Toward Simple Generic Control in Anaerobic Digestion

Giuliano C Premier

A submission presented in partial fulfilment of the requirements of the University of Glamorgan/Prifysgol Morgannwg for the degree of Doctor of Philosophy

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Award........................Doctor of Philosophy...........................

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DEDICATION

To my family...

Spero de no essar sta qua soeo par pesar so stó mondo, (paraphrasing Giuseppe Premier in his Venitian dialect).

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I would like to thank the following people for their contributions, support, help and advice.

ABSTRACT

The desirability of effective control of anaerobic digesters as a means of avoiding imbalance in the microbial population has become clearer and this can be seen from the literature in recent years. A number of published control strategies have been encouragingly successful, however the non-linear and time varying nature of the process generally requires a bespoke, engineered system dependant on the characteristics of the system. The 'cost of knowing' in employing control systems, is generally high. The ideal scenario for operators would be the availability of a generic control system at reasonable cost, which would be applicable to a large group of high rate reactor designs, operating on a limited (but broad) variety of waste streams. The system would be able to control from commissioning through to steady state and should be able to cope with reasonable expected shock loading conditions, albeit perhaps at some degree of sub-optimality. The aim of this work is to develop a control strategy, which will lead in future to this end.

Bicarbonate alkalinity (BA) is a key parameter which indicates the buffering capacity of the anaerobic digestion system and which has the potential for helping to maintain a stable system in the face of changing organic and toxic load. This is particularly the case when used in association with other informative on-line parameters such as gas production rate, %CO_2 concentration in the gas, TOC, pH and volatile fatty acids. All but the last of these have been investigated using a fluidised bed reactor and the degree to which the anaerobic process is non-linear and time varying has been assessed, as the level of complexity required to represent anaerobic digestion 'well enough' was not clear. Simple linear black box models of low order were investigated, predicting over a limited horizon and relying on current and recent data values to refine the prediction. Independent black box ARX models were identified for gas production rate, % CO_2, bicarbonate alkalinity and Total Organic Carbon using on-line data from a fluidised bed reactor at varying organic load. Model predictions looked ahead one sample step (30 minutes) and when validated using data obtained in a different time period (separated by 4-8 weeks) gave significant predictions in each case. The non-linear nature of the process was found to have little effect over the operating conditions investigated. Also the variation of the process within 4-8 weeks period was not sufficient to cause the models to predict badly.

The performance of three black box models which were parameterised and validated using data collected from the same laboratory scale fluidised bed anaerobic digester, were compared. The models investigated were all ARX (auto regressive with exogenous input) models, the first being a

linear single input single output (SISO) model, the second a linear multi-input multi-output (MIMO) model and the third a non-linear neural network based model. The performances of the models were compared and it was found that the SISO model was the least able to predict the changes in the reactor parameters (bicarbonate alkalinity, gas production rate and % CO_2). The MIMO and neural models both performed reasonably well. Though the neural model was shown to be superior overall to the MIMO model, the simplicity of the latter should be a consideration in choosing between them. A simulation with a horizon approaching 48 hours was performed using this model and showed that the method was not sufficiently accurate for use in situations where pure simulation was required.

This thesis includes the use of a two population deterministic model calibrated using data from a fluidised bed reactor operating on a simulated yeast waste, in the development of a Model Reference Adaptive Control (MRAC) strategy. The strategy uses a three term adaption mechanism, which is described in the thesis as a Fast Adaption Trajectory (FAT) strategy, as it was found to be necessary to respond to catastrophic events over short time scales, in order to maintain the viability of the bacterial population. Numerical optimisation in a simulation environment was used to parameterise the controller, and this was done on the basis of only basic design information being available for the reactor which was to be controlled.

The controller was tested on a significantly different Expanded Granular Sludge Blanket (EGSB) reactor operated on a sucrose based feed and which did not inform the controller design process beyond basic physical information. Two actuation strategies were explored over several months of operation, using a single on-line bicarbonate alkalinity monitor, which in the event proved to have significant reliability problems.

Not withstanding the problems with the alkalinity monitor, which was dominant in determining the success or failure of the control strategy, it was found that the control strategy was able to maintain control during start-up, which was the ambition of this part of the experimentation. Both actuation methodologies showed promise although the variation of loading rate was not adequately tested by the experimentation, which was conducted. The actuation by dosing with bicarbonate proved to be better at maintaining control in the face of repeated and severe perturbations caused by failure in the bicarbonate monitor system. It is believed that the FAT controller is likely to be a transferable technique provided that unmodelled dynamics are not excessively dominant and that the reactor system is comparable to a CSTR design with predominantly soluble waste in the feed.

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NOMENCLATURE

Symbol	Description	Units
Kinetic constants		
μ_a	Acidogenic bacteria growth rate	h^{-1}
μ_{amax}	Acidogenic bacteria maximum growth rate	h^{-1}
K_{sa}	Acidogenic bacteria half-velocity	$mg.l^{-1}$
k_{da}	Acidogenic bacteria decay rate	h^{-1}
μ_m	Methanogenic bacteria maximum growth rate	h^{-1}
μ_{mmax}	Methanogenic bacteria maximum growth rate	h^{-1}
K_{sm}	Methanogenic bacteria half-velocity	$mg.l^{-1}$
k_{dm}	Methanogenic bacteria decay rate	h^{-1}
K_{im}	Methanogenic bacteria inhibition concentration	$mg.l^{-1}$
Anaerobic system components		
X	Bacterial concentration	$mg.l^{-1}$
S	Substrate concentration	$mg.l^{-1}$
V	Product concentration (acetic acid) or reactor volume	$mg.l^{-1}$
HAc	Sodium acetate (and sodium hydroxide) concentration	$mg.l^{-1}$
C	Carbon dioxide concentration	$mg.l^{-1}$
P	Pressure	atmosphere
Q	Gas flow rate	$ml.min^{-1}$
B	Bicarbonate dosing	$mg.l^{-1}$
Suffices		
a	Acidogenic bacteria (2 population model)	
m	Methanogenic bacteria (2 population model)	
in	Input to the reaction vessel	
da, dm	Endogenous metabolism	
i	Generalised index for i-population model	
t	Total, as in total pressure	
(g)	Gas phase	
Yield coefficients		
y_{sa}	Substrate $\rightarrow$ Acidogenic bacteria	
y_{vfa}	Substrate $\rightarrow$ acetic acid	
y_{co2a}	Substrate $\rightarrow$ CO_2	
y_{sm}	Acetic acid $\rightarrow$ Methanogenic bacteria	
y_{ch4}	Acetic acid $\rightarrow$ methane	
y_{co2m}	Acetic acid $\rightarrow$ CO_2	
Physico-chemical constants and reactor design parameters		
C_{co2}	mole $\rightarrow$ $mg.l^{-1}$ conversion constant for CO_2	
C_{ch4}	mole $\rightarrow$ $mg.l^{-1}$ conversion constant for CH_4	
P_t	Total pressure in gas phase	atmos
V	Liquid phase volume	l
V_g	Gas phase volume	l
F	Liquid flow rate	$l.h^{-1}$
δ	Liquid/solid dilution rate ratio	
K_La	CO_2 mass transfer rate coefficient	h^{-1}
pH		
B_v	Organic loading rate	$g.COD.l^{-1}.d$
$\%CO_2$	Percentage of CO_2 in the biogas	%
TOC	Total organic carbon	$mg.l^{-1}$

Symbol	Description	Units
Parameters and constants		
K_h	Henry's constant	atmos/mol fraction
K_a	Acetic acid (CH3COOH) dissociation const.	
K_w	Water dissociation constant	
K_{co2}	H_2CO_3 (bicarbonate) dissociation constant	
K_ia	Mass transfer coefficient	
S_v	Avogadro's number	$mol.g^{-1}.mol^{-1}$
Simulation model parameter notation		
PCO2	Partial pressure of CO_2	atmos
Qch4	CH_4 fraction of biogas production rate	$l.min^{-1}$
Qco2	CO_2 fraction of biogas production rate	$l.min^{-1}$
Va, Vain	Acetic acid substrate concentration and supplied at the ingress	$mg.l^{-1}$
HAc	Undissociated part of acetic acid Va	$mg.l^{-1}$
C	Inorganic carbon concentration	$mg.l^{-1}$
X_i	Particulate concentration for fraction i	$mg.l^{-1}$
Si	Soluble substrate or product concentration for fraction i	$mg.l^{-1}$
Xm	Methanogenic bacterial concentration	$mg.l^{-1}$
Xa	Acidogenic bacterial concentration	$mg.l^{-1}$
S_{in}	Substrate concentration at ingress	$mgCOD.l^{-1}$
BA	Bicarbonate alkalinity	$mg.l^{-1}$ $CaCO_3$ equiv.
F	Flow rate to the reactor	$m^3.d^{-1}$
D	Dilution rate	d^{-1}
Bv	Organic loading rate	$gCOD.l^{-1}d^{-1}$
OLR	Organic loading rate	$kgCOD.m^{-3}d^{-1}$
Control system parameters		
R	Control system reference input	
y	Control system output	
e_m	Model error (MRAC structure)	
y_m	Model output (MRAC structure)	
f	Cost function used in numerical optimisation	
J	Loss function	
U	Control effort	
Kp, Ki, Kd	Controller adaption mechanism gains	
Modelling parameters		
G,H	General transfer functions notation	
A,B,C,D,F	Black box model polynomial notation	
na, nb	Length of regression vectors used in black box modelling	
a_i, b_i, c_i, d_i, f_i	Black box model coefficients for polynomial of order i	
x, y	Input and output vectors	
nk	Sample retardation	
$\hat{y}$	Model prediction	
θ	Parameter vector	
ζ	Feature vector	
w, W	Neural network weights	

1.0 INTRODUCTION

Biological processes occur naturally in all but the most hostile environments. The origins of the use of bacteria in the treatment of waste streams lie unrecorded in the distant past, probably owing more to fortune than any understanding on the part of our antecedents. Understanding built rapidly over the 20th century, till in this early part of the 21st century there are a large number of learned journals devoted to this field of science. The aims of biological treatment of waste include:

- the stabilisation of carbonaceous Biological Oxygen Demand (BOD),
- the removal of nutrients such as nitrogen and phosphorus,
- the elimination or reduction of pathogens,
- the production of energy (biogas) and
- removal of odour or colour before discharge to the wider environment.

These aims are achieved by virtue of the metabolic processes of the various bacterial species, and as a result, growth of biomass will occur. This growth will be achieved by the depletion of the BOD and nutrients in the waste stream that forms the substrate for the bacteria, thus reducing the pollutants. Physical and chemical separation processes generally separate the biomass from the treated waste stream in order to minimise the polluting materials, (of which the biomass would otherwise form part). These include separation processes such as settling, polymeric additives to aid settling, biomass retention by fixed film, e.g. biofilters, sludge blankets and membrane techniques. Any surplus (biomass) sludge requires disposal by routes such as incineration, agricultural or other land disposal, de-watering and land filling, amongst others.

1.1 ANAEROBIC DIGESTION

Anaerobic digestion (AD) is a subset of biological waste treatment and Graef and Andrews (1973) noted that it has been used to treat municipal and industrial wastewater since the nineteen thirties. In 1999 a survey referred to by Steyer *et al.* (2002) indicated that 1300 anaerobic digesters had been reported in the literature across the world. Anaerobic digestion occurs naturally in the digestive systems of rumen and oxygen free or depleted regions of ponds, lakes soils and marshes. With the growth in understanding following research into the field of AD and its underlying processes, there has developed a desire to improve the performance of anaerobic treatment systems, motivated by economic, environmental and operational concerns. When compared to aerobic processes, it is notable that aeration (with its associated equipment and costs) is not required and the specific production of biomass in anaerobic digestion is small compared with aerobic processes (McCarty (1964a)). This reduces the burden and cost of disposal of excess biomass generated by the process compared to aerobic processes. Many other advantages have

been attributed to anaerobic processes, such as the production of energy rich biogas, by for example Zeeman (1994) and Raizada *et al.* (2002). The high rate of start-up and improved flocculation are cited by Lettinga (1995) as further advantages. Anaerobic treatment is often used in the disposal of sludge from aerobic systems as a means of reducing the overall biomass wasted from the treatment plant. AD also finds considerable application in the treatment of primary sewage in septic tanks and relatively small municipal wastewater treatment facilities and in the treatment of a wide variety of industrial waste streams.

Organic and inorganic matter is decomposed in the absence of molecular oxygen during AD and produces various end products including carbon dioxide and methane. A large variety of bacterial species are involved in the AD process, which is often considered to be a three stage sequential process. Synergistic interaction between the micro-organisms facilitates the availability of suitable substrates and environmental conditions for all the species. The main metabolic pathways are routed through the following three bacterial stages (Pavlostathis and Giraldo Gomez (1991)):

First stage bacterial group (Hydrolysis and Fermentation)

Fermentative bacteria – relatively high molecular weight solids such as proteins, carbohydrates and lipids are hydrolysed to simpler and more soluble molecules by enzymes, possessed fermentative bacteria. Proteins and carbohydrates decompose to amino acids and sugars (monosaccharides), while lipids form fatty acids and alcohols, which can be metabolised further. The fermentative bacteria metabolise the amino acids and sugars and produce acetate, though other volatile fatty acids (VFAs) and organic acids like propionate, butyrate, valerate, lactate and others, are often produced as intermediates. Fermentative bacteria are also involved in the anaerobic oxidation of fatty acids and alcohols to produce acetate, hydrogen and CO_2. The bacteria involved in hydrolysis and acidogenesis are either facultative or obligate anaerobes. The former group could grow using molecular oxygen, so can remove oxygen entering the process, but also function anaerobically.

Second stage bacterial group (Acetogenesis)

Hydrogen producing acetogenic bacteria – this group uses the higher molecular weight VFAs (those other than acetate and including long chain fatty acids and aromatic compounds) as a substrate and produce acetate, hydrogen and CO_2. They are inhibited by hydrogen levels in excess of about 10^{-4} atmospheres.

Third stage bacterial group

Hydrogen consuming acetogenic bacteria – use hydrogen and CO_2 to produce acetate.

Fourth stage bacterial group (Methanogenesis)

CO_2 reducing methanogenic bacteria – these bacteria perform reductive methanogenesis, which involves the reduction of CO_2 by hydrogen.

Acetoclastic methanogenic bacteria – provide the alternative methanogenic path from acetate.

The third and fourth stage bacterial groups are obligate anaerobes which are inhibited by oxygen and act to maintain low hydrogen partial pressure which would otherwise inhibit the second stage acetogenic group.

The micro-organisms involved, particularly the methanogens, have a relatively limited pH range in which their metabolism is not inhibited. Over production and under consumption of volatile fatty acids may lead to reactor acidification. Under an atmosphere of CO_2 and methane, the main pH buffering agent is bicarbonate, which may be determined off-line by a simple alkalinity titration. Alkalinity is measured by reference to $CaCO_3$ and according to Speece (1996), should be above 1000 mg l^{-1} $CaCO_3$ equiv. for stable operation.

Numerous variations to this three-stage model have been postulated, some of which are reviewed by Pavlostathis and Giraldo Gomez (1991). The stability and efficiency of the entire process depends on the maintenance of balanced consumption and production rates of intermediate substrates during changes in operating conditions or disturbances. Imbalance will result in poorer treatment efficiency or, in the limit, death of one or more groups of the microbial population. Controlling the state of the reactor is therefore a desirable ambition and initial strides in this direction were based on improvements to the reactor designs and design procedures (based on simulation) as argued by Andrews and Graef (1971), Andrews (1975a) and Andrews (1975b) who considered control actions. Simulation studies would ensure that a specific reactor design would maintain bounded operation when subjected to worst case loading and disturbance scenarios. Currently AD reactors are grouped into standard and high-rate variants. The former is often used for sewage sludge, requiring retention times in the region of 30-60 days. In comparison high-rate reactors are able to reduce these retention times to a few days or less. This is achieved by heating (which increases the metabolic rate of the microbial population), mixing (which ensures good

contact with substrate and dispersion of products) and most importantly biomass retention by attached film growth or granulation/flocculation. The influent composition is also significant in determining the retention time.

In practice, the reactor is seldom at steady state, so it is not possible to assume that the loading rate is constant. This implies that appropriate methods are needed to ensure that the state of the reactor is within suitable limits, (or preferably, at the optimal conditions). Alternatively, the reactor must be designed for the worst case conditions to ensure the survival of the reactor's eco-system. Further improvement has been sought through on-line monitoring of key parameters such as pH, gas production and composition, bicarbonate alkalinity and others. Allied to this have been strategies aimed at controlling the environmental and metabolic conditions of the anaerobic bacteria, (see for example Andrews (1975a); Andrews (1975b); Rozzi and Brunetti (1980a); Rozzi and Eng (1984a); Rozzi *et al.* (1985a); Dochain *et al.* (1988); Hawkes *et al.* (1995); Guiot *et al.* (1995)). The control strategies have to date included a range of techniques from human intervention and automation, through to fuzzy techniques and expert systems. The research reported in Chapter 2 is concerned with investigating a control strategy, to determine if it is an appropriate solution for this non-linear, time varying and on occasions, somewhat brittle process.

The waste streams supplied to AD processes are widely variable, deriving from municipal or industrial sources. Their constituents are often a combination of particulate and soluble organic materials such as proteins, lipids, carbohydrates, polysaccharides, volatile organic compounds (in municipal wastes) and these are alongside a bewildering array of other compounds in industrial waste streams. A number of models of AD or its stages, have been developed in the literature. From the early work of McCarty (1964a); McCarty (1964b); McCarty (1964c) and Andrews (1968); Andrews (1969), to later developments e.g. Andrews and Graef (1971); Lawrence (1971); Costello *et al.* (1991a); Rozzi *et al.* (1985c), amongst many others. Modelling has been a key issue in AD research.

1.2 CONTROLLING ANAEROBIC DIGESTION

The desirability of effective control of anaerobic digesters as a means of avoiding imbalance in the microbial population has become clear from the literature in recent years. Steyer *et al.* (1995); Rozzi *et al.* (1994); Dochain *et al.* (1991) and Renard *et al.* (1988), have all argued the need for control on the basis that the uptake of AD is limited by the brittle nature of the process (perceived or otherwise). The resulting focus on control has been achieved by an increasing understanding of

reactor behaviour particularly in conditions of rapid changes in load. Some control strategies have been encouragingly successful (Steyer *et al.* (1999)), however the non-linear and time varying nature of the process is likely to prove taxing in situations where deviations from a tightly specified performance are undesirable, for reasons of process stability. Significant successes have been reported where adaptive strategies have been employed, such as in the work of Ryhiner *et al.* (1992) and Renard *et al.* (1988). Many of the reported control strategies have been investigated through simulations, although a fast growing body of work reports success on laboratory and pilot scale systems. The strategies employed are either based on soft computing techniques, simplified non-linear models of the biological process linearized by means of appropriate feedback, or models in which the parameters have no significance with respect to the biological or physical processes involved.

A number of anaerobic digester studies (which will be discussed further in Chapter 2) have used on-line Bicarbonate Alkalinity (BA) as a control parameter. BA is a key parameter, which indicates the buffering capacity of the system and which has the potential to help to maintain a stable system in the face of changing organic and toxic load. This is particularly the case when BA is used in association with other informative on-line parameters such as gas production rate, $\%CO_2$ concentration in the gas, and pH. Volatile Fatty Acids (VFA's) would make a good alternative and have been monitored on-line by automatic titration (commercial instruments are now available), infrared spectrometry (Steyer *et al.* (2001)), and UV adsorption techniques, but there are at this time significant problems in discriminating between the VFA species. However, on-line GC (Pind *et al.* (2001)) is capable of individual VFA determination and it is arguable that the cost of such systems is not excessive, although this technology is not in general use industrially. BA gives a measure of the buffering capacity of the reactor against the effects of VFA build up, which is analogous to a safety margin, which as usual is introduced as a precautionary measure. VFA measurements alone do not give this 'margin'.

In order to control the AD process, it is necessary to take an action, which is causal. The control actions available in anaerobic digestion are not numerous, but altering the organic loading rate or dosing with alkali are amongst the contenders. Control actions are considered in Section 2.0.1.

