

6.7.4.2 SCENARIO 1A – WITHOUT THE *A PRIORI* CONSTRAINT

Numerical results of MLR modelling without the *a priori* constraint are tabulated in Table 6.6. A typical performance of MLR modelling using auto-scaling without the *a priori* constraint is presented in Figure 6.24. A similar figure for zero-mean scaling can be found in Appendix B (Figure B. 2). The optimal window size for averaging temperature readings (Section 3.1.2) was $k = 2$ when the data was either auto-scaled or zero mean. It meant that only temperature averaged over 2 x 0.5 = 1 h should be used in these cases.
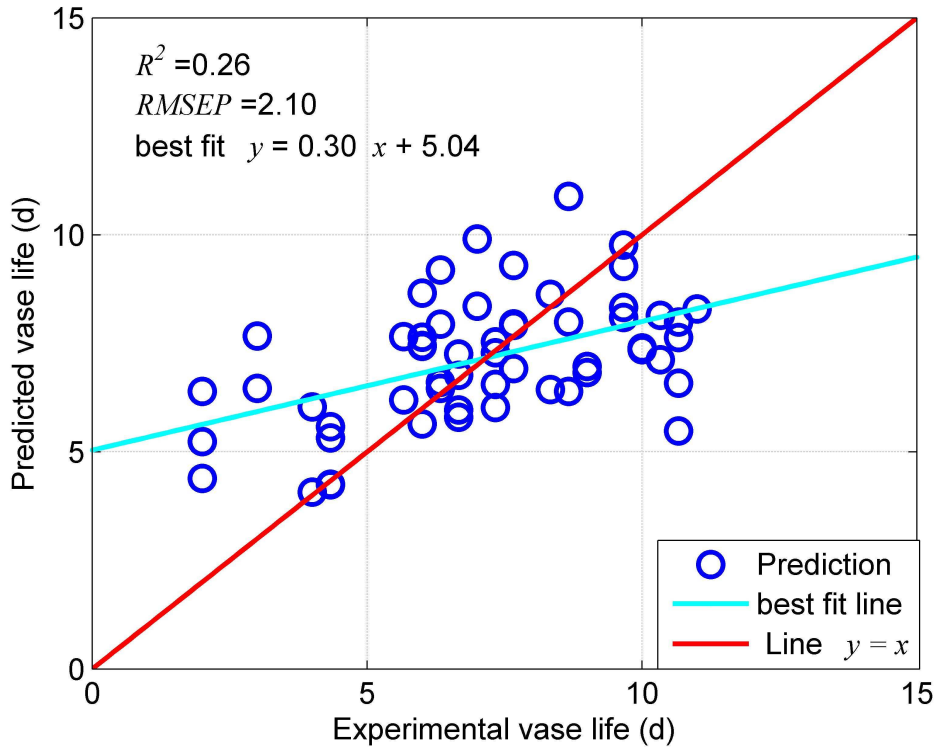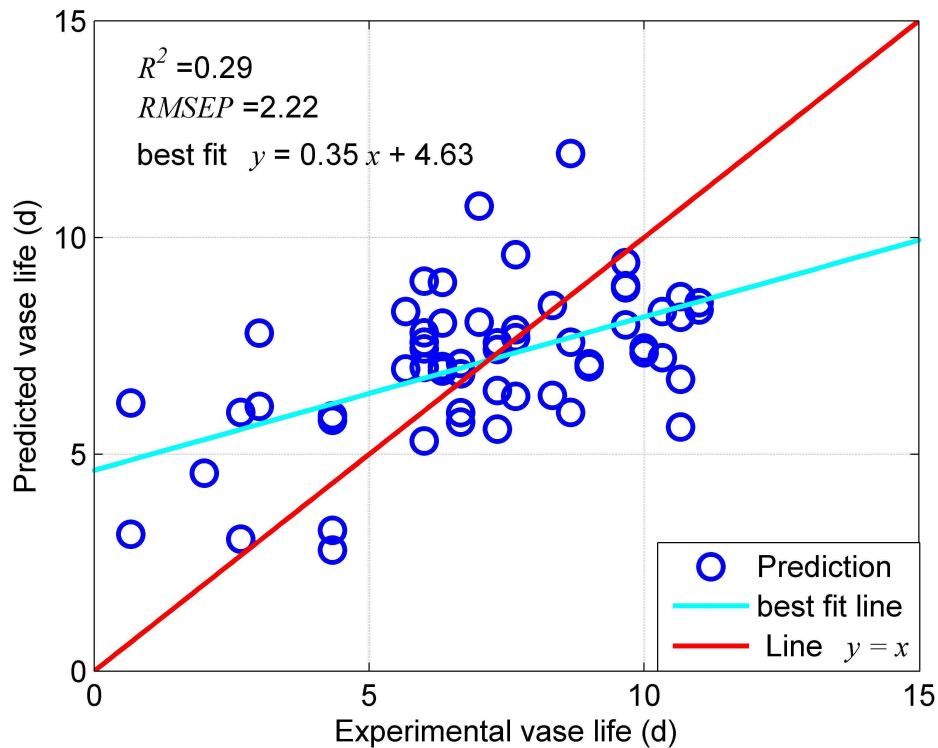
Figure 6.24: Scenario 1A – a typical MLR performance in modelling the office display period <u>without</u> the *a priori* constraint. (auto-scaling)

Comparing the actual and nonsense distributions of the selected statistics indicated that MLR performance was far from adequate. For zero-mean scaling, the actual performance was only as good as the nonsense results. In particular, both actual and nonsense MLR models produced virtually the same *RMSEP*. For auto-scaling, while the actual *RMSEP* was smaller than the nonsense one, the variations in both actual and nonsense distributions were significant, which led to substantial overlaps between the two distributions. Consequently, MLR modelling failed to make effective estimates (Section 3.2.4) for the remaining VL of the cut roses in this case.

Table 6.6: Scenario 1A – MLR performance using different scaling strategies. (100 repetitions)

Scaling strategy		Zero-mean	Auto-scaling
Predicted output		ΔVL (d) during office display (mean = 7.2; min = 2; max = 11)	
Optimal window size k		2.0 ± 1.1	2.1 ± 0.9
RMSEP	actual	2.3 ± 0.1 ^{NS}	2.3 ± 0.1
	nonsense	2.3 ± 0.1 ^{NS}	4.6 ± 1.7
	p-value	0.98	0.21
	q-value	0.93	0.11
R^2	actual	0.29 ± 0.01	0.26 ± 0.03
	nonsense	0.29 ± 0.01	0.08 ± 0.08
Slope	actual	0.31 ± 0.03	0.33 ± 0.02
	nonsense	0.24 ± 0.02	0.31 ± 0.07
Intercept	actual	4.86 ± 0.13	4.76 ± 0.12
	nonsense	5.38 ± 0.18	4.39 ± 0.94

(^{NS}: not significant i.e. the mean of the actual distribution is not smaller than that of the nonsense one at 5% significant level; see Section 3.2.4)

6.7.4.3 SCENARIO 1B – WITH THE *A PRIORI* CONSTRAINT

Similar to KLS modelling with the *a priori* constraint, slack variables were also introduced in MLR modelling to account for the non-thermal factors such as genotype and variation in conditions prior to the modelling period as well as any other effects that were not related to post-harvest temperature. The model obtained was described in Equation (3.8) (Section 3.3.1). Quadratic programming optimisation was formulated in a similar approach as that which was described in Section 4.3.4. The objective was to minimise the variance of the slack variables. Figure 6.25 shows a typical MLR performance using auto-scaling. A similar figure for zero-mean scaling can be found in Appendix B (Figure B. 3). The prediction performance is summarised in Table 6.7.
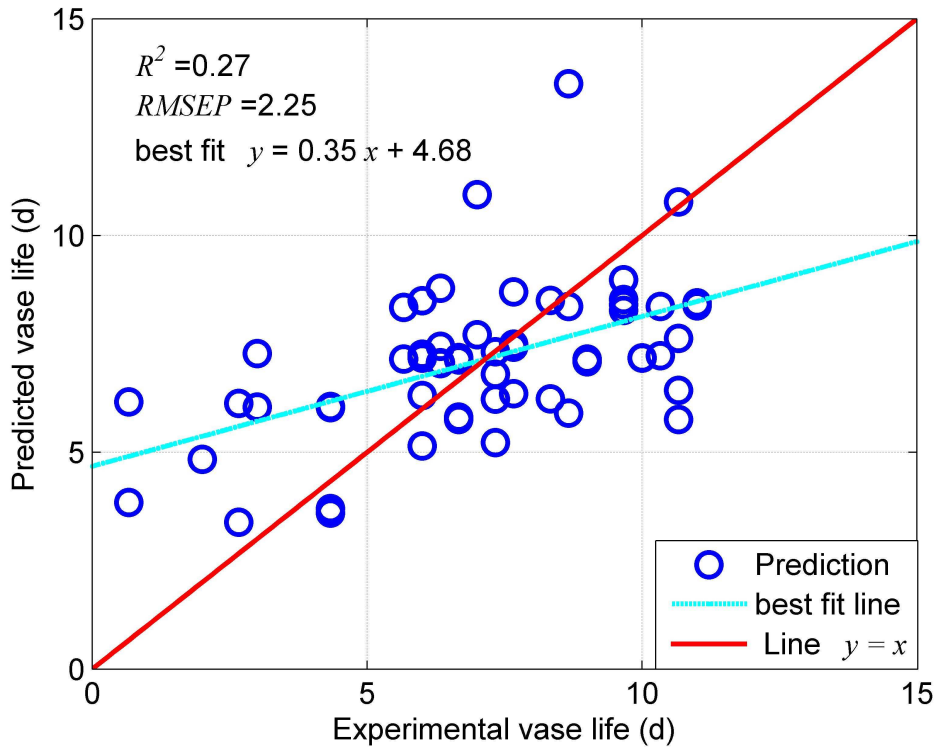
Figure 6.25: Scenario 1B – a typical MLR performance in modelling the office display period <u>with</u> the *a priori* constraint. (auto-scaling)

Table 6.7: Scenario 1B – MLR performance using different scaling strategies. (10 repetitions)

Scaling strategy		Zero-mean	Auto-scaling
Predicted output		ΔVL (d) during office display (mean = 7.2; min = 2; max = 11)	
Optimal window size k		29 ± 55	60 ± 93
RMSEP	actual	2.2 ± 0.0	2.2 ± 0.0
	nonsense	2.4 ± 0.2	2.3 ± 0.1
	p-value	0.50	0.90
	q-value	0.20	0.30
R^2	actual	0.29 ± 0.02	0.28 ± 0.02
	nonsense	0.22 ± 0.05	0.23 ± 0.03
Slope	actual	0.34 ± 0.01	0.33 ± 0.01
	nonsense	0.28 ± 0.02	0.27 ± 0.01
Intercept	actual	4.70 ± 0.06	4.74 ± 0.06
	nonsense	5.18 ± 0.07	5.19± 0.05

As shown in Table 6.7, MLR modelling with the *a priori* constraint also performed poorly. Although the mean of the actual *RMSEP* distribution was slightly smaller than that of the nonsense one, the difference was just equal to one standard deviation; the p-values and q-values were significantly greater than 0.10. So, there was considerable overlap between the real model and the nonsense one. This also occurred in the R^2 statistic. Consequently, as set out in Section 3.2.4, MLR modelling failed to make an effective prediction in this case.

In addition, in scenarios A and B (without and with the *a priori* constraint), only 100 and 10 repetitions respectively of the cross validation were performed. The reason was because MLR modelling took about 3 h (scenario A) and 16 h (scenario B) to complete an iteration. Consequently, it was not practical to increase the number of the repetitions in MLR modelling. However, the results from permutation testing indicate that the number of the repetitions was not statistically sufficient. Distributions of nonsense R^2, slopes and intercepts suggested that there was some correlation between the nonsense predictions and the observed VLs, which was not true. Increasing the number of the repetitions would eliminate this spurious correlation although significant computation time is likely involved.

6.7.5 DISCUSSION

Scenario 1, modelling the office display period, represents the scenario with the most complete data, which included the temperature stress and the corresponding loss in VL. Using the data set, KLS, PLS and MLR modelling were performed and their prediction performance was assessed based on *RMSEP*, R^2 and the slope and intercept of the best fit line, and by comparing with the results from permutation testing. In addition, the feasibility of implementing the *a priori* knowledge observed in the literature was also explored.

Table 6.8: Summary of KLS, PLS and MLR performance in Scenario 1. The best value of the actual statistics from different techniques is highlighted in blue colour.

Statistics		Scenario 1A (without the *a priori* constraint)			Scenario 1B (with the *a priori* constraint)		
		KLS	PLS	MLR	KLS	PLS	MLR
RMSEP	Actual	2.3 ± 0.1	2.1 ± 0.1	2.3 ± 0.1	2.1 ± 0.0	–	2.2 ± 0.0
	Nonsense	3.7 ± 0.0	2.4 ± 0.1	4.6 ± 1.7	3.0 ± 0.0	–	2.4 ± 0.2
	p-value	0.00	0.02	0.21	0.00	–	0.50
	q-value	0.00	0.02	0.11	0.00	–	0.20
R^2	Actual	0.32 ± 0.02	0.24 ± 0.02	0.26 ± 0.03	0.24 ± 0.02	–	0.29 ± 0.02
	Nonsense	0.00 ± 0.00	0.15 ± 0.04	0.08 ± 0.08	0.00 ± 0.00	–	0.22 ± 0.05
Slope	Actual	0.57 ± 0.02	0.31 ± 0.02	0.33 ± 0.02	0.31 ± 0.01	–	0.34 ± 0.01
	Nonsense	0.04 ± 0.02	0.27 ± 0.03	0.31 ± 0.07	0.08 ± 0.01	–	0.28 ± 0.02
Intercept	Actual	2.79 ± 0.10	4.98 ± 0.15	4.76 ± 0.12	4.90 ± 0.09	–	4.70 ± 0.06
	Nonsense	6.26 ± 0.13	5.27 ± 0.27	4.39 ± 0.94	6.53 ± 0.11	–	5.18 ± 0.07

The best performances of KLS, PLS and MLR in Scenario 1, modelling the office display period, are summarised in Table 6.8. Statistical performance assessment was described in detail in Section 3.2.4. Essentially, a distinct separation between the actual distributions of the performance indices and the nonsense ones suggests that the models are finding some features that allow for the prediction of the remaining VL. This occurred in scenarios with KLS, where there was no overlap between the actual and nonsense distributions of $RMSEP$, R^2, and the slope and intercept of the best fit line. In contrast, for PLS there was some overlap, particularly in the distributions of R^2, slope and intercept while for MLR models, the overlaps were much more significant. Therefore, MLR models did not perform adequately without or with the *a priori* constraint.

KLS without the *a priori* constraint had the best values of R^2, slope and intercept. The highest R^2 indicates that the linear correlation between the KLS predictions and the observed VLs was the strongest in this case; the best values of the slope and intercept suggest that the best fit line was closest to the line $y = x$. Although its $RMSEP$ (2.3 d) was not the smallest $RMSEP$ (2.1 d), in terms of improvement over the nonsense performance, KLS in Scenario 1A was by far the best, having its actual $RMSEP$ 1.3 d smaller the corresponding nonsense $RMSEP$. Consequently, KLS performance without the *a priori* constraint is the best among the techniques in Scenarios 1A and 1B.

Similarly, the performance of PLS in Scenario 1A was very close to that of KLS in Scenario 1B although the latter had much better distinction between the actual and nonsense performances. Therefore, it is concluded that KLS is the best technique in making effective predictions in Scenario 1 while PLS performance might still be acceptable. However, MLR was the worst of the three as it clearly could not differentiate between the original data and the nonsense (permutated) data.

However, the above performance comparison between KLS, PLS and MLR assumed that the actual and nonsense distributions of the performance

statistics were approaching their statistical population distributions. By examining the nonsense distributions, this assumption seems reasonable in KLS modelling but not in PLS and MLR. As can be seen in Table 6.8, the nonsense R^2 and the slope of KLS performance were very close to 0.0, illustrating the characteristics of the nonsense predictions: having no correlation with the observed VLs. This was not the case for PLS and MLR nonsense performances, where some spurious correlation was implied. The consequence is that increasing the number of repetitions in cross validation studies may eventually eliminate the spurious correlation. However, the computational cost and time requirement have made this exhaustive investigation for PLS and MLR modelling prohibitive in this study.

Regarding the comparison between Scenarios 1A and 1B, a number of studies suggested that the higher the storage temperature the greater the loss in VL (Section 3.3). This hypothesis was transformed into an *a priori* constraint which was implemented in Scenarios 1B for KLS and MLR techniques (no algorithm for PLS with constraints was identified and so this could not be investigated). The implementation of the *a priori* constraint slightly improved the prediction error $RMSEP$ but at a significant cost to the best fit line (i.e., moving further away from the equality line $y = x$) and R^2 (Table 6.8). The reason for a poorer performance could be associated with the validity of the assumption that was made in implementing the *a priori* constraint. It should be noted that the implementation (Section 4.3.6) required the non-thermal factors that affect the VLs of cut roses to be accounted for (Sections 3.3 and 6.7.2.3). In turn, the modelling of the non-thermal factors made an assumption of minimum variance in those factors (Section 4.3.4). While this assumption was necessary to solve for a KLS model, it may not always be reasonable. As the exploratory analysis (Figure 6.10) shows, seasonality had a clear impact on the displaying temperature. Therefore, it is expected that other non-thermal factors during the display period such as humidity could also vary with seasonality as well, which does not support the minimum variance assumption. In addition, as shown in subsequent sections growing conditions, which are expected to have significant effects on the VLs of the flowers, also varied significantly across seasons (and

hence harvests). Consequently, the assumption of minimum variance may not be strongly supported, which could lead to a poorer KLS performance.

6.8 SCENARIO 2 – MODELLING THE POSTAL DELIVERY PERIOD

In Scenario 2, the period of transport of cut roses from Cookes Rose Farm to the University of Manchester was modelled. Temperature readings recorded during the transport and VLs from the vase life tests were included in the analysis. The objective was to estimate the loss in remaining VLs of the roses during the postal delivery from Cookes Rose Farm to the University.

Data available for this Scenario included a total of 30 profiles (one from each of the 30 boxes) of temperature readings recorded during the delivery process. In addition, the remaining VL of the flowers upon receipt at the University of Manchester was estimated by the duration of their subsequent vase life tests. However, the initial VL at the farm was not available. Consequently, the assumption that all cut roses had the same initial VLs was explored. Later, this assumption was relaxed to allow the flowers in the same box to have the same initial VL, which could be different from that of other boxes.

6.8.1 EXPLORATORY STUDY

A total of 30 boxes of cut roses were sent from Cookes Rose Farm to the University of Manchester. Two data loggers were placed inside each of the boxes, with one data logger located at each end of the box, recording temperature during postal delivery. As shown earlier (Section 6.6.2), the difference in the temperature recorded by the two data loggers in each box was negligible. Consequently, the mean of the readings from the two data loggers in each box was used. As a result, there were 30 profiles of transport temperature in the data set. Figure 6.26 shows three of the 30 profiles. The blue curve corresponding to the shortest profile was from a box that took only one day to arrive at the University. On the other hand, the longest profile, shown by the red line, had 144 readings, which was equivalent to three days of transport. Most often, a box of cut roses would take two days to reach the University, as shown by the third profile.
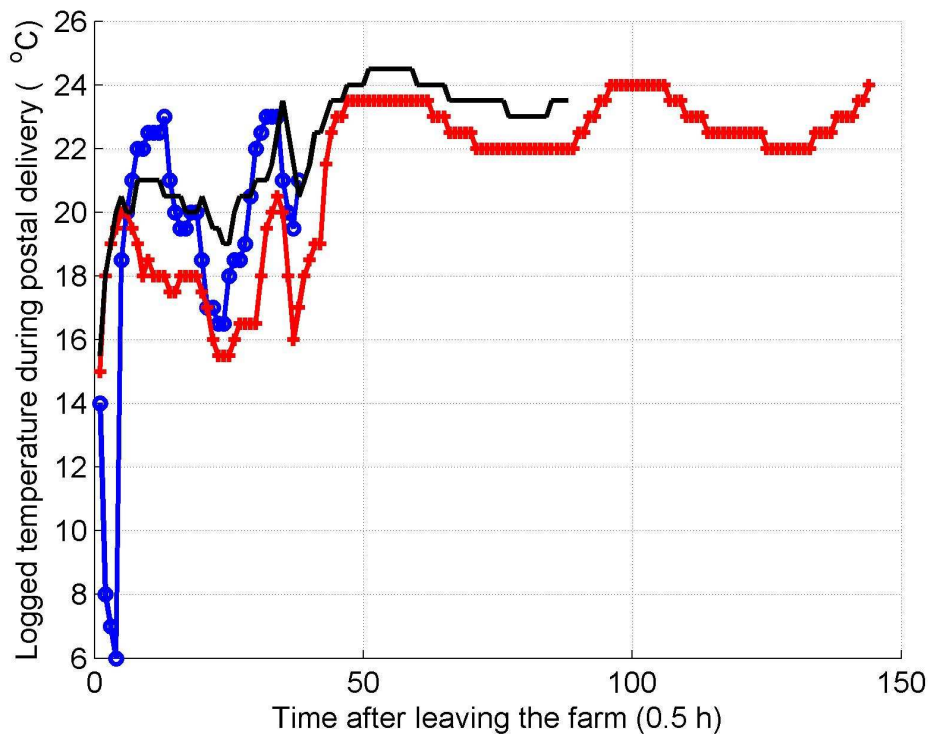
Figure 6.26: Three temperature profiles logged during postal delivery of boxes of cut roses from Cookes Rose Farm to the University of Manchester. The blue (o) and red (+) profiles correspond to the profiles with minimum and maximum lengths i.e. number of measurements respectively. The other profile is an example that had the number of readings somewhere in between.

After data pre-processing (Section 3.1.1), PCA was performed on the data set. The analysis revealed that the first two PCs accounted for more than 60% of data variance. The score plots for the first and second LVs are presented in Figure 6.27 and Figure 6.28. The observations were grouped according to the month of the delivery date of the rose samples in Figure 6.27, and according to the range of the final remaining VL (upon delivery to the University) in Figure 6.28. As seen in Figure 6.27, the September deliveries are significantly separated from the July and August ones. This separation means that the transport temperature during September was quite different from that during August and July. As the temperature was not regulated during the postal delivery, it was reasonable to expect the transport temperature to correlate with the outside air temperature, which in turn is subject to seasonal variations.
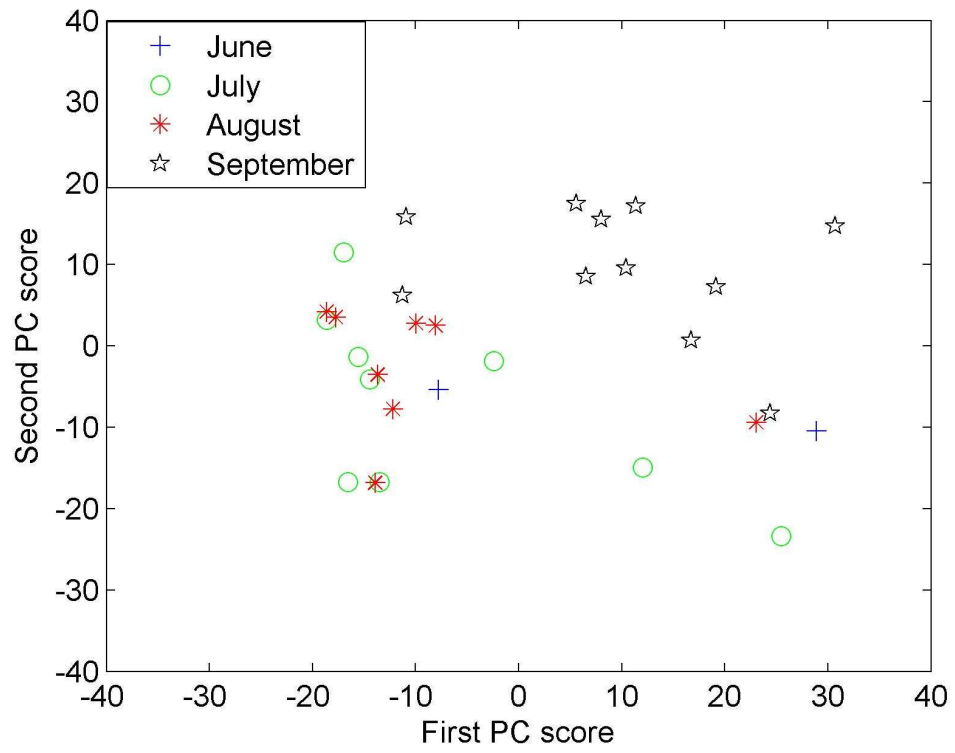
Figure 6.27: PCA score plot for the first and second PCs, which together explain 61.1% of the total variance. Different symbols represent different delivery date (month).
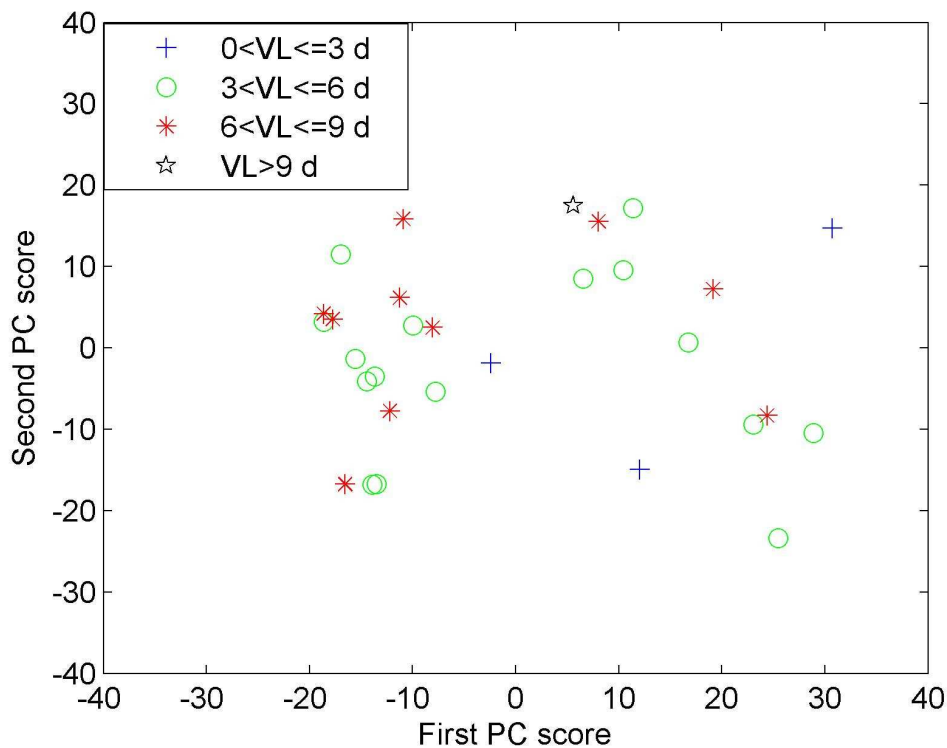
Figure 6.28: PCA score plot for the first and second PCs, which together explain 61.1% of the total variance. Different symbols represent different range in VL loss.

Figure 6.28 shows the PCA score plot (for the first and second LVs) with observations grouped according to ranges of the remaining VL of cut roses on delivery to the University of Manchester. No clear trend between the groups of VL could be observed, which suggests that estimating VL using the transport temperature would be challenging.

6.8.2 KLS PERFORMANCE

6.8.2.1 SETTING PARAMETERS

A similar procedure as described in Section 6.7.2.1 was carried out. Using the temperature profiles of the cut roses being transported from Cookes Rose Farm to the University, the lower and upper bounds of temperature in Scenario 2 were set at 14 ^{o}C and 24 ^{o}C respectively. The temperature step was set at 1 ^{o}C as a result of the data loggers' accuracy (Section 6.6.1).

6.8.2.2 SCENARIO 2A – WITHOUT THE *A PRIORI* CONSTRAINT

As the initial VLs of cut roses just before entering the postal system were not available, assumptions had to be made regarding these initial VLs (Section 4.3.5). It was assumed that all the flower samples entered the postal system with the same initial VLs, which were constant yet unknown. This assumption ignores potential variation in the VL of cut roses immediately after harvest due to pre-harvest factors such as biological variation and growing conditions. Details of the solution strategy were outlined in Section 4.3.5. KLS performance was evaluated in 1000 repetitions of cross validation; a typical performance is shown in Figure 6.29 and the numerical results are summarised in Table 6.9.

The plot shows:

$R^2 =0.05$
$RMSEP =2.51$
best fit $y = 0.12\,x + 6.37$

with axes "Experimental vase life (d)" (x-axis) and "Predicted vase life (d)" (y-axis), and a legend: Prediction, best fit line, Line $y = x$.
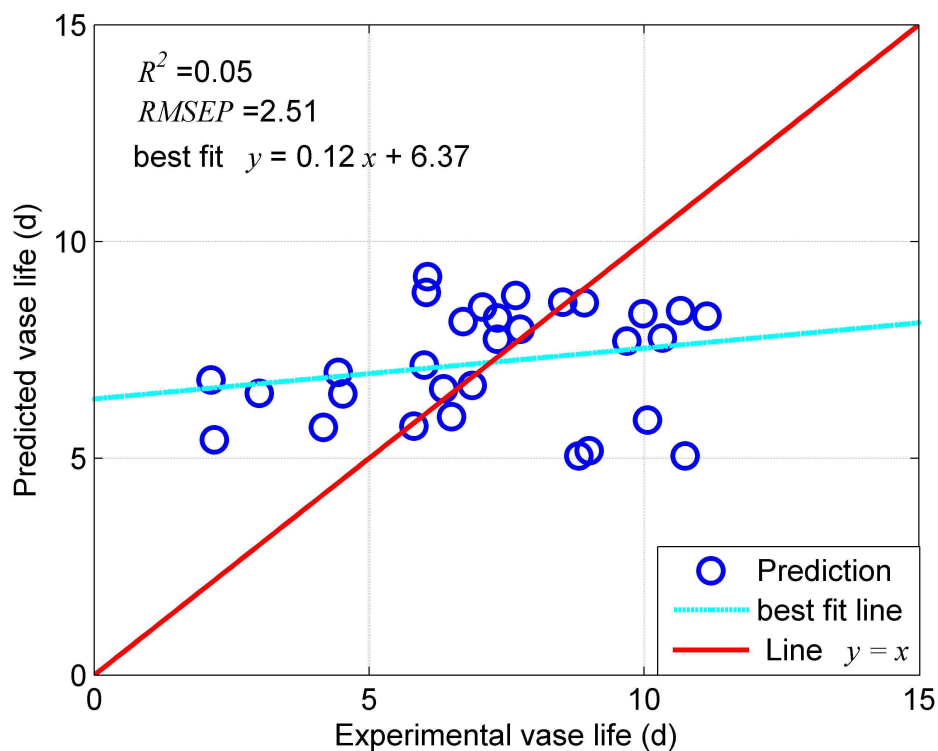
Figure 6.29: Scenario 2A – a typical KLS performance in modelling the VL upon delivery at University of Manchester assuming uniform initial VLs (<u>without</u> the *a priori* constraint).

Subsequently, the assumption of a uniform initial VL was relaxed by allowing the initial VL to vary from one harvest (i.e. box) to another. In other words, cut roses in the same delivery box had the same initial VL, which could be different from that of the flowers in another box. Consequently, there were additionally 30 unknown initial VLs (for 30 boxes) to be estimated. The removal of the

assumption of a uniform initial VL made the KLS linear system undetermined, which would normally lead to infinite number of solutions. The optimal solution was sought for such that it minimised the variance of all the initial VLs. Section 4.3.5 described briefly the solution strategy for this undetermined linear system. KLS performance was again evaluated; a typical performance is shown in Figure 6.30 and the numerical results are also summarised in Table 6.9.

Figure 6.30: Scenario 2A – a typical KLS performance in modelling the VL upon delivery at University of Manchester assuming variable initial VLs (<u>without</u> the *a priori* constraint).

The results shown in Figure 6.30 and summarised in Table 6.9 show that KLS estimates were worse than random (nonsense) guesses without the assumption of a uniform initial VL. Specifically, varying the initial VL resulted in a horizontal best fit line and a prediction error of 2.9 d while its corresponding nonsense was 2.8 d. Similarly, actual R^2 is around 0.01, which is smaller than the nonsense R^2 of 0.05. Consequently, in this case KLS estimates did not have a linear relationship with the observed VLs and hence the predictions were not effective.

On the other hand, assuming a uniform initial VL led to minimal differences between the actual performance and the nonsense one, particularly in *RMSEP* and R^2 statistics. The mean of the actual *RMSEP* distribution is 0.2 d smaller than that of the nonsense one. Nevertheless, as the difference is small compared to the standard deviations of the distributions, there are significant overlaps between the actual and nonsense distributions. This is reflected by the significant p-values and q-values. A similar observation can also be made for the R^2 statistic. The magnitude of the statistic ($R^2 \sim 0.05$) suggests that the linear relationship between the predicted and observed VLs was not significant. Consequently, KLS estimates in this case were also not effective.