1.3 OBJECTIVES OF THIS STUDY

i. AD is well known to be a non-linear process, but the degree to which this process could be modelled parsimoniously using linear and non-linear black box models was not clear from the literature. Therefore the first objective was to discover if simple models of the type

mentioned were sufficiently accurate to represent an anaerobic digester subject to relatively high loading and stressed conditions over many weeks (which would also consider time variations in the reactor behaviour). An existing fluidised bed reactor was used in this study, in the belief that the results would be reasonably transferable to any high rate reactor, which was well mixed.

ii. Having determined the success, or otherwise, of the simple black box approach, the second objective was the establishment of a suitable modelling strategy which could be used in the design of a control strategy.

iii. The third objective was to select and investigate a suitable control strategy by simulation techniques using Computer Aided Control System Design (CACSD) tools. The control strategy would be developed with an ultimate goal (partly beyond the current study), to deliver a generic control system, which could be shown to be applicable to anaerobic digesters, which are different in design and operation. The control system, based on BA as a measured variable, should require a minimum of instrumentation, expertise and prior knowledge of the reactor and should be able to control the anaerobic digester from commissioning and start-up to steady state under realistic loading conditions.

iv. The control strategy would at this point, be tested on a laboratory scale reactor and its performance investigated.

1.4 THE ORGANISATION AND STRUCTURE OF THE THESIS

The thesis has been organised in the style of a typical engineering report. The content is presented chronologically to a large extent, because of the nature of the work, which reflects the synthesis of a control system, its realisation and subsequent analysis.

Chapter 1 has introduced the reader to the wider context of AD and places the control of bicarbonate alkalinity into perspective within this field. It then goes on to state the four main objectives of the study.

In Chapter 2, the thesis considers the current state of the literature concerning the modelling and control of AD and the historical source from which it grew and from which the study draws and seeks to push forward the science in later chapters. As the control of AD is a highly multidisciplinary subject, an attempt has been made in this chapter to deal with the literature in a modular way. The chapter starts with a general look at control and modelling in AD and focuses

later on the specific parameter of interest, bicarbonate alkalinity and its use in monitoring and control.

Chapter 3 presents the materials and methods employed in the experimentation, modelling, and data analysis and control system synthesis.

Chapters 4 and 5 present the results, discussion and the conclusions drawn from the work. Appendix A contains associated software files that were used in the execution of the work and are stored on a CD. Appendix B includes publications derived from the work that have been published in journals or at conferences.

2.0 CONTROLLING ANAEROBIC DIGESTION

AD is generally considered to be a non-linear, time varying and complex process (e.g. Emmanouilides and Petrou (1997) and Simeonov *et al.* (1996)). Anaerobic digesters will eventually convert organic materials into methane and carbon dioxide, however the digesters can differ with respect to their bacterial populations, prevailing environmental conditions and sequence of reactions to obtain the end products. The bacterial species in the inoculum or seed, substrate composition, temperature, loading rate, hydraulic retention time (HRT), solids retention time (SRT), mixing and reactor design determine the final operational characteristics. Maintaining efficient operation depends on effective control (be it manual or automatic). This is particularly true in industrial waste treatment, where a build up of volatile fatty acids can occur rapidly and can lead to reactor failure. Prevention of such failures normally requires knowledge of the characteristics of the particular digester and waste, so that by monitoring specific control parameters, impending failure can be detected and information suggestive of an appropriate course of action can be extracted.

What is possible in control or what is good control in the field of AD is largely a question of opinion, though at the extremes of poor operation where there is a clear tendency to sour, consensus is likely. In aerobic systems, where a unifying model has existed since Henze *et al.* (1987), there have been benchmarks published, such as Vrecko *et al.* (2001), Vrecko *et al.* (2002) and Vanrolleghem and Gillot (2002). In the anaerobic systems, there remains little to compare with these and therefore benchmarking control strategies is not in this sense possible at this stage. The data must therefore be assessed in the context of the researchers' own expectations and against any comparable published information.

2.0.1 A perspective on monitoring and control of anaerobic digestion

A discussion of the factors which govern the nature of AD was presented by Kotze *et al.* (1969), with specific reference to control, not necessarily in the automatic sense. In the past, many others (e.g. Andrews and Graef (1971); Weiland and Rozzi (1991)), have considered the relevant parameters for controlling AD, in what has since become a rather active field of research. Early on, Andrews (1975a) and Andrews (1975b) had already gained considerable understanding of the possible approaches to control and detailed the commonly used variables including:

a) volatile acid concentration,

b) pH,

c) alkalinity,

d) gas flow rate,

e) gas composition,

f) volatile acid/alkalinity ratio,

g) unionised acid concentration and

h) rate of methane production.

The measurement of these and more recent additions and techniques such as Total Organic Carbon (TOC), turbidity/suspended solids and many others, were reviewed and presented by Guwy (1995), Vanrolleghem (1995) or specific methods for example IR spectrometry methods by Steyer *et al.* (2001). Steyer *et al.* (2002) concluded later, as a result of four years of operating a well-instrumented up-flow anaerobic fixed bed reactor of 1 m^3 volume, that current monitoring technology offered a trade off between reliability and high information content. Temperature, pH and flow could be measured reliably, but parameters such as TOC, COD and VFA were described as 'fragile'. The possibility exists to use fault diagnosis, as proposed by Genovesi *et al.* (1999), Steyer *et al.* (2001) and Lumley (2002). Andrews, as early as 1971, went on to propose the following control actions:

a) temporary halt in organic loading,

b) decrease in the rate of organic loading,

c) base addition (such as soda ash or lime),

d) dilution of the digester content,

e) addition of well digested sludge from another digester and

f) recycling and scrubbing of CO_2 from the digester gas to reduce carbonic acid.

In terms of control actions (or actuation) possible, there has been little which is fundamentally different to add to the above, though some issues are worth considering. CO_2 and hydrogen gas stripping by means of a silicon membrane was tested by Voolapalli and Stuckey (1998), during organic shock loading, demonstrating that pH could be stabilised and that improvements in acetate and VFA degradation could be improved. Biofilm build-up on the membrane was however, cited as a concern. Nitrogen sparging by Mollah and Stuckey (1992), with regulated levels of CO_2 and hydrogen in the circulating gas, affected the reaction pathways. The system for acetone-butanol production using a continuous culture of alginate-immobilised *Clostridium acetobutylicum*, showed that hydrogen biased the reaction away from acids toward solvents and CO_2 affected the acetone/butenol ratio. Similarly, Mollah and Stuckey (1993) found that stripping the product affected the reaction dynamics, but not in a straightforward manner. The prospect of controlling the methanogenesis and generally the COD removal in AD using CO_2 and hydrogen stripping by

sparging would appear to have some merit, with the former affording pH control through the carbonic acid depletion and the latter decreasing inhibition of the hydrogen producing acetogens.

Vandenheuvel *et al.* (1995), suggested that the application of fluctuating hydrostatic pressure could aid mass transfer in methanogenic granules and in as much, could improve biological processes where gas entrapment may occur.

Looking at the more speculative end of the control actions spectrum, for the related process of ruminant digestion, the use of ionophore antibiotics, methane inhibitors, inhibitors of proteolysis or deamination;, elimination of protozoa or fungi from rumen and probiotics, was investigated by Jouany (1994). The aim was to control the products of digestion available to the animal and hence tailor the growth to specific production of say, meat or milk. It is conceivable that similar dosing strategies could be adapted to AD applied to waste treatment or the production of acids etc. However with the likely cost of operation and the build-up of resistance which is likely to accrue with the overuse of such drugs, it is difficult to foresee widespread use of such techniques.

AD takes place in a three phase (solid, liquid and gaseous) environment, where each of the phases has significance for this physical, chemical and biological system. The carbonaceous material, which forms the feed in a continuous reactor, is in general a composite particulate suspension in combination with soluble components, which have associated with them a chemical oxygen demand (COD). The biodegradability of the feed is not necessarily complete, and the degree to which it is has a considerable effect on the efficiency of the system to remove COD.

Refractory, or inert (with respect to biodegradation) components, be they soluble or otherwise, will not be converted regardless of their residence time in the reactor and methods are required to either make the materials biodegradable or to perhaps chemically oxidise them. It is possible that the disintegration/hydrolysis steps can become rate limiting in the AD process overall and Pavlostathis and Gossett (1986) and Gossett and Belser (1982) discuss hydrolysis with respect to the commonly encountered problem of the digestion of sludge from aerobic systems. The use of pre-processing by heat treatment (Gossett *et al.* (1982)) or ultrasound (Tiehm *et al.* (1997)) has been considered, in order to improve the disintegration and subsequent hydrolysis, but would require specialised equipment and energy input. Separation of the acidification and methanogenic stages has been used to good effect e.g. by Ghosh (1991), Strydom *et al.* (1997) and Dinsdale *et al.* (2000), (Appendix B1). This dynamic effect derived from the hydrolysis and disintegration of particulate, which is dependent on the chemistry and physical nature of the waste, can be

significantly different between applications and it is therefore difficult to quantify this variability without empirical investigations.

There has been considerable process development, with the combination of various designs of anaerobic digester with aerobic, physical and chemical (mainly oxidation) systems in the treatment of difficult wastes such as dye waters (e.g. O'Neill *et al.* (1999)).

The composite particulate fraction is enormously variable, but will generally comprise lipids, proteins and carbohydrates, along with inert components. In industrial waste streams, processed and synthesised materials can considerably complicate the chemistry of the stream. The extracellular processes, which disintegrate and hydrolyse the solids to simpler monosaccharides and amino acids are catalytic reactions, which use enzymes secreted by bacteria in close proximity to the particulate fraction. As is stated by Batstone *et al.* (2002), modelling the disintegration from fundamental principles is not viable because of the many mechanisms by which it takes place. The disintegration process and the subsequent hydrolysis takes time and is therefore a dynamic process, which is usually represented as a first order process. Some researchers have included more complex mechanisms, such as Jain *et al.* (1992), who allowed for variation in the concentration of enzymes, within the Michaelis-Menten equation.

The physico-chemical state of a reactor depends on the bacterial consumption and products and the fluxes between the phases (Rozzi (1980b)). Parameters such as pH, BA and the partial pressures of the gases that are present are coupled to the biochemistry of the system. To describe the biochemistry of AD, without including the physico-chemical pathways is to oversimplify the process, as static operating conditions of the physico-chemical state cannot be maintained, even by complex intervention.

2.1 MODELLING OF THE ANAEROBIC PROCESS

The understanding of a system is greatly enhanced if a model can be deduced and validated and AD is no exception. Ljung (1987) gives ample justification that a model is necessarily a simplification of a real system and as such cannot comprehensively represent the behaviour of the system. The purpose to which the model is to be put will often drive the assumptions that can be made, the dynamic processes that are used (and how they are represented) and the mathematical, physical or other techniques employed. Models are often used to support our understanding of the underlying processes (Vassos (1993)). This has been very true of AD, where hypotheses have been tested with models (e.g. Bozinis *et al.* (1996)) and over time have significantly increased our

confidence to the point that the first generalised model of AD (ADM1) has been published by Batstone *et al.* (2002).

Models are usually judged on their fitness for purpose and may be used in the design of new processes and upgrades to assist in the operation of systems and the training of operators, and/or in the diagnosis of unexpected behaviour as opposed to normal operation. A common aim of modelling studies (e.g. Jones *et al.* (1992)) is to identify a dynamic model which would be suitable for on-line estimation and forecasting, providing accurate predictions of digester behaviour sufficient for use in process control and controller design. The applicability of various models is not clearly prescribed, so models such as ADM1 may be useful in a number of areas. The suitability of a model is however dependant on the application and its quality is judged by its ability to predict certain parameters over a desired time horizon. The prediction horizon will vary between applications, but the degree of difficulty in maintaining relatively accurate predictions becomes more difficult as the horizon is extended. It is often possible and desirable to improve the performance of a model by supplying the model, continually and in real-time, directly with data from the process that is the object of interest. This is much the same as weather forecasting which is indeed a dynamic model.

The basic underlying processes, which must be modelled are; hydraulic, physical (such as mass transfer), chemical and biological and are generally coupled in complex interactions. This complexity is evident in the large process rate and stoichiometry matrix for biochemical reactions and several physico-chemical rate equations of ADM1, which is itself a rationalised and simplified model.

The normal approach to the modelling of bioreactors, commonly starts with a notional reactor of fixed volume (batch or continuous) the content of which is well mixed (e.g. McCarty and Mosey (1991)). In practical terms, this is almost achieved by a well-designed Continuous Stirred Tank Reactor (CSTR). This approach simplifies the hydraulic behaviour of the process and allows the assumption that the biochemistry is straight forwardly coupled to the hydraulic regime, with assumed complete access of the bacteria to substrates and similar issues. It is clear that as the complexity of the reactor design is increased, by including, say, suspended growth, floculation, recirculation, channelling, membrane separation of phases and sequencing systems, then the simple CSTR approach will break down. For example Harmand *et al.* (2002), by using constrained optimisation to determine the trend in effective volume and biomass concentration in the reactor, produced a model to predict clogging in a fixed bed anaerobic digester and,

significantly, the work shows that the process is time varying because of clogging. Often, these complications are dealt with by modifications to the CSTR concept.

An example of unmodelled dynamics in ADM1, is the access to substrates and exposure to inhibitory agents by various species of bacteria in a floc, which is governed by the physical characteristics of the floc and the distribution of bacterial species within the floc. Access is also affected by the internal and external hydraulic and gas transfer characteristics of the floc and reactor respectively. Some of this complexity can be seen for example in Uyanik *et al.* (2001) and Tay and Show (2001).

2.1.1 Issues of complexity in the modelling of anaerobic digestion

It is not the intention of the author to produce a comprehensive treatise on the modelling of biological processes such as the work of Olsson and Newell (1999) or AD in particular, as in Bastin and Dochain (1990), however key issues are worth presenting.

The extent to which the basic processes in AD are considered determines the complexity of the model. There is a tension between the accuracy and discrimination of the model and the problems derived from complexity in the model. On the one hand, it would be desirable to have a comprehensive representation of all the processes involved, but on the other hand, this would normally be at the expense of simplicity, with large numbers of parameters. Many of the parameters would need to be calibrated or identified, (in the *system identification* sense). Ljung (1987) suggests that in situations where a large number of parameters of a non-linear model require calibration, the practical identifiability requires testing by looking at the sensitivity of the input/output relationship with respect to the parameters and the variances of the estimates (which should be related). The risk that the system becomes impossible to identify, within the noise and accuracy of available measurements, becomes higher with increasing complexity.

The principle of parsimony is a sensible approach to modelling in general and is particularly relevant in control system design and analysis. Theoretical and practical identifiability plays a key role in limiting the model complexity to the minimum number of parameters able to represent the system 'well enough' for the desired function.

In considering the anaerobic process, it is usual to define the conversion routes by which the biodegradable fraction of the feed is converted eventually to the end products of AD. With this

approach, the specific bacterial species are not defined or considered, as the mixed culture includes trophic groupings, which metabolise the various substrates to specific products along the defined conversion routes. Some bacterial species can be included in a number of trophic groups and may change their metabolism depending on the reactor conditions. This is well illustrated by a block diagram such as that shown in Figure 2.2.1 which is repeated from Batstone *et al.* (2002).
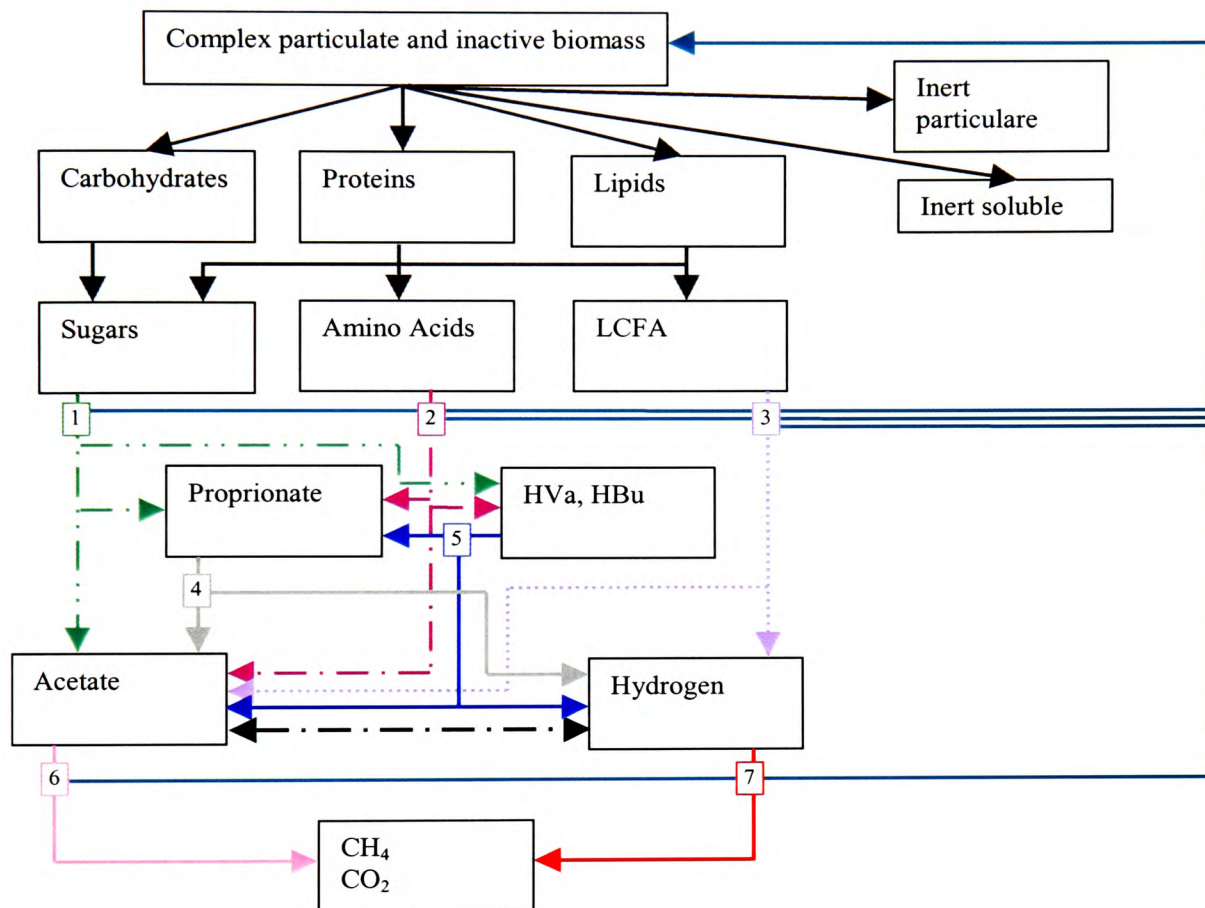
Figure 2.2.1 Biological processes included in the anaerobic model (ADM1).

(1) Acidogenesis from sugars; (2) Acidogenesis from amino acids; (3) Acetogenesis from Long Chain Fatty Acids (LCFA); (4) Acetogenesis from propionate; (5) Acetogenesis from butyrate (HBu) and valerate (HVa); (6) Acetotrophic methanogenesis; and (7) Hydrogenotrophic methanogenesis. (after Batstone *et al.* (2002))

In essence, the soluble substrates that result from hydrolysis, such as amino acids, monosaccherides and some lipids are consumed and converted to volatile fatty acids, (eventually acetic acid, balanced by their base equivalents) and CO_2, CH_4, H_2 and HCO_3^-. The possibility exists therefore, to consider different trophic groupings for each conversion path as has been done by numerous researchers and rationalised and summarised into the ADM1 presented by Batstone

et al. (2002) more recently. As all the VFAs reduce eventually to acetic acid, (though not exclusively as hydrogen can also be formed), there exists scope for simplification, normally at the cost of model accuracy.