Table 6.9: Scenario 2A – KLS performance with/without the assumption of a uniform initial VL at the farm (1000 repetitions)

Assumption		Uniform initial VL	Varying initial VL
Predicted output		VL (d) at delivery	
		(mean = 7.2; min = 2; max = 11)	
RMSEP	Actual	2.5 ± 0.1	2.9 ± 0.1 [NS]
	Nonsense	2.7 ± 0.1	2.8 ± 0.0 [NS]
	p-value	0.26	–
	q-value	0.56	–
R^2	Actual	0.05 ± 0.03	0.01 ± 0.01
	Nonsense	0.01 ± 0.01	0.05 ± 0.03
Slope	Actual	0.12 ± 0.03	0.01 ± 0.05
	Nonsense	-0.01 ± 0.03	-0.08 ± 0.01
Intercept	Actual	6.34 ± 0.25	7.24 ± 0.39
	Nonsense	7.23 ± 0.21	7.71 ± 0.04

([NS]: not significant i.e. the mean of the actual distribution is not smaller than that of the nonsense one at 5% significant level; see Section 3.2.4)

6.8.2.3 SCENARIO 2B – WITH THE *A PRIORI* CONSTRAINT

In this scenario, the *a priori* observation that a higher temperature leads to a greater loss in VLs was implemented. The observation was expressed as a mathematical constraint that the KLS coefficients must be positive and increase

with temperature. Details of the mathematical manipulation were described in Section 4.3.6

As in Scenario 2A, the initial VLs just before entering the postal delivery system were assumed uniform across all the boxes of cut roses. In other words, the initial VLs were constant, albeit unknown. Details of the solution strategy were outlined in Section 4.3.5. KLS performance was evaluated in 1000 repetitions of cross validation. A typical performance is shown in Figure 6.31 and the numerical results are summarised in Table 6.10.
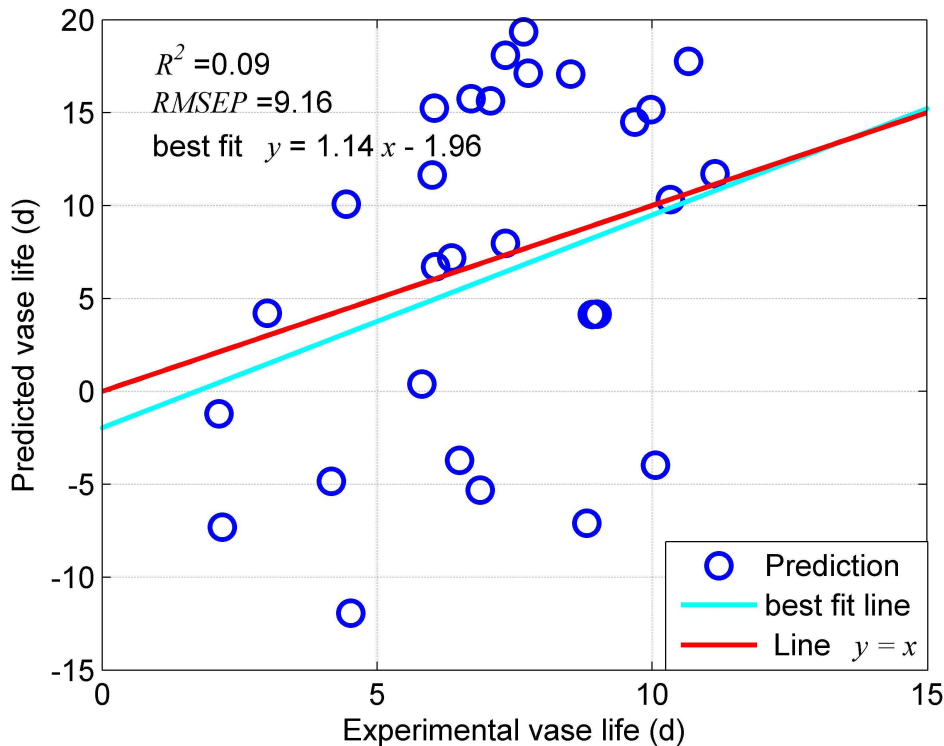
Figure 6.31: Scenario 2B – a typical KLS performance in modelling the VL upon delivery at University of Manchester assuming uniform initial VLs (<u>with</u> the *a priori* constraint).

Subsequently, the assumption of uniform initial VLs was relaxed by allowing them to vary from one delivery box to another. In this case, the initial VLs were considered as additional coefficients to be estimated. Similar to Scenario 2A, the optimal solution that minimised the variance of all the initial VLs was sought for (Section 4.3.5). KLS performance was again evaluated, illustrated in Figure 6.32 and summarised in Table 6.10.
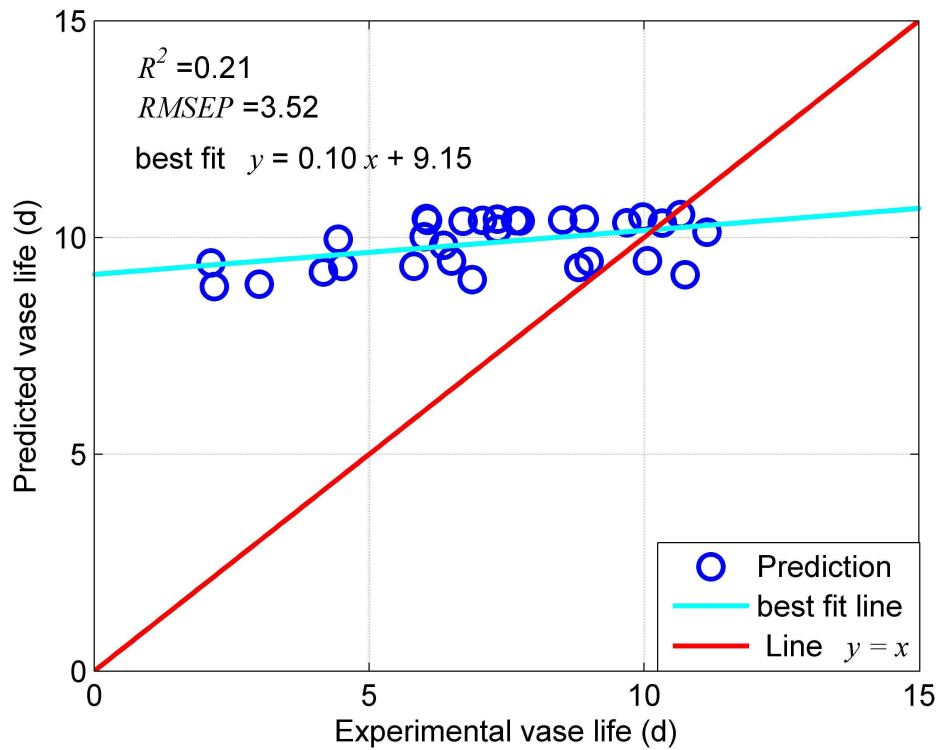
Figure 6.32: Scenario 2B – a typical KLS performance in modelling the VL upon delivery at University of Manchester assuming variable initial VLs (<u>with</u> the *a priori* constraint).

Table 6.10: Scenario 2B – KLS performance with/without assumption on initial VL at the farm (1000 repetitions)

Assumption		Uniform initial VL	Varying initial VL
Predicted output		VL (d) at delivery (mean = 7.2; min = 2; max = 11)	
RMSEP	Actual	9.1 ± 0.2	3.6 ± 0.0
	Nonsense	9.8 ± 0.2	3.8 ± 0.0
	p-value	0.06	0.00
	q-value	0.08	0.00
R^2	Actual	0.09 ± 0.01	0.19 ± 0.04
	Nonsense	0.00 ± 0.00	0.04 ± 0.02
Slope	Actual	1.12 ± 0.07	0.09 ± 0.01
	Nonsense	0.13 ± 0.06	-0.04 ± 0.01
Intercept	Actual	-1.68 ± 0.55	9.23 ± 0.01
	Nonsense	5.24 ± 0.47	10.21 ± 0.09

Figure 6.31, Figure 6.32 and Table 6.10 show that KLS performed poorly with the *a priori* constraint, regardless of whether the initial VLs were assumed uniform or variable across the boxes. Average prediction error was about 3.6 d (assuming variable initial VLs) - 9.1 d (assuming uniform initial VLs), which is rather excessive considering the average observed VLs was 7.2 d. In addition, When uniform initial VLs were assumed, the variance in the predictions was significant (Figure 6.31); in contrast, the assumption of variable initial VLs led to minimal variance in the predictions. The two cases appear to illustrate the two extremes: one with too strict an assumption (i.e. uniform initial VLs) and one with too loose an assumption (i.e. variable initial VLs). In both cases, the variance in the observed VLs was not captured and hence KLS performance was not effective.

6.8.3 PLS PERFORMANCE

6.8.3.1 DATA PRE-PROCESSING

The same data set that was previously analysed by KLS technique was studied using PLS technique. The assumption of a uniform initial VL and the two scaling strategies including auto-scaling and zero-mean scaling (Section 6.7.3.1) were also investigated.

PLS modelling technique requires a uniform number of measurements per input sample. To overcome this issue, the strategy, which was described in Section 3.1.1, was essentially to use reference temperature $T_{ref} = 18\ ^{o}\mathrm{C}$ to make up for any data samples that had fewer than the required number of measurements.

6.8.3.2 SCENARIO 2A – WITHOUT THE *A PRIORI* CONSTRAINT

Similar to Scenario 2 for KLS (Section 6.8.2.2), PLS modelling required an assumption of the initial VL of cut rose samples just before entering the postal delivery system. Under the assumption of a uniform initial VL, results of PLS modelling in Scenario 2A are tabulated in Table 6.11. A typical PLS performance using auto-scaling is shown in Figure 6.33. A similar figure for zero-mean scaling can be found in Appendix B (Figure B. 4). In addition, without being assumed constant, the initial VLs were unknown variables that were

greater than the remaining VLs as evaluated at the University. As PLS was not capable of implementing such constraints, PLS without the assumption on initial VL was not considered.
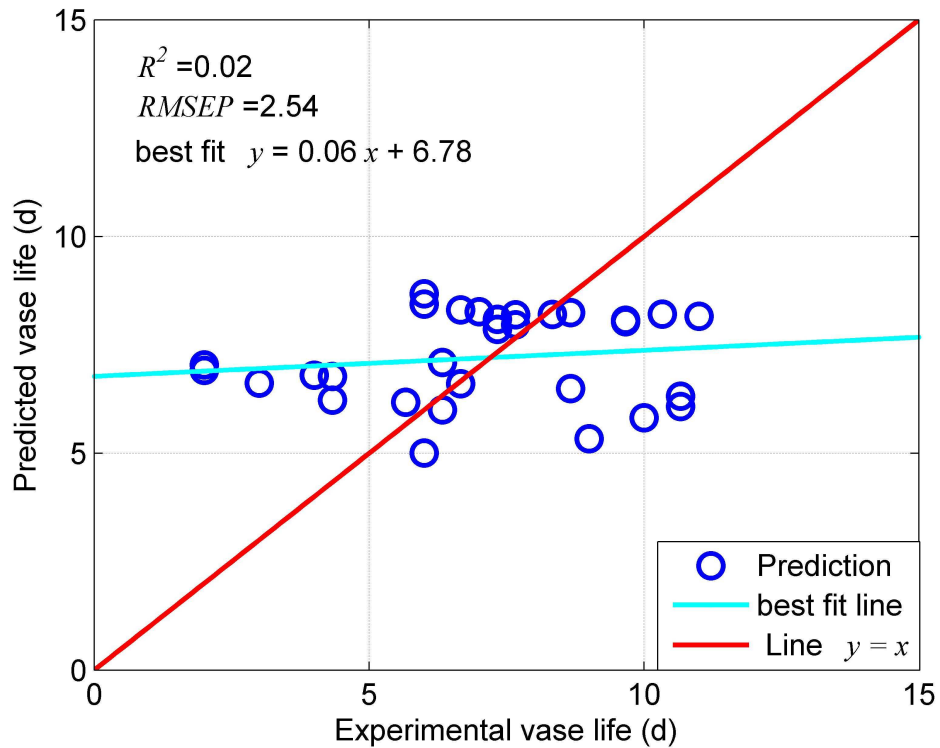
Figure 6.33: Scenario 2A – a typical PLS performance in modelling the VL upon delivery at University of Manchester assuming uniform initial VLs (<u>auto-scaling</u>).

The results in Table 6.11 show that PLS models on the actual data performed worse than on the nonsense data. For both scaling techniques, the mean of the actual $RMSEP$ distribution was greater than that of the nonsense distribution. On this basis, PLS performance was not acceptable.

Table 6.11: Scenario 2A – PLS performance under the assumption of uniform initial VL using different scaling strategies (10000 repetitions, 10^5 PLS models)

Scaling strategy		Zero-mean	Auto-scaling
Predicted output		VL (d) at delivery (mean = 7.2; min = 2; max = 11)	
Number of models (out of 10^5) that used only one PLS factor		94225	96386
RMSEP	Actual	2.5 ± 0.2 [NS]	2.6 ± 0.2 [NS]
	Nonsense	2.4 ± 0.1 [NS]	2.5 ± 0.1 [NS]
	p-value	–	–
	q-value	–	–
R^2	Actual	0.06 ± 0.04	0.05 ± 0.03
	Nonsense	0.12 ± 0.05	0.04 ± 0.03
Slope	Actual	0.12 ± 0.05	0.07 ± 0.07
	Nonsense	0.12 ± 0.03	0.07 ± 0.04
Intercept	Actual	6.27 ± 0.05	6.75 ± 0.51
	Nonsense	5.99 ± 0.25	6.58 ± 0.25

6.8.3.3 SCENARIO 2B – WITH THE *A PRIORI* CONSTRAINT

As discussed previously, as no PLS algorithm has been identified to implement the *a priori* constraint this was not tested.

6.8.4 MLR PERFORMANCE

6.8.4.1 DATA PRE-PROCESSING

Data pre-processing for MLR modelling in Scenario 2 was similar to that which was carried out in Scenario 1 (Section 6.7.4.1).

Moreover, an assumption of the initial VL at the farm was studied in a similar way as for KLS techniques (Section 6.8.2). Two data scaling techniques were explored including auto-scaling and zero-mean scaling.

MLR performance based on a uniform initial VL assumption and without the *a priori* constraint is tabulated in Table 6.12. A typical MLR performance using auto-scaling is presented in Figure 6.34. A similar figure for zero-mean scaling can be found in Appendix B (Figure B. 5). Clearly, MLR performance was not adequate. As seen in Table 6.12, the actual predictions were not better than the nonsense estimates. Prediction error based on actual data was not less than that from the permutated data. Figure 6.34 also shows that all of the predicted VLs varied around 6 d while the observed ones varied from 1 to 11 d. This indicates that minimal variance in the VL was captured by MLR modelling. This may be attributed to the fact that the MLR model was over-fitting: there were more independent variables than the number of flower samples. Consequently, MLR modelling could not produce effective estimates of the VLs in this scenario.
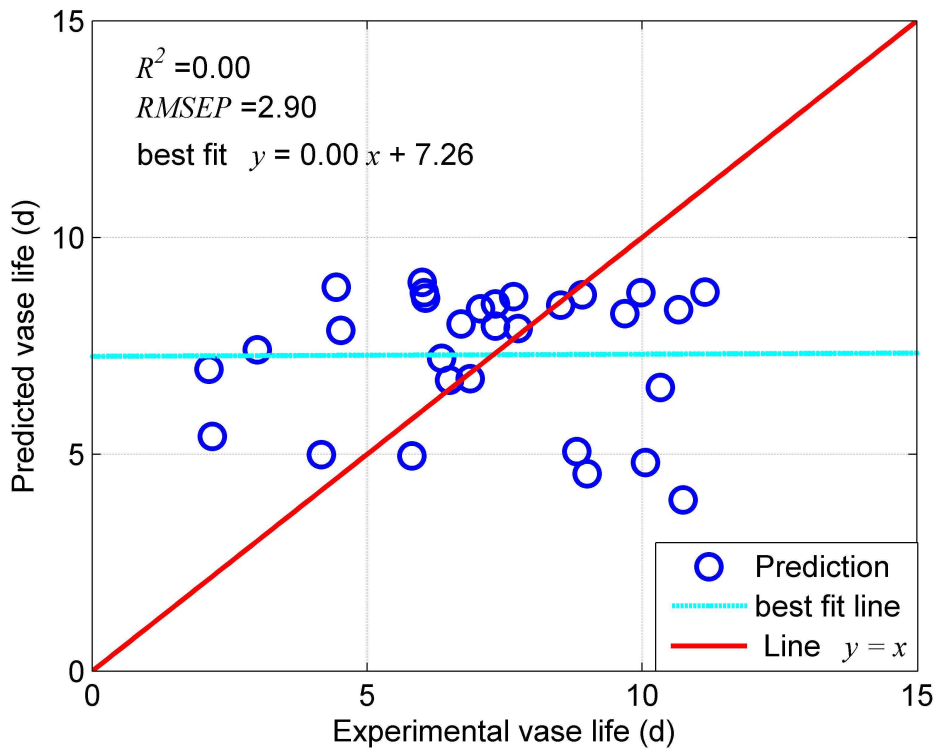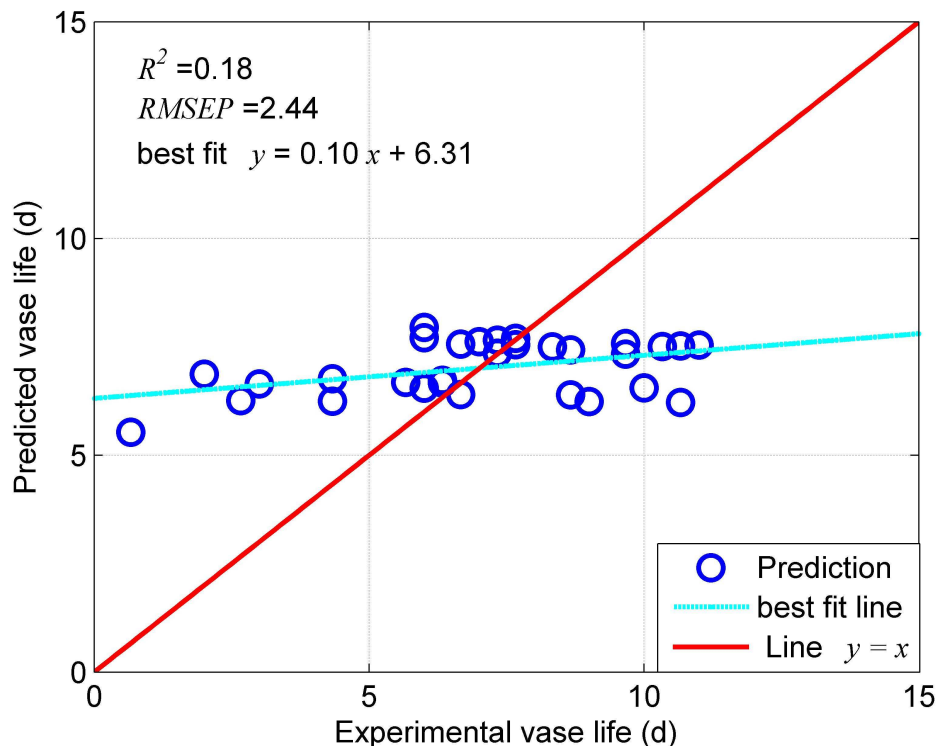

Figure 6.34: Scenario 2A – a typical MLR performance in modelling the VL upon delivery at University of Manchester assuming uniform initial VLs (<u>auto-scaling, without *a priori* constraint</u>).

Table 6.12: Scenario 2A – MLR performance using different scaling strategies. Uniform initial VLs was assumed (1000 repetitions)

Scaling strategy		Zero-mean	Auto-scaling
Predicted output		VL (d) at delivery	
		(mean = 7.2; min = 2; max = 11)	
Optimal window size k		29 ± 0	29 ± 0
RMSEP	Actual	2.5 ± 0.2 ^{NS}	2.5 ± 0.0 ^{NS}
	Nonsense	2.4 ± 0.1 ^{NS}	2.5 ± 0.0 ^{NS}
	p-value	–	–
	q-value	–	–
R^2	Actual	0.14 ± 0.04	0.14 ± 0.04
	Nonsense	0.14 ± 0.04	0.14 ± 0.04
Slope	Actual	0.12 ± 0.05	0.09 ± 0.01
	Nonsense	0.16 ± 0.03	0.09 ± 0.01
Intercept	Actual	6.27 ± 0.42	6.41 ± 0.08
	Nonsense	5.99 ± 0.25	6.41 ± 0.09

6.8.4.3 SCENARIO 2B – WITH THE *A PRIORI* CONSTRAINT

When the *a priori* constraint was implemented, MLR performance (Table 6.13) improved a little. However, for zero-mean scaling, the mean of the actual *RMSEP* distribution was not smaller than that of the nonsense distribution. For auto-scaling, while the actual mean was smaller than the nonsense one, the standard deviations of the actual and nonsense distributions also became more significant. This led to a significant overlap between the two distributions, as indicated by the significant p-values and q-values. In addition, as can be seen in Figure 6.35, the variance in the observed VLs was not effectively captured in the MLR predictions. As a result, MLR predictions were not adequate for either scaling strategy.
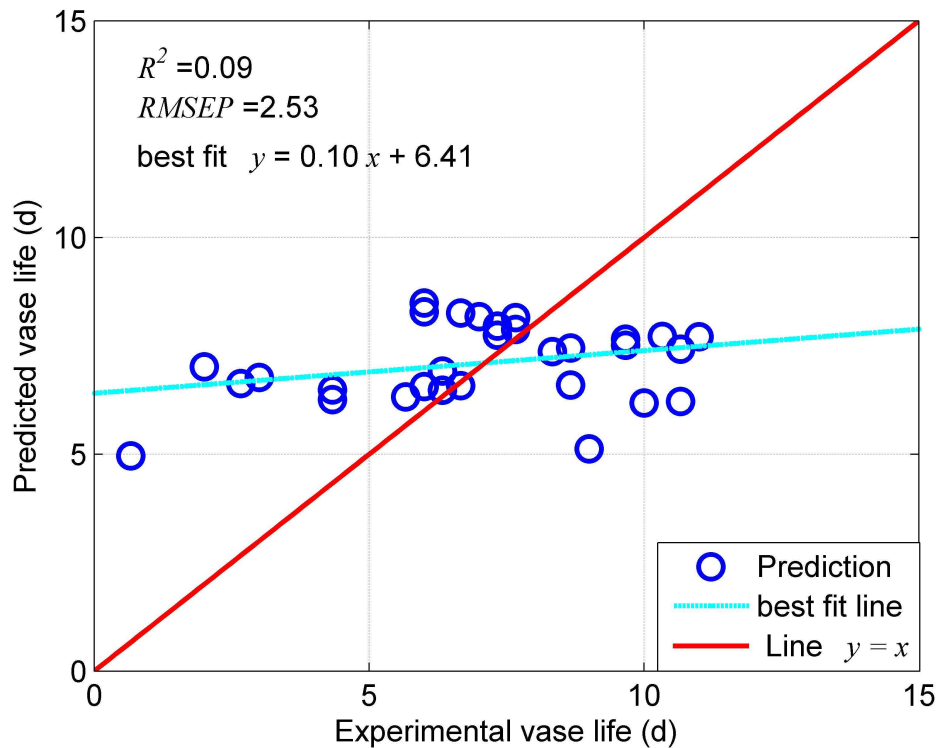
Figure 6.35: Scenario 2B – a typical MLR performance in modelling the VL upon delivery at University of Manchester assuming uniform initial VLs (<u>auto-scaling, with *a priori* constraint</u>).

It should be noted that only 100 repetitions were carried out during the cross validation study of MLR modelling. The reason was because in this case one repetition was much more time consuming than in other cases (e.g., with KLS modelling). Approximately, 100 repetitions of MLR modelling took between 5.5 h and 18 h to complete. (In comparison, 10000 repetitions of KLS modelling took less than 20 min.) This could be due to the greater number of independent variables in MLR modelling. The consequence is that the results from analysing the nonsense permutated data implied some spurious correlation between the nonsense predictions and the observed VLs. Although it is expected that a sufficiently large number of repetitions would eliminate such spurious correlation, the computation cost and hence time requirement made it impractical.

Table 6.13: Scenario 2B – MLR performance using different scaling strategies. Uniform initial VLs was assumed (100 repetitions)

Scaling strategy		Zero-mean	Auto-scaling
Predicted output		VL (d) at delivery (mean = 7.2; min = 2; max = 11)	
Optimal window size k		6 ± 0	6 ± 0
$RMSEP$	Actual	2.5 ± 0.1 [NS]	2.5 ± 0.1
	Nonsense	2.5 ± 0.0 [NS]	2.8 ± 0.5
	p-value	–	0.55
	q-value	–	0.59
R^2	Actual	0.13 ± 0.07	0.10 ± 0.07
	Nonsense	0.12 ± 0.05	0.05 ± 0.05
Slope	Actual	0.13 ± 0.02	0.15 ± 0.04
	Nonsense	0.08 ± 0.01	0.11 ± 0.04
Intercept	Actual	6.13 ± 0.21	6.05 ± 0.30
	Nonsense	6.53 ± 0.09	6.19 ± 0.48

6.8.5 DISCUSSION

Scenario 2, modelling the postal delivery period, represents the scenario with incomplete data. Only temperature during the delivery period and the final remaining VL were available; the initial VLs at the beginning of the period were not known. As a result, the assumption of a uniform initial VL was considered.

Using the data set, KLS, PLS and MLR modelling were performed and their prediction performance was assessed based on $RMSEP$, R^2, and the slope and intercept of the best fit line, and on comparison with the results from permutation testing. (Details of the performance assessment were described in Section 3.2). In addition, the feasibility of implementing an *a priori* knowledge observed in literature (Section 3.3) was also explored.

Table 6.14: Summary of KLS, PLS and MLR performance (in $RMSEP$) in Scenario 2

$RMSEP$	Scenario 2A (without the *a priori* constraint)			Scenario 2B (with the *a priori* constraint)		
	KLS	PLS	MLR	KLS	PLS	MLR
Actual	2.5± 0.1	2.5± 0.2 [NS]	2.5± 0.0 [NS]	3.6± 0.0	–	2.5± 0.1
Nonsense	2.7± 0.1	2.4± 0.1 [NS]	2.5± 0.0 [NS]	3.8± 0.0	–	2.8± 0.5
p-value	0.26	–	–	0.00	–	0.55
q-value	0.56	–	–	0.00	–	0.59

Table 6.14 summarises the best performance (i.e., having smallest $RMSEP$) of KLS, PLS and MLR in Scenario 2. The results show that prediction performance of all three techniques was not adequate. Their predictions based on the original data were often worse than those based on the nonsense data. The performance with the smallest $RMSEP$ was by KLS without the *a priori* constraint, and by MLR with the *a priori* constraint; however, in both cases the actual performance was not far from the random distribution, as indicated by the significant p-values and q-values. The performance of KLS with the *a priori* constraint was effective (Section 3.2.4) but led to excessive prediction error ($RMSEP$ = 3.6 d compared to the average VL of 7.2 d).

The inadequate performances of the three modelling techniques emphasise the importance of the initial VL data. In Scenarios 1, both the initial and final VLs were available and the VL predictions were effective, at least by KLS modelling. In contrast, the initial VLs were not available in Scenarios 2 and effective VL estimates could not be obtained.

In addition, the assumptions concerning the initial VLs seem also to contribute to the poor prediction performance in Scenarios 2. Assuming a uniform initial VL across boxes of cut roses essentially disregard any effect of growing conditions on the subsequent VL of cut roses. However, the literature review in Section 2.3.2 actually suggested that the growing conditions could have significant

effect the post-harvest VL. Moreover, as subsequent analysis shows, the meteorological conditions, which is expected to correlate with the actual growing conditions of the flowers, varied significantly over the course of the experiment. Consequently, the assumption of a uniform initial VL may not be very reasonable. In contrast, assuming variable initial VLs means that roses delivered in the different boxes had the different initial VLs and thereby recognises the VL variation between harvests due to the growing conditions. However, implementing this assumption introduced additional variables, which led to over-fitting in modelling VLs of cut roses. This can be observed in Figure 6.32 where the VL predictions varied minimally while the observed ones were from 3 to 11 d; the predicted VLs were over-fitting a straight line that is not the $y = x$ line. Clearly, the assumption of variable initial VLs needs additional information (which was not available in this study) to avoid over-fitting.

Overall, implementing the *a priori* constraint did not improve the prediction performance. For KLS, although the overlap between the actual and nonsense *RMSEP* distributions was removed, implementing the constraint also led to a significant increase in prediction error. For MLR, it increased variance in the performance. Consequently, the prediction performance was reduced in both cases. This was rather expected considering the effect of the *a priori* constraint in Scenarios 1. In other words, when sufficient data were available, implementing the constraint did not lead to any improvement in prediction performance (in Scenarios 1). Then, it is unlikely to result in any improvement when initial VLs were not available.

6.9 PRELIMINARY STUDY OF THE EFFECTS OF PRE-HARVEST CONDITIONS

6.9.1 OBJECTIVES AND ASSUMPTIONS

This preliminary study was aimed at exploring the significance of the effects of pre-harvest conditions on the remaining VL of cut roses.

As measurements from the greenhouse at Cookes Rose Farm were not available, meteorological data for the region where the farm was located were

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used for the analysis. The assumption was that the meteorological data closely reflected the conditions occurring inside the greenhouse. This assumption was reasonable because little control of the temperature, humidity or lighting for the greenhouse was implemented.

Another assumption was that the growing period for roses at Cookes Rose Farm was 6 weeks. This assumption was made based on observations by the owner of the farm.

6.9.2 EXPLORATORY STUDY

Figure 6.36 and Figure 6.37 show the daily average temperature, rainfall, sunshine period and air pressure in Jersey from 14/05/2008 to 29/09/2008. The experiment was carried out between 25/06/2008 and 29/09/2008.