Lactate for example, was considered by Costello *et al.* (1991a) and Romli *et al.* (1995), and more recently by Skiadas *et al.* (2000) in their work on the periodic anaerobic baffled reactor, (PABR). Also, the production of ethanol in preference to acetate, was discussed by Ren *et al.* (1997), in the context of a high rate acidogenic reactor. Lactate and ethanol have often been neglected from the list of products because they are only of relevance in the case of high loading and transient shocks or low pH levels. In testing control strategies, shock loading is often employed and in any case is a key reason for adopting control in the first place. It has been shown by Romli *et al.* (1995), that lactate is an intermediary product with a short life that only becomes apparent during shocks, but because of its *pKa* value, will cause an over estimate of pH if not included (Batstone *et al.* (2002)). Ethanol, according to Ren *et al.* (1997) is only produced in preference to acetic acid, in conditions where the pH<5.

The importance of hydrogenotrophs and acetate utilising bacteria was considered by Voolapalli and Stuckey (1999), to try to assess their influence in the degradation of butyrate and propionate. Spiking the reactor with cultures enriched with the trophic groups of interest, they were able to conclude that improvements in the degradation of butyrate and propionate were much greater when acetate utilising bacteria were increased as opposed to hydrogen and formate utilizers. Voolapalli and Stuckey (2001) went on to show that when the culture had acclimatised to pH>7, a shock load would cause the degradation to proceed through the formate route, while if acclimatised to pH<6.5, hydrogen production would be preferred. It is clear therefore that initial conditions are not only influential in the kinetic behaviour of AD but can redirect the metabolic pathways. Furthermore, in the case of hydrogen/formate, the conclusions of Voolapalli and Stuckey (2001) and Guwy *et al.* (1997), suggest that hydrogen is not as useful as a control variable as might be expected (e.g. Guiot *et al.* (1995)), because of its dependency on the historical state of the reactor. Ren *et al.* (1997) looked at the production of ethanol and acetic acid as opposed to propionic acid and the influence of pH on the routing. They concluded that the production of propionic acid was not necessarily related to high hydrogen partial pressure, as this parameter was high (50kPa) at about pH 4.5 when acetic acid was produced in preference to propionic acid. Ren *et al.* (2002) went on to consider the reasons for the production of propionic acid and conclude that it was a function of oxidation reduction potential (ORP) and pH and not hydrogen partial pressure. The linkage with hydrogen might be deduced from Vavilin *et al.* (1995), though they

observe only the coincidence of hydrogen partial pressure decrease with the start of propionic acid production.

A measured consideration by Batstone *et al.* (2002) and also the author, has concluded that the model resolution is relatively untouched by the exclusion of these and other degrees of freedom, provided the control strategy can be formulated to avoid the most sensitive parameters such as formate, hydrogen and lactate.

It becomes clear therefore that simplification of the model, by which one can understand the anaerobic process, leads to degradation of its predictive capacity. For example, by considering only soluble waste when particulate is present, a single volatile fatty acid species, or by assuming that the pH will be maintained above pH 5, these simplifications will limit the applicability of the resulting control strategy, which relies on the model for its development. A similar argument follows for inhibition through hydrogen, pH, toxic substances and the effect of temperature, along with any other unmodelled dynamics. However, many reactors are operated on waste streams which are not rate limited by particulate at the ingress, and that can sustain reasonably stable operation under control thus maintaining pH and avoiding lactic acid build up, or H_2 inhibition of the acetogens. Temperature is also independently controllable and as such, may be eliminated from dynamic considerations. The reactor design (Grasius *et al.* (1997)), can vary considerably, but it is often possible to find a degree of equivalence to the CSTR configuration, and as such all well mixed single stage reactors that are reasonably represented in this way, are again to a degree, equivalent.

The structures of the models, though often based on the basic underlying processes, are not necessarily so. The problem can be viewed as a 'black' or 'grey' box where the model structure is essentially a mathematical device, which will produce appropriate cause and effect relationships and the model parameters may be partially or totally unrelated to the underlying processes. Where the model structure is related to the underlying processes, the models are usually of the lumped parameter model type, while those employing grey or black box techniques can use various devices from regression models to neural networks, fuzzy modelling, wavelets and expert systems, to name some examples.

A number of dynamic and structured mathematical models have been described for AD by many researchers such as Andrews (1969); Mosey (1983); Costello *et al.* (1991a); Costello *et al.* (1991b); Jones *et al.* (1992); Vavilin *et al.* (1994)). As introduced above, the first AD model,

(analogous to the ASM models for aerobic systems) ADM1 (Batstone *et al.* (2002)), has been published. Such models may require information, such as bacterial kinetic parameters, substrate, product and bacterial concentrations (which are not easy to determine), for use in mass balance equations. A common approach adopted by for example Simeonov *et al.* (1996), was to use an identification process to estimate some of these parameters in a non-linear and time-varying scheme, or Marsili-Libelli and Beni (1996) who similarly identified parameters in mass balance type models. Hoh and Cordruwisch (1996) proposed a kinetic model which allows for the effects of substrate inhibition without the need to determine a large number of parameters experimentally. Bastin and Dochain (1990) presented a rigorous study of parameter estimation in this field, which has been central to numerous adaptive control studies. In general, model calibration is required and this usually involves considerable experimental effort and limited confidence can be maintained over a long time period because of selection and shift in the bacterial population.

When used in control, the model is not necessarily used to achieve a deeper understanding of the underlying process (though this is normally beneficial). There are significant benefits derived from the use of the simplest model, which is able to represent the system to an arbitrary accuracy specified by the designer. Furthermore the need for a non-linear model may not be paramount if the process can be represented by a piece-wise linear model, which would be the case if the model were to adapt 'rapidly enough' to represent the process at differing operating conditions and times in its life. Given that this is possible, black box adaptive control schemes could be employed. Fuzzy (Marsili-Libelli and Muller (1996); Muller *et al.* (1997)) and Expert Systems (Chynoweth *et al.* (1994); Pullammanappallil *et al.* (1998)) are two alternative approaches which like neural networks, (Boskovic and Narendra (1995)) show considerable scope. Others methods are mentioned by Olsson and Newell (1999).

The work of Premier *et al.* (1997) (Appendix B2), investigated whether a fluidised bed anaerobic digester can be represented adequately by simple linear black box models of low order. The models were employed to predict over a limited horizon and rely on current and recent data values to refine the prediction. Marsili-Libelli and Muller (1996) looked at parameterising typical lumped parameter models from data collected from the same reactor and influent as that used by Premier *et al.* (1997).

The need for modelling in the analysis and design of control systems stems from the lack of any realistic alternative. Models have the ability to enhance understanding of complex non-linear, time varying and highly coupled processes such as the AD process. It is important to differentiate

between steady state models and dynamic models, which consider the transient and steady state. The former, though often useful for system design, is limited in that it cannot predict the consequences of perturbations in the short to medium time scale, and as such is of limited use in control system design. By using a representative model and a suitable simulation environment, it is possible to rapidly investigate the characteristics of the process for a number of differing situations. The experimental costs of an equivalent laboratory based study may be prohibitive. Naturally the model's limitations and the assumptions made are crucial to the reliability of the modelled information. Never the less, in the design of control strategies for the non-linear AD process, simulation is an important tool.

2.1.2 Lumped parameter modelling and kinetics of the AD process

The principals of lumped parameter modelling are in widespread and multi-disciplinary use. Ohms law is a simple example, where the impedance is assumed to be concentrated at a point, though in reality we know that it is distributed throughout the devices and wiring. The resulting model however, is sufficiently accurate to be useful. A similar approach is often adopted to model biological process, with Andrews (1968), Andrews (1969), Andrews and Graef (1971), Andrews (1993) and Graef and Andrews (1973) being early prime protagonists. Many others such as Lessard and Beck (1991), Husain (1998), Rozzi *et al.* (1985a), Pavlostathis and Giraldo Gomez (1991), Elfadel *et al.* (1996) and Batstone *et al.* (2002), have followed.

The dynamics of the models mentioned above are usually developed by considering the mass, energy or ionic balances:

(rate of change of reactor content)=(rate of inflow)-(rate of outflow)+(rate generated)-(rate consumed),

Volumes defined by the phase boundaries and the assumption of perfect mixing are used as a starting point from which deviations can be modelled by simple mathematical mechanisms. Components of the flows may have different residence times and would therefore need to be accounted for. This is particularly true of particulate solids. The assumptions made in modelling will naturally have significant effects on the resulting model. For example, consideration of hydraulic behaviour of a reactor may assume that an increase in inflow will immediately be reflected in an increased outflow, if the liquid volume is to remain constant. The reality may be that slight volume changes occur because of a pressure drop across a restricted outflow. Dilution effects are normally considered first order, based on the fact that complete mixing exists and

component densities remain constant. Mass transfer between phases, such as the transfer of CH_4 or H_2 to the gas phase or the reversible transfer of CO_2 between the liquid and gas phases, is usually modelled as a physical (in the case of say CH_4) or physico-chemical (in the case of CO_2) effect. The physical effects are governed by a lumped factor K_{la} which is a coefficient incorporating the adsorption coefficient K_l and a factor a which is an *area/volume* ratio, (Olsson and Newell (1999)). The physico-chemical model of the CO_2, bicarbonate and pH equilibrium is set out by several authors such as Rozzi (1980b), Marsili-Libelli and Beni (1996) and Batstone *et al.* (2002) and is considered in detail in the lumped parameter model used as the basis for controller design in this study.

Kinetic models of biological systems

The kinetics of biological processes have been discussed in depth by Pavlostathis and Giraldo Gomez (1991), Olsson and Newell (1999) and Dochain and Bastin (1986), for example. A survey of kinetic models of specific growth rate is included in Bastin and Dochain (1990)). Though not exhaustive, it details models with dependence on:

> Substrate concentration
> Biomass concentration
> Substrate and biomass concentrations
> Product concentration
> Substrate and product concentrations
> Substrate and dissolved oxygen concentrations (aerobic processes)
> Substrate and dissolved oxygen and product concentrations (aerobic processes)
> Substrate concentration and inhibitory metabolite concentrations
> pH
> pH and temperature
> pH and substrate concentration

The overall specific growth rate is then calculated as the product of the specific growth rates for the various dependence factors.

The most widely used models are dependent on substrate concentration and are the *Monod*, (related to the Michaelis–Menten Law which deals with enzymes as opposed to microbial growth)

$$\mu_i(S) = \frac{\mu_{imax}S_i(t)}{K_{si} + S_i(t)}$$ (2.1)

And *Haldane* (Andrews (1968))

$$\mu_i(S_i) = \frac{\mu_o S_i(t)}{K_{si} + S_i(t) + \frac{S_i^2(t)}{K_I}}$$ (2.2)

Where $\mu_0 = \mu_{imax}\left(1 + \sqrt{\frac{K_{si}}{K_I}}\right)$ (2.3)

Equations 2.1 and 2.2 use the Monod kinetics which assumes that the biomass growth rate ($\mu_i X_i$) and the rate at which substrate is consumed ($y_i\mu_i X_i$), would be proportional to the amount of biomass in the reactor. The logical assumption from which this derives is that if the population doubles, so the requirement for nutrition doubles.

Rate limiting kinetics

The single population and single substrate CSTR described above is, for many situations, an over-simplification. In most reactors there will be a consortium of different bacterial species metabolising a number of limiting substrates and as a result, producing extra-cellular metabolites which may be substrate or inhibitory to other species and may be in the liquid or gaseous phases of the reactor. They will often affect the ionic equilibrium of the reactor. Furthermore, the notion of 'rate limiting' step in the sequential anaerobic process, as postulated by Lawrence (1971), suggests that one of the steps (usually methanogenesis or hydrolysis) is significantly slower than the other steps and will therefore dominate the dynamics. This step is effectively the weak link in the process and is the likely cause of instability within the process when it is subjected to stress (in terms of loading or disturbances). Another element of complexity is added by the endogenous respiration of bacteria resulting from death, maintenance, lysis, self-destruction or predation, but all having the effect of reducing the mass concentration of bacteria. As AD is essentially a low growth rate process, accounting for endogenous respiration is important and is often dealt with by the introduction of a *net* growth rate to include positive and negative contributions to growth.

2.2 APPLICABILITY OF CONTROL STRATEGIES TO ANAEROBIC PROCESSES

The field of automation and control is very wide and has demonstrable applicability to AD, in many ways (Vassos (1993)). There is little that one would wish to exclude from this field, as a possible tool to aid the robust and reliable control of AD. This makes a definitive study of the

control of AD beyond the reach of any single treatise. Works such as Olsson and Newell (1999) and Bastin and Dochain (1990), have a considerable impact on the direction of research, while at the same time reflecting the work that has previously been published in this area. Essentially, the research into the control of AD (without considering many underlying process issues) is aimed at several coupled outcomes (Olsson and Newell (1999)), which include:

➢ the efficient use of reactor (and even storage and sewer) volumes

➢ diagnostic systems; software sensing using model based estimation

➢ the development and management of process models and simulation tools and methodologies and protocols for calibration of models

➢ the measurement of active biomass and the development of mixed populations

There is considerable uncertainty with regard to the cost effectiveness surrounding the balance between reactor volumes and the use of control systems. The break point will be different for different situations, with considerations such as land value and labour and finance costs having major effects on the decision to adopt control. However, clear and accurate information on performance, provided at the design stage, will assist in the decision making. It is believed, (Steyer et al. (2002)) that the cost effectiveness will swing progressively towards control, with improvements derived from research. This is particularly true with regard to sensing systems, but modelling and simulation will improve confidence at the design stage. The difficulty in establishing biomass activity in anaerobic systems is a key issue in both the initial conditions for modelling and in considering the development of the microbial population. Guwy et al. (1998), have demonstrated alternatives to respirometry in aerobic activity measurement, whereby catalase present in the cells is considered to be a measure of the activity of the biomass and is measured by its ability to evolve oxygen from peroxide. Analogous measures are required for anaerobic activity.

It remains true to say that AD is a non-linear time varying process and as such, the vast literature regarding the control of such systems is to some degree applicable.

Start-up of an AD reactor can be considered to be a prolonged and particularly critical shock-loading regime and the first start-up of such a process would be accompanied by considerable uncertainty. In general, the design of the control strategy requires a representative model of the reactor and its associated processes. If a model were available, it is likely not to have been parameterised for the specific digester. Considering the likely scenario at the point of commissioning, knowledge of the specific reactor will be limited to design specifications. In the case of restart, historical operating data would also be available, but the use of these data in

parameterising a model would be at once a significant intellectual effort and an exercise which would produce dubious model performance with respect to the restart reactor characteristics. The accuracy of a model depends on the source of the data from which it is parameterised. These models may be traditional in their structure as in Andrews (1968), or fuzzy in a general sense (e.g. Marsili-Libelli and Muller (1996) or Premier et al. (1999)). On-line identification would take care of time variations, but usually depends on a number of on-line measurements, and consequently, and not withstanding the exceptions mentioned in the review of literature, may involve considerable instrumentation.

It would be beneficial to the AD operator and commissioner to be able to control the start-up over its entire duration, using a minimum number of on-line sensors and relying as far as possible on the generation of model information from a system other than the one being commissioned. The benefit of such an approach would be reduced commissioning costs from the reduced 'cost of knowing' and reduced instrumentation requirements. It could be postulated that start-up can be accelerated compared with a manual approach and that risk of failure might be reduced.

Controlled start-up of AD is considered to be an important objective of AD reactor control and is not necessarily unrelated to normal operation. Start-up control of biological reactors has been considered by a number of authors such as Moller and Jorgensen (1997); Renard et al. (1991); Rozzi et al. (1994); Weiland and Rozzi (1991). As is the focus of this work, Rozzi et al. (1994) in particular used Bicarbonate Alkalinity (BA) as a control variable, but used a markedly different control strategy. Maintaining a BA buffering margin is a means of controlling the pH drop caused by a build up of Volatile Fatty Acids (VFAs), (McCarty (1964b); Rozzi et al. (1985a)). When the seed is introduced to a digester at start-up/commissioning, it is often derived from systems operating on waste streams with significantly different characteristics. The size of the population could also be relatively small and in any case the viable fraction of the biomass and its distribution in terms of trophic groups would be difficult to ascertain. The combination of these factors means that feeding can be increased only slowly, with the expectation that the microbial population is time varying, in its ability to treat the waste. This time variation is not necessarily restricted to start-up, so that a controller suitable for start-up may be able to cope with disturbances during normal operation.

2.2.1 Automatic control strategies used in anaerobic digestion

There have been several hundred publications with direct relevance to the control of AD. These are spread widely, from those concerned with the parameters of significance, such as the work of

McCarty (1964a), Kotze *et al.* (1969) and Andrews (1975a) and Andrews (1975b), in the earlier work in this field to those concerned with highly specific applications and/or techniques such as Alcaraz-Gonzalez *et al.* (2001), Tay and Xiyue (1999), Hilgert *et al.* (2000) and Tartakovsky *et al.* (2002) more recently. Apart from this 40 year spread, there is also a significant spread in complexity of approaches. Control strategies which had simplicity as a positive ambition have been considered by a number of authors e.g. Ryhiner *et al.* (1993), Swamy *et al.* (1997), Steyer *et al.* (1999), Muller *et al.* (1997), Perrier and Dochain (1993) and Marsili-Libelli and Beni (1996). The latter looked at the feasibility of PID control using bicarbonate alkalinity as a control parameter, and thus has relevance to the current study. Steyer *et al.* (1999) adopted pH and gas flow rate as measured variables and adjusted the loading rate to regulate the system. This approach has the major advantage that the reliability and cost of the sensors involved are of an order that they would be likely to be used industrially. The philosophical approach and execution have resonance to this study, which seeks to minimise the instrumentation and has as a goal widespread adoption of control in anaerobic digester operation. A small number of measured variables would give an incomplete indication of the state of the process and would be sensitive to sensor failures, with less possibility for associated diagnostics and correction.

Hybrid systems sometimes help by increasing the possibility to actuate (and so control) the process, as was reported by Polito-Braga *et al.* (2002), demonstrating a system which had an anaerobic UASB followed by an activated sludge process. Control of the effluent COD and suspended solids concentrations were maintained by using two independent PI controllers to manipulate the flow rate of recycled sludge from the clarifier.

Hydrogen has been considered as a control parameter and early warning indication of reactor failure by Cord-Ruwisch *et al.* (1997), who used a silicon tube and trace gas analyser to determine the dissolved hydrogen concentration in the liquid phase. Others e.g. Strong and Cord-Ruwisch (1995), Guiot *et al.* (1995) have also considered hydrogen as a control variable. The control strategies used by Cord-Ruwisch *et al.* (1997) were simple set point bang-bang control (20% steps in feed rate) and a proportional only controller. The feed used was glucose based and the resulting control was comparatively good. The use of hydrogen as a control parameter remains a concern in cases of more complex and variable waste for the reasons that the metabolic pathways can change depending on reactor history as mentioned in Section 2.1.1.

In recent years, efforts to establish adaptive control strategies, have been seen by some research groups as a promising line of investigation, as have the 'fuzzy' approaches associated with soft computing techniques, which have gained in popularity across the spectrum of process control.

A generalised and comprehensive lumped parameter modelling approach has been presented by Bastin and Dochain (1990), which is developed into a treatise for adaptive linearizing control in biological processes and relies on on-line estimation of unknown parameters associated with the reaction kinetics. These are notoriously difficult to model accurately because of their time varying non-linear characteristics. Furthermore, consensus exists regarding models of reaction kinetics, only in so far as Batstone et al. (2002) has assumed as much in the publication AMD1. Several kinetic reactions are not included, as evidenced by the numerous functions in Appendix 1 of Bastin and Dochain (1990), which do not find application in ADM1. The problems of identifiability of the reaction constants within these functions are also discussed by Bastin and Dochain (1990), further justifying their on-line estimation approach.

The techniques presented by Bastin and Dochain (1990) are reported with reference to specific control variables in Dochain et al. (1988), who present the control strategy investigated by simulation, using volatile fatty acids, BA and H_2 concentration (again considered by Dochain et al. (1991)) as control variables. The H_2 was considered at this stage to be promising because of its rapid dynamics and the assumption was made that equilibrium would exist between the gas and the liquid phases, thus on-line measurement of gaseous H_2 would be the only requirement. More recently, Bernard et al. (2001) investigated a combined linearizing controller and fuzzy controller the objective of which was to maintain the ratio of total to intermediate alkalinity at a pre-set value. Renard et al. (1988) sought to maintain a constant substrate concentration by altering the feed dilution rate on a pilot scale plant CSTR. The controller (based on a non-linear model of the fermentation process) was implemented using off-line COD measurements with a sampling time of 2 hours. Since then, Steyer et al. (2001) has shown the practicality of directly measuring COD and others including Aubrun et al. (2001) have used software sensor techniques. Renard et al. (1991) continued to employ an adaptive algorithm for 161 days (including start-up) on a completely mixed, once through reactor, by using the propionate concentration as a control variable, with promising results. The propionate concentration in the reaction vessel was compared to a prescribed level, and the error between them minimised over time exponentially. The adaptation came from the fact that the conversion yield factor from substrate to propionate needed to be estimated on-line.