A PCA exploratory study was performed on the meteorological data. As the growing period was assumed to be 42 days, for each cut rose sample all the weather measurements within a 42 days prior to its harvest were included in the PCA study. This resulted in 253 weather measurements for each cut rose sample. As the samples from one delivery box had the same set of measurements, there were 30 data samples in total. Auto-scaling was carried out before the PCA operation.
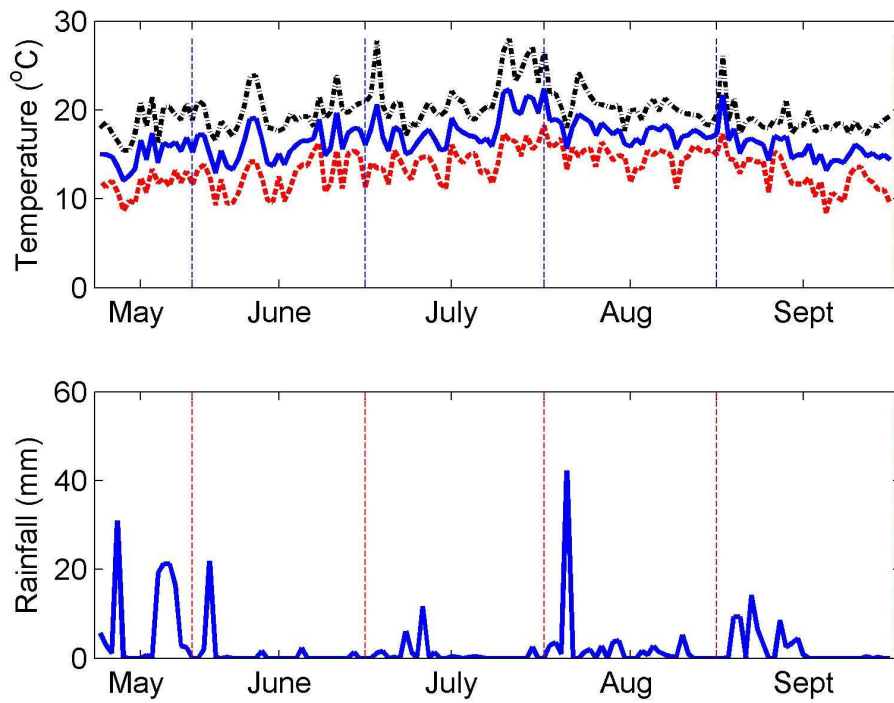
Figure 6.36: Daily maximum, mean, and minimum air temperatures and rainfall levels in Jersey from 14/05/2008 – 29/09/2008. All cut rose samples in the study were harvested between 25/06/2008 – 29/09/2008. Growing period was 42 days (e.g. 14/05 – 25/06).
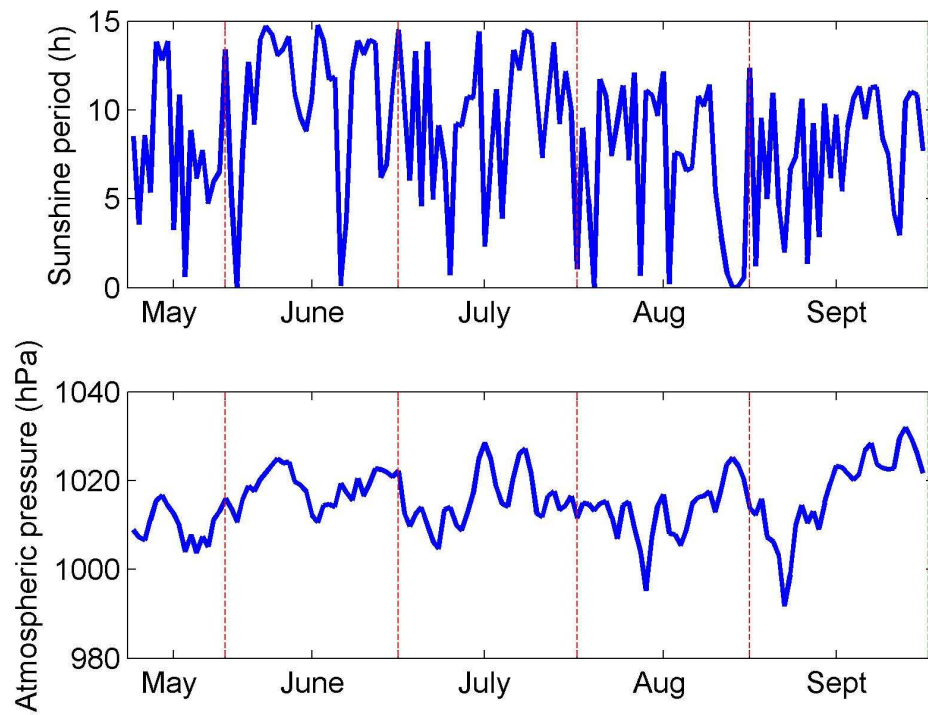
Figure 6.37: Sunshine period and air pressure in Jersey from 14/05/2008 – 29/09/2008.
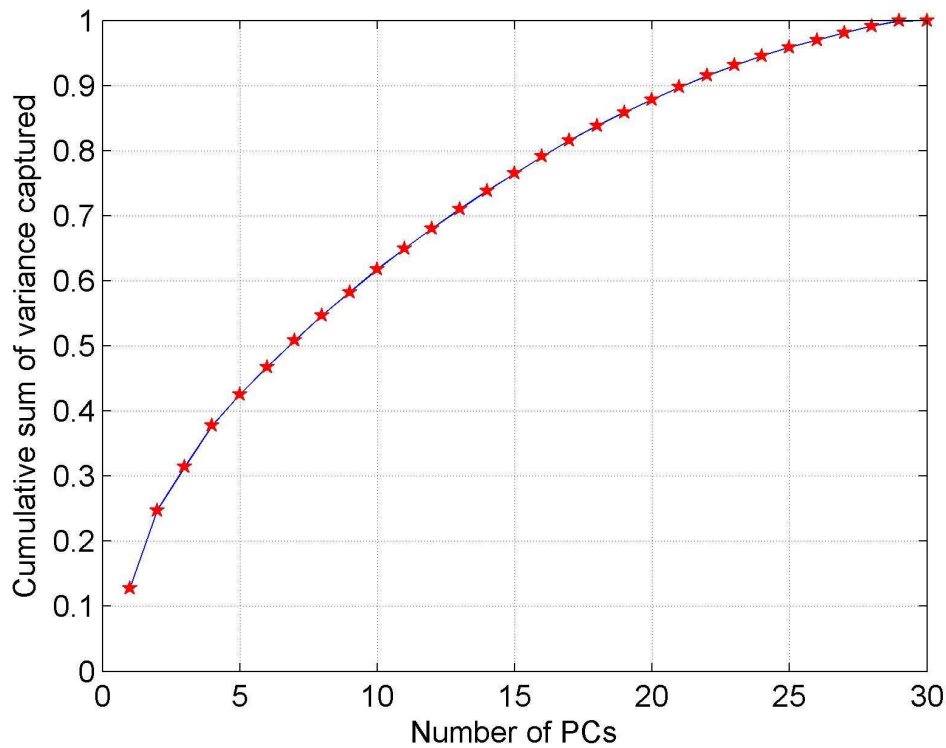
Figure 6.38: Scree plot showing the cumulative sum of variance that was captured versus the number of PCs used.

Figure 6.38 shows the cumulative sum of captured variance for the first 30 PCs. As can be seen, all of the variance of the data would be retained using these first 30 PCs. The reason was that there were only 30 different samples of meteorological measurements (i.e., one for each delivery box).

Figure 6.39 shows the PCA scatter plot (for the first and second PCs) with observations grouped according to ranges of VL loss. No clear trend between the groups of VL could be observed, which seems to suggest that estimating the remaining VL using the meteorological data would be challenging.
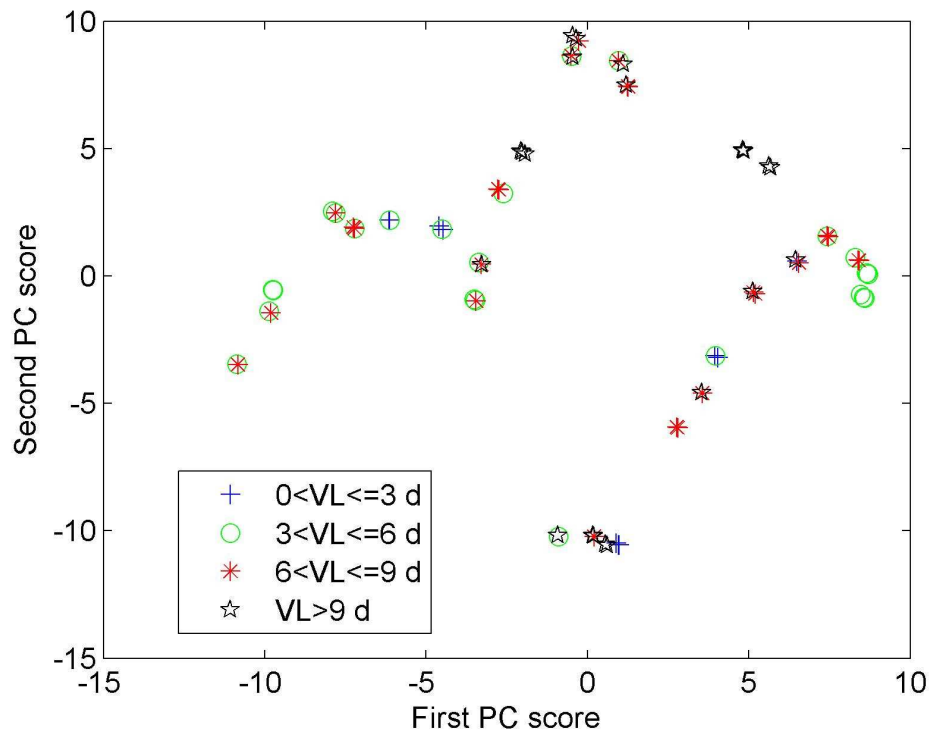
Figure 6.39: PCA scores plot for the first and second PCs, which together explain 24.7% of the total variance. Different symbols represent different range in remaining VL upon delivery at the University of Manchester.

6.9.3 MODELLING RESULTS AND DISCUSSION

6.9.3.1 MODELLING TECHNIQUES AND SUB-SCENARIOS

As MLR prediction performance was consistently inadequate in previous scenarios, MLR was not considered in this analysis of the pre-harvest measurements. Consequently, only KLS and PLS were used for the modelling of the pre-harvest effects on the remaining VL of cut roses.

As KLS only works on temperature, the daily average air temperatures collected over 6 weeks prior to harvest was used in KLS modelling. In contrast, PLS could analyse other meteorological measurements such as rainfall level, sunshine period and atmospheric pressure in addition to the average air temperature. The corresponding post-harvest VL was the same as that which was observed in Scenario 1, the office display test. Specifically, two levels of modelling were considered. For modelling at *box level*, the VL loss for each box was equal to the initial VL at delivery, which was estimated by averaging the

VLs of the three stems from the box that were used for the vase life test in the incubator. This led to 30 data samples, one for each box of cut roses. Additionally, modelling was carried out at *stem level*. In this case, the loss in VL corresponding to each stem could be equal to the VL of any of the three stems that were placed in the incubator. Consequently, there were a total of 90 data samples (3 from each box).

6.9.3.2 DATA PRE-PROCESSING

The pre-harvest data used in this analysis contain meteorological measurements reported in different units and ranges (see Section 6.4). Consequently auto-scaling was applied to the data prior to performing PLS modelling. No scaling was performed prior to KLS modelling.

6.9.3.3 KLS PREDICTION PERFORMANCE

KLS prediction performance in box-level modelling is presented in Figure 6.40; a similar figure for stem-level modelling can be found in Appendix B (Figure B. 7). Corresponding numerical results are summarised in Table 6.15. As can be seen in the distributions of the statistics, the performance based on the actual data was slightly better than that based on the permutated nonsense data for *RMSEP*, slope and intercept but not for R^2. However, the slope of the best fit line was very close to zero i.e. the best fit line approached a horizontal line. R^2 was also close to zero and smaller than the nonsense R^2, suggesting there was no (linear) correlation between the predicted and observed VLs. In addition, as the *p*-values and *q*-values indicated, there was significant overlapping between the actual and nonsense *RMSEP* distributions, which indicates low statistical confidence. Consequently, KLS predictions at both box level and stem level were not effective.
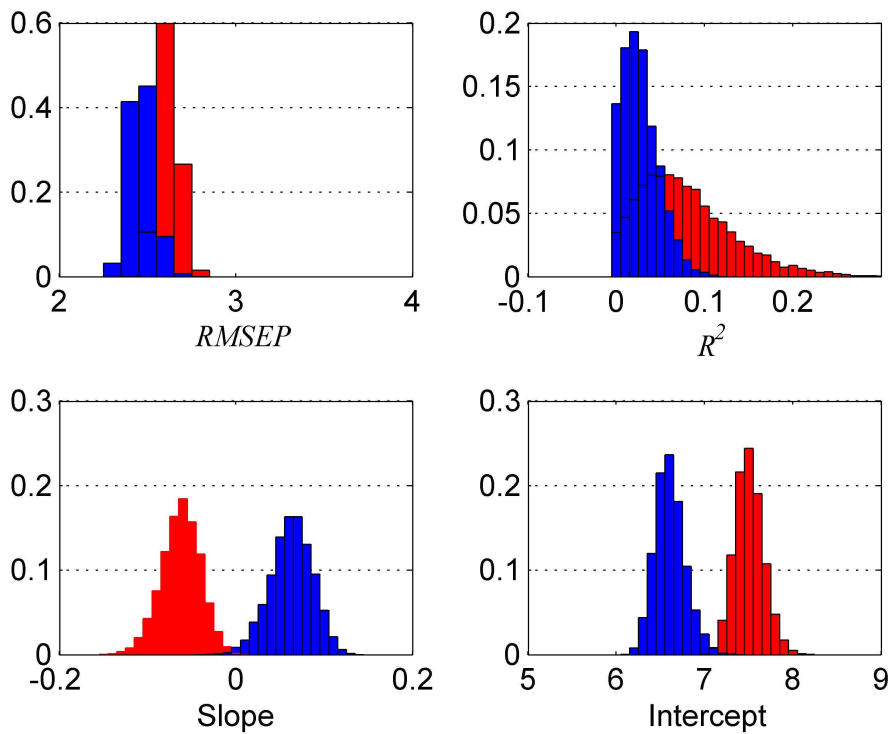
Figure 6.40: Performance of KLS in pre-harvest modelling at box level. X-axis shows the performance indices while y-axis plots the fraction of the total number of samples. Blue distributions were based on actual data while the red distributions were from nonsense permutated data.

Table 6.15: Pre-harvest modelling – KLS performance. (10000 repetitions of double cross validation studies were performed.)

Modelling level		*RMSEP*	R^2	Slope	Intercept
Box level	Actual	2.5 ± 0.1	0.03 ± 0.02	0.07 ± 0.02	6.66 ± 0.17
	Nonsense	2.7 ± 0.1	0.08 ± 0.05	-0.06 ± 0.02	7.55 ± 0.16
	p-value	0.15	(not applicable)		
	q-value	0.27			
Stem level	Actual	3.2 ± 0.1	0.01 ± 0.01	0.02 ± 0.02	6.90 ± 0.13
	Nonsense	3.3 ± 0.1	0.04 ± 0.01	-0.04 ± 0.02	7.33 ± 0.16
	p-value	0.34	(not applicable)		
	q-value	0.59			

6.9.3.4 PLS PREDICTION PERFORMANCE

For comparison with KLS, PLS modelling was performed with only pre-harvest air temperature, and with all meteorological measurements.

Table 6.16: Pre-harvest modelling – PLS performance. I: only daily average air temperature was used; II: all pre-harvest data (air temperature, rainfall level, sunshine period, atmospheric pressure) were used. (1000 repetitions)

	Modelling level		$RMSEP$	R^2	Slope	Intercept
I	Box level	Actual	3.0 ±0.2	0.03 ±0.03	-0.07 ±0.06	7.68 ±0.51
		Nonsense	3.3 ±0.2	0.03 ±0.04	-0.09 ±0.07	7.85 ±0.50
		p-value	0.33	(not applicable)		
		q-value	0.63			
	Stem level	Actual	3.6 ±0.2 [NS]	0.02 ±0.02	-0.06 ±0.05	7.67 ± 0.35
		Nonsense	3.2 ±0.1 [NS]	0.04 ±0.02	0.09 ± 0.03	6.54 ±0.21
		p-value	–	(not applicable)		
		q-value	–			
II	Box level	Actual	3.2 ±0.1 [NS]	0.02 ±0.02	-0.09 ±0.05	7.62 ±0.34
		Nonsense	3.0 ±0.2 [NS]	0.05 ±0.05	-0.10 ±0.06	8.00 ±0.46
		p-value	–	(not applicable)		
		q-value	–			
	Stem level	Actual	3.6 ±0.1 [NS]	0.02 ±0.02	-0.06 ±0.03	7.54 ±0.22
		Nonsense	3.3 ±0.1 [NS]	0.00 ±0.00	0.00 ±0.02	7.32 ±0.14
		p-value	–	(not applicable)		
		q-value	–			

The combination of types of meteorological data being considered (only temperature or all available measurements) and modelling levels resulted in four different scenarios. The results of PLS performance in these scenarios are shown in Table 6.16. In three out of those four scenarios, PLS performance was not adequate as its prediction error based on the actual data was worse than that based on randomised data. The only case which produced some distinction between the actual and nonsense performances was PLS modelling at box level with daily averaged temperature. However, as the p-values and q-values indicated, significant overlapping between the actual and nonsense *RMSEP*

distributions was present. Further, the slope of the best fit line was very close to zero. Consequently, the PLS prediction was also not effective in this case.

6.9.3.5 DISCUSSION AND CONCLUSION

Meteorological data were analysed to examine the effects of pre-harvest factors on post-harvest loss in the VL of cut roses. The data included daily temperature (maximum, minimum and average), rainfall level, sunshine period and atmosphere pressure. Based on information from the farm's owner, the pre-harvest period was assumed to be 6 weeks.

The results in Table 6.15 and Table 6.16 show that both KLS and PLS did not perform adequately in modelling pre-harvest temperature. There was significant overlap between the actual and nonsense $RMSEP$ distributions; the best fit lines for the actual performance were approaching a horizontal line; and the actual R^2 was very small.

For comparison, modelling at the box level led to a better performance than at the stem level. This was observed both in KLS and in PLS modelling. The two modelling levels differed in one aspect: what was represented by each data sample. For a box of cut roses, the flowers were harvested on the same day and hence had the same meteorological measurements for 42 days before harvest. In box level modelling, that set of meteorological measurements corresponds to one vase life loss which was estimated by the average of the VLs of the three cut roses from the box that were placed in the incubator. However, in stem level modelling, the same set of meteorological measurements corresponds to any of the three VLs of the roses in the vase life test. In other words, the same values of independent variables (i.e., meteorological measurements) had (three) different values of dependent variable (i.e., the vase life loss). This "data inconsistency" is believed to be responsible for the poorer performance of modelling at the stem level.

In conclusion, KLS and PLS techniques could not make effective estimates of the post-harvest loss in VL using pre-harvest air temperature and other meteorological measurements.

6.10 MODELLING PRE- AND POST- HARVEST TEMPERATURES

6.10.1 OBJECTIVES AND TECHNIQUES

This section investigates whether or not combining pre-harvest and post-harvest temperatures could lead to a better prediction performance. Specifically, the modelling in Scenario 1, the office display test period, is re-examined where both pre-harvest and post-harvest temperatures are analysed to estimate the loss in VL of cut roses.

As in Section 6.9, only KLS and PLS are used in this section. In addition, modelling at stem level is not considered as it was shown (Section 6.9) to produce poorer performance compared to modelling at box level.

6.10.2 DATA DESCRIPTION

In this scenario, pre-harvest meteorological temperature during the growing period, and post-harvest temperature recorded during the office display test were combined to estimate the post-harvest loss in VL. A detailed description of the post-harvest data set was presented in Section 6.7.1. Similarly, pre-harvest data were described in Section 6.9.2. The combined pre-harvest and post-harvest data set contained 60 data samples (two cut roses from each box were displayed in the office display test). Each data sample consists of a temperature profile and a VL loss. The temperature profile was formed by combining pre-harvest 42-day meteorological temperature readings with post-harvest temperature collected during the office display period. The loss in the VL was equal to the initial VL for the box at delivery, which was estimated by averaging the VLs of the three stems that were placed in the incubator for the vase life test.

KLS modelling was performed with the same parameter settings (lower and upper temperature thresholds) as those used in Section 6.7.2.1 for post-harvest temperature. For PLS modelling, two scaling strategies including auto-scaling (PLS(**I**)) and zero-mean (PLS(**II**)) were investigated.

6.10.3 RESULTS

Numerical results of estimating the VL loss using the combined pre-harvest and post-harvest temperature are presented in Table 6.17 for KLS and PLS techniques. Typical performances of KLS and PLS modelling can be found in Appendix B (Figure B. 8 and Figure B. 9)

Table 6.17: Results of pre-harvest and post-harvest modelling for KLS and PLS. (PLS(I) corresponds to results with auto-scaling; PLS(II) corresponds to results with zero-mean scaling) (10000 repetitions)

Modelling technique		*RMSEP*	R^2	Slope	Intercept
Predicted output		ΔVL (d) during office display			
		(mean = 7.2; min = 2; max = 11)			
KLS	Actual	2.2 ± 0.1	0.23 ± 0.03	0.33 ± 0.02	4.87 ± 0.15
	Nonsense	3.0 ± 0.1	0.00 ± 0.00	-0.00 ± 0.02	7.21 ± 0.16
	p-value	0.00	(not applicable)		
	q-value	0.00			
PLS (I)	Actual	2.2 ± 0.0	0.23 ± 0.02	0.33 ± 0.01	4.81 ± 0.11
	Nonsense	2.3 ± 0.1	0.18 ± 0.04	0.31 ± 0.03	4.97 ± 0.28
	p-value	0.07	(not applicable)		
	q-value	0.06			
PLS (II)	Actual	2.2 ± 0.1 [NS]	–	–	–
	Nonsense	2.2 ± 0.1 [NS]	–	–	–
	p-value	–	(not applicable)		
	q-value	–			

For KLS technique, the inclusion of pre-harvest temperature into the modelling slightly lowered the prediction error by 0.1 days (Table 6.4 in Section 6.7.2) at the cost of reducing the expected best fit line.

For PLS with auto-scaling (i.e., PLS(**I**)), the same prediction error was obtained with a small improvement in the best fit line (Table 6.5 in Section 6.7.3). However, the difference between the actual and nonsense distributions of performance statistics became smaller. Effectively, this reduced the statistical

confidence in the PLS prediction, as suggested by the increase in p-values and q-values. For PLS with mean centering (i.e., PLS(**II**)), the prediction performance was not effective.

Additional results (not shown) from analysing the combined data set of temperature during the postal delivery and the office display test periods did not lead to any significant improvement in prediction performance for both KLS and PLS.

6.10.4 DISCUSSION

Comparing between KLS and PLS, both techniques produced similar prediction performances for actual data (Table 6.17). All of the performance statistics including $RMSEP$, R^2, slope and intercept based on the actual data were virtually the same for both KLS and PLS actual performances. Consequently, it may seem that there was no better technique between the two. However, inspecting their performances on nonsense data argues otherwise. As Table 6.17 shows, the KLS nonsense performance reflects the characteristics of nonsense data. There is no correlation between the nonsense predictions and the nonsense outputs as R^2 is zero and the best fit line is a horizontal line at the mean of the observed VLs. In contrast, the PLS nonsense performance implied some spurious correlation between the nonsense predictions and the nonsense outputs. This may be because the number of repetitions of cross-validation study was not sufficiently big. Therefore, the statistical distributions of the performance indices have not converged to their population distributions.

On the basis of relative improvement over nonsense performances, KLS would be preferred to PLS. As shown in Table 6.17, the difference between the actual and nonsense performances was much more significant in KLS results than in PLS. In fact, from nonsense data to actual data RMSEP was improved by 0.8 d using KLS modelling but only 0.1 d using PLS. Similar observations can be made for other statistics.

Overall, combining the pre-harvest and post-harvest temperatures did not significantly improve the KLS and PLS prediction performance, as compared to the performance based only on the post-harvest temperature. One of the reasons could be that for each box the initial VL, which was estimated by the average of the VLs of the three cut rose stems placed in the incubator, could have effectively captured the effects of the pre-harvest meteorological measurements. As the initial VL was incorporated in the analysis, the subsequent inclusion of the pre-harvest measurements could be more or less redundant, and hence did not improve the prediction performance. The second reason could be that the correlation between the pre-harvest air temperature and post-harvest VL was quite weak. This could be inferred from the results of modelling the pre-harvest data (Section 6.9).

Although no significant improvement in prediction performance was achieved in this case, it should not preclude the use of pre-harvest measurements in any subsequent prediction exercise. The reason is that this analysis of pre-harvest factors was only a preliminary study. Meteorological conditions, instead of actual pre-harvest measurements, were analysed and shown to have a weak correlation with post-harvest VL. Since actual pre-harvest measurements describe more accurately what happens to the rose plant, it is reasonable to expect that using the actual pre-harvest measurements would result in a stronger correlation, which could improve the estimation of the post-harvest VL.

6.11 FURTHER DISCUSSION

6.11.1 WHY KLS WAS BETTER THAN PLS AND MLR

KLS, PLS and MLR represent different modelling strategies that could be used in estimating the loss in remaining VLs of cut roses. KLS is a novel technique developed from kinetic modelling principles (Chapter 4). PLS, probably the most common technique in chemometrics, is based on the regression of a specifically chosen subset of linear combinations of the original variables to the target VL. MLR is based on the linear regression of the original variables.

In Scenario 1, KLS produced the best prediction performance while PLS performance may be acceptable; none of the techniques worked in Scenario 2. There were three major reasons that may explain the difference in performance of the three techniques. The first reason is that PLS and MLR are purely data-driven while KLS originates from kinetic modelling. The difference in the origins here could be a key factor. It is known that important processes (e.g. respiration) that could contribute to the loss in remaining VL of cut roses are governed by kinetic principle. Some information relevant to the kinetics of these processes may have been captured by KLS technique and therefore enabled it to perform better at estimating the VL loss. In fact, KLS models are in the forms of mathematical vectors of the rates at which the remaining VLs of cut roses would diminish at specified temperatures. Based on such KLS models, kinetics of VLs of cut roses in terms of temperature can also be deduced. In contrast, PLS and MLR were purely mathematical techniques. They are not capable of capturing any information regarding the actual chemical processes occurring within the flowers. Consequently, this difference could contribute to KLS superior performance.

The second reason for better performance in KLS modelling lies in its formulation. Both PLS and MLR techniques model the loss in VL of cut roses as a linear combination of temperature readings. On the other hand, KLS expresses the overall VL loss as the sum of the losses at each temperature state. Therefore, PLS and MLR assume the VL loss varies linearly with temperature while KLS solves for the (rate of) loss at every temperature state, which could be nonlinear. As the literature review in Section 2.3.3 discovered, the relationship between temperature stress and VL of cut roses is complex and hence unlikely to be linear. On this basis, KLS is more flexible than the other two methods. In fact, as KLS solutions indicated (Figure 6.14), the effect of temperature on VL of cut roses could very well be nonlinear. As a result, the linearity assumption that MLR and PLS make might be partly responsible for their worse performance compared with KLS.

The third reason relates to the number of independent variables that each modelling technique has to deal with. PLS and MLR models the data along the

time axis while KLS does so along the temperature axis. In other words, both PLS and MLR designate an independent variable for temperature at each time point. This led to the number of independent variables being equal to the total number of temperature readings which in turn depended on the time duration and the frequency of data collection. On the other hand, KLS only had one independent variable for each temperature state, which is a design parameter i.e. can be pre-selected. As a result, while both MLR and PLS had to deal with more than 240 independent variables, KLS was content with no more than 11. This clear advantage in data reduction capability is likely to be an important factor contributing to the superiority of KLS over the other two techniques.

In short, KLS outperformed MLR and PLS because:

1) It is originated from kinetic modelling.

2) It does not make a linearity assumption for temperature effect on the loss in VL.

3) It has a better capability in data reduction and hence a KLS model has fewer independent variables.

6.11.2 VASE LIFE ESTIMATION USING POST-HARVEST TEMPERATURE

Using the Cookes Rose data set, this chapter investigated the hypothesis of using post-harvest temperature to estimate the corresponding loss in the remaining VL of cut roses. With regard to this objective, the study has compared the prediction performance of KLS, PLS and MLR using the actual data, with the performance obtained from the permutated nonsense data. Results from KLS, the best of the three techniques, show that there were distinct differences between the two actual and nonsense performances. This indicates that the VL loss estimates based on post-harvest temperature are better than nonsense guesses. In other words, post-harvest temperature data contain embedded information that is useful in estimating the vase life loss.

In addition, meteorological data were also used to build models for estimating the loss in VL in Scenario 1 but their performance was not effective. This was because significant overlap between the actual and nonsense *RMSEP*

distributions was present. Nevertheless, in some cases the *RMSEP* based on the actual data was better than that based on the nonsense data. As a result, there was some correlation between the pre-harvest meteorological conditions and the loss in VL of cut roses but it was too weak for an effective prediction performance

In summary, while other conditions such as pre-harvest meteorological temperature may also play a part, post-harvest temperature was a major factor in estimating the post-harvest loss in the VL of cut roses.

6.11.3 COMPARISON BETWEEN SCENARIOS 1 AND 2

Scenario 1 corresponded to the office display test, where cut roses were placed in vases and observed until they died. This scenario had the most complete data set, which consisted of initial VLs (estimated by the VL test), final VLs =0 (displayed until death), and the temperature stress during the office display test (recorded by attached data loggers). By contrast, Scenario 2 corresponded to the postal delivery period where the flowers were transported from Cookes Rose Farm to the University of Manchester. For practical reasons, initial VLs to this period were not known and hence the data set in Scenario 2 was incomplete. Although an assumption about initial VLs could be made, the lack of real data seemed to be the major reason as to why overall prediction performance in Scenario 1 was better than in Scenario 2.

6.12 CHAPTER CONCLUSION

In this chapter, KLS, PLS and MLR modelling techniques were used to analyse the Cookes Rose data set. Two post-harvest scenarios were considered, including Scenario 1, the office display period, and Scenario 2, the postal delivery period. The conclusion is that in Scenario 1, where a complete data set was available, KLS performed better than PLS and MLR. In Scenario 2, where the initial VLs were not available, KLS, PLS and MLR performances were all inadequate.

The study also concludes that effective estimates of post-harvest VL could be obtained based on post-harvest temperature. In addition, preliminary analysis indicated that pre-harvest meteorological temperature appeared to contain information that is predictive of the post-harvest loss in the VL of cut roses, but the correlation was too weak for an effective estimation.

7 AN INTERNATIONAL CHILLED SUPPLY CHAIN CASE STUDY

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This chapter analyses the data collected from an experiment with World Flowers Ltd. During the experiment, boxes of cut roses of Tropicana, Red Calypso and Armani varieties were transported in a chilled supply chain from a farm in Kenya to a distribution centre in Hook (UK). For each box of flowers, two VL tests were performed; one was at the farm and the other was at the distribution centre. Pre-harvest measurements including growing temperature, rainfall and radiation levels were retrieved from records at the farm. Post-harvest temperature was collected using RFID tags and data loggers. KLS and PLS techniques were used to analyse the data.

A number of modelling scenarios and sub-scenarios were considered. Based on input data, there were three scenarios including modelling pre-harvest measurements, modelling post-harvest temperature, and modelling the combination of pre- and post-harvest temperatures. In terms of the estimated output, there were three sub-scenarios corresponding to estimating the VL at the farm, the VL at the distribution centre and the loss in VL (i.e. the difference between the two VLs). It was found that the growing temperature could be used to obtain effective estimates of the VLs at the farm, at the distribution centre and the in-between loss; using post-harvest temperature would lead to a smaller prediction error for the VL at the distribution centre and the VL loss. In addition, combining both pre-harvest and post-harvest temperatures led to a slight improvement in KLS estimates but not in PLS ones. Nevertheless, the estimates of the VL loss may still not be useful practically due to the excessive relative prediction error. Overall, KLS was more robust than PLS in modelling post-harvest temperature although the latter seemed to have a smaller prediction error.

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7.1 BACKGROUND

This chapter investigates a chilled supply chain of cut roses from a Kenyan farm to a distribution centre in United Kingdom. At one end of the supply chain is the Oserian farm which is located close to Lake Naivasha in Kenya; its area is about 84 hectares, which makes it the largest flower farm in Kenya. At the other end is the distribution centre owned by World Flowers Ltd, which is located in Hook, Hampshire (UK). Boxes of different varieties of cut roses were transported in 40-ft trailers to Nairobi airport, which is about 126 km from the farm. The flower boxes were then flown to either the UK or the Netherlands and then trucked to the distribution centre in Hook. The whole journey took approximately 2-3 days but substantial variation (in the duration) was possible, due to the changes in destination airport.

7.2 OBJECTIVES AND SCOPE OF THE STUDY

As part of the overall work, this chapter continues investigating the hypothesis of estimating the loss in remaining VL of cut roses using post-harvest temperature stress. This chapter uses KLS and PLS to analyse the experimental data collected from the Oserian-to-Hook chilled supply chain.

In terms of scope, this chapter continues focusing on analysing post-harvest temperature stress. However, results in the previous chapter have shown that pre-harvest weather conditions may correlate, albeit weakly, with the remaining VL of cut roses. Consequently, this chapter also considers thoroughly all pre-harvest factors that are available from the greenhouses at the farm.

This study consists of two parts: data collection and data analysis. In the data collection experiment, boxes of cut roses were transported from the farm in Kenya to the distribution centre in Hook (UK). Throughout this experiment, various data such as post-harvest temperature, remaining VL at the farm and at the distribution centre, and other pre-harvest and at-harvest measurements were collected. Details of the data collection experiment are explained in

Section 7.3; the modelling scenarios and techniques are described in Section 7.5. Results from the data analysis are presented and discussed in Sections 7.7 – 7.9, which is followed by discussions (Section 7.10) and conclusions (Section 7.11).