The measurement of VFAs has been demonstrated by Steyer *et al.* (2001) using IR, but can be determined by titrometric methods (e.g. Dehaas and Adam (1995)) and commercial on-line GC devices, though the cost of the latter is as yet relatively high. The principle was extended to batch fed reactors in a general treatise by Dochain and Bastin (1990). Further, Dochain *et al.* (1991) undertook a simulation study looking at the adaptive control of AD by using hydrogen concentration. This simulation did not include the formate/hydrogen path selection resulting from acclimatisation, which was described in Section 2.1.1. Dochain and Perrier (1993) then went on to publish accounts of the design and evaluation of adaptive non-linear control algorithms (model reference adaptive linearizing control law) for activated sludge and AD processes, with the controller validation again performed by simulation. Van Breusegem *et al.* (1990) used simulations to investigate the technique with BA as a control variable, comparing it with the L/A control strategy. The L/A technique involves the use of a logarithmic function to ensure positive control actions at all times, and is described in the paper. Adaptive linearizing control strategies were adopted by Monroy *et al.* (1996), though altered to avoid the need for on-line bio-gas flow rate measurement.

The work of Alcaraz-González *et al.* (1999), Alcaraz-Gonzalez *et al.* (2000) and Alcaraz-Gonzalez *et al.* (2001), showed the application of an adaptive scheme which regulated to its nominal target value. The system settled exponentially and did so in the accepted presence of uncertainties and Alcaraz-Gonzalez *et al.* (2001) went on to demonstrate the approach by simulation and experimentally on a 1 m³ anaerobic reactor. The idea that the process is liable to experience uncertain inputs is important, as they may lead to an undetectable (i.e. cannot be identified) system. The control is handled by a non-linear observer which requires that the inputs such as mass, energy and feeding rates be known. The fact that they are not, but *a priori* knowledge of their bounds is available, allows a second observer (so called interval observer), to estimate these uncertain inputs and thus makes the overall control become bounded and guaranteed to converge exponentially. The methodology was applicable to SISO situations and demonstrated that with an estimation of the input variations, the reactor performance could be predicted and controlled within well-defined bounds. This would appear to be a powerful technique in the presence of *a priori* knowledge, from which the bounds could be set. The applicability could extend to more general application where the bounds could include typical anaerobic digesters, though the wider the bounds of certainty, it is expected that the bounds of prediction will also widen.

Adaptive optimal control was employed by Ryhiner *et al.* (1992). The technique employed a performance index, which was used to adjust the control conditions of the ever-changing reactor and process. Under simulated conditions, the control strategy was reported to have performed well. Again, however, the shortcomings of simulation studies are essentially that the unmodelled dynamics are not considered and equally, the noise and aberrations which are expected with a degree of resignation, are assumed not to exist, or else are instigated in a predictable model.

Self-tuning PID control of a fermentation process was considered by Dostal *et al.* (1994) and Jones *et al.* (1996), however the former considered reaction temperature and the latter was in order to control the dissolved oxygen in a *Saccharomyces cerevisiae* fermentation. Self-tuning systems are essentially automated controller design systems based on a model of the process, which is recursively identified. To this extent, the techniques of Bastin and Dochain (1990) have similarities. In the broadest sense, all these systems 'learn' by parameterising a model with data measured in the past and at each sample interval. Self-tuning systems rely on the integrity of the data to converge on a representative model and spurious data can cause them to deviate from this. In essence there is little difference between model reference adaptive techniques and self-tuning in this regard.

Some researchers such as Punal *et al.* (2002) have given attention to so called 'soft computing' techniques such as expert systems, fuzzy logic and neural networks, in order to implement control strategies. The primary attraction of these methods is that they are able to represent systems with non-linear characteristics, without the, often difficult, task of dealing with deterministic non-linear mathematics. Fuzzy logic and expert systems rely on rules which have very intuitive basis such as if<condition> then<outcome>, although there are significant differences in implementation. Toxic substances in the feed will cause the efficiency of the bacterial population to treat the waste, to become reduced and is evident as inhibition. The difficulty in measuring toxicity with regard primarily to aerobic systems is discussed by Fearnside and Caffoor (1998) and Brown *et al.* (1996), though the arguments are relevant to anaerobic systems. They suggest that there is no way to comprehensively test the ingress for toxicity as the range and effect of substances is very large and complex. An approach analogous to respirometry for anaerobic systems which uses a Ranter, was proposed by Rozzi *et al.* (1995); Rozzi *et al.* (1997). The consistent criticism of such systems is that the microcosm does not represent the reactor ecosystem with fidelity, though this may be mitigated by renewing the culture in the Ranter from the main reactor periodically. The control system employed should consider the special nature of toxic loading in the control action which is taken. A reduction in say, gas production may be

considered to warrant increased loading, but may be the result of inhibition which may require the reverse action. Methane production rate was used by Pullammanappallil *et al.* (1998) as the measured variable, along with an expert system, which was employed to ensure safe operation of a digester. The essential argument presented by Pullammanappallil *et al.* (1998) was that previous control research could not cope with the gain inversion, which is possible with shock loading of an inhibitory (or toxic) nature. When tested on an actual live process, the control system prevented failure when the reactor was dosed with phenol as well as other shocks. Broadly fuzzy control strategies have been adopted by Polit *et al.* (1995), Muller *et al.* (1997), Steyer *et al.* (1997), Estaben *et al.* (1997) and Flores *et al.* (2000), all reporting some success.

Neural networks rely on supervised or unsupervised learning, which avoids the need for modelling fundamental physical, biological and chemical laws of the underlying process. Control of anaerobic digesters using neural networks has been reported by Guwy *et al.* (1997) and Wilcox *et al.* (1995) who used bicarbonate alkalinity as a measured variable. Fell and Wheatley (1995) conducted a comparative study between neural and adaptive control, though the study was not exhaustive in its scope. The possibility exists to consider the measurement space as a series of fields, which are indicative of the state of the reactor. Rosen *et al.* (2002) applied principle component analysis and fuzzy c-means clustering to classify the operating status of a simulated aerobic system to then change set points in essentially a gain scheduling fashion. This principle should be applicable to anaerobic systems just as well. The 'soft computing' techniques above are in general non-linear in nature, and gain much of their usefulness from this fact. As far as the AD process is concerned, the degree to which it is non-linear and time varying has not been explicitly investigated, as this would require exhaustive experimentation.

An indication as to whether non-linear techniques are in fact desirable can be seen in Premier *et al.* (1997), which is discussed in some detail in section 5.0 of this document.

2.3 CONTROL USING BICARBONATE ALKALINITY

The definition of the state of an AD system relies on the state variables however they are defined, with variables such as pH and BA coupled, as has been intimated above in Section 2.1.1. The assumptions made in modelling can make the coupling very strong, to the point that one or other becomes redundant. Techniques like principle component analysis, as described by Bishop (1995) and Freeman and Skapura (1991), can be used to determine the interdependence of measured data. Consideration of the underlying mechanisms is however an important part of determining the relevance of calibrating a particular on-line parameter such as gas production rate, %CO_2 and temperature. If a single measured variable is desired, for reasons of simplicity or economy, then the selection of this variable or parameter (on-line measurement) is constrained by the information content of possible measured variables and the available measurement technology. Bicarbonate alkalinity compares favourably with others that have been proposed.

The physico-chemical equilibria considered by Rozzi (1980b), indicated that VFAs, CO_2, total inorganic carbon and carbonic acid, bicarbonate, pH and cations such as Na^+, the solubility and partial pressures of the gas species (particularly CO_2) and OH^- from the dissociation of water, are all implicated. Rozzi concluded that parameters such as pH and the partial pressure of CO_2 have high sensitivity to cations, VFAs, temperature and substrate concentration of the influent. This means that the simple measurement of pH or gas production rate or %CO_2 individually will not give an indication of the true state (be it partially defined) of the system, because of their coupled interactivity. The measurement of VFAs will however give a direct measure of any imbalance between volatile acid production by the acidogens and consumption by the methanogenic bacteria. This is particularly true if the VFA species can be quantified. Bicarbonate alkalinity is similarly indicative of the imbalance because its reduction is as a consequence of an increased presence of VFAs, given that the total cations must be in equilibrium with the HCO_3^- and the acid anions.

Many anaerobic systems are employed in the degradation of materials rich in natural buffers such as NH_4HCO_3, which would increase the bicarbonate available in the reactor, which could then tolerate higher VFA levels without dropping the pH and risking souring. Considering VFAs would not account for the added intrinsic stability whereas considering the bicarbonate alkalinity (or buffering capacity) would. The information content of bicarbonate alkalinity is very high, structurally including many of the other measurable parameters within the physico-chemical

equilibrium model, and at the same time being a relatively straight forward parameter to measure on-line, as discussed below.

The special case of start-up, reviewed by Hickey *et al.* (1991), is often a period of high risk and uncertainty with regard to the loading regime. As has been the case in this work, Rozzi *et al.* (1994) are notable for having used Bicarbonate Alkalinity (BA) as a control variable. However, they used a controller which dosed the reactor with alkali at a fixed rate, for a time proportional to the error, which in essence combines continuos and bang-bang control strategies. Maintaining a BA buffering margin is a means of controlling the pH drop caused by a build up of Volatile Fatty Acids (VFAs) (McCarty (1964b); Rozzi *et al.* (1985a)).

The use of VFAs as a control variable has been shown to be practically achievable (as demonstrated by Renard *et al.* (1991), using propionate concentration), particularly since titration based, on-line measurement of VFAs has been shown to be feasible (Dehaas and Adam (1995)). The total VFAs that are measured do not discriminate between the species, whereas individual VFA measurement could indicate stress in the different bacterial groups within the biomass. Nevertheless, a measure of VFAs does indicate the balance between acidogenesis and methanogenesis, such that a build up in VFAs indicates a propensity to sour. BA gives similar information to the VFAs but is affected by the carbon dioxide equilibrium in the reactor (Rozzi (1980b)), through carbonic acid. The activity or stress levels, (particularly of the methanogens) is therefore intrinsically part of the BA measurement. The information content of BA measurement in the reactor makes it a good candidate for monitoring and control by a single variable. This is particularly true because it has been shown to be readily measured on-line, (Guwy *et al.* (1994); Hawkes *et al.* (1993); Rozzi and Labellarte (1984b); Tomei *et al.* (1994), amongst others).

2.3.1 Indicators of stability with particular reference to bicarbonate alkalinity

A great deal of effort has been expended in order to characterise the process and determine the most informative control parameters that could be measured on-line, (e.g. Steyer *et al.* (1995); Jones *et al.* (1992); Ryhiner *et al.* (1993); Denac *et al.* (1988); Ross and Louw (1987)). BA, and VFAs have, in the estimation of the author, emerged as important control variables. McCarty (1964b) considered the environmental conditions for anaerobic populations and the means by which the environment could be controlled. The issue of digester unbalance was central to the discussion of parameters, which may be suitable as indicators of unbalance or which showed promise as control variables. McCarty discussed the use of bicarbonate 'buffering capacity' in order to mitigate against the effect of increased volatile acid, without a large drop in pH, the

corollary being that BA should be controlled. McCarty also looked at the CO_2 in gas and liquid phases according to Henry's law and showed a strong link between pH, BA and CO_2 partial pressure. Graef and Andrews (1973) went on to produce computer simulations to investigate the sensitivity of a number of process variables, including BA, which confirmed the buffering action of increasing levels of BA, as the reactor could tolerate commensurately greater substrate loading variations. Consideration was given to the modelling of BA by Rozzi et al. (1985a) and Rozzi and Passino (1985b) where it was argued that good stability indicators were not necessarily good control variables. They mentioned specifically the partial pressure of CO_2 with its dependence on the 'stored' CO_2 as bicarbonate and its reliance on the volatile acid levels in the system. They went on to propose BA as a control variable for its ability to indicate buffering capacity at any concentration and the plausibility of online measurement. Di Pinto et al. (1990) placed the use of BA as a control variable into an historical perspective, showing the importance of the use of BA as a control variable, was not widely understood till on-line measurement became available in the 1980's. They along with Rozzi and Passino (1985b) further illustrated the connection between the partial pressure of CO_2, HCO_3^- and pH.

Weiland and Rozzi (1991) compared the characteristics of three high-rate anaerobic treatment systems, with particular emphasis on the start-up phase of operation which they viewed as a particular problem in control terms and conceptualised as a prolonged overload. The focus of their treatise was on the monitoring and control of the systems, and as such, their paper establishes a good general review of the field. In their discussion on control variables in the liquid phase, BA is seen as a strong contender, again since the practicality of BA on-line monitoring has subsequently been demonstrated to be a feasible proposition.

2.3.2 On-line monitoring of bicarbonate alkalinity

The on-line monitoring of BA has had a crucial bearing on the use of BA as automatic control variables. Rozzi and Brunetti (1980a) proposed a simple procedure for the measurement of HCO_3^- alkalinity to avoid the protracted effort of determining total acids and volatile acids. This was developed in Rozzi and Brunetti (1981) to determine BA from volumetric CO_2 measurements and Rozzi and Labellarte (1984b) by measuring CO_2 pressure, as did Anstice et al. (1995). Subsequently Rozzi et al. (1985a) proceeded to discuss anaerobic process control by bicarbonate monitoring looking at the advantages of doing so and the available techniques for BA measurement at the time. Further developments are reported in Tomei et al. (1994). A similar approach to the measurement of BA was adopted by Guwy et al. (1994) using a sensitive gas flow meter developed for the purpose. This BA instrument was used subsequently in experimentation

for process modelling and control (e.g. Hawkes *et al.* (1995)). The latter proved it to be reliable and robust, but later in the work of Premier *et al.* (2000) and Premier *et al.* (2001), and in experimental work included in this thesis, reliability became an issue. The carryover of particulate would seem to be the main reason for the differences in performance. A titrometric method was proposed by Pauss *et al.* (1990) and Dehaas and Adam (1995), who also showed that VFAs could be determined in a similar way. A manual method presented by Lahav *et al.* (2002), may be automated, however has yet to be considered so far, to the author's knowledge.

2.3.3 Controlling the anaerobic process using bicarbonate alkalinity as a control variable

The desirability of controlling anaerobic digesters using BA is long established (Andrews (1975a); Andrews (1975b); Rozzi and Brunetti (1980a); Rozzi and Eng (1984a); Rozzi *et al.* (1985a); Dochain *et al.* (1988)). The use of modelling again has been significant in establishing BA as a suitable control parameter. In Rozzi (1980b), the biological considerations of AD are modelled as an ideal catalyst, while the overall process is considered to include a physico-chemical dimension. The equilibrium between the gas and liquid phases is modelled by assuming that CH_4 is insoluble and CO_2 remains in solution according to Henry's law. Furthermore, the ionic balance in the digester governs the substrate conversion to CO_2. The simulations conducted by Rozzi (1980b) sought to show the variations in pH and CO_2 partial pressure resulting from physico-chemical factors, while accepting that changes could arise from the biological process. The conclusions of the study were that parameters such as pH and CO_2 partial pressure were quite sensitive to concentrations of cations, substrate and volatile acids. The implication is that in process control, parameters which are sensitive to physico-chemical variations will perhaps be more useful as indicators of instability than as control variables, which strengthens the case for parameters such as volatile acids and arguably BA for control variables, as BA is indirectly affected.

Testing control strategies in AD is a long and difficult task. Simulations were used by Rozzi and Eng (1984a), modelling a digester degrading carbohydrates to acetic acid by acetogenic bacteria, which were further degraded by methanogenic bacteria (acetoclastic) to produce CH_4 and CO_2, to simulate ramped organic overloading. They went on to test and compare control strategies based on pH or bicarbonate-concentration monitoring and alkali dosing by simulation and investigated CO_2 partial pressure as a stability indicator. They concluded that the best control would be a multi-variable system with CO_2 scrubbing controlled by CO_2 partial pressure and BA or pH control. Furthermore, BA and pH control would give comparable results and the choice would

depend on the availability of sensors and their characteristics. Multi-variable control would naturally require appropriate sensors and current technology offers robust solutions for these parameters.

Dochain *et al.* (1988) describe a simulation based on an adaptive control strategy which is comprehensively described in Bastin and Dochain (1990). The justification for using BA is given as the lack of suitable reliable instruments for the on-line measurement of volatile acids. The situation is no longer as clear, with the advent of titrometric and IR methods already mentioned. This control strategy maintained stable operation in the presence of a toxic shock, which would otherwise have destabilised the reactor. As mentioned earlier, further BA control strategies were proposed by Van Breusegem *et al.* (1990) and supported by simulation studies. Adaptive linearizing and L/A controllers were investigated, considering alkali addition and dilution rate as control actions. The simulation showed that control of the influent dilution rate would control the volatile acid concentration and was suitable for this objective, whereas alkali addition did not control volatile acids, but did maintain them within admissible bounds.

2.3.4 Previous applications of bicarbonate alkalinity as a control variable

Some practical applications of automatic control of AD using BA are to be found in the literature, notably, Di Pinto *et al.* (1990) describing an on-line BA sensor which is then used in the control of two olive oil effluent reactors. These authors looked at the reaction to shock loading with and without BA control. They concluded that BA could be monitored cost effectively and BA control maintained stable performance using proportional control, which was not the case without the control of BA. This work was followed up in Rozzi *et al.* (1994) with similar results with respect to process stability, however the control was also active over the start-up phase of the digestion process and showed control could reduce start-up time.

Control experimentation using BA as a control variable was performed by Hawkes *et al.* (1995) who controlled a fluidised bed system using an on-off control strategy and compared this to a neural network, both controlling alkali addition and both displaying a measure of success. The neural network control study was published in more detail (Wilcox *et al.* (1995); Guwy *et al.* (1997)) and consisted of a feed forward network trained by back propagation. Work conducted in preparation for the control experimentation reported in this thesis, using the same reactor and fundamental control strategy, were presented by Premier *et al.* (2000) and Premier *et al.* (2001).

2.4 A WAY FORWARD

In light of the preceding discussion, it can be seen that numerous researchers have, with varying success, applied a number of approaches to the control of anaerobic digesters. Even in the case of reactor start-up, some successes have been reported. The control variables adopted have been many and varied, often as single inputs and often as multiple input. Similarly, the actuation techniques have spanned the range of possibilities and have included special features in the reactor design, such as recirculation pathways and membranes. The take up of these techniques has been low in general, with the literature reporting very few full-scale applications of control in AD.

It is believed that the critical issues to making the application of control to AD attractive to operators are to minimise the cost and complexity by minimising the instrumentation and expertise required to set-up and operate the system. A SISO system, with a single control variable and a controller that requires little or no parameterisation by the operator, is most likely to be considered. The operator would expect the system to operate with minimal maintenance through start-up, restart, and shock loading of various types and also at steady state. The control strategy would not necessarily need to be transparent to the operator, but this would help to dispel doubt and aid diagnosis should failure occur. The research reported here takes these ambitions as a philosophical starting point.

3.0 EXPERIMENTAL EQUIPMENT, MATERIALS AND METHODOLOGY

The experimentation detailed in this thesis used two reactor systems, which will be described below. The first was a fluidised bed reactor system used to determine the ability of black box models to represent the AD process, which were reported in Premier *et al.* (1997) and Premier *et al.* (1999). The same system generated the data used to parameterise the model reported by Marsili-Libelli and Beni (1996), whose model was used as the basis for the controller design reported herein. The second was an EGSB system, which was used to investigate the controllers, designed and optimised on the model of the fluidised bed system.