7.3 EXPERIMENTAL METHOD AND EQUIPMENT

7.3.1 OVERVIEW

The purpose of the experiment was to collect relevant data that could be used to estimate the post-harvest loss in the remaining VL of cut roses. The experiment consisted of four stages including pre-harvest growing period, post-harvest transport and storage, the VL test at the farm and the VL test at the distribution centre. The order of these stages is described in Figure 7.1 below.
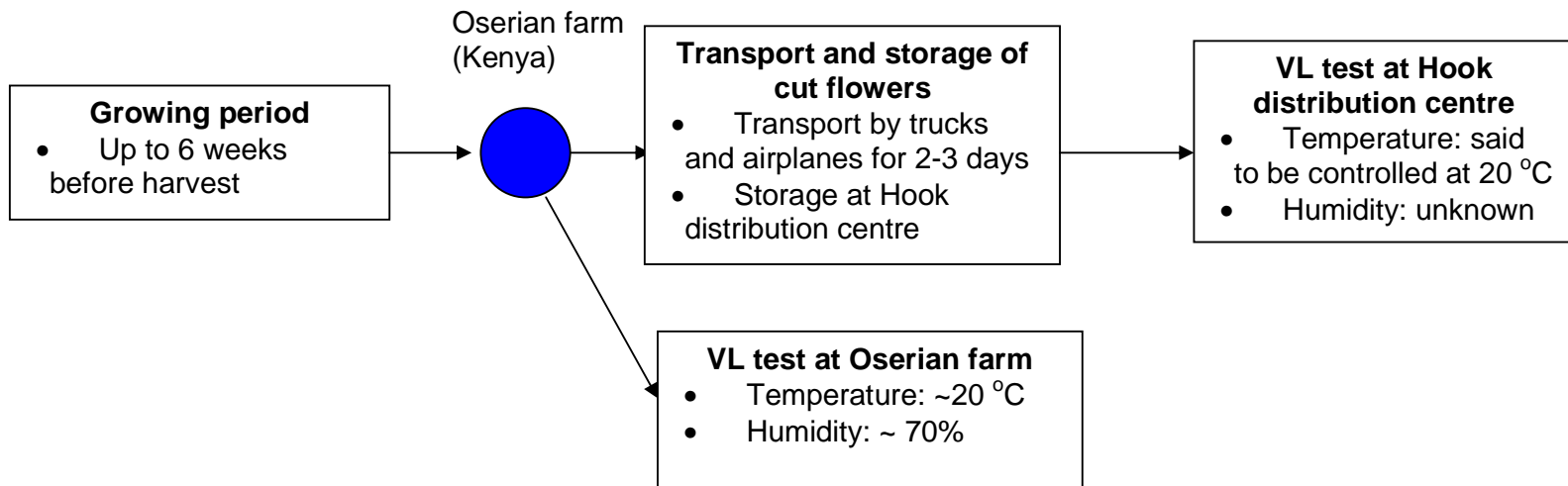
Figure 7.1: Different stages in the World Flowers data collection experiment

7.3.2 MATERIALS AND EQUIPMENT

The data collection experiment involved three rose cultivars including Tropicana, Calypso and Amani. Photos of these rose cultivars are shown in Table A. 2 in Appendix A. Two boxes of cut roses were delivered from the farm to the distribution centre almost every day from 17/06/2008 to 23/10/2008.

iButton data loggers (DS1921L-F52), products of Maxim Integrated Products Ltd (http://www.maxim-ic.com/), were used to record temperature measurements. The data loggers were programmed to record a temperature measurement every 30 min. These loggers were activated at the University of Manchester and then sent to the farm. One data logger was placed on the middle layer in the centre of every box.

MTsens RFID tags were used in many occasions in this study to demonstrate the concept of employing a wireless sensor network for data collection. The tag is a semi-passive RFID tag that is marketed by Montalbano technology Ltd. (http://www.montalbanotechnology.com/) and is designed to monitor the temperature of perishable products.

An RS-1365 temperature and humidity meter, which was described in Section 6.3.2, was also used to validate the accuracy of the data loggers and the MTsens RFID tags.

7.3.3 EVALUATION OF REMAINING VL

As described in Section 1.2.3, remaining VL is defined as the time period that a cut rose takes under a pre-specified standard condition to reach the end of its useful life. For the flower industry, the display temperature for the reference condition is 20 ^{o}C (Floral Solutions 2006).

During the data collection experiment, for each box of cut roses being studied two VL tests were performed; one was at the farm and the other was at the distribution centre. Detailed procedure of the tests was described in (Floral

Solutions 2006). It should be noted that in the tests, subjective criteria were used to determine when a flower was dead, and the exercise was performed once a day. Consequently, the vase life test results were subject to a measurement resolution of 1 d.

7.4 DESCRIPTION OF EXPERIMENTAL DATA

Figure 7.2 summarises the data that were collected at the different stages of the experiment. For the pre-harvest growing period, meteorological measurements including daily maximum, minimum and average temperature (^{o}C), daily rainfall (mm) and daily radiation (J/cm^2) between 01/05/2008 and 19/11/2008 were recorded. In addition, the at-harvest conditions including temperature, humidity and lighting condition were also measured. From a randomly selected box of cut roses, a bunch, which consisted of 12 stems, was weighted and subjected to a VL test at the farm. A data logger was placed within the selected box to record the post-harvest temperature stress during the transport from the farm to the distribution centre and during subsequent storage. At the end of the storage period, one bunch consisting of 12 stems was subjected to a VL test at the distribution centre. Table 7.1 tabulates the data that were collected during the experiment.

At harvest
- Temperature, humidity, fresh weight and lighting

Oserian farm (Kenya)

Growing period
- Temperature, rainfall and radiation

Transport and storage of cut flowers
- Temperature

VL test at the distribution centre
- Remaining VL at distribution centre

VL test at farm
- Remaining VL at the farm
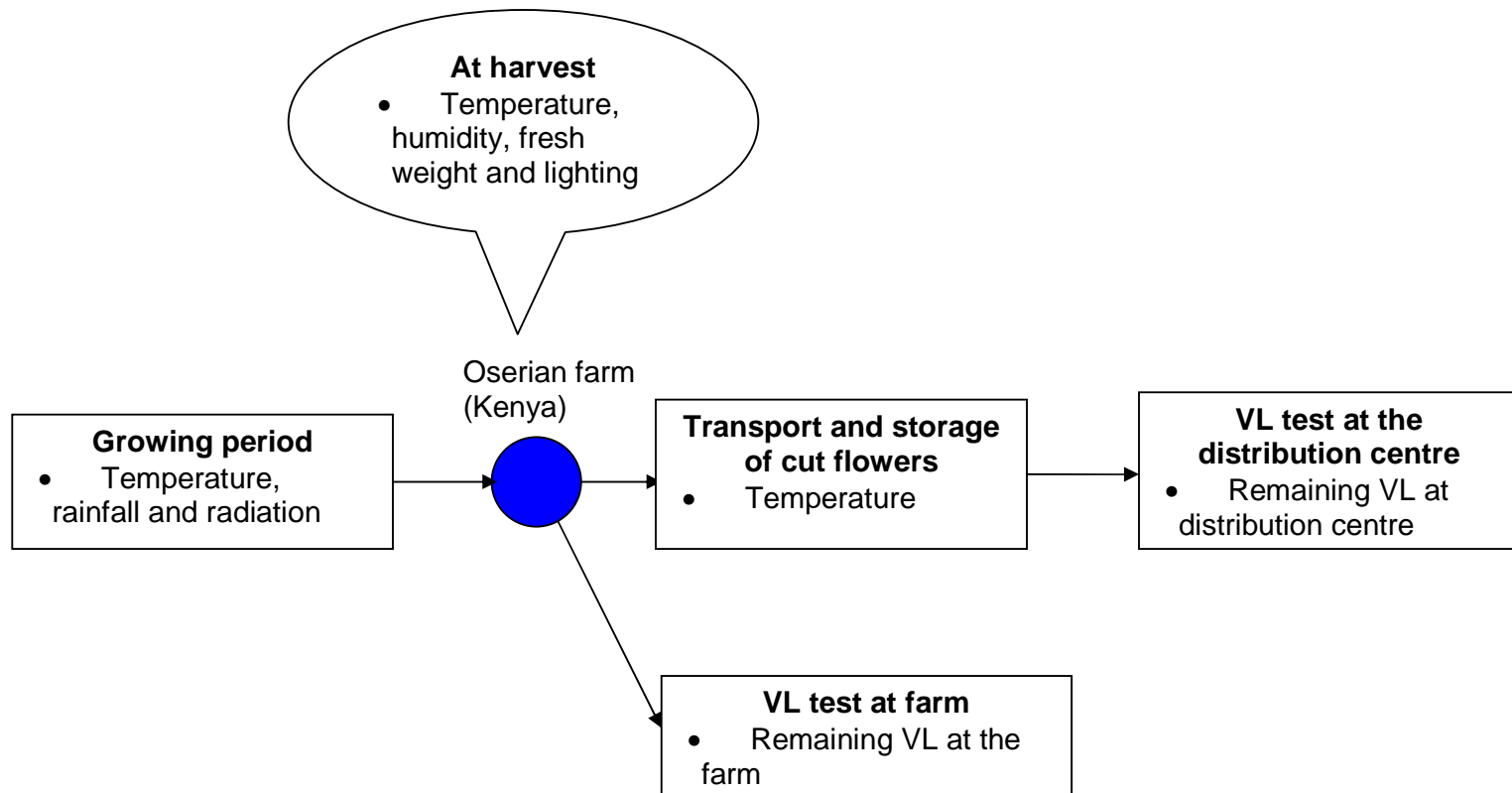
Figure 7.2: Data collected at different stages in the World Flowers case study

Table 7.1: Experimental data collected during the World Flowers case study

Data and quantity	Description
Pre-harvest data • Up to 6 weeks (i.e. 42 daily measurements) before harvest	The measurements included daily maximum, minimum, and average temperature, daily rainfall and daily radiation.
At-harvest data • 154 sets of measurements	The measurements included harvest time, temperature, humidity, lighting condition and fresh weight
Post-harvest temperature stress during transport and storage • 154 temperature profiles by data loggers. • 97 temperature profiles by RFID tags.	Data loggers were used. One profile corresponded to a box of cut roses.
	RFID tags were used. Each box had one RFID tag in addition to a data logger. However, due to the limited number (10) of the RFID tags, many boxes only had one data logger i.e., without an MTsens RFID tag.
Post-harvest humidity stress during transport • 3 humidity profiles	Humidity was recorded for 3 boxes from two different harvest by data loggers
VL at the farm • 154 sets	A set is consisted of daily observations of 12 cut roses until 6 of them were judged as dead. Average temperature and humidity during the test were also recorded.
VL at the distribution centre • 154 sets	

7.5 MODELLING OVERVIEW

7.5.1 MODELLING OBJECTIVE

The modelling objective in this chapter is similar to that of Chapter 6; i.e., to obtain a model that captures the effect of post-harvest temperature stress on subsequent changes in the VL of cut roses. Moreover, as had been found in Chapter 6, the pre-harvest conditions could potentially provide meaningful

estimates of the post-harvest loss in the VL of cut roses. Consequently, the effects of such measurements in the estimation are also investigated.

7.5.2 ASSUMPTIONS

This study made two major assumptions. The first assumption was that the bunches of cut rose stems which were subjected to the VL tests were representative of the box from which they were removed. In essence, this assumption neglected the potential variation in the remaining VL of cut roses within a box. As a result, before leaving the farm, the cut roses would have the same remaining VL, which was evaluated by the VL test at the farm; at the end of the storage period, the cut roses would have the same VL, as evaluated by the VL test at the distribution centre. This assumption was necessary so that the initial and final remaining VLs of the (transport and storage) period under study could be estimated and used in subsequent modelling.

The second major assumption was that the temperature recorded by a data logger was representative of the box to which the logger was attached. Essentially, the assumption neglected the temperature variation within a box. However, as shown in Section 7.6.3 this assumption was not validated.

7.5.3 MODELLING SCENARIOS

There are two ways to group the modelling scenarios in this chapter; one is based on the input data and the other is based on the output information. From the viewpoint of input data, the major modelling scenarios in this chapter were:

    I. Scenario 1: using the pre-harvest (and at-harvest) measurements.

    II. Scenario 2: using the post-harvest temperature stress.

    III. Scenario 3: using both the pre-harvest (including at-harvest) measurements as well as the post-harvest temperature.

In turn, based on the output to be estimated, the three major sub-scenarios were:

    a. Estimating the remaining VL at the farm immediately before dispatching.

    b. Estimating the remaining VL at the end of the storage period at the distribution centre.

c. Estimating the post-harvest loss in VL during transport from the farm to the distribution centre and during the subsequent storage.

Except for the combinations of II.a and III.a, all other combinations of modelling scenarios were considered and are indicated by a tick mark in Table 7.2. The exceptional combinations (II.a and III.a) are marked by a cross (X) in Table 7.2 and were not considered. The reason is that the remaining VL of cut roses at the farm and the post-harvest conditions during transport and storage of the flowers are independent. The remaining VL at the farm is only influenced by the factors that affect the flowers before leaving the farm; in contrast, the post-harvest conditions only affect the flowers after leaving the farm.

Table 7.2: Summary of modelling scenarios considered

Input scenario / Output sub-scenario	I. Scenario 1 – Pre-harvest modelling	II. Scenario 2 – Post-harvest modelling	III. Scenario 3 – Pre- and Post-harvest modelling
(a) Remaining VL at the farm	✔	X	X
(b) Remaining VL at the distribution centre	✔	✔	✔
(c) The loss in the remaining VL during transport and storage	✔	✔	✔

7.5.4 MODELLING TECHNIQUES

In this chapter, KLS and PLS techniques are used for data analysis. Details of their mathematical formulations and the solution techniques were described in Chapter 4 for KLS and Chapter 3 for PLS.

Results in Chapter 6 had consistently indicated that MLR performance was inferior to that of PLS, and hence MLR technique was not considered.

7.5.5 PERFORMANCE EVALUATION

The approach to performance evaluation was described in detail in Section 3.2. Basically, it involves the evaluation of R^2, *RMSEP*, and the slope and intercept of the best fit line on the predictions in a (double) cross validation strategy.

Permutation testing was performed to obtain the lower performance limits for R^2, *RMSEP*, and the slope and intercept of the best fit line. Details of permutation testing are described in Section 3.2.

7.6 DATA RELIABILITY

7.6.1 TEMPERATURE MEASUREMENTS

7.6.1.1 DATA LOGGERS

The accuracy of data loggers has been investigated in Section 6.6.1. The conclusion was that only 74.6% of the data logger readings were within 1 ^{o}C of the corresponding RS-1365 meter (Section 6.3.2).

7.6.1.2 RFID TAGS

10 MTSens RFID tags and an RS-1365 meter were used to generate data for validating the reliability and accuracy of the RFID tag measurements. All devices, RFID tags and the RS-1365 meter, were placed at the same location (within 10 cm of each other) and recorded 26 readings at frequency one reading per 15 min.

Analysis of variance (ANOVA) for the readings from the RFID tags resulted in a p-value of 0.9999, suggesting that the readings had the same mean. This meant that the RFID measurements were consistent with each other and hence were considered to be reliable.

The difference between the readings from each of the RFID tags and the corresponding ones from the RS-1365 meter was evaluated. Figure 7.3 shows the box plot and the distribution of all of the deviations with their statistics. As can be seen, the deviations were likely to be negative, indicating that the RFID

readings were smaller than the corresponding readings from the RS-1365 meter. Numerical results showed that only 45% of the RFID readings were within 1 ^{o}C difference from that of the RS-1365 meter; 94% were within 2 ^{o}C difference. This suggested that the RFID tags were ±2 ^{o}C accurate. This is in contrast with the product datasheet for MTsens RFID tags, available online at http://www.montalbanotechnology.com/images/docs/MTSENS-BROCHURE-EN.pdf, which states that the tag accuracy is ±1 ^{o}C.
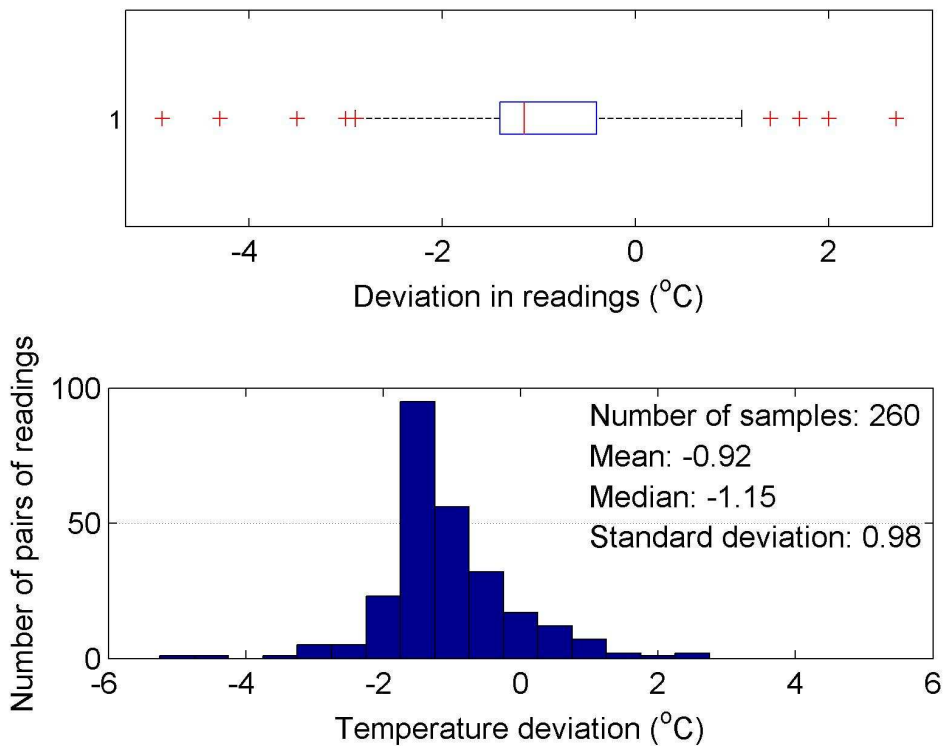
Figure 7.3: Deviation of the readings by MTsens RFID tags from the readings from the RS-1365 meter

The above exercise was also repeated at higher data collection frequency (1 reading per min). Analysis of the collected data led to a similar conclusion and hence was omitted.

7.6.2 REMAINING VASE LIFE MEASUREMENTS

As explained earlier, the variation in remaining VL within one box was assumed to be negligible. The assumption implied that the flowers in the same box had the same remaining VL at the farm and the same remaining VL at the end of the

storage period at the distribution centre. Consequently, due to post-harvest deterioration during transport and subsequent storage, the flowers would have shorter VLs at the end of the storage period than at the farm. Figure 7.4 shows both remaining VLs for all Tropicana samples. While most were consistent with the assumption, a few samples showed contradiction: the VL at the farm was shorter than at the distribution centre. Clearly, the assumption of negligible variation in VL of cut roses within a box was not reasonable in those cases. This is because the roses may have different growing conditions and other biological factors such as plant age. The more significant the variation was, the less accurate the estimate of the VL by any deterministic value would be, which as a consequence led to observations that were inconsistent with the assumptions. As the factors that lead to the VL variation within a box were not within the scope of this study, it was not possible to include the inconsistent samples in the subsequent data analysis. Consequently, those samples were removed before data analysis was performed.
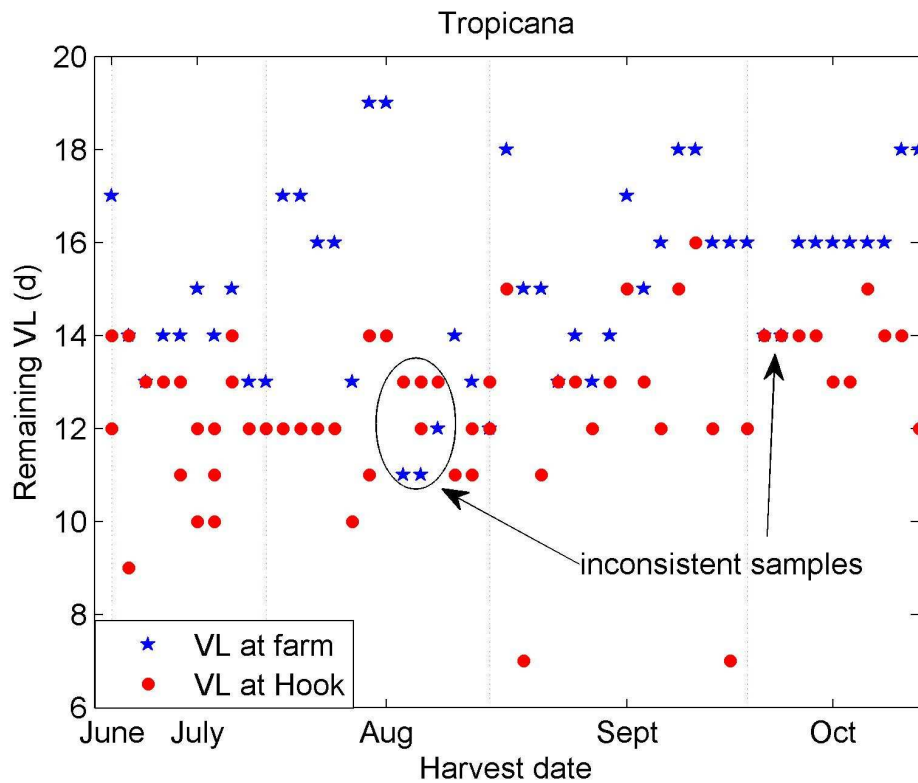
Figure 7.4: Remaining VL of cut roses at the farm and at the distribution centre; the samples that were inconsistent with the assumption of negligible variation in the remaining VL within a box are indicated.

7.6.3 TEMPERATURE VARIATION IN A BOX OF CUT ROSES

Variation of temperature within a box of cut roses was investigated. Nine data loggers were placed at different positions in a box of cut roses which departed Nairobi at 02:25 hours on the 26th June 2008 and arrived in Hook at 22:00 hours on the same day. Figure 7.5 illustrates the physical locations of the data loggers in the box. The first data logger was placed at one layer from the top of the box and toward one end. The second logger was one layer further down and toward the centre of the box. The third, fourth and fifth data loggers were one layer from the bottom of the box, where the remaining loggers were located.
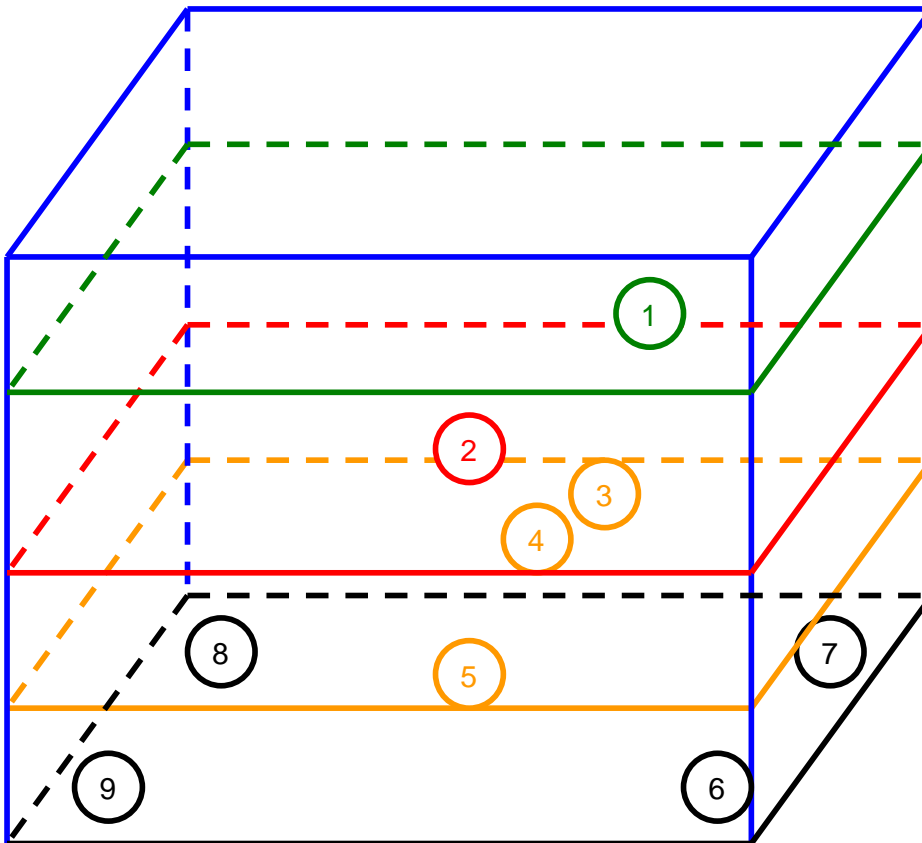
Figure 7.5: Physical locations of the nine data loggers in a box of cut roses

The box plots from analysis of the data are shown in Figure 7.6. Analysis of variance gave a p-value of 0.0, which strongly suggested that temperature varied across the box of cut flowers.
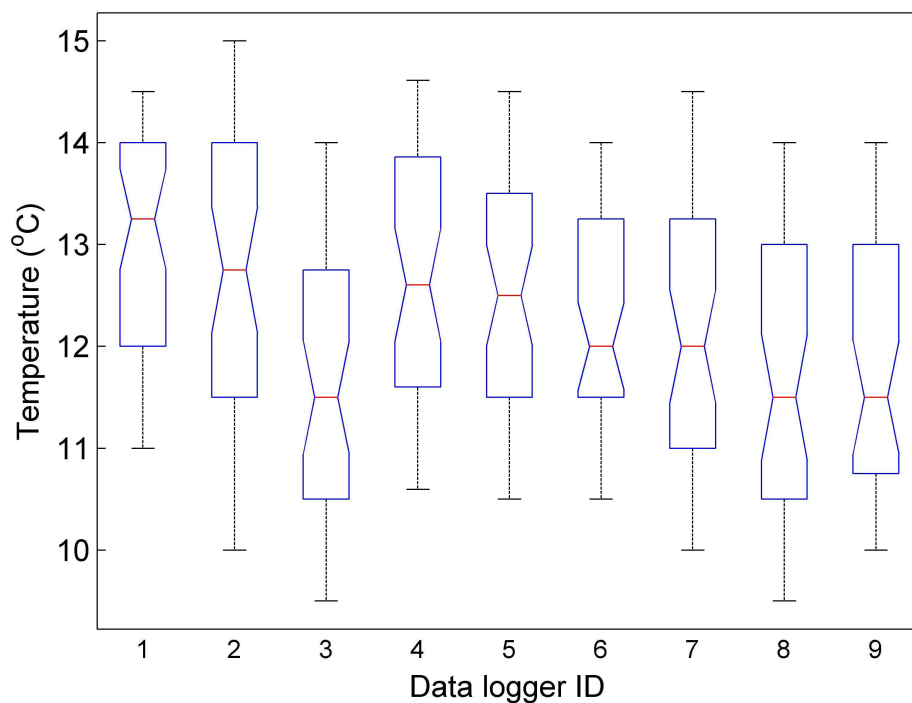
Figure 7.6: Analysis of temperature readings from 9 data loggers placed at different positions in the same box of cut roses.

The exercise was repeated for another box of cut roses with different data loggers. The collected data was analysed and a similar result was obtained. Therefore, it was concluded that temperature variation within a box was significant.

A notable trend in Figure 7.6 is that except for the third data logger, the average temperature of the other loggers seemed to decrease from the first logger to the ninth. Referring to the physical location in the box (Figure 7.5), this suggested that temperature decreased from the top to the bottom of the box of cut roses. However, this trend was not confirmed using data from the repeated exercise.

7.7   SCENARIO 1 – MODELLING PRE-HARVEST CONDITIONS

As described in Section 7.5.3, analysis of pre-harvest and at-harvest data was performed in Scenario 1. The data consisted of pre-harvest daily measurements including average growing temperature, rainfall and radiation,

and at-harvest measurements including temperature, humidity, lighting and fresh weight (Table 7.1). The objective was to examine the effect of the pre-harvest and at-harvest conditions on the remaining VL just before leaving the farm and on the remaining VL at the distribution centre.

Scenario 1 led to a number of sub-scenarios studying the effects of two parameters including data input and the size of the historical window. The former parameter referred to whether only pre-harvest temperature data or all pre-harvest and at-harvest data were analysed. The latter controlled how far back from harvest the pre-harvest data would be included in the analysis. Up to 6 weeks of pre-harvest data were available but it would not be necessary nor optimal to analyse all. The three values of this parameter that were considered were 2, 4 and 6 weeks.

7.7.1 EXPLORATORY STUDY

7.7.1.1 IS THERE A TREND IN PRE-HARVEST DATA?
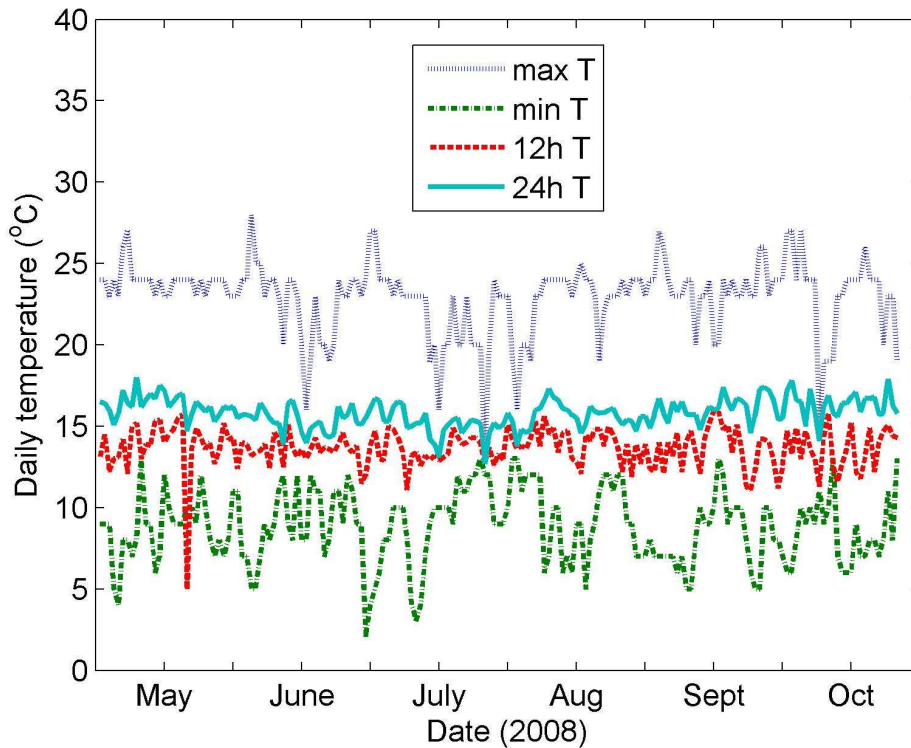
Figure 7.7: Variation in growing temperature during pre-harvest period (01/05-23/10)

Maximum, minimum, 12 hour-average and whole-day average growing temperatures during pre-harvest period (01/05/2008 – 23/10/2008) are shown in Figure 7.7. The figure indicates that the average temperatures were stable around 15 ^{o}C with little variation. On the other hand, the daily maximum and minimum temperatures experienced more fluctuations from day to day but showed no sign of any trend on a bigger time scale such as from month to month.

Figure 7.8 shows similar information for daily average rainfall and radiation level. While no clear trend could be identified for the daily radiation measurements, the rainfall data confirm the existence of a rainy season which started in late July and was in full effect from late August till the end of the study period (23/10/2008).
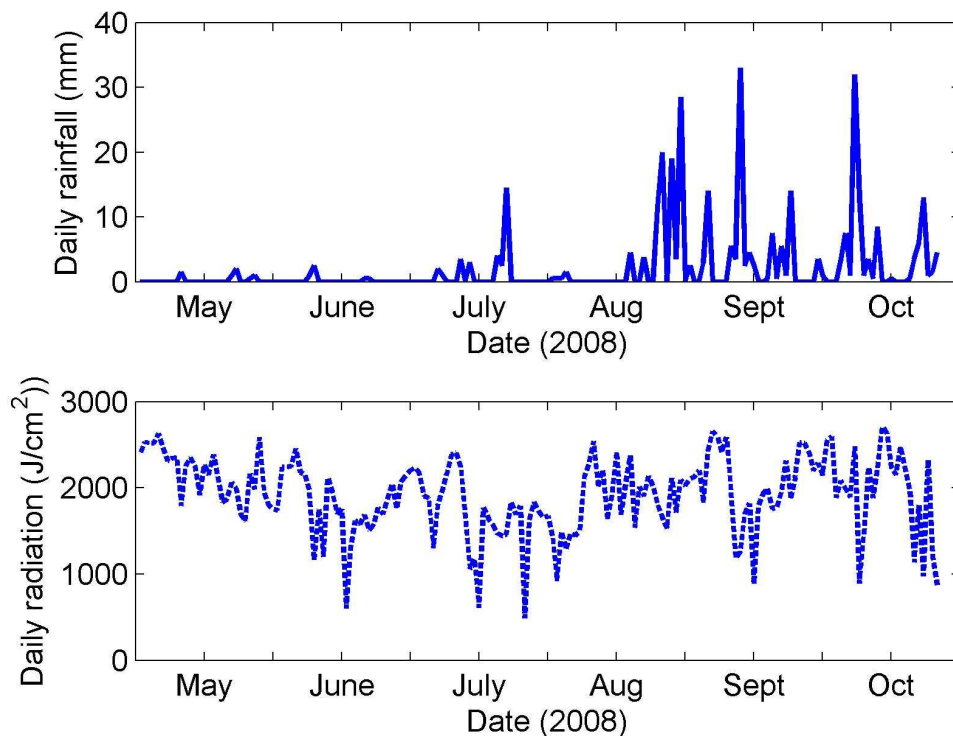
Figure 7.8: Daily rainfall and radiation level during pre-harvest period

7.7.1.2 Is there a trend in VL measurements against harvest time?

Figure 7.4 plots remaining VL evaluated at the farm and at the distribution centre against the date of harvest. As shown, variation in longevity of cut roses

across seasons was not obvious. However, it seemed that the roses that were harvested after the beginning of September appeared to last longer. Statistical hypothesis testing confirmed that the average VL of those flowers harvested before September was slightly smaller than those harvested from September onward. This conclusion applies to both VL at the farm and VL at the distribution centre. Interestingly, the harvests of longer lasting roses seems to coincide with the full onset of the rainy season, considering that the growing period is typically up to 6 weeks. Consequently, rainfall level during the growing period could be an important factor that correlates with the post-harvest VL of cut roses.