The development of the models and the testing of the control system are split into four tasks and to assist the reader, these are summarised in Table 3.1. Included in this table are section references to the descriptions of the experimental equipment and materials used. Furthermore, each task will be explained in turn in the section indicated in the table.

Table 3.1 Model development and controller testing tasks

Task	Task description	Materials and equipment used
1	**Section 3.3.1** Low order linear black box models ability to predict one sample (30 minute) ahead on a fluidised bed reactor.	**Section 3.1** Fluidised bed reactor and operating regime. **Section 3.1.1** Instrumentation associated with the Fluidised bed reactor.
2	**Section 3.3.2** Comparing the ability of low order linear and non-linear (neural network) ARX models to represent a fluidised bed reactor.	
3	**Section 3.3.3** The implementation of a deterministic model capable of representing appropriate control parameters in an anaerobic digester	
4	**Section 3.4** The development and implementation of control strategies capable of maintaining a different reactor (in design and operation) to that which parameterised the deterministic model. *Start-up 1* to *Start-up 4*	**Section 3.2** EGSB reactor and operating regime for control by feed strength actuation and BA dosing actuation

3.1 FLUIDISED BED REACTOR SYSTEM FOR BLACK BOX MODELLING

The fluidised bed reactor used (Figure 3.1.1) in Tasks 1 and 2 (Table 3.1), was used in earlier control experimentation by Guwy *et al.* (1997), and is presented in their paper. The information contained, with some variation (particularly in the feeding arrangement), is presented here for convenience, though the reactor configuration and feed make-up were virtually the same.

HEAD VOLUME = 1.5 Litres

VOL = 1.7 Litres

VOLUME = 0.9 Litres

Ø 16.2 cm

(60°)

7.6 cm

Ø 7.4 cm

$V = 0.2618 \, h \, (D^2 + Dd + d^2)$
$V = 0.2618 \times 7.6 \, (16.2^2 + 16.2 \times 7.4 + 7.4^2)$
$V = 870 \, cm^3 \simeq 0.9 \, Litres$

TOTAL VOLUME = 5.5 Litres
(1.7 + 0.9 + 2.2 + 0.08 + 0.6 Aux Volume)

VOL = 2.2 L

60°

Ø 7.1 cm

5.3 cm

Ø 1 cm

$V = 0.2618 \, h \, (D^2 + Dd + d^2)$
$V = 0.2618 \times 5.3 \, (7.1^2 + 7.1 \times 1 + 1^2)$
$V = 81.2 \, cm^3 \simeq 0.08 \, Litres$

VOL = 0.08 L

Scale 1:5 @ A4   Drawn by AJ E

5.5 Litre EGSB REACTOR
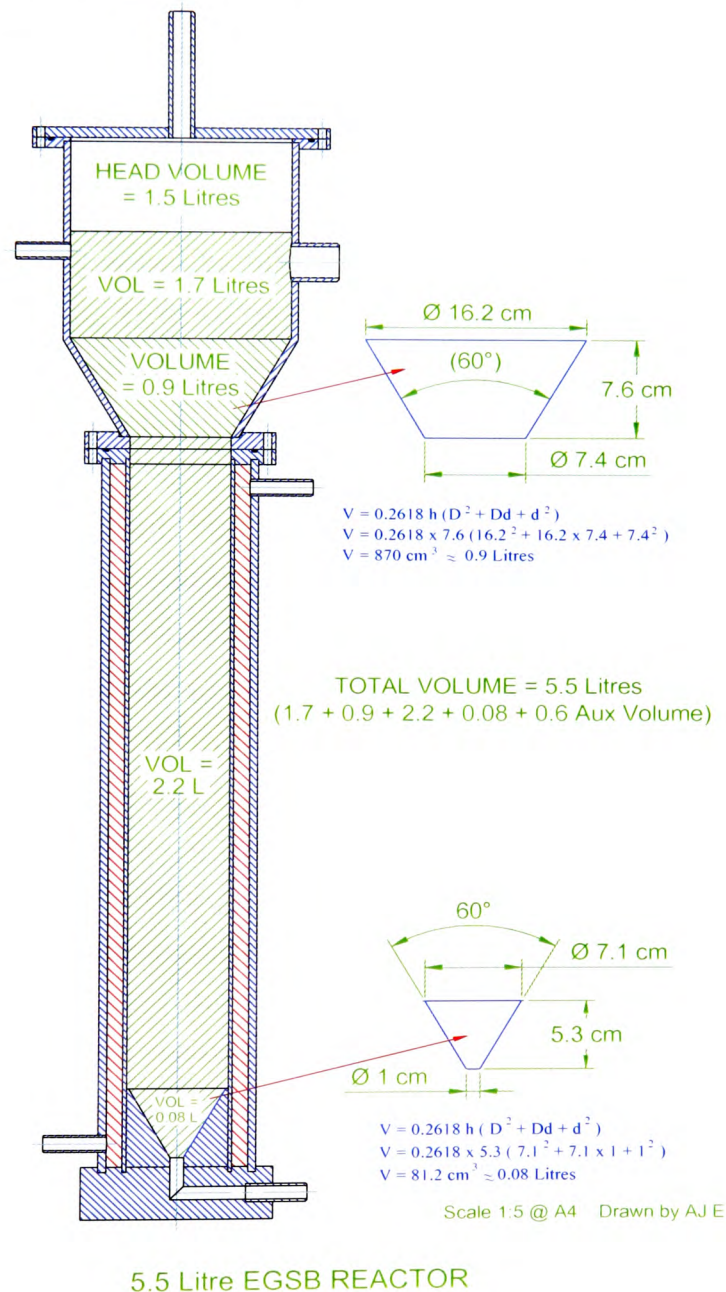
Figure 3.1.1 Fluidised bed anaerobic reactor.

In the interest of clarity, it should be stated that Dr. A. J. Guwy, Dr. R. M. Dinsdale conducted the day to day operation and off-line sampling and analysis of the fluidised bed system and Dr. Guwy particularly was instrumental in its initial construction and instrumenting. The author, (with the exception of the software required to access the TOC data, written by Dr. S J Wilcox), did the computerised data collection system and process excitation and advised on the experimental requirements.

In previous experimental work conducted by Guwy *et al.* (1997), the reactor was operated using similar influent, which was made up every 4-5 days and stored in a refrigerated feed tank. This caused changes in biogas H_2 and CO_2 content thought to be due to changes in VFA content of the feed. Concentrated feed and dilution water delivery at the point of ingress eliminated these changes and stable baseline values for BA, gas flow and biogas H_2 and CO_2 content were achieved. The TOC:COD ratio for the effluent was 1:3.1 and the attached biomass content of the reactor system was determined to be 16.6 $g.l^{-1}$VSS, with some loss of biomass noted during the washing of the Siran carrier prior to measuring the volatile solids carried by it.

The system consisted of two Perspex™, 7 l fluidised bed reactors connected in parallel as shown in Figure 3.1.2. The recirculatory and effluent configuration ensured that the reactor vessels were well connected and in contact with similar substrates as far as was possible. The reactors had previously been operated independently but were connected during the study (Guwy *et al.* (1997)), so that sufficient sample could be extracted for use in the BA monitor. The reactor had been operated on the same influent for two years prior to the experiments reported here, and supplied the data for Tasks 1 and 2. At the end of the experimental period the biomass content of the bed was measured by taking samples which were washed in deionised water and analysed for volatile suspended solids (VSS) by standard methods APHA (1989).

The total liquid volume of the connected reactor was 11 l, giving a head volume of 3 l. The reactor was operated at a temperature of 37°C, which was maintained by a water heating jacket system connected to a thermostatically controlled water pump/heater (Grant Instruments, Cambridge, U.K.). The support medium was a Siran® sintered glass carrier (Schott Glaswerke, Germany) which gave a total collapsed bed volume of 3 l, when allowed to settle. Recirculation of the liquor and consequent fluidisation was effected by a 1031 EHEIM recycle pump (supplier Monside Ltd, Letchworth, Herts., UK), with an up-flow velocity of approximately 0.55 $m.min^{-1}$, from a flow-rate of about 25 $l.min^{-1}$. The feed was pumped into the reactors through a connection into the recycle line common to both reaction vessels, by using a Watson-Marlow (Falmouth, UK)

pump (type 503u) and diluted with water delivered by a Watson-Marlow 503u pump at the point of delivery to the reactor. The interconnection of the reaction vessels was such that the effluent from the top of each was recycled (through a small separation system to prevent Siran® carry-over and pump erosion), to the bottom of the other. This was done using two 1031 EHEIM recycle pumps (Monside Ltd, Letchworth, U.K.). The effluent was discharged through a manometer arrangement connected in common with both vessels, to points 5 cm below the level of the liquid.
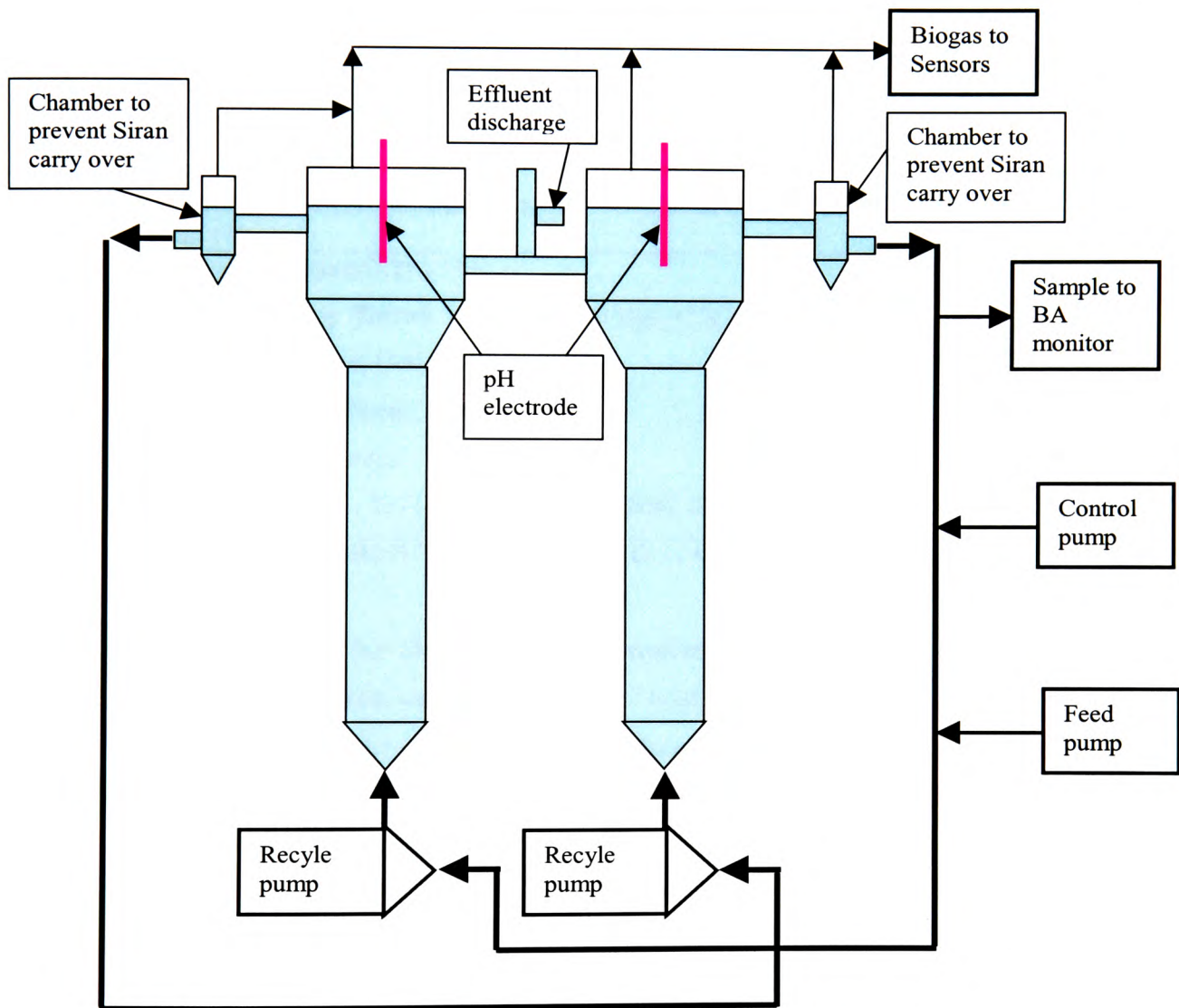
Figure 3.1.2 Schematic diagram of the fluidised-bed anaerobic digester. (after Guwy *et al.* (1997))

The influent feed was a simulated baker's yeast wastewater, the composition of which is detailed in Table 3.2, with a COD of approximately 6,700 $mgO_2.l^{-1}$ and a steady state loading rate to the reactor between 17.6 - 18.8 $kgCODm^{-3}$ day^{-1} with a corresponding hydraulic retention time 9.1 -

8.2 hours. The influent was made up in a concentrated form with a COD of approximately 247,000 $mgO_2.l^{-1}$, delivered using a Watson-Marlow (Falmouth, UK) pump (type 503u) and diluted, with water at the point of delivery to the reactor. It was not considered necessary to refrigerate the feed, even though it had been cooled by a Grant Flow Cooler (type FC15/FC20) during previous work, as at this concentration no COD reduction with time or acidification due to microbial growth was detected. The pump delivering dilution water remained at a fixed rate (19.5 - 21.7, average 20.8 $ml.min^{-1}$) so that hydraulic retention time decreased by a maximum of 10% from a nominal average of 8.5 hours during the overloading evident from the data presented in Chapter 4. The feed pump voltage was directly related to the flow and hence the digester's loading rate (Bv).

Table 3.2 Composition of the simulated baker's yeast wastewater in 100 l tap water (after Guwy *et al.* (1997))

1200 g Yeastex (yeast extract) (CPC, U.K.)
310 g of molasses beet syrup (British Sugars, Cambridge, U.K.)
29 cm^3 of 90% ethanol (Fisons, U.K.)
39 cm^3 of 99.8% acetic acid (Fisons, U.K.)
0.5 cm^3 of trace metal supplement[a]
2.5 cm^3 of anti-foam (Dehysan 32111, Henkle, Dusseldorf, Germany)

[a] $NiCl_26H_2O$ 11.6 g l^{-1}, $CoCl_26H_2O$ 7.0 g l^{-1}, $MnSO_4H_2O$ 11.0 g l^{-1}, $Na_2MoO_42H_2O$ 8.0 g l^{-1}.

3.1.1 Instrumentation for the fluidised bed reactor system

The on-line instrumentation data were logged by a PC equipped with an interface card (MIO 16) and LabVIEW™, propriety virtual instrumentation programming software, (which were both supplied by National Instruments, Newbury, U.K.). Time and date, along with the data generated by the online sensors, were pre-processed and logged to a file periodically at a sampling interval of 2 minutes. This sample rate was very fast and although high sampling helps to increase confidence in the sampling of a continuous data stream it can lead to the deduced discrete time model having poles clustered close to $z=1$ on the complex z plane as discussed by Wellstead and Zarrop (1991). The data was post-processed off-line using a separate software application, MatLAB™, to improve the resulting models identified from it. This involved filtering to eliminate what was perceived to be sensor noise (or noise unrelated to the process). The sampled data were filtered in both chronological directions in order to remove any phase effects and then re-sampling to produce a more appropriate sampling rate for the process dynamics. The digital filtering used a zero phase, forward and reverse low-pass Butterworth filter of 5th order, which was parameterised

by the Yule/Walker recursive least squares approach as described in the MatLAB™ signal processing toolbox (Krauss *et al.* (1995)). The data were then re-sampled at 30-minute intervals, which was considered at this stage to be a reasonable compromise with respect to the digester dynamics. In the case of Task 2, the data were normalised with respect to their mean and standard deviation, with a particular view to improving the performance of the neural network training as discussed by Bishop (1995). A different set of data was required to effect the parameter estimation (and network training), from that used in validation. The 'training' and 'validation' sets were chosen for their significant temporal separation (approximately four weeks, during which time the digester was fully operational), which might have allowed process time variance the opportunity to develop.

Measurement of gas stream parameters included the percentage of carbon dioxide and the hydrogen concentration in the biogas. An ADC monitor type SBG100-002-15290 (ADC Ltd. Hodderson, UK) and a GMI Exhaled Hydrogen Monitor (Gas Measurements Ltd., Renfrew, Scotland) respectively, monitored these on-line. It was necessary to remove the hydrogen sulphide from the biogas in order to measure hydrogen. This was achieved by passing the gas through a saturated solution of copper sulphate and by calibrating the monitor with standard gases on a monthly basis. The biogas flow-rate was measured with an on-line, low flow gas meter, (Guwy *et al.* (1995)). A bespoke bicarbonate alkalinity (BA) monitor developed and described previously by Guwy *et al.* (1994), was used on-line in the effluent stream to measure the BA as $mgCaCO_3.l^{-1}$ equivalent. A Kent EIL9142 meter using an Ingold Xerolyte electrode (type HA405-DXK-S8/120) was used to measure the pH in each reaction vessel.

A high temperature IR method supplied by Rosemount-Dohrmann DC 190 (Sartec Ltd., Borough Green, UK), was used to measure the Total Organic Carbon (TOC). The instrument was automated by using an auto sampling, $(50\mu l)$ injection system. A nylon fabric filter filtered effluent from the reactor, at a rate of 20 ml.min^{-1}. The filter had a pore size of 15μm, (Sericol Industrial Fabrics, Broadstairs, UK), and was contained in a specially designed (by the Institute for Biotechnology, KFA, Julich, Germany), chamber and fitted into the system, with a rotating brush for automatic cleaning. This filter reduced the measured COD by 15 fold, an amount equivalent to settling the effluent for an hour, or filtering with a Whatman G/FC filter. Unused filtrate was returned to the reactor in order not to remove any more effluent from the system than was necessary. The TOC measurement required the equivalent to 6.3 ml.min^{-1} of filtrate, which passed through a 9 ml, mixed continuous flow cell on the auto-sampler tray. The sampling frequency was not constant and depended on the time taken by the machine to determine the

Inorganic Carbon (IC), Total Carbon (TC) and the difference being them, the TOC. This took between 8 and 11 minutes and the data was logged by proprietary software from Rosemount-Dohrmann, from which it was transferred to a spreadsheet for further processing.

3.2 EXPANDED GRANULAR SLUDGE BED (EGSB) REACTOR SYSTEM FOR CONTROL STRATEGY TESTING

The EGSB reactor employed in the testing of control strategies detailed in Table 3.4.1 and developed in this thesis, was a 38 l Perspex™ vessel as shown in Figure 3.1.3, which had (for most of its height), a jacket heating arrangement, which was also constructed from Perspex™. A conical diffuser, (with a volume of 1.3 l) was placed in the bottom of the reactor to ensure even flow across the reactor, which reduced the total volume. However, the liquid volume was nominally 30 l, leaving a headspace of 6.7 l. The headspace was further reduced by other equipment, (such as sensors and pipe-work), such that a nominal headspace volume of 5 l was used in the modelling of the reactor. The temperature of the reactor was controlled at a nominal 35°C, by hot water circulated through the heating jacket using a FH-15 thermostatically controlled Flow Heater (Grant Instruments Ltd., Cambridge, U.K.). Peristaltic pumps (505S or 503U) and tubing (Watson and Marlow Ltd., Falmouth, UK) were used throughout the system to effect circulation or for the metering of fluid flows. The system is shown schematically in Figure 3.1.4.

Again in the interest of clarity, it is emphasised that the author was not involved with the day to day running of the EGSB reactor, and had only an advisory/discursive role in parameters associated with its establishment. The author was once more, instrumental in establishing the software and interfacing required to monitor and control the process. The operation and maintenance, as well as the offline sampling and analysis was conducted by Mr K Monson, or under his supervision, by the ERASMUS students listed in the acknowledgements of this thesis.

The reactor was initially seeded (with approximately 25% by volume of the liquid phase i.e. a settled height of 0.41m from the diffuser at the bottom of the reactor – 7.5 l), granules taken from a UASB reactor at Davidson's Paper Mill (Aberdeen, Scotland). The seed had been kept refrigerated for over 1 year prior to their use in this work. The total solids (TS) concentration of this sludge was 74.78 g.l^{-1} and the volatile solids (VS) concentration was 50.21 g.l^{-1}, at the time of seeding. These bacteria were used in experimentation, which was conducted over a ten-month period, some of which has been reported in Premier *et al.* (2000) and Premier *et al.* (2001).

VOLUME C = 11 litres

VOLUME B = 5 litres

VOLUME A = 14.14 litres

Ø 34 cm

86.4°

Ø 15 cm

10.11647 cm

$V = .2618h (D^2 + Dd + d^2)$ $V = .2618 \times 10.11647 (34^2 + 34 \times 15 + 15^2)$ cm^3
$V = 2.6484918 (1156 + 510 + 225)$ cm^3
$V = 2.6484918 \times 1891$ cm^3
$V = 5008.2979$ cm^3 = 5 litres

TOTAL VOLUME = 30 litres

Scale 1:5 @ A4   Drawn by AJ Evans   20 Aug '98

30 litre EGSB REACTOR
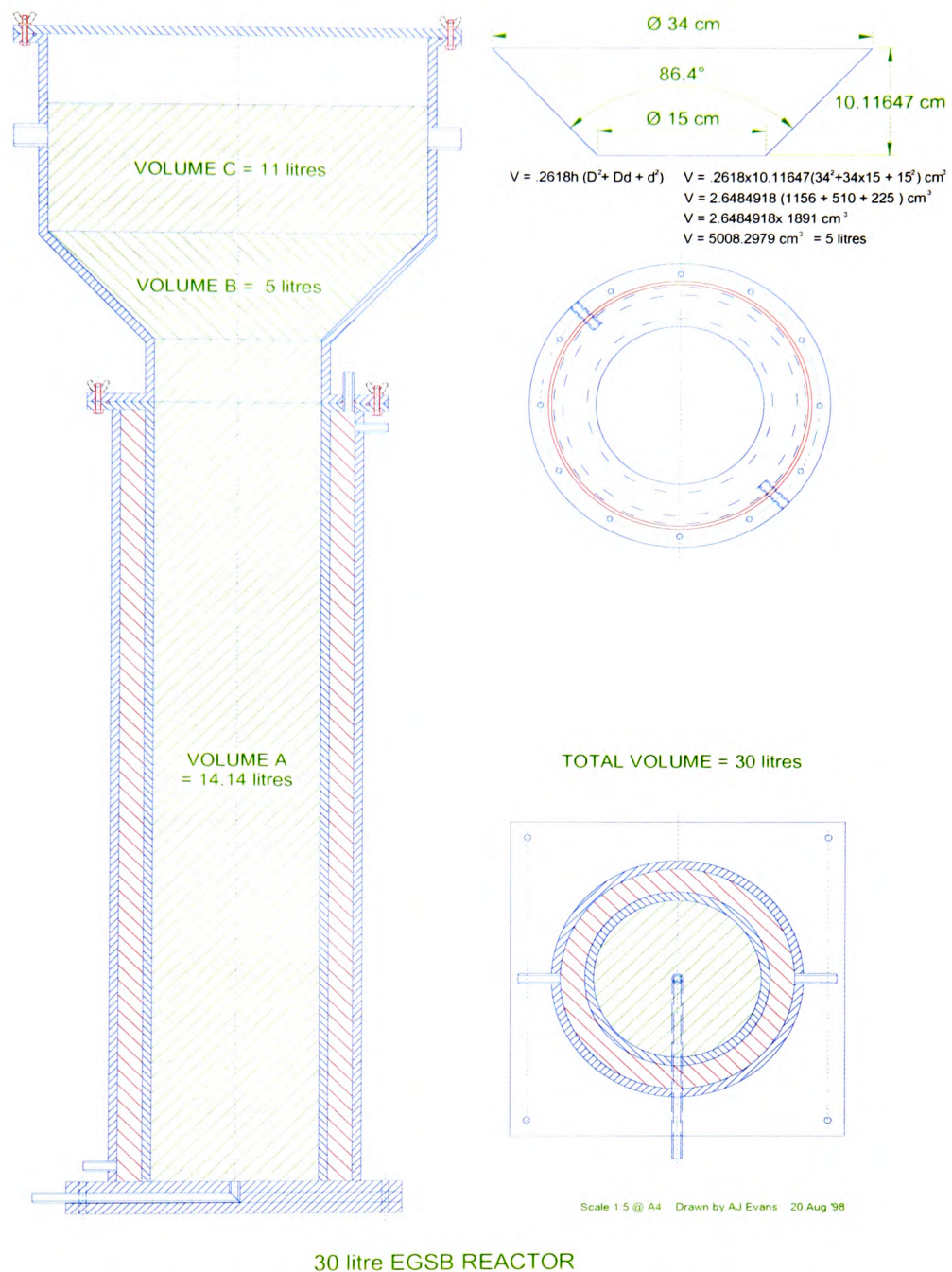
Figure 3.1.3 Expanded Granular Sludge Bed (EGSB) anaerobic reactor.

The first of these papers is not an integral part of this treatise, though the second forms part of *Start-up 1*, the first of four start-up experiments to test the optimised adaptive control strategies developed by the author. In fact, *Start-up 1* and *Start-up 2* used the bacterial seed described above, but the reactor was re-seeded for experiment *Start-up 3* and again for experiment *Start-up 4*. The final two start-up experiments were conducted on the same reactor system, which had been seeded by approximately 15 l of sludge before each Start-up, from a UASB reactor used to treat molasses waste from a citric acid producing plant, (Tate and Lyle Citric Acid, Selby, N.

Yorkshire). In the case of *Start-up 3*, a sample of the sludge revealed the total solids (TS) concentration was 104.9 g.l^{-1} and the volatile solids (VS) concentration was 36.6 g.l^{-1}. For *Start-up 4*, the total solids (TS) concentration of this sludge was 109.7 g.l^{-1} and the volatile solids (VS) concentration was 67.1 g.l^{-1}. This was after the reactor had been filled with tap water and recirculated at 61% of the rate used in *Start-up 1* and *2*, while dosing with BA at 2222 mg.l^{-1} CaCO$_3$ equiv. for four days. The seed for *Start-up 4* had been sourced at the same time as that for *Start-up 3* and was stored in a refrigerator for approximately seven months.
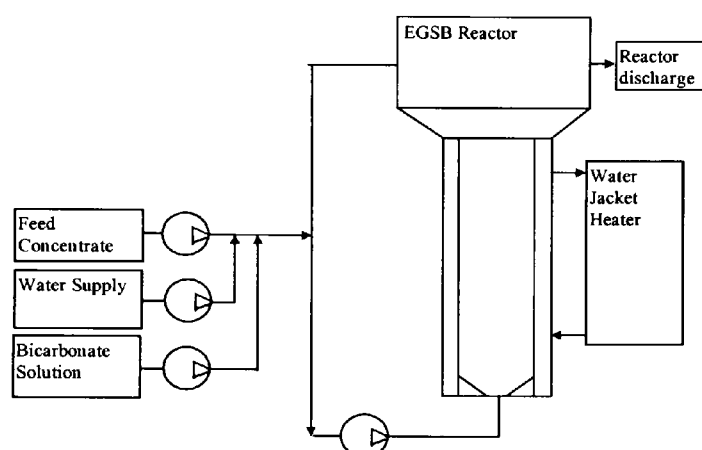
Figure 3.1.4 Schematic diagram of EGSB reactor, showing feed and circulatory arrangements.

The reactor was fed on an idealised synthetic waste with sucrose as its key constituent. The sucrose was diluted with tap water and to maintain reasonable concentrations of BA and sodium bicarbonate was added at the above concentration of 2222 mg.l^{-1} CaCO$_3$ equiv., by continually pumping the solution into the reactor feed line using a peristaltic pump. Two fundamentally different control actuation strategies were adopted. The first of these was to alter the loading rate in order to affect the measured effluent BA and the second was the use of BA dosing dependant on the effluent BA measured.

3.2.1 Instrumentation for the EGSB reactor system

The personal computer (Macintosh Quadra 650) based monitoring system was arranged to log data from a number of on line sensors and was equipped with a virtual instrument software package (LabVIEW^{TM}). The control system was implemented on a separate PC (Viglen, Pentium), for convenience and to make the data logging system independent of the control and hence able to continue should failure occur in the control system. The on-line parameters (sampled at 1-minute intervals) were:

- BA,

- pH,

- gas phase hydrogen concentration,

- gas production rate,

- % carbon dioxide in the biogas and

- reactor temperature.

BA, the most important parameter with regard to the control system, was measured on-line as described by Guwy et al. (1994). A constant flow of reactor effluent was saturated with CO_2 in a well-mixed (saturation) chamber. The saturated sample was transferred to the instrument's acidification chamber, where the pH was dropped to about pH 2, but in any case below pH 4, which causes all the HCO_3^- to evolve CO_2. A sensitive gas meter measured the evolved gas volumetric flow-rate, which was proportional to the HCO_3^- in the sample. The low flow gas meter consisted essentially of a ballast chamber, which was pressurised to approximately 5 mmH_2O by the evolved gas. At this point a 3-way solenoid valve was activated releasing the pressure in the ballast chamber while sealing the acidification chamber, until a low threshold pressure was achieved. This process was repeated at a rate dependent on the gas flow-rate and indeed, the gas release rate was calibrated (periodically with standard solutions), to indicate BA concentration. A microprocessor-based system designed and programmed by the author, to give frequency to voltage conversion with an output in the range 0-5 V.

The pH was measured using a temperature compensated ABB Kent-Taylor pH meter/controller (model EIL9142) connected to a Mettler Toledo HA405-DXK-S8/225 probe. The system required weekly calibration with pH buffer solutions at pH 4 and pH 9.2. The instrument supplied a voltage signal in the range 0-5 V which represented pH 0-14.

The rate at which biogas was produced by the reactor, was measured by a low-flow gas meter (Alexander Wright Low Flow Meter, LFM300, supplied by G H Zeal Ltd., London, U.K.), which had a range of 0.2 – 4.0 $l.hr^{-1}$. The output of the meter was in the range 0-5 V. In operation, the reactor could and did produce biogas in excess of the maximum range of the LFM300. It was therefore necessary to include an instrument capable of measuring flows at higher rates. The available flow meters were not able to cover the complete range adequately, so both the LFM300 and a mass flow meter (Honeywell AWM 3300V Mass Air Flow Sensor, Farnell, Leeds, U.K.), were used. The flow-rate was used in a subroutine in LabVIEW™, to activate a solenoid valve,

which selected between the flow meters. Some hysteresis was included in the programming to avoid rapid and continual switching.

The % CO_2 was measured using a Gascard II Infra-Red Monitor. Absorption of the IR by CO_2, CO and CH_4 are frequency dependent. By measuring the characteristic frequency and intensity of absorption, the concentration of CO_2 as a percentage can be determined. Once again, the output from the instrument was arranged to be 0-5 V, calibrated using 100% Nitrogen, 100% CO_2 and 40% CO_2 sequentially.

The reactor temperature was measured by a single temperature sensing semiconductor device (LM35DZ, RS Electronics, U.K.) suspended in the liquid phase of the reactor, with a sensitivity of $10 \text{ mV.}^{\circ}\text{C}^{-1}$

The Monitoring Computer had both A/D and D/A I/O facilities, (MIO 16 data acquisition card from National Instruments, UK). The data from the on-line instrumentation were connected to the I/O card and read by a program created in LabVIEW^{TM}. Facility to calibrate the signals was included and pre-processing such as filtering manipulation or correction, were also embedded in the software. The Monitoring Computer was also required to take some control actions, such as selecting flow-meters, switching to manual control, sending the BA signal to and receiving the control effort signal from the Control Computer and outputting control effort signals to the variable speed, feed and dosing pumps. However its primary function was to log the data to an ASCII file along with time and date information, every minute. The sampling-rate of the Control Computer was independent of the Monitoring Computer and was 1 sample.h^{-1}. The BA signal was provided to the Control Computer, which in turn provided the Monitoring Computer with the control effort calculated by the controller at each sample. The control strategy determined if the OLR varied or if the BA dosing of the reactor varied. The control effort was converted to appropriate voltage signals to run the water, BA dosing and/or concentrate feed pumps such that the volumetric flow-rate reflected the desired HRT, but the feed strength varied, or the BA dosing rate varied accordingly. The Control Computer used a Lab PC+ I/O card (National Instruments, UK) and LabVIEW^{TM} virtual instrument package to effect the I/O function. The control algorithm was programmed using a graphical, block oriented Computer Aided Control System Design (CACSD) package, (MatLAB/Simulink^{TM}, The Mathworks, U.K.). Communications between the software packages was achieved using the Dynamic Data Exchange (DDE) facilities provided by both. In the system created in this work, MatLAB/Simulink^{TM} was configured as a Client, whereby a number of functions were available for use in initiating the DDE conversation,

requesting data and terminating the DDE conversation etc, while LabVIEW™ acted as the Server. The Client was established by writing an M-File function, which included the DDE functions which established communication, requested data, checked to see if the data had changed (which was assumed to be the point at which LabVIEW™ had sampled, before passing the data to Simulink™ through a Function Block. Within LabVIEW™, the DDE was initiated and serviced through standard functions (check.vi and set.vi) provided by National Instruments Inc. The M-Files, Function Blocks and LabVIEW™ used are included in Appendix A1 and A2, particularly in Figures A2.2 and A2.3. The BA set point could be adjusted within LabVIEW™ on the Control Computer. The set point and measured value (BA) were then provided to the control algorithm (presented in Section 3.4), at each sampling interval as illustrated by in Figure 3.1.5.
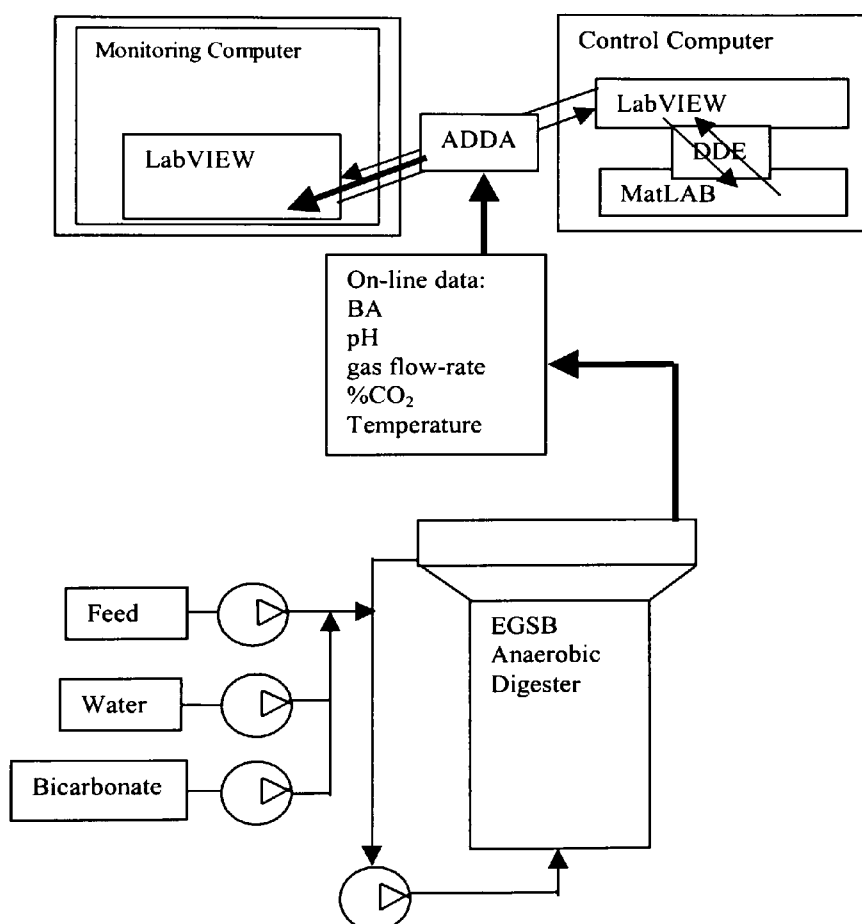
Figure 3.1.5 Schematic diagram of the communication between LabVIEW™ MatLAB/Simulink™ via DDE.

The current control effort was passed back to LabVIEW™ for delivery to the Monitoring Computer. All communications to and from the computers was through the Analogue to Digital/Digital to Analogue conversion (ADDA) facilities of the I/O cards used.

Arrangement for actuation through Loading Rate (Start-up 1,2 and 3)

A constant 18 ml.min^{-1} of a 3733 mg.l^{-1} NaHCO$_3$ solution, equivalent to BA of 2222 mg.l^{-1} CaCO$_3$ equiv. was fed to the reactor. A summary is shown in Table 3.3 of a variable (according to the control effort), flow of a simple salts medium at a ×20 concentration, (as in Cohen *et al.* (1979)) which was input to the reactor. The feed included a concentrate containing 1% glucose (W/V) which was mixed with tap water (tested to show negligible BA), so that a constant inflow volume of 21.5 ml.min^{-1} was delivered to the reactor. Trace elements were added to the concentrate at a rate of 1 ml.l^{-1}, according to the recipe of Table 3.4. The up-flow velocity (V_{up}) was kept constant at 4.78 m.h^{-1} and similarly, the retention time was maintained at 24 hours.

Table 3.3 Summary of the feed composition for EGSB reactor

Constituent solution	Concentration [ml.l^{-1}]
2M NaH$_2$PO$_4$.2H$_2$O	1.25
4M NH$_4$Cl	6.25
2M KCl	1.5
1M Na$_2$SO$_4$	0.4
1M Citric acid	0.5
0.25M MgCl$_2$.6H$_2$O	1.25
0.02M CaCl$_2$.2H$_2$O	0.25
0.001M Na$_2$MoO$_4$.2H$_2$O	0.025

The constant flow-rate to the reactor was achieved by regulating the flow from two feed pumps (one supplying feed concentrate, the other tap water), such that the sum of the flows was constant at a rate of 21.5 ml.min^{-1}. The algorithm used to control the pumps was configured to adjust the flows to maintain a specified though changeable HRT. The 21.5 ml.min^{-1} flow-rate corresponded to a 24 hour HRT.

Table 3.4 Summary of trace elements added to feed for EGSB reactor

Trace element	Concentration [ml.l^{-1}]
HCl	5.1
Fe$_2$Cl$_2$.4H$_2$O (dissolved in acid)	1500
H$_3$BO$_3$	60
MnCl$_2$.4H$_2$O	100
CoCl$_2$.6H$_2$O	120
ZnCl$_2$	70
NiCl$_2$.6H$_2$O	25
CuCl$_2$.2H$_2$O	15
Na$_2$MoO$_4$.2H$_2$O	25

Arrangement for actuation through BA dosing (Start-up 4)

In the experiment where BA dosing was used as the control action, an algorithm similar to that for actuation through loading rate was used. In this case, the loading rate was manually set at a constant level (which was changed as the requirement to do so arose). A concentrated BA solution of 2222 mg.l $^{-1}$ $CaCO_3$ equiv. was supplied (according to the control effort), and mixed with tap water from a separate pump, again configured to maintain a constant inflow to the reactor. In the case of the BA dosing, the HRT was not always kept at 24 hours (in experiments beyond those reported here), so the flow-rate was changed as a consequence. The feed composition, with respect to trace elements and salts, remained the same as Tables 3.3 and 3.4, as did the recirculation rate and *Vup*.

3.3 MODEL DEVELOPMENT FOR CONTROLLER DESIGN

The choice of a model, for use in the design of a control strategy for AD is not necessarily obvious or straightforward. AD is known to be non-linear and time varying, but the extent to which this is of relevance within a model, is dependant on the use to which the model is to be put and the operational characteristics of the system it represents. As no techniques for rational and efficient elimination of alternative approaches could be discovered from the literature, it became necessary to investigate the possibilities presented by what was perceived to be the most promising of the different modelling approaches. Considering and comparing all the different modelling approaches would prove to be a prohibitive strategy. It was decided therefore, to consider the simplest approaches first and attempt to discover the point at which a sufficiently representative model was obtained. The strategy sought to determine if simple black box models could be made to represent the process with a 'good enough' degree of accuracy. In this work, several black box models were parameterised from measured data and investigated using separate validation data in order to find the most appropriate of these models. The apparent stability of the process begged the question; whether linear models could represent the process as accurately as non-linear models. To try to answer this, a comparison was made between linear and non-linear (neural network) models of similar structure. The parameterisation of the black box models relies entirely on identification and the parameters have little or no physical meaning.