7.7.1.3 IS THERE A CORRELATION BETWEEN PRE-HARVEST DATA AND VL?
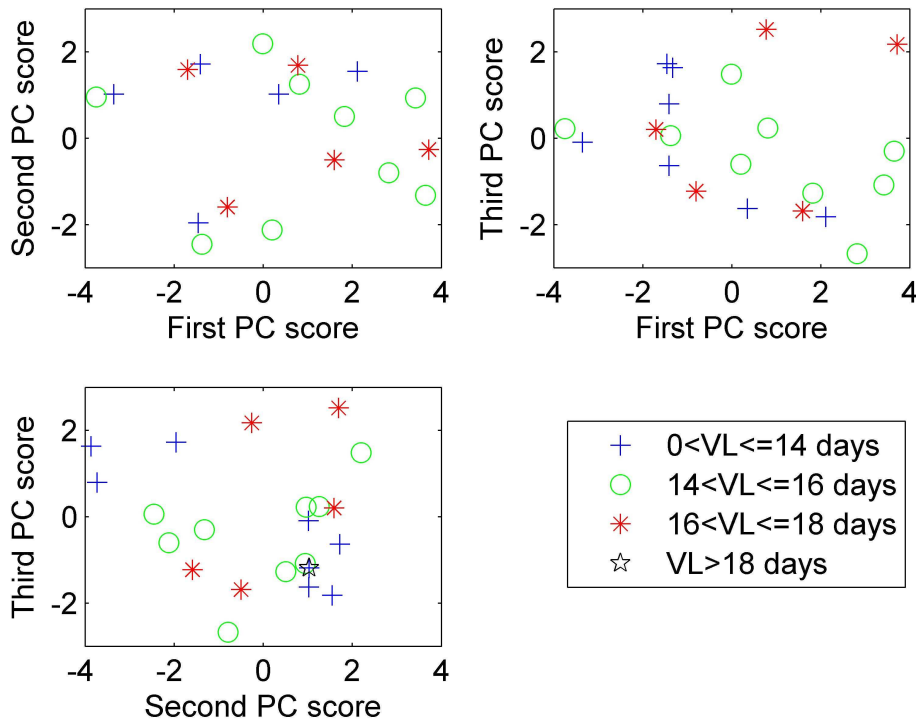
Figure 7.9: PCA score plots based on 4-week pre-harvest growing temperature. The first three PCs captured 54% variance. Data was grouped according to ranges in VL at the farm

PCA was performed on pre-harvest and at-harvest measurements, and the scores were grouped according to the corresponding VL at the farm, at the distribution centre and according to the loss in VL due to transport, which was the difference between the two VL values.

Initially, only growing temperature during the 4 weeks prior to harvest was analysed. Figure 7.9 shows representative results for Tropicana samples. In the figure, the scores were grouped according to VL at the farm. As can be seen, the indication from the figure was that the pre-harvest temperature measurements did not seem to have any correlation with the remaining VL evaluated at the farm.

Adding other measurements such as rainfall level and radiation did not reveal any correlation between the pre-harvest measurements and the remaining VL. Neither did varying the size of the historical window (from 4 to 6 or 2 weeks). Similar analysis with grouping in VL at the distribution centre or in the loss in VL led to a similar conclusion.

7.7.2 KLS PERFORMANCE

7.7.2.1 SETTING PARAMETERS

Figure 7.10 shows the variation of the daily average growing temperature at the farm from 01/05/2008 to 23/10/2008. From this figure, the lower and upper temperature bounds for KLS modelling were set at 14 ^{o}C and 17 ^{o}C respectively. The temperature step was set at 0.5 ^{o}C.
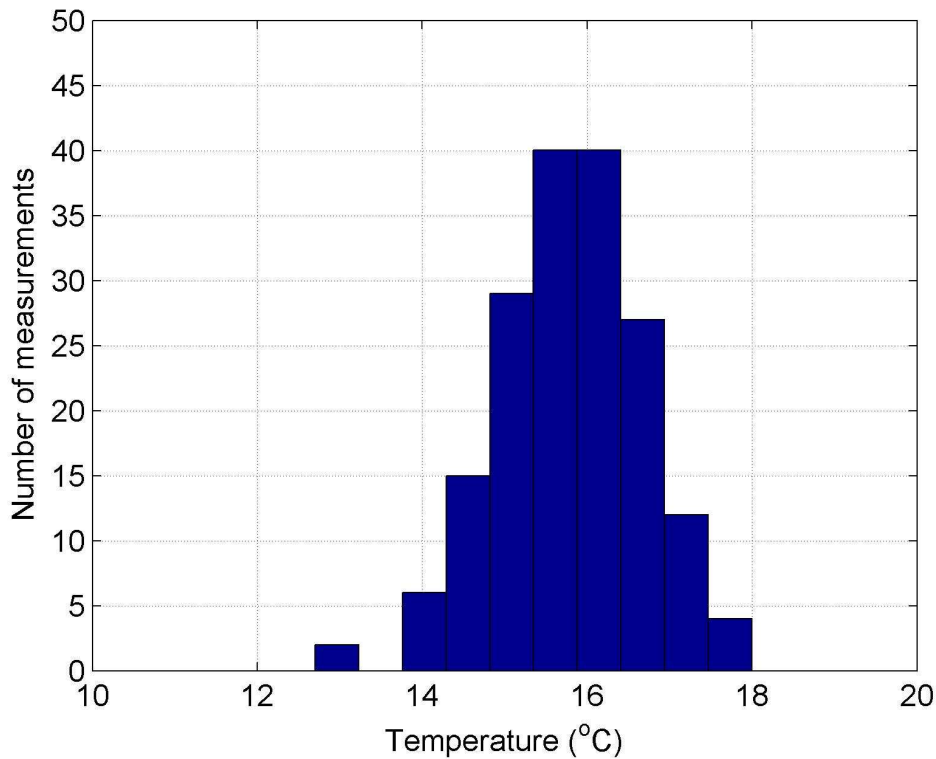
Figure 7.10: Variation in pre-harvest daily average temperature

7.7.2.2 ESTIMATING REMAINING VL AT THE FARM

Following the procedure described in Section 4.4, KLS was applied to daily average growing temperatures to estimate the remaining VL at the farm. Cross validation (with $N_{test} = 10$ segments) was repeated 10000 times and *RMSEP*, R^2 and the slope and intercept of the best fit lines were evaluated. A typical KLS performance is shown in Figure 7.11 for Tropicana variety. Permutation testing was also carried out to obtain the corresponding nonsense distributions of the same statistics. The whole procedure was repeated for three varieties including Tropicana, Red Calypso and Amani at three different sizes of data window: 2, 4 and 6 weeks. Figure 7.12 plots KLS performance for Tropicana based on 2-week pre-harvest temperature data. Prediction performance (as measured by *RMSEP*) in every case is summarised in Table 7.3.
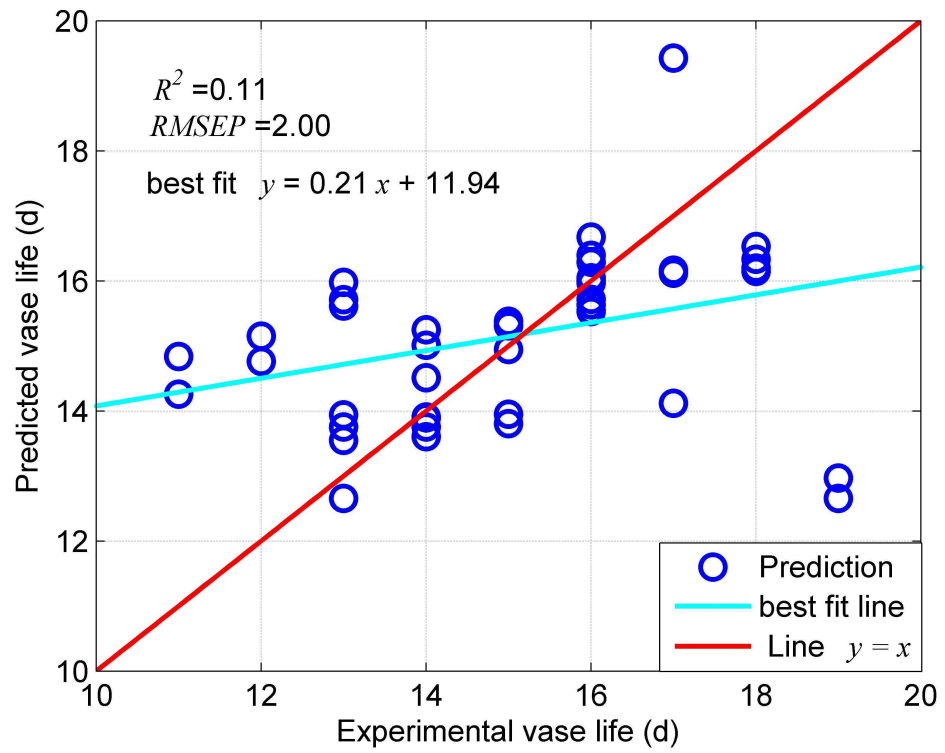
Figure 7.11: A typical KLS performance in estimating (Tropicana) VL at the farm based on 2-week pre-harvest temperature measurements.
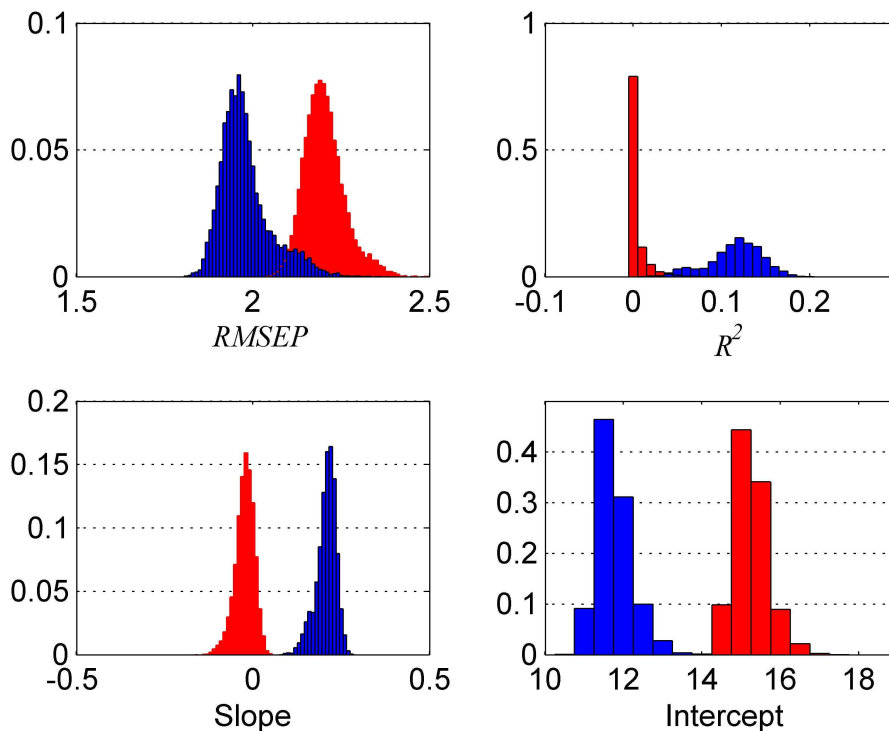
Figure 7.12: Cross-validated KLS performance in estimating (Tropicana) VL at the farm based on 2-week pre-harvest temperature measurements. Blue distributions represent the actual performance; Red distributions show the nonsense performance from permutation testing. Y-axes show statistical densities of the performance indices.

Figure 7.12 and Table 7.3 show that the estimates from KLS modelling were effective (Section 3.2.4). The distinction between the actual and nonsense distributions of the performance indices was visible in Figure 7.12. Further statistical tests confirmed that the actual errors were smaller than the nonsense ones for all but one case (Amani with 6-week data). All of the p-values and q-values (shown in Table 7.3) were small except for those of Amani variety with 6-week data, which were not evaluated because the estimation was not significant. Considering that the results of the VL tests had a resolution of 1 d, an estimation error of 1.3-2.0 d (Table 7.3) may seem reasonable. However, the linear correlation between the predicted and observed VLs was not very strong as indicated by R^2 statistic.

Further, Table 7.3 also shows the effect of pre-harvest window size on the VL estimation of KLS. The worst performance came from the modelling of 6-week pre-harvest growing temperature, which produced the biggest estimation errors

in each of the three varieties. For the other two window sizes, 2 weeks and 4 weeks, there was little difference although the latter outperformed the prior in estimating VL of Tropicana cut roses.

Table 7.3: $RMSEP$ in KLS estimation of VL at the farm using growing temperature

Pre-harvest window size		2 weeks	4 weeks	6 weeks
Tropicana (average VL=15.7 d; min=13 d; max=19 d)	Actual	2.0 ± 0.1	1.8 ± 0.1	2.0 ± 0.1
	Nonsense	2.2 ± 0.1	2.2 ± 0.1	2.4 ± 0.1
	p-value	0.06	0.00	0.00
	q-value	0.09	0.00	0.00
Red Calypso (average VL=15.4 d; min=13 d; max=18 d)	Actual	1.3 ± 0.0	1.3 ± 0.0	1.6 ± 0.0
	Nonsense	1.9 ± 0.1	1.9 ± 0.0	1.8 ± 0.0
	p-value	0.00	0.00	0.00
	q-value	0.00	0.00	0.00
Amani (average VL=15.9 d; min=14 d ; max=18 d)	Actual	1.3 ± 0.0	1.3 ± 0.0	1.5 ± 0.0[NS]
	Nonsense	1.6 ± 0.0	1.5 ± 0.0	1.5 ± 0.0[NS]
	p-value	0.00	0.01	-
	q-value	0.00	0.00	-

([NS]: not significant i.e. the mean of the actual distribution is not smaller than that of the nonsense one at 5% significant level; see Section 3.2.4)

Across the three varieties Tropicana had the biggest estimation error. This may suggest that the correlation between Tropicana VL and the pre-harvest temperature was weaker, compared to that of Red Calypso and Amani. Consequently, for the same pre-harvest temperature, the Tropicana variety had greater variation in VL at the farm than that of the other two.

7.7.2.3 ESTIMATING REMAINING VL AT THE DISTRIBUTION CENTRE

Similarly, KLS was also used to estimate the remaining VL at the end of the storage period at the distribution centre based on the growing temperature. A similar procedure was carried out and results are tabulated in Table 7.4.

Table 7.4: *RMSEP* (d) in KLS estimation of VL at the distribution centre using growing temperature

Pre-harvest window size		2 weeks	4 weeks	6 weeks
Tropicana (average VL=12.5 d; min=7 d; max=16 d)	Actual	1.9 ± 0.1 [NS]	1.8 ± 0.0 [NS]	1.8 ± 0.0 [NS]
	Nonsense	1.9 ± 0.1 [NS]	1.9 ± 0.0 [NS]	1.7 ± 0.0 [NS]
	p-value	-	-	-
	q-value	-	-	-
Red Calypso (average VL=12.7 d; min=10 d; max=14 d)	Actual	1.2 ± 0.0 [NS]	1.2 ± 0.0 [NS]	1.2 ± 0.0 [NS]
	Nonsense	1.2 ± 0.0 [NS]	1.3 ± 0.0 [NS]	1.2 ± 0.0 [NS]
	p-value	-	-	-
	q-value	-	-	-
Amani (average VL=11.4 d; min=6 d; max=15 d)	Actual	2.7 ± 0.1 [NS]	2.5 ± 0.0	2.6 ± 0.1
	Nonsense	2.8 ± 0.1 [NS]	2.6 ± 0.1	2.8 ± 0.1
	p-value	-	0.05	0.04
	q-value	-	0.05	0.04

The results suggest that the KLS technique did not perform well. In most cases, on average the actual *RMSEP* was not smaller than its nonsense counterpart. The only two exceptions were in the Amani variety with 4 and 6 weeks of pre-harvest temperature data. In those cases, the means of the actual *RMSEP* were smaller than the means of the nonsense distributions. This suggested that the VL estimates were better than nonsense. In addition, the corresponding *p*-values and *q*- values were also small, indicating little overlap between the actual and nonsense distributions and hence high statistical confidence in the estimation.

7.7.2.4 ESTIMATING THE LOSS IN REMAINING VL DURING TRANSPORT

Similarly, based on the growing temperature KLS was also used to estimate the post-harvest loss in VL during the transport of cut roses from the farm to the distribution centre and the subsequent storage there until the VL test took place. The results are tabulated in Table 7.5.

Table 7.5: *RMSEP* (d) in KLS estimation of the loss in VL during chilled transport and storage using growing temperature

Pre-harvest window size		2 weeks	4 weeks	6 weeks
Tropicana (average loss in VL = 3.2 d; min=1 d; max=9 d)	Actual	2.3 ± 0.0 [NS]	2.1 ± 0.1	2.0 ± 0.1
	Nonsense	2.0 ± 0.1 [NS]	2.2 ± 0.1	2.3 ± 0.1
	p-value	-	0.23	0.01
	q-value	-	0.25	0.00
Red Calypso (average loss in VL = 2.7 d; min=1 d; max=7 d)	Actual	1.8 ± 0.1	1.7 ± 0.0	1.8 ± 0.0 [NS]
	Nonsense	2.1 ± 0.1	2.0 ± 0.1	1.9 ± 0.0 [NS]
	p-value	0.02	0.00	-
	q-value	0.00	0.00	-
Amani (average loss in VL = 4.5 d; min=1 d; max=10 d)	Actual	3.0 ± 0.1	2.8 ± 0.1	2.8 ± 0.0
	Nonsense	3.2 ± 0.1	3.0 ± 0.1	3.2 ± 0.1
	p-value	0.21	0.00	0.00
	q-value	0.29	0.00	0.00

Results in Table 7.5 show that the actual *RMSEP* distribution was significantly smaller than the nonsense for Amani and possibly Red Calypso but not for Tropicana roses. Further, the excessive p-values and q-values for the Amani variety with 2-week data indicated that there was significant overlapping between the actual *RMSEP* distribution and the nonsense one, and hence the estimates had low statistical confidence. For other Amani and Red Calypso cases, the p-values and q-values were low, which suggested high statistical confidence in the estimation. Given that the average loss in VL of Amani roses was about 4.5 d (min=1; max=10 d), an average *RMSEP* of 2.8 d may not be very useful. For Red Calypso roses, which had an average VL loss of 2.7 d (min=1; max=7 d), the estimation errors were 1.7-1.8 d. Considering that the data for the remaining VL was subject to a measurement resolution of 1 d, further improvement on the estimation error may require vase life data of better quality.

7.7.3 PLS PERFORMANCE

7.7.3.1 PLS IMPLEMENTATION

In addition to the analysis with all available data, PLS analysis with only temperature data is also carried out for comparison purposes as KLS can only work with temperature data. Consequently, two sub-scenarios are explored, including:

       1) Applying PLS to only the growing temperature.

       2) Applying PLS to all pre-harvest data.

In both sub-scenarios, double cross validation (Section 3.2.2) is performed to identify the optimal number of PLS factors and to assess the prediction performance.

7.7.3.2 ESTIMATING REMAINING VL AT THE FARM

Using only growing temperature

The prediction errors obtained when using PLS to estimate the remaining VL of cut roses at the farm are presented in Table 7.6 for growing temperature only. The p-values and q-values of the actual and nonsense $RMSEP$ distributions are also shown. A typical PLS performance is presented in Figure 7.13.

As shown in Table 7.6, for all combinations of varieties and pre-harvest window sizes, the means of the actual $RMSEP$ distributions were smaller than the means of the corresponding nonsense distributions. However, in two combinations including Tropicana with 2-week data and Amani with 2-week data, high p-values and q-values existed, indicating significant overlap between the actual and nonsense distributions. Moreover, the R^2 statistic was small (*ca.* 0.1), indicating that the linear correlation between the predicted and observed VLs was not very significant.
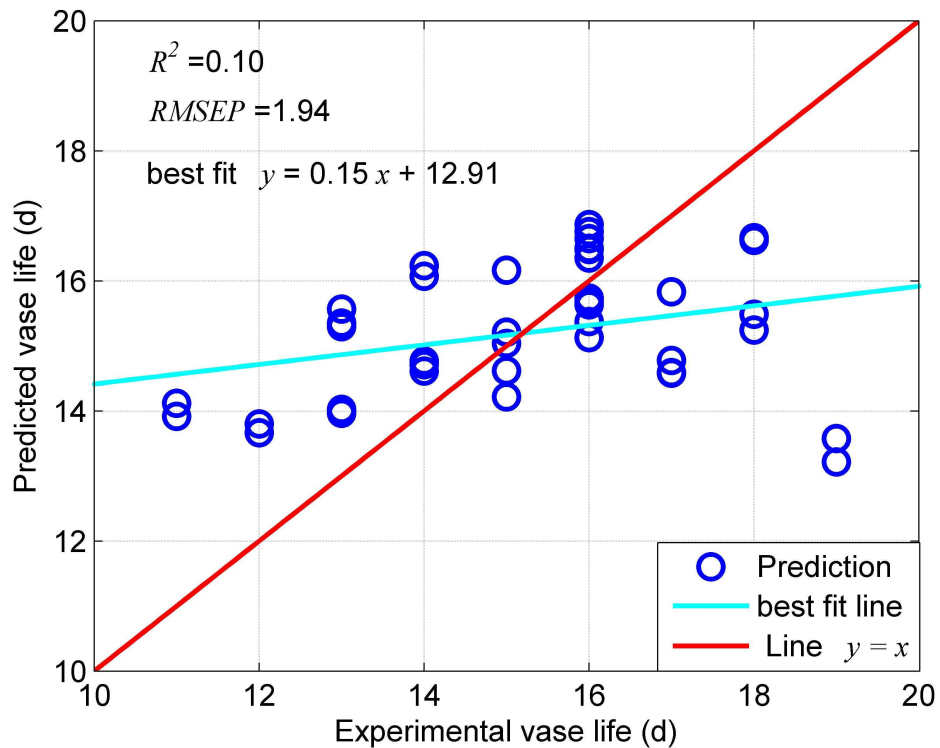
Figure 7.13: A typical PLS performance in estimating (Tropicana) VL at the farm based on 4-week pre-harvest temperature measurements.

Table 7.6: *RMSEP* in PLS estimation of VL at the farm using growing temperature

Pre-harvest window size		2 weeks	4 weeks	6 weeks
Tropicana (average VL=15.7 d; min=13 d; max=19 d)	Actual	2.1 ± 0.1	2.0 ± 0.2	2.0 ± 0.1
	Nonsense	2.2 ± 0.1	2.3 ± 0.1	2.4 ± 0.1
	p-value	0.31	0.05	0.02
	q-value	0.42	0.02	0.00
Red Calypso (average VL=15.4 d; min=13 d; max=18 d)	Actual	1.4 ± 0.1	1.5 ± 0.1	1.3 ± 0.1
	Nonsense	1.8 ± 0.1	1.9 ± 0.1	2.0 ± 0.1
	p-value	0.01	0.02	0.00
	q-value	0.00	0.00	0.00
Amani (average VL=15.9 d; min=14 d; max=18 d)	Actual	1.5 ± 0.1	1.1 ± 0.2	1.1 ± 0.1
	Nonsense	1.6 ± 0.0	1.8 ± 0.1	1.8 ± 0.1
	p-value	0.12	0.00	0.00
	q-value	0.43	0.00	0.00

Using all pre-harvest data

All the pre-harvest data including growing temperature, radiation and rainfall levels were analysed, and the results for PLS performance are tabulated in Table 7.7. The results show that the mean of the actual *RMSEP* distribution was smaller than that of the nonsense distribution for all combinations of varieties and window sizes studied. However, significant overlaps between the two distributions were present in three combinations including Amani with 2-week data and Tropicana with 2- and 4-week data.

Table 7.7: *RMSEP* **(d) in PLS estimation of VL at the farm using all pre-harvest measurements**

Pre-harvest window size		2 weeks	4 weeks	6 weeks
Tropicana (average VL=15.7 d; min=13 d; max=19 d)	Actual	2.1 ± 0.5	2.1 ± 0.2	1.9 ± 0.2
	Nonsense	2.6 ± 0.1	2.4 ± 0.1	2.6 ± 0.1
	p-value	0.06	0.12	0.02
	q-value	1.00	0.40	0.00
Red Calypso (average VL=15.4 d; min=13 d; max=18 d)	Actual	1.4 ± 0.1	1.0 ± 0.1	0.8 ± 0.1
	Nonsense	2.0 ± 0.1	1.9 ± 0.0	2.1 ± 0.1
	p-value	0.00	0.00	0.00
	q-value	0.00	0.00	0.00
Amani (average VL=15.9 d; min=14 d; max=18 d)	Actual	1.3 ± 0.1	1.1 ± 0.1	1.0 ± 0.1
	Nonsense	1.5 ± 0.1	1.7 ± 0.1	1.7 ± 0.0
	p-value	0.14	0.00	0.00
	q-value	0.80	0.00	0.00

In terms of input data, the tabulated results (Table 7.6 and Table 7.7) suggest that using all pre-harvest measurements seemed to produce a smaller estimation error than using only growing temperature. The most significant difference was observed in the Red Calypso variety. Using all pre-harvest data with window sizes of 4 and 6 weeks led to estimation errors of 1.0 and 0.8 d respectively. On the other hand, using only growing temperature gave errors of 1.5 and 1.3 d with the same window sizes. This suggested that additional data such as rainfall level and radiation intensity seemed to improve the PLS

estimation performance. This conclusion appears to agree with an earlier observation (see Section 7.7.1.2). The only exception was in Tropicana with 4-week data where using only growing temperature led to a smaller estimation error and higher confidence i.e., lower p-values and q-values.

In terms of the duration of the pre-harvest period, PLS seems to perform better with the bigger window size. Table 7.6 and Table 7.7 show that increasing the window size reduces the error in estimating the VL at the farm. For example, as the window size increased from 2 weeks to 4 weeks and then to 6 weeks, the error was lowered from 1.3 to 1.1 and then to 1.0 d for Amani (using all pre-harvest data, Table 7.7). The only exception was observed in estimating the VL of Red Calypso using 2 and 4 weeks of growing temperature where the difference in estimation error, 1.4 and 1.5 d, was mostly due to rounding errors. Furthermore, increasing the window size also reduced the p-values and q-values and hence the overlapping between the actual and nonsense *RMSEP* distributions.

Across the three varieties, Tropicana seems to have the worst error in VL estimation by PLS modelling. This occurred consistently across the three window sizes regardless of whether only growing temperature (Table 7.6) or all pre-harvest data (Table 7.7) was analysed.

7.7.3.3 ESTIMATING REMAINING VL AT THE DISTRIBUTION CENTRE

PLS was applied to the pre-harvest data to estimate the remaining VL at the end of the storage at the distribution centre. The results are presented in Table 7.8. In most cases the remaining VL was not well predicted by PLS modelling of pre-harvest data. The actual errors were often not significantly smaller than the nonsense ones. However, exceptional cases existed in the Amani variety where its VL was effectively estimated with high statistical confidence (low p-values and q- values) by PLS modelling of growing temperature. An example of the exceptional cases is presented in.
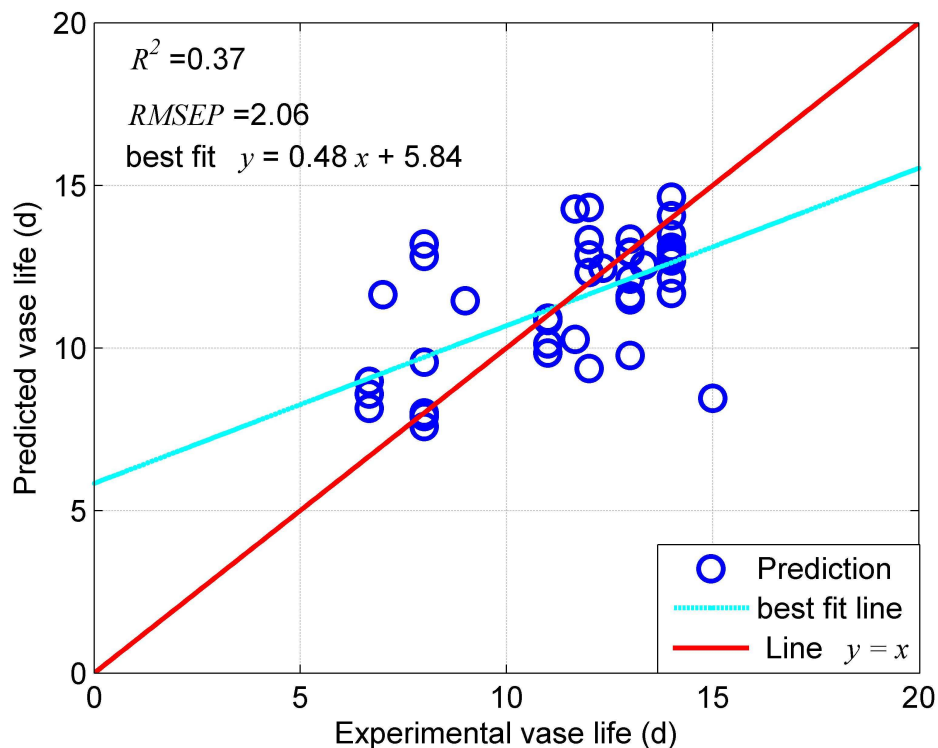
Figure 7.14: A typical PLS performance in estimating (Amani) VL at the distribution centre based on 4-week pre-harvest temperature measurements.

Using additional pre-harvest data seems to worsen PLS prediction performance. This was supported by the observation that the estimation error for Amani VL using only growing temperature was smaller than that from using all available pre-harvest data regardless of the size of the pre-harvest window period.

7.7.3.4 ESTIMATING THE LOSS IN REMAINING VL DURING TRANSPORT

The post-harvest loss in remaining VL of cut roses during transport and subsequent storage at the distribution centre was predicted by PLS modelling of the pre-harvest data. The prediction error and corresponding p-values and q-values are tabulated in Table 7.9. The results suggest that PLS prediction of the loss in VL during transport was effective in some but not all cases. For example, for Red Calypso variety with any of the three window sizes being studied, minimal overlap between the actual and nonsense $RMSEP$ distributions occurred; the mean of the actual errors was smaller than the nonsense one. Consequently, effective predictions were achieved in those cases. On the other

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hand, cases such as Amani with 2-week data led to high p-values and q-values, indicating significant overlapping between the actual and nonsense $RMSEP$ distributions. The predictions in those cases were not reliable.

The magnitude of the prediction errors reveals a practical concern. As shown in Table 7.9, in most cases for Tropicana and Amani, the average $RMSEP$ exceeds 2 d. However, the observed average losses in remaining VL of the two varieties were 3.2 and 4.5 d, respectively. As a result, while PLS predictions of the post-harvest loss in remaining VL could be effective in some cases, the associated prediction error may be excessive for practical applications.