The discussions of the development of such models are not easily divorced from the data and experimentation from which they are parameterised because the model is essentially a regression fit of the data (using least squares approaches in general). The model development for the ARX modelling will be presented as an identification process after having elaborated the model

structures that were used. As the overarching conclusions of these studies showed significant differences between the model predictions and the real behaviour of the process, it was necessary to consider the use of non-linear lumped parameter models as are commonly used in AD research. These models had been validated in several studies, some of which are mentioned in Section 2.1.

Presented here are the modelling procedures used in the development of simple linear black box models of various structures and then proceeds to present the techniques (Task 1), and non-linear ARX model structures with which they are compared (Task 2). As the performance of these models was not considered sufficiently high with respect to predictions over large horizons, the section presents a suitable deterministic model (Task 3), which was then integrated with the control system and strategies adopted in Section 3.3, (Task 4). A summary of these tasks was presented in Table 3.1

3.3.1 Low order linear black box models (Task 1)

The model of a system need not be a complete description of its properties and seldom is. The accuracy is similarly context dependent in as much as the purpose of the model is the final arbiter of the accuracy of the model and consequently its suitability. The user of the model need not believe that the model is a true representation of the system, though some knowledge of the limitations of the model are useful *a priori* knowledge in its application. Given that broad agreement seems to exist that the AD process is a non-linear process and is time varying to some extent, which is not quantifiable and is system specific, the search for a suitable model can take a number of philosophical directions. Should the complexity derived from the process non-linearly be considered or not? Would the assumption of Linear Time Invariance (LTI) cause the resulting model to predict poorly, in the context of a specific application? Or, would the search for a suitable model from within a set of LTI structures yield a model with adequate performance? These questions would appear only to be answerable in specific (but hopefully representative) exemplar systems, though their analysis. It is therefore appropriate to attempt to predict the condition (in terms of at least some state variables) of the AD process in various states of excitation, for a laboratory scale fluidised bed AD reactor, as an example process.

Black box modelling

A similar analysis to that presented by Ljung (1987) on black box modelling and identification follows. LTI systems can be represented by Equation 3.3.1.

$$y(t) = G(z^{-1})u(t) + H(z^{-1})e(t)$$
3.3.1

With the added knowledge of the probability distribution function (PDF) of the disturbance $e(t)$, denoted $f_e(.)$, and where $G(z^{-1})$ represents the discrete transfer function to which the input is subject and similarly, the $H(z^{-1})$ represents the discrete transfer function to which the disturbance is subject. Specifying any particular model becomes a matter of specifying the three functions $G(z^{-1})$, $H(z^{-1})$ and $f_e(.)$. Typically, the transfer functions G and H are specified as reasonably low order polynomials in z^{-1} for practical reasons. They may also be defined in state-space representation of finite dimension. The PDF of $e(t)$ is often assumed to be Gaussian and as such, the *expectation* or *mean* value of $e(t)$ and its *variance* are respectively the first and second moments:

$$Ee(t) = \int x f_e(x)dx = 0$$
3.3.2

$$Ee^2(t) = \int x^2 f_e(x)dx = \lambda$$
3.3.3

When the transfer functions G and H have coefficients, which are unknown, they become the object of interest in an *identification* process. We can assemble these *parameters to be identified* into a vector and denote it as θ. Equation 3.3.1 then becomes:

$$y(t) = G(z^{-1}, \theta)u(t) + H(z^{-1}, \theta)e(t)$$
3.3.4

and $e(t)$ is white noise. From this, a one step ahead prediction which does not depend on the PDF can be derived (as has been done by Ljung (1987) which he called the *predictor model*) to give:

$$\hat{y}(t, \theta) = H^{-1}(z^{-1}, \theta)G(z^{-1}, \theta)u(t) + [1 - H^{-1}(z^{-1}, \theta)]y(t)$$
3.3.5

LTI Model Identification is the process of producing a linear mathematical model which is able to predict future values of the data to an arbitrary degree of accuracy. Perhaps the most obvious parameterisation of Equation 3.3.4, is to replace G and H with rational quotients of polynomials where the *parameters to be identified* are the coefficients of these polynomials. These model structures are known as black box models.

A black box approach was adopted in Task 1, because of its simplicity and flexibility. In so doing, an input (U) and Gaussian white noise (e) were mapped through transfer functions $G(z)$ and $H(z)$ and added to give a resulting output (y), as discussed by Ljung (1987) or Soderstrom and Stoica (1989). The structure is shown schematically in Figure 3.3.1 (a)
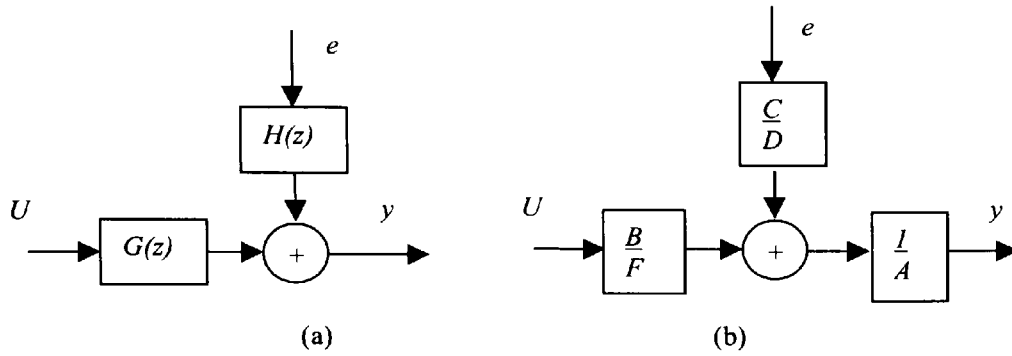
Figure 3.3.1 (a) Black box model structure and (b) General family of model structures.

The black box model can be represented more flexibly as a *General Family of Model Structures* by representing the transfer functions as ratios of polynomials in z^{-1} (which can be considered as the delay operator), as shown in Figure 3.3.1 (b).

The family of models can be written as:

$$A(z^{-1})y(t) = z^{nk}\frac{B(z^{-1})U(t)}{F(z^{-1})} + \frac{C(z^{-1})e(t)}{D(z^{-1})}$$

3.3.6

Where: $A(z^{-1}) = 1 + a_1 z^{-1} + a_2 z^{-2} \dots + a_{na} z^{-na}$, $B(z) = b_1 + b_2 z^{-1} \dots + b_{nb} z^{-nb+1}$ and similarly for $C(z^{-1})$, $D(z^{-1})$ and $F(z^{-1})$, and where z^{-nk} represents a pure delay as a multiple of sample periods. The model structure can be selected to include as many or as few of these black box parameters as is necessary to produce a sufficiently accurate model. Soderstrom and Stoica (1989), Ljung (1987) and Ljung (1993) discuss model structures at length. A synopsis of the types of LTI black box model structures available are shown in Table 3.3.1

Table 3.3.1 Standard LTI black box model structures (after Ljung (1987))

Polynomial used, from Equation 3.3.6	Model Structure
B	Finite Impulse Response (FIR)
AB	Auto Regressive with Exogenous input (ARX)
ABC	Auto Regressive with Moving Average and Exogenous input (ARMAX)
AC	Auto Regressive with Moving Average (ARMA)
ABD	Auto Regressive with Auto Regressive Exogenous input (ARARX)
$ABCD$	Auto Regressive with Auto Regressive Moving Average Exogenous input (ARARMAX)
BF	Output Error (OE)
$BFCD$	Box-Jenkins (BJ)

These models (Equation 3.3.6), if they could predict digester behaviour sufficiently accurately, could be used in process control. Although the process is generally considered to be non-linear, it could possibly be represented by a recursively parameterised linear model, where the model adapts rapidly enough to represent the process at differing conditions and times in its operating life. Simple linear black box models of low order are investigated here, (without recursion) and predicting over a limited horizon, relying on current and recent data values to refine the prediction.

After considering several of the structures presented in Table 3.3.1, black box ARX Single Input, Single Output (SISO) models were adopted and identified for gas production rate, % CO_2, bicarbonate alkalinity and Total Organic Carbon. This was done using on-line data from the fluidised bed reactor described in Section 3.1, which was subjected to varying organic load. More complex model structures were able to reduce the sum of squared errors when tested against validation data, however the added complexity of the model was not justified by the improvement in forecasting. The model structure reduced to:

$$A(z^{-1})y(t) = B(z^{-1})U(t - nk) + e(t) \qquad\qquad 3.3.7$$

in which $(t-nk)$ represents the number of samples by which the input was retarded, or most generally:

$$\hat{y}(t) = \hat{f}(U(t)) \qquad\qquad 3.3.8$$

where:

$\hat{y}(t)$ Represents the model prediction,

$U(t)$ Represents the regression vector of current and past inputs, outputs and additive pre-filtered noise,

$\hat{f}(.)$ Is some function of $U(t)$

Parameter estimation of the linear ARX models followed a standard minimisation of the Sum Squared Errors approach (Wellstead and Zarrop (1991)). In the absence of noise, the model could be determined directly from linear algebra from very few data points, in a relatively trivial manner. In the ARX structures, it is assumed that the noise, which is always in evidence in experimental data (to a varying degree), is equivalent to pre-filtered white noise where the poles of the filter are identical to those of the resulting ARX model. Practically, this means that iteration may be necessary to ensure that deviation from this assumption does not have a deleterious effect on the model predictions. Again because of the noise we are forced to use an overly determined data set, and to solve using the least square approach.

The Linear SISO ARX Model

$$\hat{y}(t) +y(t)(a_1z^{-1} +a_2z^{-2} +........ a_{na}z^{-na}) = U(t-nk)(b_1 +b_2z^{-1} +...b_{nb}z^{(-nb+1)}) +e(t) \qquad 3.3.9$$

Where:

$a_1, a_2, ...a_{na}$ and $b_1, b_2, ...b_{nb}$ are constant coefficients which form the *parameters to be identified*

$\hat{y}(t)$ is the one-step-ahead prediction of $y(t)$ the actual output.

z^{-1} represents the delay operator.

$U(t)$ is the input

$e(t)$ is the additive noise

nk number of delayed samples (minimum $=1$)

na length of the output regression vector

nb length of the input regression vector $+1$

Data sets for the parameterisation and validation of black box models

Model predictions looked ahead one sample step i.e. 30 minutes. The experiments reported here were performed over an 8-week period during which the fluidised bed reactor was run continually. Data used in parameter estimation for the modelling of %CO_2, BA and gas responses, were separated by one month from the model validation data and for modelling TOC model the data were separated by two months. Changes in organic loading rate (Bv) were brought about with minimal changes in hydraulic retention time by adjusting the feed pump flow delivering the concentrated feed to the reactor. The pump delivering dilution water remained at a fixed rate as described in Section 3.1. The feed pump voltage was directly related to the flow and hence Bv. Table 3.3.2 shows the experiments used for parameter estimation and validation of the predictive models.

Table 3.3.2 Experiments used for parameter estimation and validation of models

Expt.No.	Min. Bv [gCOD.l^{-1}.d]	Max. Bv [gCOD.l^{-1}.d]	Description
1	26.5	70.2	Series of step changes in Bv of varying amplitude and duration; black box parameter estimation for BA, %CO_2 and gas production rate models
2	17.8	38.6	Series of step changes in Bv of varying duration; black box parameter estimation for TOC model; validation of the models of BA, CO_2, and gas production rate
3	16.1	69.9	Two step changes in Bv of similar duration and amplitude; validation of TOC model
4	17.6	75.0	Single step change in Bv (8.8h duration); validation of the models of BA, CO_2, and gas production rate

3.3.2 A COMPARISON OF THE ABILITY OF BLACK BOX AND NEURAL NETWORK MODELS OF ARX STRUCTURE, TO REPRESENT A FLUIDISED BED ANAEROBIC DIGESTION PROCESS (TASK 2)

Linear black box models described so far are all LTI and independent in so far as the coupling between say BA and %CO_2, or any other couplings are not considered. The question arises as to whether considering such couplings would improve the predictions of the model. Furthermore, the LTI approach does not attempt to represent the underlying non-linearity of the process and an intrinsically non-linear approach such as neural network modelling (given sufficient non-linear activation functions), would tend to do this.

Using the data collected from the fluidised bed reactor system, three different black box models were parameterised and validated so that their performance could be compared. The three models were all based on the ARX (auto regressive with exogenous input) structure, and were:

1. linear SISO model,

2. linear Multi-Input, Multi-Output (MIMO) model and

3. non-linear neural network based model.

The linear independent SISO, ARX model is that described above in Section 3.3.1, and the basic structure remains the same as Equation 3.3.8, repeated here for convenience:

$$\hat{y}(t) = \hat{f}(U(t)) \qquad\qquad 3.3.8$$

In the case of linear black box models, this function $\hat{f}(.)$ consists of linear polynomial quotients. In the multivariable case (MIMO), Equation 3.3.8 represents a matrix equation with definable cross coupling between the data sets. The model parameterisation follows the same procedure for both the SISO and MIMO linear structures as described in 3.3.1. For the case of the non-linear connectionist (or neural network) model, the function is a neural network of Multi-layer Perceptron architecture with a single hidden layer of non-linear squashing activation function neurones and a linear output layer, (Norgaard (1995)).

The Linear ARX Models

The Linear SISO ARX Model—This is of the form:

$$\hat{y}(t) + y(t)(a_1 z^{-1} + a_2 z^{-2} + \ldots\ldots a_{na} z^{-na}) = U(t-nk)(b_1 + b_2 z^{-1} + \ldots b_{nb} z^{(-nb+1)}) + e(t) \qquad 3.3.9$$

The Linear MIMO ARX Model—Similarly, the MIMO ARX model is of the form:

$$A(z^{-1})y(t) = B(z^{-1})U(t) + e(t) \qquad 3.3.10$$

where:

$$A(z^{-1}) = I_{ny} + A_1 z^{-1} + \ldots + A_{na} z^{-na}$$
$$B(z^{-1}) = B_0 + B_1 z^{-1} + \ldots + B_{nb} z^{-nb}$$

As detailed in Ljung (1993)), the parameter vector is determined in a similar way to the SISO ARX, with the difference that the parameter vector $\theta = [A_1, \ldots, A_{na}, B_1, \ldots, B_{nb}]$, consists of matrices (bold type). θ will include parameters which cross couple the data streams, such that the effect of past values of % CO_2 for example can be made to have an effect on the prediction of bicarbonate alkalinity and gas production rate.

The Non-linear Neural Network ARX Model

This model is after Norgaard (1995)

$$\hat{y}_i(w, W) = F_i\left(\sum_{j=1}^{q} W_{ij} f_j\left(\sum_{l=1}^{m} w_{jl} \zeta_l + w_{j0} \right) + W_{i0} \right) \qquad 3.3.11$$

Where:

$\hat{y}_i(w, W)$ is the prediction of the model as a function of network weights.

F_j is the output layer activation function, which is linear in this thesis.

W_{ij} are the weights through which the hidden layer is connected to the output layer. W_{i0} acts as a bias.

f_j is the hidden layer activation function, which is a tanh function in this paper.

w_{jl} are the weights through which ζ_l is connected to f_j. therefore w_{j0} acts as a bias.

ζ_l represents the feature vector of length m, presented to the input of a feed forward Neural Network.

Training and validation data

The data used in parameter estimation (and training) is described by Premier *et al.* (1997)) and is shown in Figure 3.3.2. The data are normalised by subtracting their mean and dividing by their standard deviation (by using the M-File bishnorm.m in Appendix A), according to

$$Data_i^{norm} = \frac{Data_i - \overline{Data}}{DataSD}.$$ Where *Data* is the data vector with each element i being normalised to give the vector $Data_i^{norm}$. However the ranges of the absolute values of the data are shown in Table 3.3.3. The normalised data can be returned to its original state by applying the inverse procedure.

The same data gathered from these experiments were used to determine the linear model parameters and the neural network model weights. Model validation was performed using the same validation data set (Figure 3.3.3) in all cases.
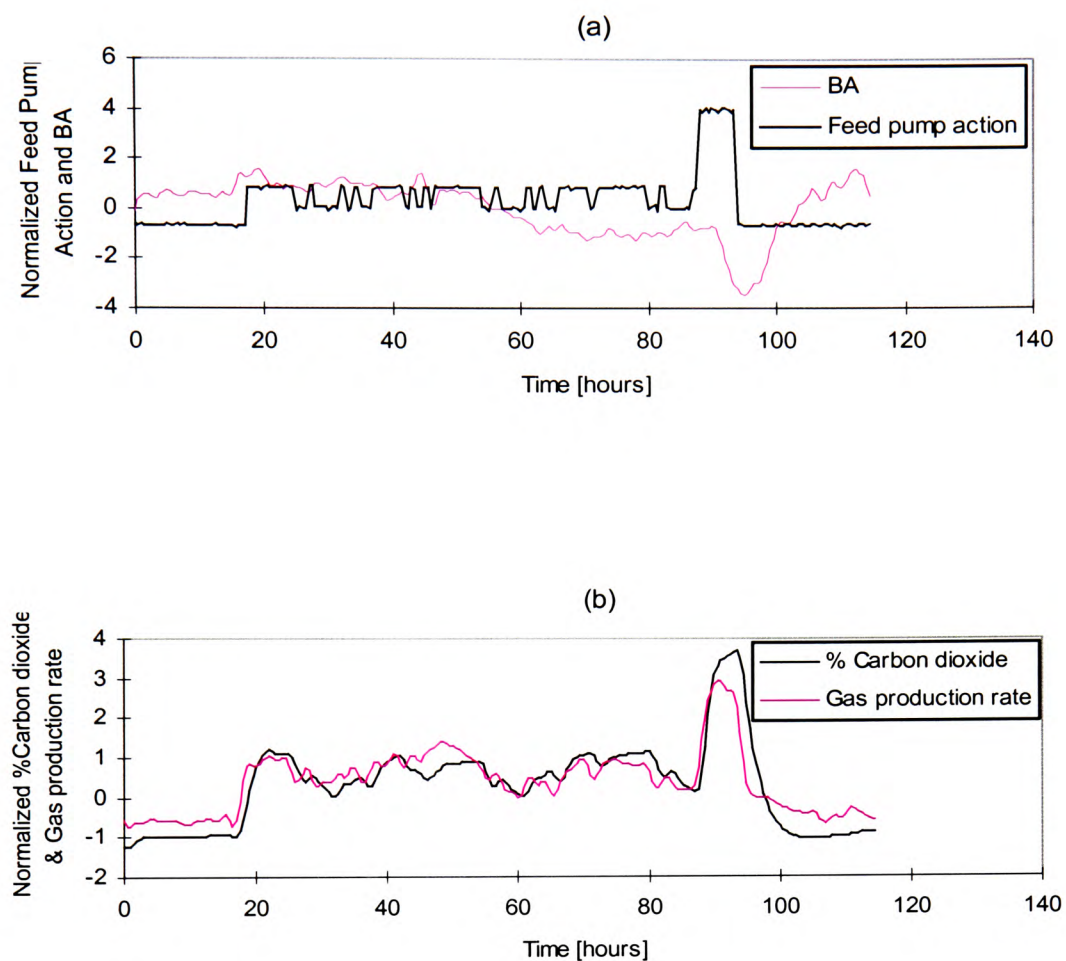
Figure 3.3.2. Data used in Parameter Estimation and Neural Network Training for System Identification

(a) Normalised Feed Pump Control Voltage and Bicarbonate Alkalinity. (b) Normalised % CO_2 and Gas Production Rate.
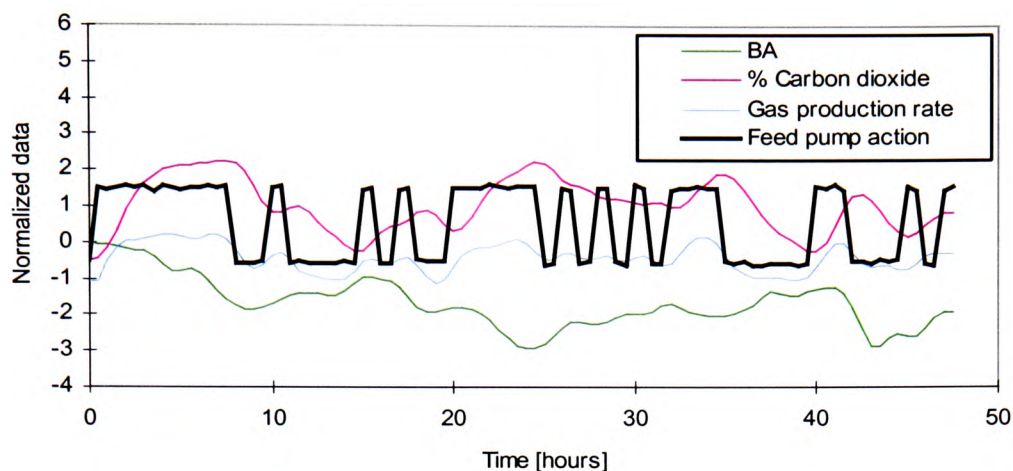
Figure 3.3.3. Normalised Bicarbonate Alkalinity, %CO₂, Gas Production Rate and Feed Pump Data used in the Validation of the ARX Models for System Identification.