Table 7.8: *RMSEP* (d) in PLS estimation of VL at the distribution centre

Input data	Pre-harvest window size		2 weeks	4 weeks	6 weeks
Growing temperature	Tropicana (average VL=12.5 d; min=7 d; max=16 d)	Actual	2.0 ± 0.1 NS	1.9 ± 0.2 NS	1.9 ± 0.1 NS
		Nonsense	1.9 ± 0.1 NS	1.9 ± 0.1 NS	2.0 ± 0.0 NS
		p-value	-	-	-
		q-value	-	-	-
	Red Calypso (average VL=12.7 d; min=10 d; max=14 d)	Actual	1.3 ± 0.1 NS	1.3 ± 0.1 NS	1.3 ± 0.1 NS
		Nonsense	1.2 ± 0.0 NS	1.3 ± 0.1 NS	1.2 ± 0.1 NS
		p-value	-	-	-
		q-value	-	-	-
	Amani (average VL=11.4 d; min=6 d; max=15 d)	Actual	2.3 ± 0.1	2.1 ± 0.1	2.2 ± 0.1
		Nonsense	2.8 ± 0.1	2.9 ± 0.1	3.0 ± 0.1
		p-value	0.01	0.00	0.00
		q-value	0.00	0.00	0.00
All pre-harvest data	Tropicana (average VL=12.5 d; min=7 d; max=16 d)	Actual	2.1 ± 0.3 NS	2.1 ± 0.1 NS	1.7 ± 0.1
		Nonsense	2.0 ± 0.1 NS	2.1 ± 0.1 NS	1.8 ± 0.0
		p-value	-	-	0.37
		q-value	-	-	0.95
	Red Calypso (average VL=12.7 d; min=10 d; max=14 d)	Actual	1.3 ± 0.1 NS	1.3 ± 0.1	1.4 ± 0.1 NS
		Nonsense	1.1 ± 0.0 NS	1.4 ± 0.1	1.2 ± 0.0 NS
		p-value	-	0.57	-
		q-value	-	0.70	-
	Amani (average VL=11.4 d; min=6 d; max=15 d)	Actual	2.7 ± 0.3 NS	2.3 ± 0.1	2.3 ± 0.1
		Nonsense	2.6 ± 0.1 NS	2.8 ± 0.1	2.9 ± 0.1
		p-value	-	0.00	0.00
		q-value	-	0.00	0.00

Table 7.9: *RMSEP* (d) in PLS estimation of the loss in remaining VL (i.e., ΔVL) during transport and storage

Input data	Pre-harvest window size		2 weeks	4 weeks	6 weeks
Growing temperature	Tropicana (average ΔVL = 3.2 d; min=1 d; max=9 d)	Actual	2.0 ± 0.1	2.3 ± 0.2 [NS]	2.2 ± 0.1
		Nonsense	2.5 ± 0.1	2.2 ± 0.1 [NS]	2.5 ± 0.1
		p-value	0.02	-	0.14
		q-value	0.01	-	0.44
	Red Calypso (average ΔVL = 2.7 d; min=1 d; max=7 d)	Actual	1.6 ± 0.1	1.6 ± 0.1	1.4 ± 0.1
		Nonsense	2.1 ± 0.1	2.1 ± 0.1	2.1 ± 0.1
		p-value	0.01	0.00	0.00
		q-value	0.00	0.00	0.00
	Amani (average ΔVL = 4.5 d; min=1 d; max=10 d)	Actual	2.9 ± 0.2	2.4 ± 0.1	2.5 ± 0.2
		Nonsense	3.4 ± 0.1	3.6 ± 0.1	3.2 ± 0.1
		p-value	0.10	0.00	0.00
		q-value	0.29	0.00	0.00
All pre-harvest data	Tropicana (average ΔVL = 3.2 d; min=1 d; max=9 d)	Actual	2.5 ± 0.3 [NS]	2.3 ± 0.1 [NS]	1.9 ± 0.1
		Nonsense	2.2 ± 0.3 [NS]	2.0 ± 0.1 [NS]	2.3 ± 0.1
		p-value	-	-	0.05
		q-value	-	-	0.05
	Red Calypso (average ΔVL = 2.7 d; min=1 d; max=7 d)	Actual	1.7 ± 0.1	1.8 ± 0.1	1.4 ± 0.1
		Nonsense	2.3 ± 0.1	2.1 ± 0.1	2.8 ± 0.2
		p-value	0.02	0.01	0.00
		q-value	0.00	0.02	0.00
	Amani (average ΔVL = 4.5 d; min=1 d; max=10 d)	Actual	3.2 ± 1.1	2.8 ± 0.2	2.5 ± 0.1
		Nonsense	3.5 ± 0.2	3.5 ± 0.1	3.0 ± 0.1
		p-value	0.07	0.01	0.00
		q-value	0.34	0.00	0.00

7.7.4 DISCUSSION

In this scenario, where the pre-harvest conditions were modelled, various sub-scenarios were investigated.

The smallest estimation errors from different sub-scenarios are reproduced in Table 7.10. Only results in Table 7.3 - Table 7.9 where effective predictions were achieved are summarised. A hyphen is used to indicate that such an effective prediction was not available.

Table 7.10: Smallest *RMSEP* from various sub-scenarios of Scenario 1

Sub-scenarios		KLS (temperature only)	PLS (temperature only)	PLS (all pre-harvest data)
Remaining VL at the farm	Tropicana	1.8 ± 0.1	2.0 ± 0.2	1.9 ± 0.2
	Red Calypso	1.3 ± 0.0	1.3 ± 0.1	0.8 ± 0.1
	Amani	1.3 ± 0.0	1.1 ± 0.1	1.0 ± 0.1
Remaining VL at the distribution centre	Tropicana	-	-	-
	Red Calypso	-	-	-
	Amani	2.5 ± 0.0	2.1 ± 0.1	2.3 ± 0.1
Loss in remaining VL	Tropicana	2.0 ± 0.1	2.0 ± 0.1	1.9 ± 0.1
	Red Calypso	1.7 ± 0.0	1.4 ± 0.1	1.4 ± 0.1
	Amani	2.8 ± 0.1	2.4 ± 0.1	2.5 ± 0.1

7.7.4.1 COMPARISON BETWEEN KLS AND PLS PERFORMANCES

From Table 7.10, PLS seems to be a better modelling technique than KLS in terms of estimation error. Except for estimating the remaining VL of Tropicana at the farm, in all other cases the best *RMSEP* from PLS was smaller than that from KLS. This is also true regardless of whether PLS was applied to growing temperature only or to all pre-harvest data.

The reason that PLS outperformed KLS in this scenario is that KLS is not built as a regression technique. As detailed in Chapter 4, KLS was developed from kinetic principles to describe the loss in shelf life or VL in terms of the temperature condition that the perishable item experiences. Consequently, the KLS development was only valid for the modelling of the quality (shelf life, VL) deterioration during the period that the temperature measurements were collected. However, procedurally KLS could be applied to temperature data recorded outside that period, like a regression technique (Section 4.3.3); this was demonstrated in this section where growing temperature was used to estimate the VL at the farm, at the distribution centre and the VL loss in between. Nevertheless, such KLS implementation was not supported by the original mathematical development from kinetic principles. Without the link to kinetic principles, the KLS regression technique did not perform as well as PLS.

7.7.4.2 PREDICTION PERFORMANCE IN THE THREE VL SUB-SCENARIOS

Table 7.10 also reveals that in modelling the pre-harvest conditions, estimating the VL at the farm was the sub-scenario with the smallest error. This is expected, in view of the assumptions that were made implicitly regarding the many factors that could affect the remaining VL of cut roses. As the literature review in Chapter 2 revealed, those factors included biological factors (e.g., flower variety, flower age), pre-harvest growing conditions (e.g., temperature, humidity, light intensity), and post-harvest conditions (e.g., temperature, humidity, ethylene exposure). Compared to the other two sub-scenarios, the estimation of the remaining VL at the farm made the most reasonable assumption. No assumption of the post-harvest conditions was necessary while most important biological (i.e., flower variety) and pre-harvest (temperature, rainfall level, sunlight radiation level) factors were considered.

For the remaining VL at the distribution centre and the VL loss during post-harvest transport and storage, their estimations in Scenario 1 did not consider post-harvest conditions. In doing so, important factors such as post-harvest temperature were implicitly assumed to be uniform across the flower samples; i.e., all samples were exposed to the same post-harvest temperature during transport and storage. However, this assumption may not necessarily be

reasonable, as shown by the profiles of logged post-harvest temperature (Figure 7.15). Consequently, the performances in these sub-scenarios were lower compared to the estimation of the VL at the farm.

7.7.4.3 USING ALL PRE-HARVEST DATA OR ONLY GROWING TEMPERATURE

Moreover, the results in Table 7.10 confirmed that using rainfall and sunshine radiation levels, in addition to the growing temperature, reduced errors in estimating the remaining VL at the farm, at the distribution centre, and the loss in between. An explanation for this could be that during the growing period of the roses the two additional factors correlated very well with the humidity and sun light intensity, which in turn were shown to have important roles in the growth, development and senescence of roses (Section 2.3.2).

7.8 SCENARIO 2 – MODELLING POST-HARVEST TEMPERATURE

As described in Section 7.5.3, modelling of the post-harvest transport of cut roses from the farm to the distribution centre was performed in Scenario 2. The post-harvest data included the temperature recorded during transport and storage, and the remaining VLs as evaluated at the farm and at the distribution centre. The objective was to investigate the effect of post-harvest temperature stress on the loss in the remaining VL of cut roses.

In this scenario, two sub-scenarios were considered depending on whether or not the remaining VL at the farm was used. In addition, for KLS technique, the effect of the *a priori* constraint that higher temperature leads to greater loss in VL was also examined.

7.8.1 EXPLORATORY STUDY

7.8.1.1 PROFILES OF POST-HARVEST TEMPERATURE
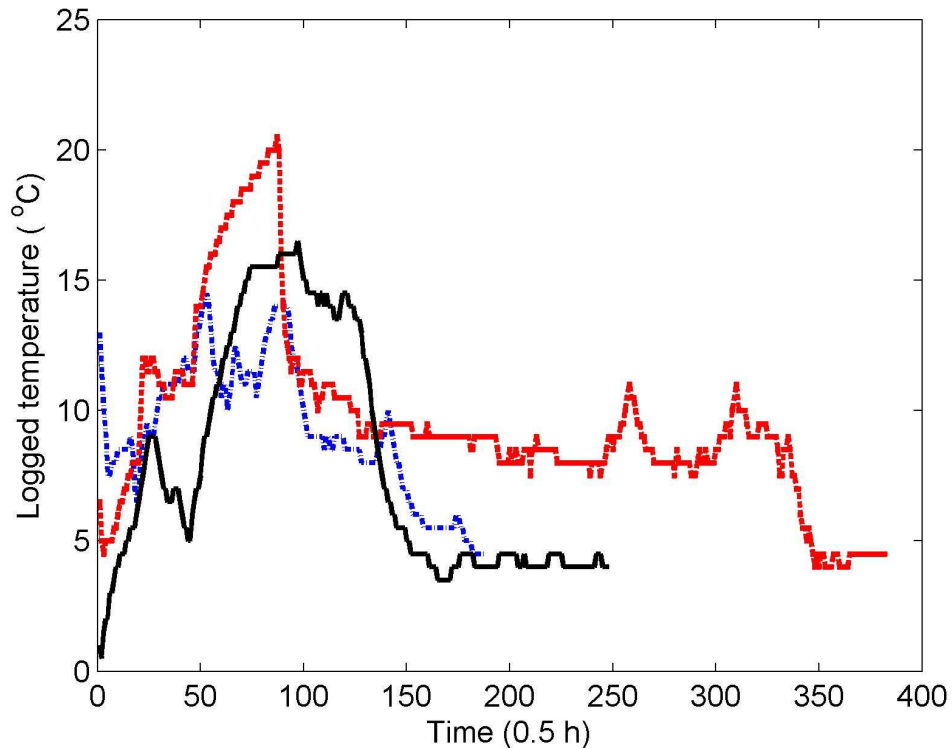
Figure 7.15: Typical logged temperature profiles for Tropicana

Figure 7.15 shows typical temperature profiles logged during the transport of cut roses (Tropicana variety) from the farm to the distribution centre and the subsequent storage prior to the vase life tests. The shortest profile, which lasts 4 days, is represented by the blue curve; the longest, almost 8 days, is shown by a red curve. A typical temperature profile, visualised by the black solid line in Figure 7.15, shows significant temperature variation in the first part, which was believed to correspond to the transport from the farm to the distribution centre. The temperature during the second half of the profile was more stable, which seems to relate to the storage period before the vase life test at the distribution centre.

7.8.1.2 CORRELATION BETWEEN POST-HARVEST TEMPERATURE AND LOSS IN REMAINING VL
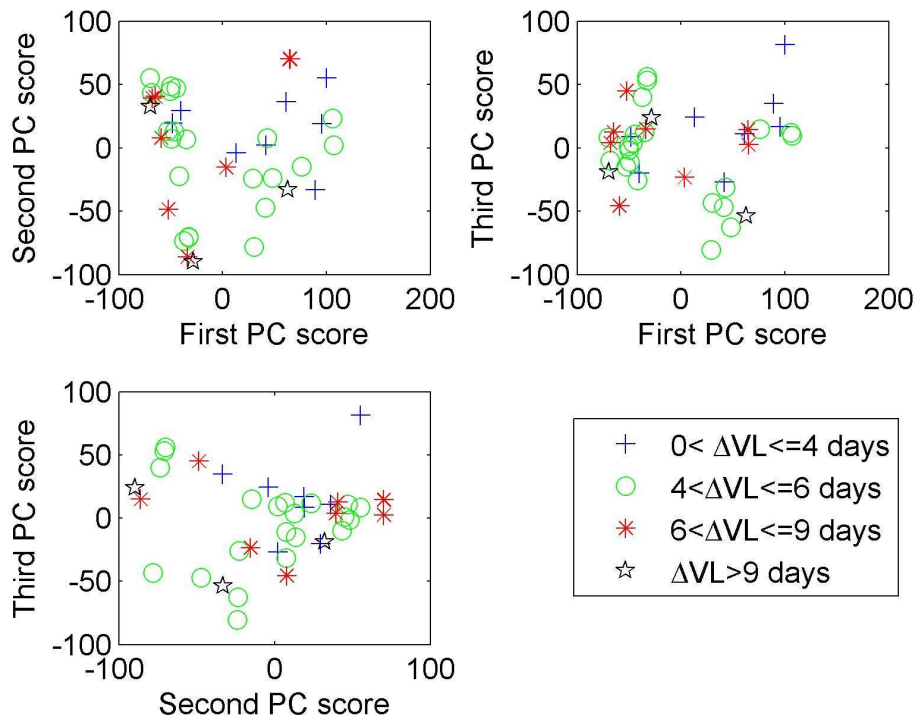
Figure 7.16: PCA score plots based on post-harvest temperature. The first three PCs captured 76% variance. Data were grouped according to post-harvest vase life loss

The logged post-harvest temperature was pre-processed to obtain a uniform number of measurements in each profile. The procedure of the pre-processing was described in details in Section 3.1.1. The pre-processed temperature profiles were then analysed using PCA technique. Figure 7.16 showed the results for Tropicana samples. In this figure, the scores were grouped according to the loss in VL during post-harvest transport and storage, which was the difference between the remaining VLs at the farm and at the distribution centre. As can be seen, the figure shows that the PCA scores for different groups in the VL loss spread quite randomly. This suggests that the correlation between the logged temperature and the loss in VL during transport would not be strongly linear and hence linear techniques such as MLR and PLS may not perform very well.

Similar analyses for Red Calypso and Amani varieties, or with grouping in remaining VL at the distribution centre led to a similar conclusion.

7.8.2 KLS PERFORMANCE

7.8.2.1 SETTING PARAMETERS

Based on the variation in logged temperature, the lower and upper temperature bounds for KLS modelling were set at 5 ^{o}C and 20 ^{o}C respectively. The temperature step was set at 1 ^{o}C.

7.8.2.2 ESTIMATING THE POST-HARVEST LOSS IN VL

Following the procedure described in Section 4.4, KLS was applied to the logged temperature to estimate the loss in VL during transport from the farm to the distribution centre and the subsequent storage before the vase life test. Cross validation (with $N_{test} = 10$ segments) was repeated 10000 times and $RMSEP$, R^2, and the slope and intercept of the best fit line were evaluated. Permutation testing was also carried out to obtain the corresponding nonsense distributions of the same statistics.

The procedure was performed for three varieties including Tropicana, Red Calypso and Amani. KLS performance without the *a priori* constraint for Tropicana variety is shown in Figure 7.17; results for the other varieties are summarised in Table 7.11.
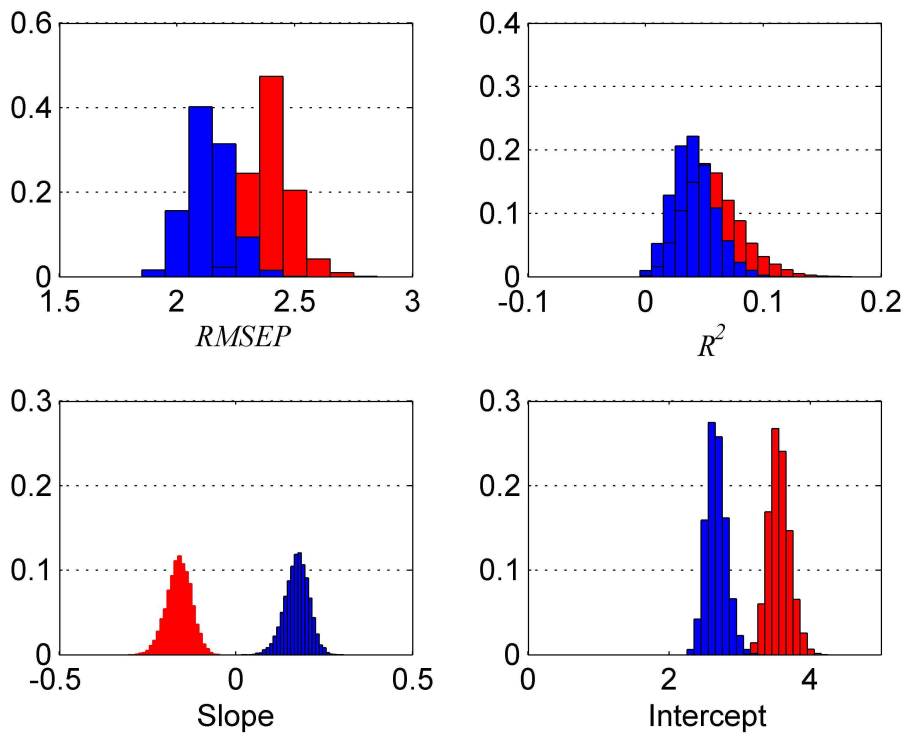
Figure 7.17: KLS performance in estimating the loss in VL of cut roses (Tropicana variety) during transport and storage using logged temperature. Blue distributions represent the actual performance; Red distributions show the nonsense performance from permutation testing. Y-axes show statistical densities of the performance indices

As can be seen in Figure 7.17, the actual distributions of the performance statistics, *RMSEP*, and the slope and intercept, do not coincide with their corresponding nonsense distributions. The peaks of the distributions are distinct; the overlaps in *RMSEP*, as reflected by p-values and q- values in Table 7.11, are relatively small. This indicates that the estimates were effective (Section 3.2.4), which in turn suggests that the logged temperature indeed contained information predictive of the VL loss, and that information was captured by the KLS model. However, the linear correlation between the observed and predicted loss was not justified by R^2, which was almost the same as its nonsense distribution (Figure 7.17).

Nevertheless, as compared to the average loss in VL for each variety the magnitude of the prediction error seemed quite big. From Table 7.11, the average losses were 3.2, 2.7 and 4.5 d; yet, the average estimation errors

(without the *a priori* constraint) were 2.2, 1.7 and 2.7 d for Tropicana, Red Calypso and Amani respectively.

Table 7.11: *RMSEP* (d) in KLS estimation of the loss in VL during transport and storage using post-harvest temperature

Sub-scenarios		Without *a priori* constraint	With *a priori* constraint
Tropicana (average ΔVL = 3.2 d; min=1 d; max=9 d)	Actual	2.2 ± 0.1	1.9 ± 0.0 [NS]
	Nonsense	2.5 ± 0.1	1.9 ± 0.0 [NS]
	p-value	0.07	-
	q-value	0.09	-
Red Calypso (average ΔVL = 2.7 d; min=1 d; max=7 d)	Actual	1.7 ± 0.0	1.9 ± 0.0 [NS]
	Nonsense	2.1 ± 0.2	1.8 ± 0.0 [NS]
	p-value	0.00	-
	q-value	0.00	-
Amani (average ΔVL = 4.5 d; min=1 d; max=10 d)	Actual	2.7 ± 0.1	2.6 ± 0.0
	Nonsense	3.6 ± 0.1	3.0 ± 0.0
	p-value	0.00	0.00
	q-value	0.00	0.00

The performance of KLS with the *a priori* constraint was also evaluated and is shown in Table 7.11. According to the tabulated results, implementing the constraint reduces the prediction performance of KLS technique. KLS with the *a priori* constraint could not produce effective estimates for Tropicana and Red Calypso as it did without the constraint. In the exceptional case, the estimation error for Amani variety from the constrained KLS (2.6 d) seemed smaller than that from the unconstrained one (2.7 d). Nevertheless, further analysis of the numerical results confirmed that this reduction of 0.1 d in *RMSEP* was not statistically significant.

7.8.2.3 ESTIMATING THE REMAINING VL AT THE DISTRIBUTION CENTRE

Similar to Section 7.8.2.2, KLS was implemented to estimate the remaining VL of cut roses at the distribution centre.

Table 7.12 presents the KLS performance in estimating the remaining VL based on post-harvest temperature. The results suggest that implementing the *a priori* constraint worsened KLS prediction performance. When the constraint was implemented, KLS could not make effective estimates of the remaining VL from the post-harvest temperature. On the other hand, without the constraint, effective estimates were possible for all three varieties. However, the linear correlation between the predicted and observed VLs, as measured by R^2, was not very strong, as shown in Figure 7.18.

Table 7.12: KLS prediction error $RMSEP$ (d) in estimating the remaining VL at the distribution centre using logged temperature

Sub-scenarios		Without *a priori* constraint	With *a priori* constraint
Tropicana (average VL=12.5 d; min=7 d; max=16 d)	Actual	1.8 ± 0.1	2.8 ± 0.0 [NS]
	Nonsense	2.1 ± 0.1	2.8 ± 0.0 [NS]
	p-value	0.03	-
	q-value	0.03	-
Red Calypso (average VL=12.7 d; min=10 d; max=14 d)	Actual	1.1 ± 0.1	2.6 ± 0.0 [NS]
	Nonsense	1.3 ± 0.1	2.2 ± 0.0 [NS]
	p-value	0.04	-
	q-value	0.04	-
Amani (average VL=11.4 d; min=6 d; max=15 d)	Actual	2.1 ± 0.2	4.0 ± 0.1 [NS]
	Nonsense	3.1 ± 0.1	2.8 ± 0.0 [NS]
	p-value	0.01	-
	q-value	0.00	-
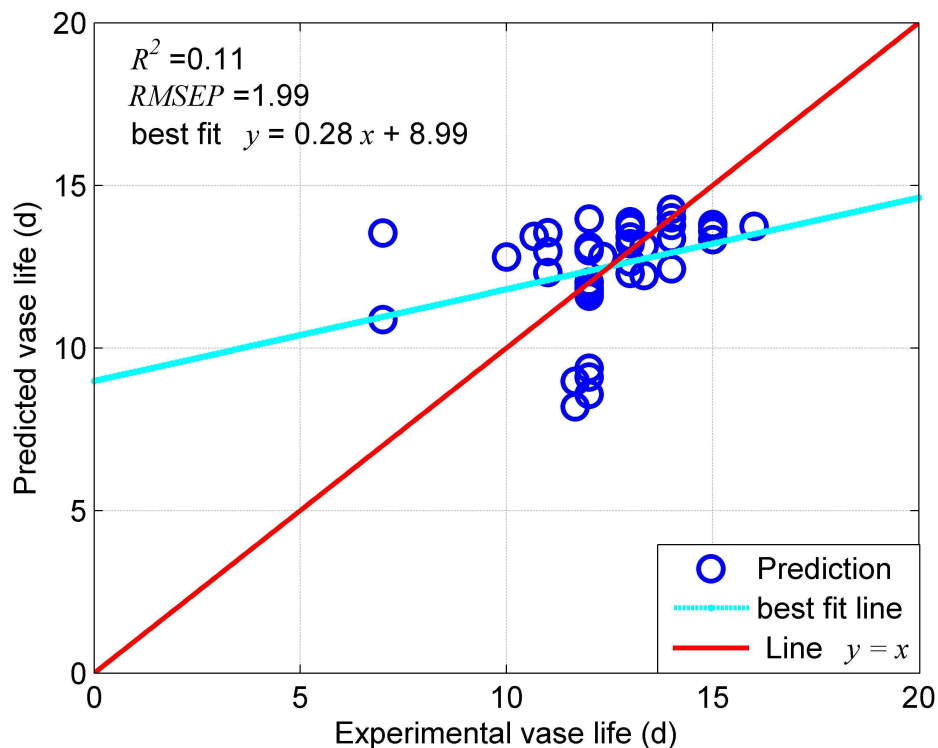
Figure 7.18: A typical KLS performance in estimating (Tropicana) VL at the distribution centre based on post-harvest temperature measurements (without *a priori* constraint).

In addition, relative to the average VL for each variety as well as its range (i.e., min and max), the magnitude of the prediction error seems reasonable. For example, for Red Calypso with an average VL of 12.7 d (min=10 d; max=14 d), the average *RMSEP* was 1.1 d. Given that the remaining VL was evaluated in the vase life tests with a measurement resolution of 1 d, any improvement in the prediction error may require VL data of better quality. Similar observations can be made for Tropicana and Amani roses.

7.8.3 PLS PERFORMANCE

7.8.3.1 PLS IMPLEMENTATION

PLS was used to model the post-harvest temperature. Double cross validation (Section 3.2.2) is performed to identify the optimal number of PLS factors and to assess the prediction performance.

In addition, the *a priori* constraint that was previously explored in KLS modelling was not implemented with PLS. This was because no PLS algorithm to implement constraints was found in literature.

7.8.3.2 Estimating the post-harvest loss in VL and the remaining VL at the distribution centre

Table 7.13 tabulates the performance of PLS in two sub-scenarios: estimating the loss in VL during transport and subsequent storage, and estimating the remaining VL at the end of the storage period. In the first sub-scenario, the means of the actual $RMSEP$ distributions were smaller than those of the nonsense ones. However, the p-values and q-values for Tropicana and Amani roses were significant, indicating excessive overlaps between the actual and nonsense distributions. Consequently, only PLS estimates for the loss in VL of Red Calypso were effective. In the second sub-scenario of estimating the VL at the end of the storage period at the distribution centre, only estimates for Tropicana roses were effective. For the other two varieties, either the mean of the actual $RMSEP$ distribution was greater than that of the nonsense one, or the excessive p-values and q-values indicated significant overlapping between the two distributions.

Table 7.13: PLS prediction error $RMSEP$ (d) in Scenario 2

Sub-scenarios		Post-harvest VL loss	VL at the distribution centre
Tropicana	Actual	2.1 ± 0.1	1.6 ± 0.1
	Nonsense	2.3 ± 0.1	1.9 ± 0.1
	p-value	0.47	0.01
	q-value	0.66	0.00
Red Calypso	Actual	1.5 ± 0.1	1.3 ± 0.1 [NS]
	Nonsense	2.2 ± 0.1	1.2 ± 0.0 [NS]
	p-value	0.01	-
	q-value	0.00	-
Amani	Actual	2.9 ± 0.2	2.3 ± 0.1
	Nonsense	3.3 ± 0.1	2.5 ± 0.1
	p-value	0.24	0.13
	q-value	0.84	0.89

7.8.4 Discussion

In this section, two sub-scenarios analysing the post-harvest temperature were considered. In the first one, the estimation of the remaining VL at the end of the storage at the distribution centre was studied; in the second, the VL loss during the transport (from the farm to the distribution centre) and the subsequent storage was estimated. The estimation errors in the two sub-scenarios are summarised in Table 7.14. Only errors from effective estimates (Table 7.11-Table 7.13) are presented. A hyphen is used to indicate that such an effective estimate was not available.

7.8.4.1 THE EFFECT OF THE *A PRIORI* CONSTRAINT

Studies in the physiology of cut flowers suggest that a higher temperature may lead to a greater loss in the remaining VL of cut flowers (Section 3.3). This *a priori* knowledge was investigated by implementing a constraint that satisfied the suggestion. As no PLS algorithm with constraints was identified, only KLS with the *a priori* constraint was explored. However, as can be seen from Table 7.14, the results of KLS modelling with the *a priori* constraint only gave effective estimates for the loss in VL of Amani. Yet, even in that case, the estimation error $RMSEP$ (2.6 d) was quite significant relative to the average loss in VL (4.5 d). Recall that (Section 3.3) the implementation of KLS with the *a priori* constraint has to accommodate a mathematical constraint (Section 4.3.6) as well as account for the non-thermal factors (Section 4.3.4). It is believed that significant variations in the factors such as daily rainfall (Figure 7.8) was present, which may make the assumption of minimum variance in those factors (Section 4.3.4) unreasonable.

Table 7.14: *RMSEP* (d) from different sub-scenarios in Scenario 2

Sub-scenarios		KLS (without the *a priori* constraint)	KLS (with the *a priori* constraint)	PLS
Remaining VL at the distribution centre	Tropicana (average VL=12.5 d; min=7 d; max=16 d)	1.8 ± 0.1	-	1.6 ± 0.1
	Red Calypso (average VL=12.7 d; min=10 d; max=14 d)	1.1 ± 0.1	-	-
	Amani (average VL=11.4 d; min=6 d; max=15 d)	2.1 ± 0.2	-	-
Loss in remaining VL	Tropicana (average ΔVL = 3.2 d; min=1 d; max=9 d)	2.2 ± 0.1	-	-
	Red Calypso (average ΔVL = 2.7 d; min=1 d; max=7 d)	1.7 ± 0.0	-	1.5 ± 0.1
	Amani (average ΔVL = 4.5 d; min=1 d; max=10 d)	2.7 ± 0.1	2.6 ± 0.0	-

7.8.4.2 COMPARISON BETWEEN KLS AND PLS PERFORMANCES

Table 7.14 also reveals that KLS seems to be more robust than PLS although the later can produce smaller estimation errors. Based on post-harvest temperature, for all three rose varieties, KLS can be used to obtain effective estimates of the remaining VL at the distribution centre as well as the loss in VL during the transport and storage. In contrast, PLS only gave effective estimates of the remaining VL of Tropicana rose and the loss in VL of Red Calypso; for the other cases, the PLS estimates were not effective. Nevertheless, in the cases where PLS estimates were effective, the corresponding estimation errors were smaller than those of the KLS estimates.

7.9 SCENARIO 3 – MODELLING PRE-HARVEST AND POST-HARVEST TEMPERATURE

In Scenario 3, both pre-harvest and post-harvest temperatures were analysed. The objective was to investigate whether the combination of both pre-harvest and post-harvest temperatures would lead to better estimates of the loss in remaining VL of cut roses.

7.9.1 KLS PERFORMANCE

7.9.1.1 KLS IMPLEMENTATION AND PARAMETERS

Intuitively, pre-harvest and post-harvest stages represent two fundamentally different stages for roses (and other flowers in general). The former stage associates with the accumulation and possibly deterioration in biological structures and in contents of micronutrients and carbohydrates that would determine the remaining VL of the flower just after being harvested. In the latter stage, the post-harvest period, the cut rose, which had been detached from its plant, was using up its stored nutrients and carbohydrates, and hence its remaining VL diminished with time. (The effect of any vase life solutions in extending the VL of cut flowers was not investigated in this study). Consequently, for KLS implementation in modelling both pre-harvest and post-harvest temperatures, two sets of parameters were used; one was for pre-harvest and the other was for post-harvest. The values of the parameters including upper and lower temperature bounds, and the temperature step were the same as those used in modelling pre-harvest temperature (see Section 7.7.2.1) and in modelling post-harvest temperature (see Section 7.8.2.1) independently.

7.9.1.2 ESTIMATING THE POST-HARVEST LOSS IN VL AND THE REMAINING VL AT THE DISTRIBUTION CENTRE

Table 7.15 shows the statistics associated with the actual and nonsense *RMSEP* distributions in estimating the post-harvest vase life loss and in estimating the remaining VL at the distribution centre. As can be seen, in estimating the vase life loss, KLS could not make effective estimates for Tropicana variety. For the

other two varieties, the average of the actual *RMSEP* was significantly smaller than the nonsense one. In addition, the p-values and q-values for the actual and nonsense *RMSEP* distributions in those cases were small, indicating little overlapping between the two distributions. A typical KLS performance is shown in Figure 7.19. Consequently, the KLS estimates for Red Calypso and Amani were effective although the linear correlation between the estimates and the observed VL loss was not very strong.
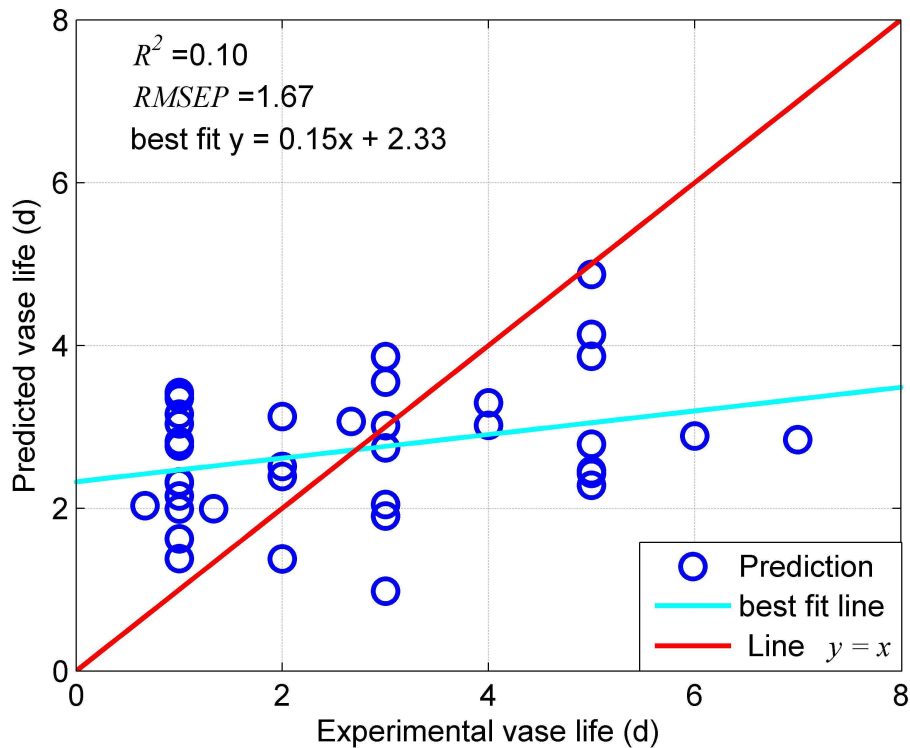
Figure 7.19: A typical KLS performance in estimating the loss in VL of Red Calypso roses during transport and storage based on pre-harvest and post-harvest temperature measurements.

Table 7.15: KLS prediction error *RMSEP* (d) in Scenario 3

Scenarios		Post-harvest VL loss	VL at the distribution centre
Tropicana	Actual	2.1 ± 0.1 [NS]	2.2 ± 0.7
	Nonsense	2.1 ± 0.1 [NS]	2.7 ± 1.2
	p-value	-	0.74
	q-value	-	0.85
Red Calypso	Actual	1.6 ± 0.1	1.6 ± 0.8
	Nonsense	2.1 ± 0.1	2.0 ± 1.3
	p-value	0.00	0.96
	q-value	0.00	0.85
Amani	Actual	2.5 ± 0.1	2.9 ± 1.4
	Nonsense	2.8 ± 0.1	3.9 ± 1.8
	p-value	0.03	0.32
	q-value	0.03	0.86

In estimating the remaining VL at the end of the storage period at the distribution centre, KLS produced estimates with the actual *RMSEP* distributions having smaller means than the nonsense ones. However, the p-values and q-values were excessively large, suggesting that significant overlapping between the actual and nonsense *RMSEP* distributions were present. Therefore, the statistical confidence in those KLS estimates was low and hence the predictions were considered not to be effective.

7.9.2 PLS PERFORMANCE

7.9.2.1 PLS IMPLEMENTATION

Pre-processing of the temperature profiles (so that they all have a uniform number of measurements) was carried out in the same way as performed in Section 7.8.3.1.

Double cross validation was also employed in determining the optimal model dimension and subsequently in assessing its predictive performance.

7.9.2.2 ESTIMATING THE POST-HARVEST LOSS IN VL AND THE REMAINING VL AT THE DISTRIBUTION CENTRE

Table 7.16 shows the PLS performance in Scenario 3. The results indicate that in all but one case, the actual PLS estimates had smaller average errors than the nonsense ones from the permutation test. (The exceptional case was in estimating the vase life loss for Tropicana roses, where the estimate was not significant). However, in the cases of Amani roses, the p-values and q-values were exceeding the significant level of 0.10, suggesting that significant overlapping was present between the actual and the nonsense $RMSEP$ distributions.

Table 7.16: PLS prediction error *RMSEP* (d) in Scenario 3

Scenarios		Post-harvest VL loss	VL at the distribution centre
Tropicana	Actual	2.1 ± 0.1 [NS]	1.6 ± 0.0
	Nonsense	2.0 ± 0.1 [NS]	2.0 ± 0.1
	p-value	-	0.00
	q-value	-	0.00
Red Calypso	Actual	1.6 ± 0.1	1.3 ± 0.1
	Nonsense	2.1 ± 0.1	1.4 ± 0.0
	p-value	0.00	0.07
	q-value	0.00	0.08
Amani	Actual	2.4 ± 0.2	2.2 ± 0.1
	Nonsense	2.7 ± 0.1	2.5 ± 0.1
	p-value	0.20	0.10
	q-value	0.37	0.36

7.9.3 DISCUSSION

In this section, two modelling sub-scenarios were studied. In the first sub-scenario, the estimation of the remaining VL at the end of the storage at the distribution centre was studied; in the second, the vase life loss during the transport and the subsequent storage was estimated. In both of the sub-scenarios, the pre-harvest and post-harvest temperatures were used as input. The estimation errors from the sub-scenarios are summarised in Table 7.17. Only errors from the effective estimates (Table 7.15 and Table 7.16) are reproduced. When an effective estimate was not available, a hyphen is shown.

As shown in Table 7.17, of the six cases, for two sub-scenarios involving three varieties each, KLS and PLS could only make effective estimates in two cases each; in the other cases, the estimation was not effective, meaning that either the mean of the estimation error was greater than that from a permutation test, or the statistical confidence was low as indicated by significant p-values and q-values.

Table 7.17: *RMSEP* from different sub-scenarios in Scenario 3

Sub-scenarios		KLS	PLS
Remaining VL at the distribution centre	Tropicana (average VL=12.5 d; min=7 d; max=16 d)	-	1.6 ± 0.0
	Red Calypso (average VL=12.7 d; min=10 d; max=14 d)	-	-
	Amani (average VL=11.4 d; min=6 d; max=15 d)	-	-
Loss in remaining VL	Tropicana (average ΔVL = 3.2 d; min=1 d; max=9 d)	-	-
	Red Calypso (average ΔVL = 2.7 d; min=1 d; max=7 d)	1.6 ± 0.1	1.6 ± 0.1
	Amani (average ΔVL = 4.5 d; min=1 d; max=10 d)	2.5 ± 0.1	-

An interesting observation was that while the vase life loss could be estimated effectively (e.g., for Amani and Red Calypso roses), the corresponding VL at the distribution centre may not, and vice versa. Further investigation is required to explain why that was so.

7.10 FURTHER DISCUSSION

In terms of input data, this chapter investigated three scenarios including:

1) Scenario 1: modelling of the pre-harvest conditions.
2) Scenario 2: modelling of the post-harvest temperature.
3) Scenario 3: modelling of the combined pre- and post-harvest temperature.

Furthermore as shown in Table 7.2 Scenario 1 had three sub-scenarios while Scenarios 2 and 3 only had two. These sub-scenarios corresponded to the output variables including the remaining VL at the farm, the VL at the distribution centre and their difference i.e. the loss in VL during transport to and storage at the distribution centre. The prediction errors of KLS and PLS in all modelling scenarios are summarised in Table 7.18.

Table 7.18: Prediction error *RMSEP* (d) in all modelling scenarios

Scenarios		1) Pre-harvest modelling		2) Post-harvest modelling		3) Pre- and post-harvest modelling	
		KLS	PLS (temperature only)	KLS	PLS	KLS	PLS
Remaining VL at the farm	Tropicana (average VL=15.7 d; min=13 d; max=19 d)	1.8 ± 0.1	2.0 ± 0.2	*na*	*na*	*na*	*na*
	Red Calypso (average VL=15.4 d; min=13 d; max=18 d)	1.3 ± 0.0	1.3 ± 0.1	*na*	*na*	*na*	*na*
	Amani (average VL=15.9 d; min=14 d ; max=18 d)	1.3 ± 0.0	1.1 ± 0.1	*na*	*na*	*na*	*na*
Remaining VL at the distribution centre	Tropicana (average VL=12.5 d; min=7 d; max=16 d)	-	-	1.8 ± 0.1	1.6 ± 0.1	-	1.6 ± 0.0
	Red Calypso (average VL=12.7 d; min=10 d; max=14 d)	-	-	1.1 ± 0.1	-	-	-
	Amani (average VL=11.4 d; min=6 d; max=15 d)	2.5 ± 0.0	2.1 ± 0.1	2.1 ± 0.2	-	-	-
Loss in remaining VL	Tropicana (average ΔVL = 3.2 d; min=1 d; max=9 d)	2.0 ± 0.1	2.0 ± 0.1	2.2 ± 0.1	-	-	-
	Red Calypso (average ΔVL = 2.7 d; min=1 d; max=7 d)	1.7 ± 0.0	1.4 ± 0.1	1.7 ± 0.0	1.5 ± 0.1	1.6 ± 0.1	1.6 ± 0.1
	Amani (average ΔVL = 4.5 d; min=1 d; max=10 d)	2.8 ± 0.1	2.4 ± 0.1	2.7 ± 0.1	-	2.5 ± 0.1	-

na: not applicable i.e., this sub-scenario was not considered.

7.10.1 COMPARISON BETWEEN KLS AND PLS

As Section 2.5.2 revealed, PLS is one of the most commonly used regression techniques and is designed to deal with data sets in which the number of measurement variables per sample is large. By contrast, KLS was developed from a general differential equation describing the kinetics of the quality of a perishable product (Chapter 4). Results in Table 7.18 show that PLS produced estimates of the remaining VLs and the vase life loss that were slightly more accurate than those from KLS. The most significant difference between KLS and PLS was in estimating the vase life loss for Amani roses using growing temperature. In that case, $RMSEP$ of KLS estimates averaged 2.8 d while that of PLS ones was only 2.4 d.

Despite being slightly less accurate, KLS is more robust and flexible compared to PLS. The robustness of KLS was evident in Scenario 2 (see Table 7.18) where KLS was able to give effective predictions in all six cases while PLS could only do so for two cases. In addition, KLS is more flexible as it was able to implement *a priori* constraints as demonstrated in Section 7.8.2 while PLS could not do so. Although this KLS capability did not lead to any estimation improvement, it may be valuable in other applications where appropriate *a priori* knowledge and data sets exist.

7.10.2 PRE-HARVEST OR POST-HARVEST TEMPERATURE

Post-harvest temperature was suggested as the most important factor in the post-harvest life of cut roses (Section 2.3). However, this study found that growing temperature could be equally important. As can be seen in the results from Scenarios 1 and 2 (Table 7.18), using post-harvest temperature to estimate the remaining VL at the distribution centre and the vase life loss led to prediction errors that were similar to those from using growing temperature. In some cases, using growing temperature led to smaller $RMSEP$ (e.g., estimating the loss in VL of Tropicana); in other cases, more accurate predictions were obtained based on post-harvest temperature e.g., estimating the remaining VL of Amani roses at the distribution centre. The only notable difference in the

prediction performance in Scenario 1 (using growing temperature) and Scenario 2 (using post-harvest temperature) was in estimating the remaining VL at the distribution centre for Tropicana and Red Calypso. In those two cases, the post-harvest modelling produced effective estimates of the remaining VL but the pre-harvest modelling could not.

The potential benefit of combining pre-harvest and post-harvest modelling was investigated in Scenario 3. Intuitively, it was expected that such combination would result in an improved performance compared to Scenarios 1 and 2. However, as the results in Table 7.18 show, only KLS performance was improved while PLS performance was slightly worsened. More importantly, the improvement in KLS performance was at the expense of its robustness as effective estimates were only obtained in two out of six cases.

For PLS, although the combined data set had many more measurements for each data sample than the individual pre-harvest or post-harvest data sets, little change in PLS prediction performance was observed compared to Scenario 2. The performance was not reduced significantly because PLS is capable of dealing with data sets having many more measurements compared to the number of samples. On the other hand, it is believed that the performance was not improved because the number of data samples was not increased.

7.10.3 PREDICTION PERFORMANCE IN THE SUB-SCENARIOS

In each Scenario, two VL sub-scenarios were considered including the estimation of the remaining VL at the distribution centre and the estimation of the vase life loss during transport and storage. For Scenario 1, an additional sub-scenario was the estimation of the remaining VL at the farm. As shown in Table 7.18, of the three sub-scenarios, estimating the loss in VL had the biggest estimation error. This could be explained using the fact that the vase life loss was the mathematical difference between the remaining VL at the farm and the remaining VL at the distribution centre. Errors existed in evaluating the remaining VL both at the farm and at the distribution centre, regardless of which evaluation technique (i.e. experimental testing or numerical estimation) was

used. Such errors would mathematically propagate to the estimation of their difference i.e. the vase life loss, leading to a greater estimation error.

7.10.4 USEFULNESS OF THE VL ESTIMATION

Table 7.18 showed that estimates of the remaining VLs and the vase life loss during transport and storage were possible using either growing temperature or post-harvest temperature. Such estimates were effective, meaning that there was high statistical confidence that their errors were smaller than that of a random guess from the permutation testing. However, for the estimation of the vase life loss, the relative estimation errors were rather significant. Specifically, the minimum relative errors based on the means of *RMSEP* were 2/3.2 (63%), 1.4/2.7 (52%) and 2.4/4.5 (60%) for Tropicana, Red Calypso and Amani, respectively. It is likely that such excessive relative errors would make the estimation of the vase life loss not useful practically. For the estimation of the remaining VLs (at the farm or at the distribution centre), the relative estimation errors were much more modest (based on the minimum of *RMSEP* means: 11%, 8% and 7% for Tropicana, Red Calypso and Amani respectively). Consequently, those estimates could still be useful practically.

The excessive relative error in estimating the loss in VL of cut roses should be expected. This was because the average of the vase life loss was rather small (2.7-4.5 d). Further, the absolute error of the estimation of the vase life loss is always greater than those from estimating the individual VLs (Section 7.10.3), which in turn are greater than 1 d due to the measurement resolution of the vase life test results (Section 7.3.3). For those reasons, using other techniques for the estimation may not significantly improve the relative error.

7.11 CHAPTER CONCLUSION

This chapter reported a case study in a chilled supply chain of cut roses. It found that not only post-harvest temperature but also pre-harvest temperature and other environmental factors could be used to obtain effective estimates of the remaining VLs and their difference (i.e. loss) during transport and storage of cut roses. However, the estimation of the vase life loss had high relative error and hence may not be practically useful. This was due to the (small) magnitude of the vase life loss as well as the measurement resolution of the vase life test results. In addition, it was found that PLS led to smaller prediction errors although KLS was demonstrated to be more robust and flexible.

8 CONCLUSION AND FURTHER WORK

8.1 CONCLUSION

This thesis reports the investigation of the hypothesis that multivariate data analysis techniques can be used to estimate the loss in the quality of fresh fruits, fresh vegetables and cut flowers in chilled supply chains based on the data collected using advanced sensors. Cut roses were selected as an exemplar system although it is expected that the findings will also be applicable to other produce.

Literature review in the senescence of cut flowers, particularly cut roses, and in their vase life prediction was undertaken. Simulation studies of various perishable products such as tomato, mushroom, seasoned soybean sprout, cooked shrimp, and other seafood products were performed. For real supply chain data, two large scale experiments with cut roses, one with Cookes Rose Farm (Jersey) and the other with World Flowers Ltd. (UK), were performed. The outcomes of the two experiments were two original data sets that are considered as an original contribution of this work. In addition, a new technique termed KLS, and existing ones including PLS and MLR were implemented for the data analysis. Detailed results, discussions and conclusions were presented in Chapters 5, 6, and 7. The essential conclusions are summarised below.

1. A novel data-driven technique termed Kinetic Linear System (KLS) was developed for modelling the effect of temperature on the remaining shelf life of perishable products. The technique is based on kinetic principles and hence is applicable to perishable products the shelf life of which is governed by chemical, biochemical, microbial and physical processes. Simulation studies showed that a KLS model could "learn" and subsequently reproduce the output of traditional kinetic models in shelf life prediction. Consequently, it can be applied to products which do not normally have a traditional kinetic model. This was demonstrated by using KLS for the analysis of the data from the Cookes Rose and the World Flower experiments.

2. With respect to the research hypothesis KLS, PLS and MLR were investigated for the analysis of the data from the two experiments with cut roses. MLR was shown to have poor estimation performance whereas KLS and PLS could generate estimates of the loss in VLs of cut roses during transport and storage. These estimates are effective, having a smaller error than that of nonsense guesses with a high statistical confidence. However, the estimation of the losses in VLs may not be useful practically due to the magnitude of the associated relative error. This was demonstrated in the Cookes Rose Farm case study (Chapter 6), where the minimum *RMSEP* was 2 d for an average loss of 7.2 d; and in World Flowers case study (Chapter 7), where the *RMSEP* was from 1.4 to 2.8 d for average VL losses of 2.7-4.5 d.

In addition, PLS technique had a slightly smaller *RMSEP* than KLS technique. However, the latter was more flexible as it can work with constraints and does not require a uniform number of measurements in its input. KLS is more robust as it worked effectively in many cases where PLS failed to. KLS also has a better capability in data reduction because it uses temperature states rather than the actual temperature measurements as its independent variables (Section 6.11.1).

3. In terms of the physiological understanding of cut roses, the studies reported in this thesis confirmed an expert opinion that temperature is one of the most important post-harvest factors for cut roses. In addition to post-harvest temperature, the literature review in this thesis also found that other factors including genotype, pre-harvest (growing) conditions, post-harvest non-thermal factors (e.g. humidity) could also have influential effects on the post-harvest longevity of cut roses. The effect of the pre-harvest conditions was indeed confirmed by the results from the data analysis in the Cookes Rose and the World Flowers case studies. Effective estimates of the VLs of cut roses at the farm, at the distribution centre, and the loss in VLs were obtained based on the growing temperature using KLS and PLS techniques.

In conclusion, multivariate data analysis techniques can be used to generate effective estimates of the loss in VLs of cut roses based on post-harvest temperature collected by data loggers. However, the estimates of the VL loss may not be useful practically due to high relative errors. Of the three techniques that were studied, PLS and KLS performed effectively while MLR could not. Although PLS had slightly smaller errors than KLS, the latter was more robust and flexible. In addition, either post-harvest temperatures or pre-harvest temperatures could be used for the estimation although the post-harvest measurements may lead to slightly smaller errors.

8.2 FURTHER WORK

The work reported in this thesis has presented a number of possibilities for further work. These include studies to improve the quality of the experimental data, investigations of alternative techniques and the application of KLS and multivariate data analysis techniques in a real-time decision support system.

8.2.1 IMPROVED DATA SETS

Reducing measurement error

In this study, measurement error, particularly for the evaluation of the remaining VL of cut roses, could be significant. As described in Sections 6.3.4 and 7.3.3, the VL was evaluated based on human judgement which could be subjective and recorded with a measurement resolution of 1 d. Clearly, the remaining VL values were susceptible to judgemental error and as a consequence were likely to have an accuracy of ±1 d. It should be noted that any data analysis technique can not eliminate such error in the data for the experimental VL i.e., its estimates of the remaining VL would have an error that is always greater than 1 d. Considering that the minimum *RMSEP* reported in this study was around 1.4-2 d, the contribution of the measurement error represents a major portion of the *RMSEP*. As a result, reducing the measurement error using more objective criteria could significantly improve the prediction performance of any data analysis technique.

A trivial way to reduce the measurement error is to employ additional experts and perform the evaluation task (of determine whether the flower sample has reached its end of its useful life) multiple times a day. In that way, human error can be reduced and the measurement resolution is improved. However, this approach may not be very practical due to the cost associated with employing additional experts to perform the VL tests. Alternatively, the remaining VL may be assessed using gene expression analysis techniques, as discussed in Section 2.4.2. Nevertheless, because the techniques are not publically available, either further research must be carried out to correlate the expression levels of the relevant genes to the potential VL or a commercial service such as that from NSure Ltd. (2007a) must be employed.

Another approach to evaluate objectively the VL could be potentially developed in metabolic studies of the cut flowers. The idea would be to identify one or more metabolites associated with the senescence process in cut roses, and subsequently correlate the concentration of such metabolite(s) to the VL of the flowers. As reviewed in Section 2.5.2, this idea was already explored in studying the spoilage of food products such as milk (Nicolaou and Goodacre 2008), minced beef (Ammor *et al.* 2009) and others as mentioned in (Nicolaï *et al.* 2007). Nevertheless, no application in cut flowers have been reported, which is possibly because their quality attributes have not been successfully linked to any particular plant metabolite(s).

Reducing pre-harvest and biological variation

Figure 6.7 and Figure 6.8 showed the variation in VL of cut roses that were exposed to the same post-harvest temperature stress profile. As this VL variation was not due to post-harvest temperature, its presence would reduce the accuracy of any VL estimation using post-harvest temperature. Consequently, it may be desirable to minimise such VL variation.

It is believed that the variation in the pre-harvest conditions and the genetic variation in the flower samples are the two major sources that contribute to the VL variation shown in Figure 6.7 and Figure 6.8. Consequently, a thorough study would start with using genetic engineering technology to generate flower plants having identical genetic materials. These genetically identical plants

would be grown under a well-controlled greenhouse so as to minimise the variation in their pre-harvest conditions. (The idea of manufacturing genetically identical plants and growing them in controlled greenhouse has been proposed under the concept of "sustainable plant factory"). Subsequently, the flowers from these plants would be used for data collection experiment. In other words, some would undergo at-harvest VL testing while others would be subjected to various post-harvest temperature profiles and subsequent VL testing. The data collected can then be used to develop models such as in Chapters 6 and 7.

8.2.2 ALTERNATIVE DATA ANALYSIS TECHNIQUES

MLR and PLS were selected in this project to explore the capability of linear regression techniques in estimating the (loss in) VL of cut roses. As a result, the performance of other linear techniques such as principal component regression could be potentially inferred from that of either MLR or PLS. On the other hand, the performance of nonlinear techniques such as artificial neural networks (ANNs), support vector machine (SVM), and nonlinear (kernel) PLS need further study.

As an example, ANNs were selected to demonstrate the potential of nonlinear techniques in estimating the vase life loss using post-harvest temperature. A multilayer perceptron model with as many input nodes as the number of measurements in each temperature profile was calibrated. Figure 8.1 shows the preliminary performance of ANNs for Tropicana roses in World Flowers case study (Chapter 7). Although its performance still needs to be optimised and statistically assessed, the technique produced lower prediction error ($RMSEP$ = 1.3 d) than either KLS ($RMSEP$ = 2.2 d, Table 7.11) or PLS ($RMSEP$ = 2.1 d, Table 7.13). As a result, nonlinear regression techniques and ANNs in particular may be worth further consideration.
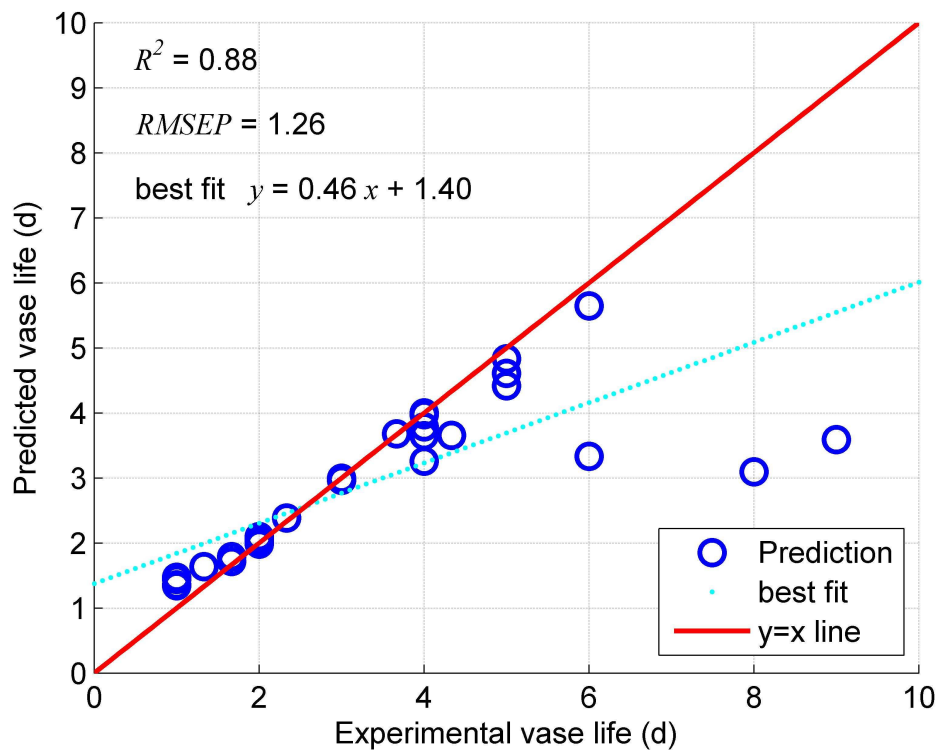
Figure 8.1: Performance of ANNs in estimating the loss in VLs of Tropicana roses in World Flowers case study.

Alternatively, survival analysis techniques may also be considered for future studies. These techniques were developed to evaluate the times until an event of interest (e.g., the death of cut flowers), taking into account the effects of censorships as well as the effects of external factors (e.g., post-harvest temperature). Methods of survival analysis have been used extensively in various fields such as clinical studies (Sanz *et al.* 1989; Fleming and Lin 2000) and reliability studies (Wang *et al.* 2005; Bradley and Kohler 2007). For modelling shelf life of food, Hough *et al.* applied survival analysis techniques to study the spoilage of yogurt stored at 42 $^\circ$C (Hough *et al.* 2003). While the study successfully illustrated the concept in the modelling of sensory shelf life of food products, the example it used was rather simple. As the researchers noted, additional challenges e.g., accounting for the effects of storage temperature and humidity are expected in more practical studies (Hough *et al.* 2003). The data collection would also become more challenging when the conditions e.g., temperature and humidity vary during storage.

8.2.3 VL ESTIMATION FOR A REAL-TIME DECISION SUPPORT SYSTEM

Decision support systems (DSS) refer to any computer-based information systems that are developed to improve any decision-making process and its outcome (Arnott 2004). Since its introduction in 1970s, DSS has been implemented in a wide range of applications such as healthcare (Shin and Markey 2006; Berner and Lande 2007; Shebl *et al.* 2007), environmental management (Jones *et al.* 2002; Mysiak *et al.* 2005), urban development management (Quattrochi *et al.* 2000), and agriculture (Bange *et al.* 2004; Bazzani 2005). A real-time DSS is a system that supports decision making at any point in time.

As mentioned in Section 1.3, in a quality-controlled logistics system, decisions are made based on the quality of the products. Consequently, the estimation of the quality (loss) of horticultural produce was to facilitate making such decisions. This thesis demonstrated that the effective estimates of the VL loss in cut roses were obtained at the end of their transport or storage. Such estimates are valuable in making decisions regarding the subsequent management of the flowers and the optimal distribution policy e.g., which quality class do they belong to? which customers should they be sold to, and at which price? However, in a logistics system it is often necessary to make many decisions at any time point, particularly before the end of the transport or storage. For examples, when a produce is deteriorating too fast, decisions must be made as to which remedial actions e.g., adjusting temperature conditions, changing transport route, or selecting alternative destinations should be performed. For such decisions, real-time quality estimation for a real-time DSS is required.

While real-time quality estimation is not a novel concept, its application in perishable goods supply chain has not been identified. The reason is that there are several difficulties in addition to the already-challenging task of quality estimation. The first additional challenge would be the collection of the data that are suitable and reliable for the real-time estimation. The desired data set would consist of not only the measurements of the conditions e.g., temperature but

also the corresponding assessments of the product quality during transport and storage. Accurate quality assessments are believed to be the most time-consuming and costly task in the data collection exercise. The second additional challenge is of more technical nature i.e. the quality estimation must be made based on an incomplete set of real-time data. For this challenge, KLS implementation in a real-time context must be explored while applications of dynamic PLS were reported in many studies (e.g. (Chen *et al.* 1998; Komulainen *et al.* 2004; Doan *et al.* 2006)).

From the above three areas for further research, the accurate determination of product quality (e.g., vase life or shelf life) is probably the most important. The reason for that is because data sets of better accuracy enable a more objective evaluation of the capability of the data analysis techniques. Such an evaluation may subsequently provide further insights into the feasibility of the relevant practical application, and hence raises the importance of the research not only in academia but also in industry. Within this area of further work, it is believed that preferences should be toward automatic and objective evaluation techniques, which do not heavily involve human judgement. Consequently, gene expression analysis and metabolic studies would be the preferred options.

8.3 FINAL REMARKS

The work reported in this thesis has opened a new research area in using multivariate data analysis techniques to estimate the loss in quality of in-transit product based data collected by advanced sensors. As the cost of deploying advanced sensors continues decreasing, their applications in logistics and the supply chains of perishable products in particular are drawing more and more interest from various stakeholders. Therefore, it is apparent that multivariate data analysis techniques will continue to be at the centre of further research and applications in this area.

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APPENDICES

A.   USING PHOTOS TO DETERMINE THE END OF THE USEFUL LIFE OF CUT ROSES

For the Cookes Rose Farm study, photos were taken daily during the office display tests and the VL tests of cut roses. These photos and a number of criteria as set out in Section 6.3.4 were subsequently used to determine the end of the useful life of the flowers. The following photos demonstrate an example of the evaluation task.

Table A. 1: Observation photos for flower ID 17 during the office display test

Date	Sample ID 17 in the office display test
08/07/2008 The flower is delivered, processed and displayed in a cylinder in an office environment.	
09/07/2008	

10/07/2008	
11/07/2008	

12/07/2008 The flower shows the first sign of bent neck.	
13/07/2008 The flower is dead. The display test is ended.	

B. **ADDITIONAL RESULTS IN COOKES ROSE CASE STUDY**
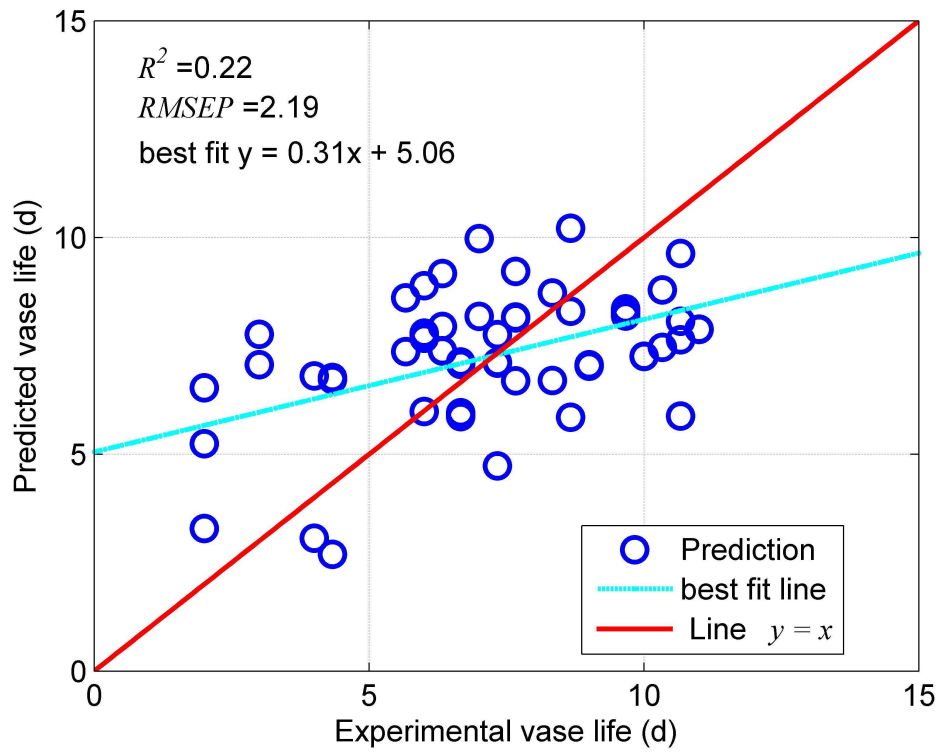
Figure B. 1: Scenario 1A– a typical PLS performance in modelling the office display period <u>without</u> the *a priori* constraint. (zero-mean)
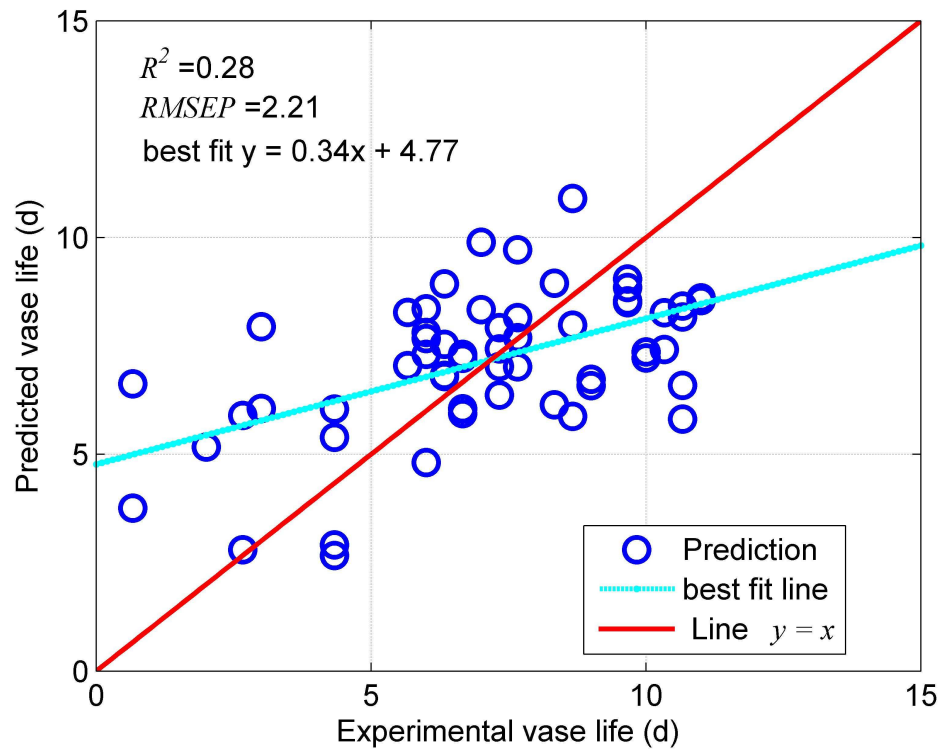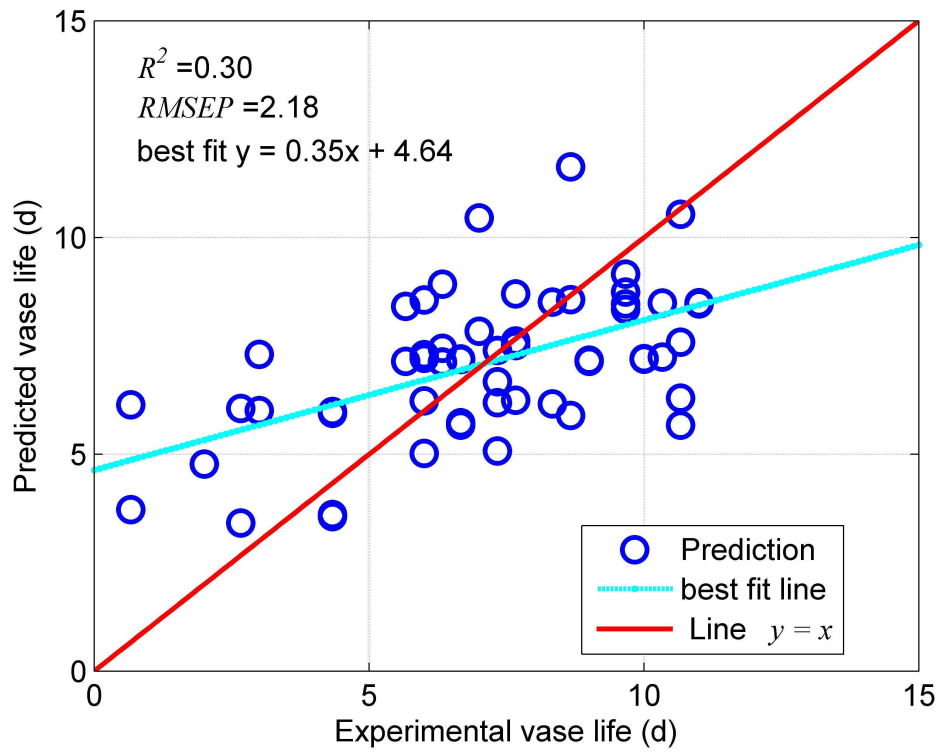
Figure B. 2: Scenario 1A– a typical MLR performance in modelling the office display period <u>without</u> the *a priori* constraint. (zero-mean)

Figure B. 3: Scenario 1B – a typical MLR performance in modelling the office display period <u>with</u> the *a priori* constraint. (zero-mean)
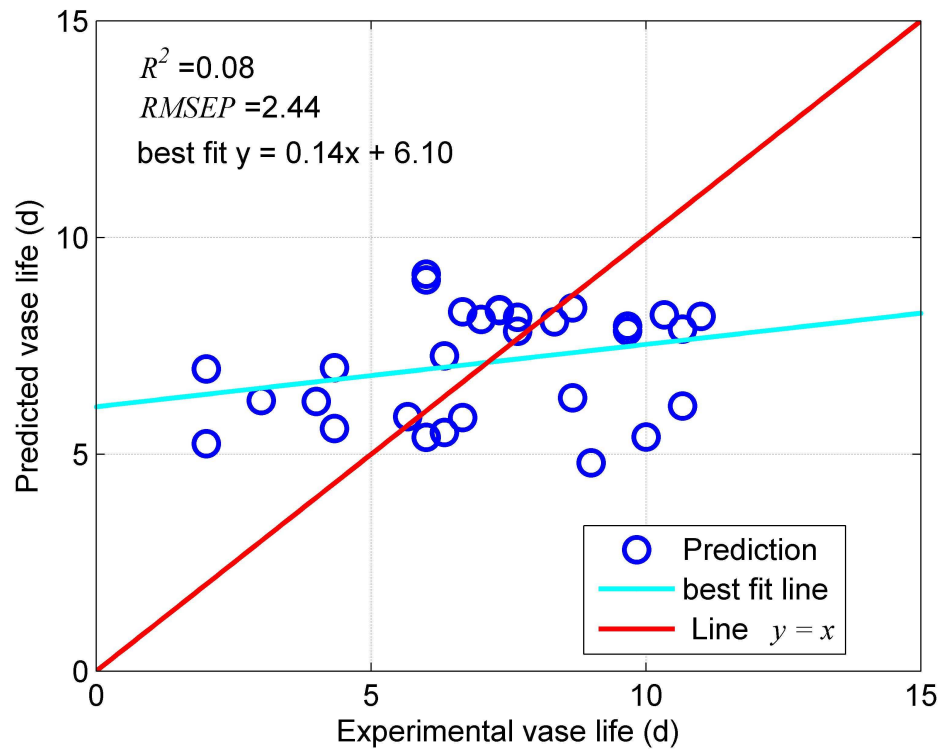
Figure B. 4: Scenario 2A – a typical PLS performance in modelling the VL upon delivery at University of Manchester assuming uniform initial VLs (<u>zero-mean scaling</u>).
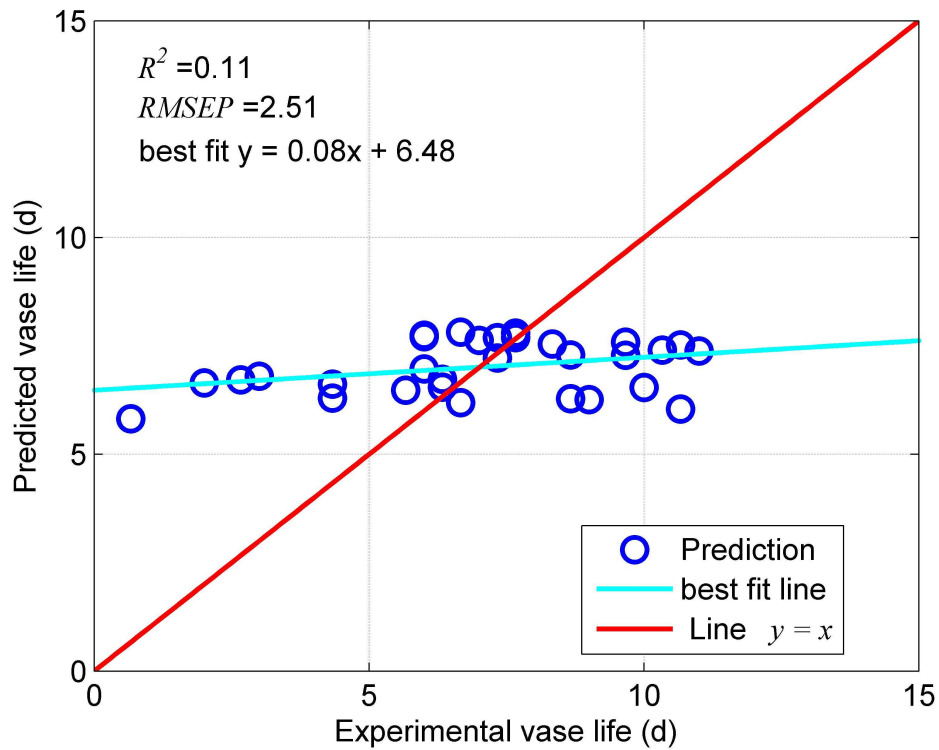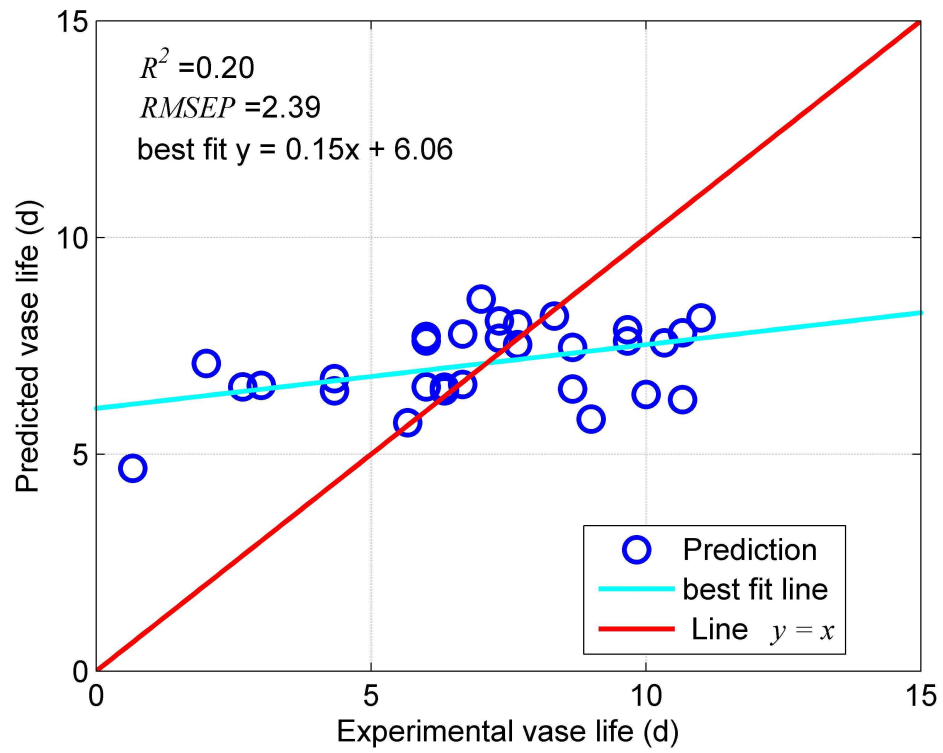
Figure B. 5: Scenario 2A – a typical MLR performance in modelling the VL upon delivery at University of Manchester assuming uniform initial VLs (<u>zero-mean scaling, without _a priori_ constraint</u>).

R^2 =0.20
$RMSEP$ =2.39
best fit y = 0.15x + 6.06

Figure B. 6: Scenario 2B – a typical MLR performance in modelling the VL upon delivery at University of Manchester assuming uniform initial VLs (<u>zero-mean scaling, with a priori constraint</u>).
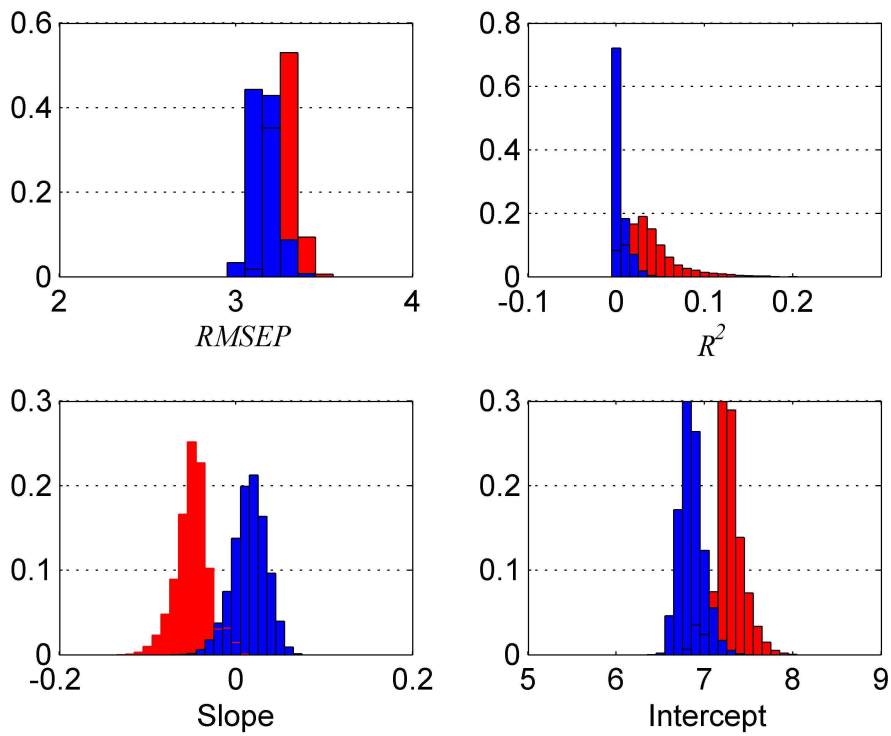
Figure B. 7: Performance of KLS in pre-harvest modelling at stem level. X-axis shows the performance indices while y-axis plots the fraction of the total number of samples. Blue distributions were based on actual data while the red distributions were from nonsense permutated data.
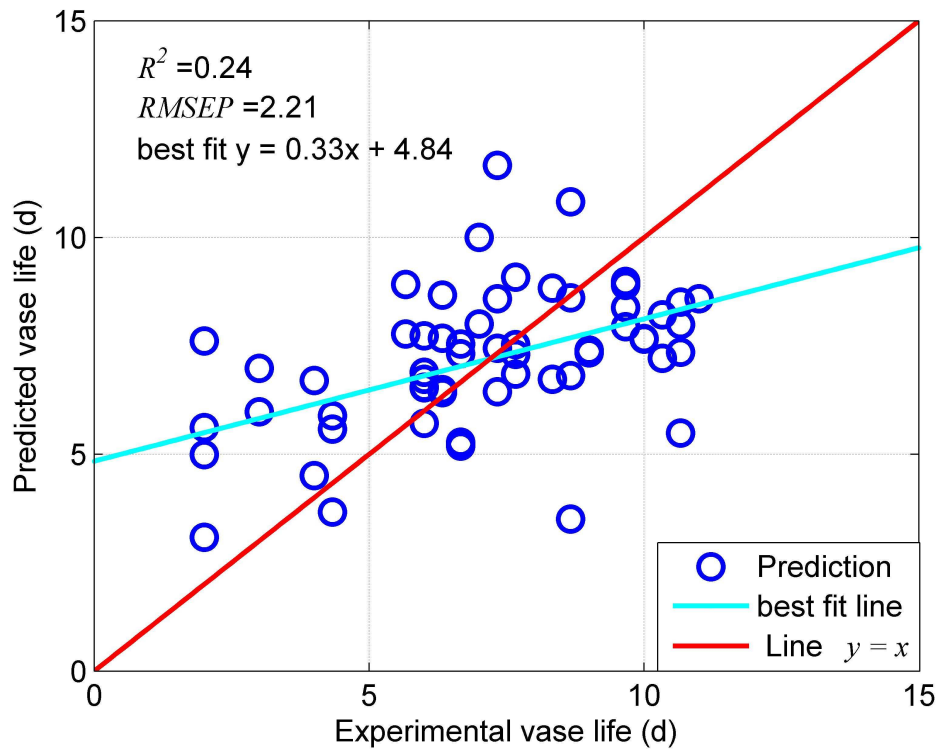
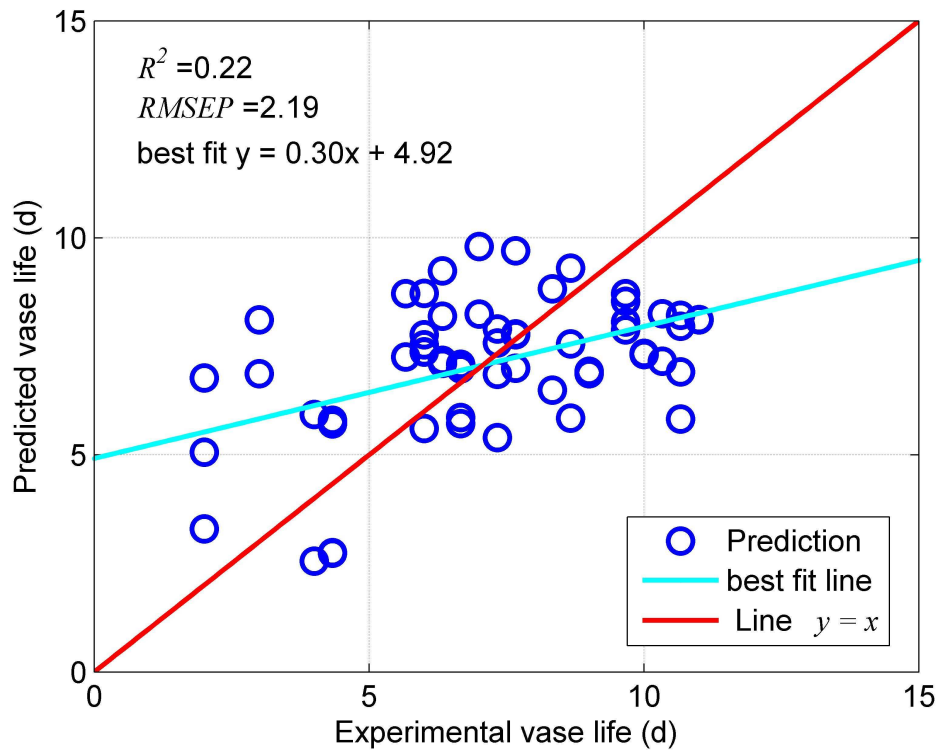**Figure B. 8: A typical performance of KLS in pre-harvest and post-harvest modelling.**

Figure B. 9: A typical performance of PLS in pre-harvest and post-harvest modelling (auto-scaling)

C. ROSE CULTIVARS IN WORLD FLOWERS STUDY

In the World Flowers case study, three roses cultivars were used; these included Red Calypso, Amani and Tropicana. Table A. 2 below shows photos of the roses.

Table A. 2: Rose cultivars in World Flowers study

Red Calypso	Amani	Tropicana

D. PUBLISHED PUBLICATION

As a result of the work reported in this thesis, a paper was submitted and accepted for an oral presentation at the International Conference on Signal Processing 2008 in China. Its manuscript was subsequently published in the conference proceedings and is available online at http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=4697709 (subscription to IEEE Xplore digital library is required). A copy of the paper is attached at the end of the thesis.

Further publications are being prepared and will be submitted in the near future.

Regression analysis for supply chain logged data: A simulated case study on shelf life prediction

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Abstract

The paper illustrates that valuable information can be mined from temperature data collected along the perishable food produce supply chain. Three regression techniques: Ordinary Least Square (OLS), Principal Component Regression (PCR) and Latent Root Regression (LRR) have been used to predict remaining shelf life of tropical seafood products. The results show that LRR is the best of the three regression techniques and works well in predicting remaining shelf life for tropical seafood. The results demonstrate the potential usefulness of utilizing automated temperature data collection (e.g. using RFID sensors) to help achieve a challenging business objective–remote real-time prediction of remaining shelf life of chilled foods.

1. Introduction

RFID has been seen as a technology to revolutionize the supply chain and the retail industry, but early adopters have found the technology expensive. It has been argued that to achieve the full benefits of RFID technology, valuable information must be mined from raw RFID data, interpreted, and then shared both internally and externally with supply-chain partners, to achieve a specific business objective.

One such objective for the food industry is *shelf life* monitoring, prediction and control for chilled foods. Generally, *shelf life* of a food product is defined as the time duration it can be stored until becoming unacceptable for human consumption. The concept of *Shelf life* relates to a number of terms such as *best before*, *use by*, and *freshness date,* all of which are in common use. Remaining shelf life is basically the shelf life as evaluated at the time of assessment. As food quality depends significantly on the conditions under which it is stored, remaining shelf life varies greatly with environmental factors; temperature being a key variable. Traditionally, determination of remaining shelf life is carried out in laboratory studies which are now considered as time consuming and expensive. Increasing customer demand for high quality food and safety assurance as well as rapid market expansion are the main motivating factors in developing novel techniques for estimating remaining shelf life of fresh food products.

This paper illustrates the idea of using regression technique to analyze data and then predicting the remaining shelf life of chilled foods. Three regression techniques are used for data analysis: Ordinary Least Square (OLS), Principal Component Regression (PCR) and Latent Root Regression (LRR). The work is based on temperature data collected from an international fresh produce supply chain.

2. Material and methods
2.1. Temperature data from field trial

Temperature measurements gathered from field trials in an international supply chain were made available for analysis. Whilst this temperature data relates to non-sea food produce, it is used in the research reported here as a generic data set to investigate the usefulness of the three regression techniques considered. In effect, the working assumption, as a starting point for the research, is that the data represents seafood that has been shipped through a chilled supply chain, rather than the normal $0^{o}C$ conditions. The purpose was to use this data for the regression analysis, and also to generate simulated

shelf life data using public domain software available for this purpose.

Two sets of temperature measurements were available. The first consists of 80 temperature profiles recorded over 22 hours (one measurement per hour). This data set was used to construct a training data set. The second data set, consisting of 37 temperature profiles recorded over the same duration and frequency, was used as the test data set.

2.2. Seafood Spoilage and Safety Prediction (SSSP) software

As remaining shelf life measurements corresponding to the provided temperature profiles were not available, Seafood Spoilage and Safety Predictor (SSSP) v2.0 software was used to generate this data.

SSSP was developed by P. Dalgaard and colleagues at The Danish Institute for Fisheries Research. SSSP originates from the Seafood Spoilage Predictor (SSP) software and has been available online (for free download) since February 1999 [1]. The software predicts shelf life and growth of bacteria in a number of fresh and lightly preserved seafoods under dynamic storage conditions (e.g. temperature, CO_2 concentration, water activity). There are basically two classes of models in the SSSP v2.0 software: relative rate of spoilage (RRS) models; and microbial spoilage (MS) models. For fresh seafood, RRS models are of empirical nature, which means that they are developed using shelf life data obtained at different storage temperatures. On the other hand, MS models are based on the concepts of specific spoilage organism (SSO) and the range of conditions (pH, temperature, water activity and atmosphere) under which a SSO can grow and produce spoilage metabolites [2].

In this study, RRS models have been used as only temperature measurements were available for analysis.

2.3. Ordinary Least Square (OLS)

OLS is probably the most basic technique for multiple linear regression. Its mathematical development is covered in numerous textbooks and hence will not be reproduced here. The formulation of the technique is summarized as follows:

Let y be the dependent variable and $\mathbf{x}$ represent the independent predictors. The multiple linear regressions can be expressed as

$$y = \mathbf{x}^T \cdot \boldsymbol{\beta} + \varepsilon \qquad (1)$$

Where: $\boldsymbol{\beta}$ is the parameter vector and ε is the residual error. For a set of training data $\{\mathbf{X}_{train}; y_{train}\}$, the OLS estimate of the coefficient vector is

$$\hat{\boldsymbol{\beta}}_{OLS} = \left(\mathbf{X}_{train}^T \mathbf{X}_{train} \right)^{-1} \mathbf{X}_{train}^T \mathbf{y}_{train} \qquad (2)$$

If the inverse matrix does not exist, a pseudo inverse could be used. Given the OLS estimate, the prediction can be performed as

$$\hat{y}_{OLS} = \mathbf{x}_{test}^T \cdot \hat{\boldsymbol{\beta}}_{OLS} \qquad (3)$$

2.4. Principal Component Regression (PCR)

PCR has a long history dating back to Kendall's and (independently) Hotelling's work in 1957. Recently PCR has received increasing interest. For details of PCR mathematical development, readers are referred to [3]. The technique is essentially based on using principal components (PCs) in regression. The estimate of the coefficient vector is:

$$\hat{\boldsymbol{\beta}}_{PCR} = \mathbf{A}\mathbf{L}^{-2}\mathbf{A}^T \mathbf{X}_{train}^T \mathbf{y}_{train} \qquad (4)$$

$\mathbf{A}$ consists of eigenvectors of $\mathbf{X}_{train}^T \mathbf{X}_{train}$ that correspond to the PCs retained for regressions; $\mathbf{L}$ is a diagonal matrix whose diagonal elements are the square root of the corresponding eigenvalues of $\mathbf{X}_{train}^T \mathbf{X}_{train}$. Similar to Equation (3), the prediction is:

$$\hat{y}_{PCR} = \mathbf{x}_{test}^T \cdot \hat{\boldsymbol{\beta}}_{PCR} \qquad (5)$$

Note that $\mathbf{A}$ does not necessarily include all of the eigenvectors of $\mathbf{X}_{train}^T \mathbf{X}_{train}$. In fact, by excluding some eigenvectors that are deemed insignificant PCR prediction performance may be improved compared to OLS technique. The decision of which eigenvectors (and hence PCs) to retain is a challenging task and a lot of work has been done to address this issue. Readers are referred to [3] and the reference therein for a detailed discussion.

2.5. Latent Root Regression (LRR)

Latent Root Regression (LRR), also known as Ridge Regression, is, like PCR, related to Principal Component Analysis (PCA). However, the main difference is that while PCR uses PCs evaluated from the predictor variables $\mathbf{X}_{train}$, the LRR technique calculates the PCs based on both predictor variables $\mathbf{X_{train}}$ and the dependent variable $\mathbf{y_{train}}$. Under the same LRR framework, there are a number of different LRR

techniques. In a recent study, Bertrand et al. [4] proposed a version of LRR by utilizing the latent roots of $\begin{bmatrix} \mathbf{Z}_{train} & y_{train} \end{bmatrix}$ for regression where $\mathbf{Z}_{train}$ is the PCs of $\mathbf{X}_{train}$. This LRR version leads to a simple expression for mean square error of the estimator and makes variable selection easier, as noted by Jolliffe [3]. However, the original LRR seems to have been proposed by Webster et al [5], where latent roots of the correlation matrix of the matrix $\begin{bmatrix} \mathbf{X}_{train} & y_{train} \end{bmatrix}$ are used in regression. According to Webster's LRR technique, the estimate of the coefficient vector is:

$$\hat{\beta}_{LRR} = \sum f_k \boldsymbol{\delta}_k \quad (6)$$

$$f_k = -\delta_{0k} \left(\sum_{i=1}^{n} y_i^2 \right)^{\frac{1}{2}} \tilde{l}_k^{-1} \left(\sum \delta_{0k}^2 \tilde{l}_k^{-1} \right)^{-1} \quad (7)$$

Here $\boldsymbol{\delta}_k$ is the vector of coefficients of the predictor variables corresponding to the kth PC; and δ_{0k} represents the coefficients of the dependent variable y to the kth PC. The summation in Equation (6) and the second summation in Equation (7) are over a subset of PCs for which either the corresponding eigenvalues $\tilde{l}_k$ or the coefficient δ_{0k} are largest.

2.6. Performance statistics

A number of statistics were calculated to evaluate the performance of the regression techniques. They include mean square error (MSE), coefficient of determination, and maximum relative absolute error (RAE_{max}). Letting $\boldsymbol{\varepsilon}$ denote the error vector for the prediction of the test data set, where $\boldsymbol{\varepsilon}$ is defined as:

$$\boldsymbol{\varepsilon} = \hat{\mathbf{y}} - \mathbf{y}_{test} \quad (8)$$

Here $\hat{\mathbf{y}}$ and $\mathbf{y}_{test}$ are respectively the predicted and simulated shelf life vectors. Then

$$MSE = \frac{1}{m} \boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon} \quad (9)$$

$$R^2 = 1 - \frac{\boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon}}{\mathbf{y}_{test}^T \mathbf{y}_{test}} \quad (10)$$

$$RAE_{max} = \max \left(100 \left| \frac{\boldsymbol{\varepsilon}}{\tilde{\mathbf{y}}_{test}} \right| \right) \quad (11)$$

Here m is the number of test samples in the data set (for the case of the data considered in this paper, m = 37); $\tilde{\mathbf{y}}_{test}$ represents the raw simulated shelf life before scaling (i.e. not yet normalized to zero mean); and the vector division in Equation (11) is defined as an element-by-element division operator.

3. Results and Discussion

The SSSP v2.0 software was used to generate shelf life data for the temperature profiles from the field trial. Tropical seafood simulation in SSSP was selected for the study. This simulation is based on an exponential RRS model:

$$shelf\ life\left(T\ ^{o}C\right) = \frac{shelf\ life\left(T_{ref}\ ^{o}C\right)}{\exp\left[a\left(T - T_{ref}\right)\right]} \quad (12)$$

Where $a = 0.12$ for tropical seafood is a model parameter; T and T_{ref} are storage and reference temperatures respectively. In this study, T_{ref} was set at $0^{o}C$ and the corresponding shelf life at reference temperature is 14 days i.e., 336 hours.

The temperature profiles and the simulated shelf life data are mean-centered before all analysis. As the matrix $\mathbf{X}_{train}^{T}\mathbf{X}_{train}$ is full rank and hence its inverse exists, OLS analysis is quite straightforward: estimate $\hat{\boldsymbol{\beta}}_{OLS}$ by Equation (2) and use it for prediction as in Equation (3). In PCR analysis, the first two PCs are retained, which together account for 87.5% of total variance. Different combinations of PCs were also examined but they seemed to lead to lower prediction performance.

For LRR analysis, the temperature profiles and the simulated shelf life data were scaled to unit standard deviation. PCA was then performed on the scaled data matrix $\begin{bmatrix} \mathbf{X}_{train} & y_{train} \end{bmatrix}$. The strategy is to retain both the first few PCs that together accounts for up to 90% total variance and the PCs for which magnitudes of the coefficients to the dependent variable y exceed a threshold. Using a threshold of 0.05, a total of 12 PCs were retained for regression.

Figure 1 shows the prediction performance of the three regression techniques being studied. The x-axis corresponds to the simulated shelf life (from the SSSP software) and the y-axis corresponds to the predicted shelf life (from the regression technique). The line y = x is also shown for visual reference. The figure indicates that while there is not much difference between results from PCR and OLS, the LRR performance is the best of the three. This observation is numerically supported by the performance statistics

tabulated in Table 1. These statistics show little difference between OLS and PCR techniques. On the other hand, LRR is shown to be a much better regression technique, with substantial improvement in all three performance statistics (MSE, R^2 and RAE_{max}).
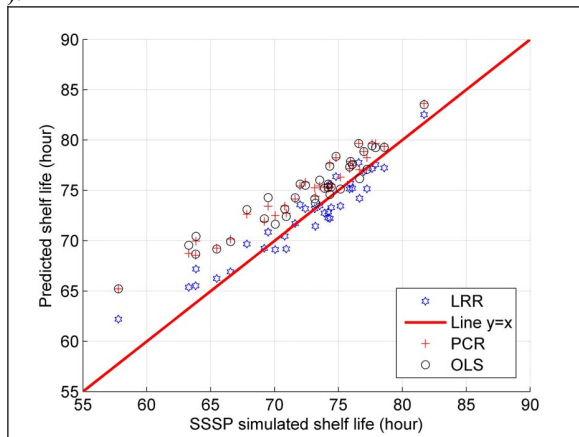

Figure 1: Tropical seafood shelf life prediction by OLS, PCR and LRR techniques

The observation that LRR performs significantly better than OLS and PCR is surprising. It should be noted that LRR (and PCR) is designed to deal with multi-collinearities in the predictor data. A quick check on the rank of X_{train} and X_{test} revealed that they are both full rank and hence multi-collinearities should not be an issue. Therefore, it is reasonable that PCR did not offer any advantage in using PCs for regression. However, LRR surprisingly improves the prediction performance. The reason could be that LRR takes into account the correlation between the predictor variables x and the dependent "y" variable

Table 1: Performance statistics in tropical seafood simulation study

	OLS	PCR	LRR
MSE (hour)	9.51	9.10	2.43
R^2	0.61	0.63	0.90
RAE_{max}	12.90%	12.88%	7.66%

The good performance of LRR technique is an interesting result. It should be noted that the simulated data sets are non-linear (cf. Equation (12)). Yet LRR, which is essentially a linear regression technique, is capable of producing a good prediction performance. Although further validation with experimental shelf life data is necessary, this preliminary result indicates the potential usefulness of linear regression techniques in the challenging task of predicting shelf life of perishable food products.

4. Conclusion

Three regression techniques (Ordinary Least Square (OLS), Principal Component Regression (PCR) and Latent Root Regression (LRR)) were used to predict remaining shelf life of tropical seafood products. The results show that LRR is the best of the three regression techniques for the data and produce considered, and it works well in predicting remaining shelf life for tropical seafood.

This preliminary study has used data that was collected using data loggers to prove the concept. In addition, shelf life information was not experimentally determined (hence the reason for using the simulated values from SSSP v2.0 simulation software). The next step in the research is to extend the study to the use of RFID tags to enable automated data collection and remote real-time prediction, and to undertake experimental assessment of the shelf life for comparison with the shelf life predictions provided by the regression techniques.

5. References

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2. Gram, L. and P. Dalgaard, *Fish spoilage bacteria - problems and solutions.* Current Opinion in Biotechnology, 2002. **13**(3): p. 262-266.
3. Jolliffe, I.T., *Principal Component Analysis.* 2nd ed. 2002: Springer.
4. Bertrand, D., E.M. Qannari, and E. Vigneau, *Latent root regression analysis: an alternative method to PLS.* Chemometrics and Intelligent Laboratory Systems, 2001. **58**(2): p. 227-234.
5. Webster, J.T., R.F. Gunst, and R.L. Mason, *Latent Root Regression Analysis.* 1974, American Statistical Association and American Society for Quality. p. 513-522.

6. Acknowledgement