Table 3.3.3. Maximum and minimum true values of parameter estimation and validation data.

Data series	Maximum	Minimum
Parameter estimation data		
Feed pump (volts)	2.5	1.6
Bicarbonate alkalinity (g.l^{-1})	1.8	1.3
%CO$_2$	60	32
Gas production rate (ml.min^{-1})	80	40
Validation data		
Feed pump (volts)	1.5	0.7
Bicarbonate alkalinity (g.l^{-1})	1.7	1.38
%CO$_2$	52	33
Gas production rate (ml.min^{-1})	39	19

System identification procedure

Having determined appropriate data sets for the training and validation, all the selected models were trained and validated with the same data sets, to allow a basis for comparison. The number of previous samples in the regression vectors for inputs and outputs (lag space) was determined using a function implemented by Norgaard attributed to He and Asada (1993)). This confirms a heuristic approach taken in Premier *et al.* (1997)) on the basis of observation of the data time series. A MatLAB™ function (*LIPSCHIT*) implemented by Norgaard, determines an index which is high when the regression space is insufficient and becomes constant at a lower value when

increasing the lag space has no further significant effect on accuracy in representing the data. The number of regressors effectively defines the model structure for the SISO linear ARX model. The MIMO linear ARX model however, still requires a decision as to the cross coupling between a particular output prediction ($\%CO_2$ for example) and previous samples of the other time series (BA and gas production rate in this example). In all cases, second order polynomials (in the delay operator) were used. In the case of the neural network model, the training algorithm was based on the Levenberg-Marquadt non-linear least squares technique, while the remaining models were parameterised using a linear least squares approach, as implemented by Ljung (1993)).

3.3.3 The implementation of a deterministic model capable of representing appropriate control parameters in an anaerobic digester (Task 3)

The parameterisation of the MRAC control system developed in Section 3.4 is reliant on the use of a representative model of the AD process, so that by means of optimisation and simulation (at worst, using an heuristic approach), the parameters may be determined. The models considered above in Sections 3.3.1 and 3.3.2 turned out not to be sufficiently representative over long (virtually infinite) prediction horizons, as is required in controller design. It became necessary therefore, to use a deterministic model which had parameters based on the underlying physical/chemical/biological processes found in the AD process. A large quantity of literature is available on the subject of AD modelling, with numerous variations on trophic groupings and their associated kinetics and interrelationships, some of which have been discussed in Chapter 2.0. The model, which was to be used, must have a useful and representative description of the parameters used in the control of the process. In particular, BA should be considered, as this was to be the measured variable in the SISO control system investigated in this work. Models such as that of Costello *et al.* (1991a), which includes verification in Costello *et al.* (1991b), would be appropriate, had it not included unnecessary details and omitted others.

Verification of modelling techniques and application software

As a starting point and as a means of verifying the modelling tools and techniques adopted, the model used in the work of Alcaraz-González *et al.* (1999), was described in MatLAB™ using the Cauchy and Simulink™ representations. Sufficient data was available to verify the coding, by comparing it to the simulations produced by Alcaraz-González *et al.* (1999) model (although initial conditions were not available). BA in this model was considered dynamically, only in so far as the hydraulic characteristics of the system were concerned. The correlation between the published simulations and those carried out by the author was good and afforded considerable

confidence in the modelling technique. The Simulink™ mdl-File description of the model allowed its easy inclusion with control strategies, and allowed the full functionality of this application to be made available. Appendix A contains the M-File narbonne.m used to verify the Cauchy methodology and includes the assumed initial conditions. This file calls the model admodel_1.m which is essentially that from Alcaraz-González *et al.*, which was taken in turn from Bernard *et al.* (1998). This model was then implemented as a Simulink™ model (narbonne_model.mdl) and is included in Appendix A.

Lumped parameter deterministic model for controller design

A model was developed by the University of Florence as part of an EC funded project "Integrated Process Control for Carbon and Nitrogen Removal by Wastewater Treatment Plants", in which the University of Glamorgan was a partner institution. The model was later published by Marsili-Libelli and Beni (1996), in which data generated by the fluidised bed reactor described in Section 3.2 was used to parameterise the model. The model included an ionic equilibrium treatment of the $BA/VFA/CO_2$ system and as such was a suitable model for the design of the control system based on BA as a measured variable. Two interim reports written during the execution of the EC project (Marsili-Libelli and Beni (1993a); Marsili-Libelli and Beni (1993b)), which develop the model are somewhat different to the model published by Marsili-Libelli and Beni (1996). The model which was used is detailed below.

The model was developed on the following basis:

Hydraulic characteristics

The Hydraulic characteristics of the reactor were approximated by a CSTR configuration, although the reactor was in fact the fluidised bed reactor presented in Section 3.1, (Marsili-Libelli and Beni (1996) describe the reactor as an anaerobic filter with recycle). The need to develop a new model stemmed from the lack of a model in the literature, which would be suitable to represent the BA monitor developed by Guwy *et al.* (1994). The BA was to be modelled with a view to employing it to detect the onset of overload and to develop a local on-line regulator, which would determine the required dosing of BA to the reactor.

Acidogens

The rate of change of the concentration of acidogenic bacteria is related to the instantaneous concentration of the same, the substrate available to these bacteria and their endogenous decay. The retention of the bacteria will also affect their growth or otherwise.

$$\frac{dX_a}{dt} = \mu_a X_a - (k_{da} + \delta \frac{F}{V})X_a$$

3.3.12

Where $\quad \mu_a = \frac{\mu_{a\,max} S}{K_{sa} + S} \cdot \frac{S_{in} + K_{sa}}{S_{in}}$

3.3.13

kd_a endogenous decay term

δ a factor to take account of the solids retention time

The first term of Equation 3.3.12 is the classical Monod substrate limited growth kinetics, with a multiplying term, to make the half velocity constant (K_{sa}), have proportionality to the incoming substrate. The second term includes the endogenous growth and a term, which takes account of the retention of biomass, in a sense deviating from the CSTR assumption (that solids and hydraulic retention times are the same), by the factor δ.

Methanogens

$$\frac{dX_m}{dt} = \mu_m X_m - (\delta \frac{F}{V} + k_{dm})X_m$$

3.3.14

Where $\quad \mu_m = \frac{\mu_{m\,max}}{1 + \frac{K_{sm}}{HAc} + \frac{HAc}{K_{im}}}$

3.3.15

In this case, Haldane kinetics are used, which differ from the Monod kinetics by including an inhibition factor K_{im} where increasing the VFA's beyond a certain level causes the inhibition term to become more dominant, effectively reducing the population of methanogens compared to an uninhibited dynamic. The substrate for this group of bacteria (recalling that the model assumes only two populations, lumping all methanogens into the acetoclastic methanogenic grouping and ignoring the hydrogenotrophic methanogens), is in the undissociated part of the acetic acid (HAc and not CH_3COO^-). Rozzi *et al.* (1997) noted that acetoclastic methanogens are the most important as about 70% of the converted COD mass flow is routed through acetic acid. Acetic acid (V_a) is assumed by the model to be the only product of the acidogens. Again, endogenous growth and retention of the bacteria also affect their rate of concentration growth.

Volatile fatty acids

The conversion of the feed to volatile acids is simplified in this model, to include only acetic acid. The higher molecular weight acids, though they would be produced, are assumed to be acetic acid. For the model to take these (butyric, propionic, lactic etc. acids), into account, each would need to be described by a differential equation, and have a bacterial population associated with it, thus

increasing the number of parameters and model complexity, probably without significant advantage. The concentration of acetic acid (V_a) is dependent on its presence in the influx, its production by the acidogenic bacteria and its consumption by the methanogens to grow, or to yield biogas.

$$\frac{dV_a}{dt} = \frac{F}{V}(V_{ain} - V_a) + \mu_a X_a y_{vfa} - \mu_m X_m (\frac{1}{y_{sm}} + y_{co2m} + y_{ch4})$$

3.3.16

The undissociated acetic acid can be determined from the total acid concentration as follows:

$$HAc = V_a \left(1 + \frac{K_a}{[H^+]}\right)^{-1}$$

3.3.17

Where K_a is the dissociation constant of acetic acid.

Organic substrate

The organic substrate available for use would normally be a complex combination of soluble and particulate biodegradable material. This model assumes that hydrolysis is not limiting, or in fact that all the carbonaceous material is soluble and available for metabolism by the acidogenic bacteria. The first term in Equation 3.3.18 considers the hydraulic behaviour of the system in the usual way, while the second term considers the consumption of substrate by the acidogens to grow or to produce acetic acid and CO_2.

$$\frac{dS}{dt} = \frac{F}{V}(S_{in} - S) - \mu_a X_a (\frac{1}{y_{sa}} + y_{vfa} + y_{co2a})$$

3.3.18

Carbon dioxide dynamics

The first term of Equation 3.3.19 describes the loss of CO_2 from the system by way of the biogas. Carbon dioxide is generated by both bacterial groups, depending on the usual Monod and Haldane kinetics and is considered in the second and third terms. The final term considers the gas transfer between the gas and liquid phases according to Henry's law, and depends on the partial pressure of CO_2 in the system.

$$\frac{dC}{dt} = -\frac{F}{V}C + \mu_a X_a y_{co2a} + \mu_m X_m y_{co2m} + K_{l^a}(K_h P_{CO2} - C)$$

3.3.19

Partial pressure of carbon dioxide

The solubility of CO_2 in water (the main constituent of the effluent), is significant and cannot be ignored as it will affect the acid/alkali equilibrium of the reactor. The CO_2 partial pressure and Henry's law govern its concentration in the liquid phase, and the rate at which it is transferred into the gas phase is governed by the CO_2 mass transfer coefficient $(K_l a)$. The bracketed term which

includes S_v (Avogadro's number), determines the proportion of CO_2 in the gas phase. The second term in Equation 3.3.20 quantifies the CO_2 lost from the reactor system through the outflow of biogas.

$$\frac{dP_{co2}}{dt} = -P_t\left(\frac{S_vV}{C_{co2}V_g}\right)K_1a(K_hP_{co2}-C)-\left(\frac{Q}{V_g}\right)P_{co2}$$

<div align="right">3.3.20</div>

Production of carbon dioxide gas

As in Equation 3.3.20 the production of CO_2 (Equation 3.3.21) and similarly CH_4 in Equation 3.3.22 are governed by partial pressure and mass transfer considerations.

$$Q_{co2}=-\left(\frac{S_vV}{C_{co2}}\right)K_1a(K_hP_{co2}-C)$$

<div align="right">3.3.21</div>

Production of methane gas

Methane is considerably less soluble in the liquid phase than is carbon dioxide and the mass transfer rate is assumed to be irrelevant, although its production rate by the methanogenic bacteria must be considered, as can be seen by the inclusion of the Haldane kinetics through μ_m.

$$Q_{ch4}=\left(\frac{S_vV}{C_{ch4}}\right)\mu_mX_my_{ch4}$$

<div align="right">3.3.22</div>

Bicarbonate input

The bicarbonate supplied to the reactor through the feed is subject to the same transport dynamics, so that its concentration in the reactor is defined by Equation 3.3.23.

$$\frac{dB}{dt}=\frac{F}{V}(B_{in}-B)$$

<div align="right">3.3.23</div>

pH and alkalinity

The pH and alkalinity depend on the ionic distribution in the liquid phase which are assumed to balance and which also depends on the CO_2 equilibrium between the gas and liquid phases. Knowledge of the instantaneous $[H^+]$ ion concentration will determine the pH and the alkalinity expressed as sodium bicarbonate molarity will be determined from the $[HCO_3^-]$ ion concentration. The algorithm is developed fully in Marsili-Libelli and Beni (1996), but is considered here in the interests of understanding.

The distribution of CO_2 between the liquid and gas phases is in accordance with Henry's law $K_h = CO_{2(aq)}/CO_{2(g)}$. When in the liquid phase, CO_2 forms carbonic acid, which dissociates (dissociation constant for CO_2 is K_{co2}), in accordance with the equilibrium Equation 3.3.24.

$$K_{co2} = \frac{[H^+][HCO_3^-]}{H_2CO_3} = 4.5 \times 10^{-7} \qquad 3.3.24$$

So that from Henry's law, $[H_2CO_3] = K_h CO_{2(g)}$

Partial dissociation of $CO_{2(g)}$ requires that an ionic balance exists, yielding Equation 3.3.25.

$$[H_2CO_3] = [HCO_3^-] + \frac{[H^+][HCO_3^-]}{K_{co2}} = [HCO_3^-]\left(\frac{[H^+]}{K_{co2}} + 1\right) \qquad 3.3.25$$

If all the $[H^+]$ ions come from the carbonic acid, then electrical equilibrium would mean that $[H^+] = [HCO_3^-]$, then by substituting and by rearranging Equation 3.3.25, it would give:

$$[H^+]^2 + K_{co2}[H^+] - K_h K_{co2} CO_{2(g)} = 0 \qquad 3.3.26$$

If we assume that the entire BA is derived from H_2CO_3, then the middle term of Equation 3.3.26 is eliminated giving:

$$[H^+]^2 = K_h K_{co2} CO_{2(g)} \qquad 3.3.27$$

Which is used throughout the modelling of pH and BA in Marsili-Libelli and Beni (1996), who incrementally proceed to model the inclusion of a weak acid such as acetic acid (CH_3COOH), the effect of CO_2 partial pressure and other ionic species.

The dissociation of the weak acid HA is governed by Equation 3.3.28.

$$K_a = \frac{[H^+][A^-]}{HA} \qquad 3.3.28$$

and similarly the ion product of water:

$$K_w = [H^+][OH^-] = 10^{-14} \qquad 3.3.29$$

The ion concentrations should balance to give:

$$[H^+] + [Na+]_{bic} + [Na+]_{NaAc} = [A^-]_{HAc+NaAc} + [OH^-] + [HCO_3^-] \qquad 3.3.30$$

Where the suffices bic refers to sodium bicarbonate and $NaAc$ and HAc refer to sodium acetate and acetic acid respectively. Equation 3.3.30 can be written:

$$[A^-]_{HAc+NaAc} = [H^+] + [Na+]_{bic} + [Na+]_{NaAc} - [OH^-] - [HCO_3^-] \qquad 3.3.31$$

and from Equation 3.3.29

$$[OH^-] = \frac{K_w}{[H^+]}$$

3.3.32

also from Equation 3.3.24

$$[HCO_3^-] = \frac{K_{co2}K_hCO_{2(g)}}{[H^+]}$$

3.3.33

The total acid HA_o becomes the sum of the CH_3COOH and others acetic species (sodium acetate (and sodium hydroxide).

$$[HA_0] = \frac{[H^+][A^-]_{Hc+NaAc}}{K_a} + [A^-]_{Hc+NaAc}$$

3.3.34

Combining Equations 3.3.31 to 3.3.34

$$[H^+]^3 + A1[H^+]^2 + A2[H^+] + A3 = 0$$

3.3.35

where:

$$A1 = (K_a + [Na^+]_{bic} + [Na^+]_{NaAc})$$

$$A2 = (-K_a([HAc^o] - [Na^+]_{bic} - [Na^+]_{NaAc}) - K_w - \alpha)$$

$$A3 = -K_a(K_w + \alpha)$$

and

$$\alpha = K_{co2}K_hCO_{2(g)}$$

Equation 3.3.35 was encoded in a MatLAB™ M-File which was based on the work of Marsili-Libelli and Beni (1993a) and which determines the pH and [HCO$_3$] (bicarbonate alkalinity). The function was embedded in a Simulink™ 'MATLAB Function' block, and the function is included in Appendix A as pH_BA.m.
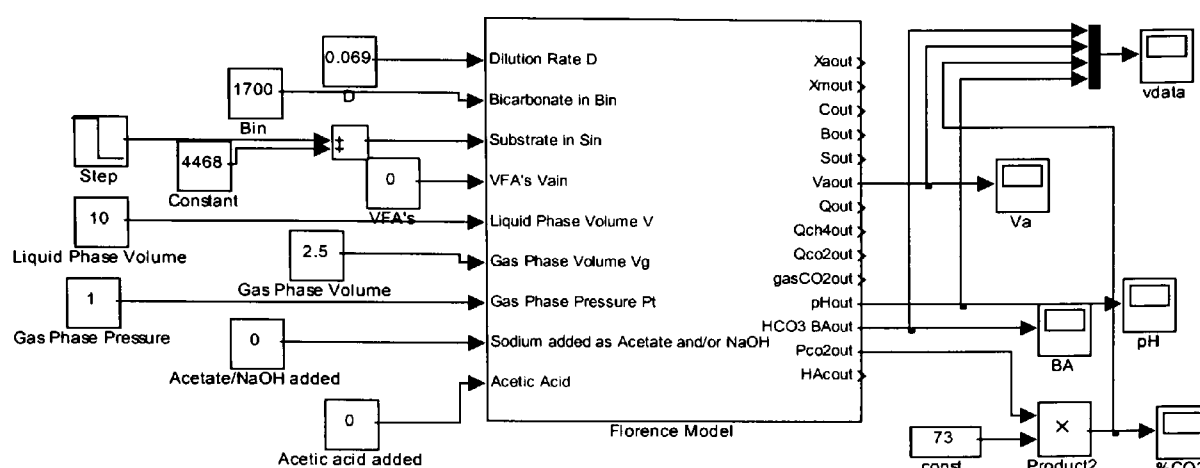
Figure 3.3.4 Simulink™ block representation (top level) of a two-population lumped-parameter AD model showing inputs to and outputs from the block (for verification purposes).

The complete two-population lumped parameter model of the AD Process, including a model of BA was constructed in Simulink™, and Figure 3.3.4 shows the top level of the model with all available input (with arbitrary signals connected) and output connections as listed in Table 3.3.4 (after Marsili-Libelli and Beni (1996)). The two-population model is included in Appendix A and has the filename florence_model_verification.mdl.

Table 3.3.4 List of input and output parameters

Parameter	Symbol [units]	Input-I Output-O
Dilution rate	D [m^3.d^{-1}.m^{-3}=d^{-1}]	I
Sodium bicarbonate NaHCO$_3$	B_{in} [mgCaCO$_3$.l^{-1}]	I
Organic substrate	S_{in} [mgCOD.l^{-1}]	I
Volatile fatty acids supplied	Va_{in} [mg.l^{-1}]	I
Liquid phase volume	V [m^3]	I
Gas phase volume	Vg [m^3]	I
Acetic acid added	$Acetic\ Acid$ [mg.l^{-1}]	I
Sodium acetate or Sodium hydroxide (NaOH) added	HAc [mg.l^{-1}]	I
Acidogenic bacteria	Xa [mg.l^{-1}]	O
Methanogenic bacteria	Xm [mg.l^{-1}]	O
Inorganic carbon	C [mg.l^{-1}]	O
Bicarbonate (considering transport dynamics)	B [mgCaCO$_3$.l^{-1}]	O
Substrate in effluent	S [mgCOD.l^{-1}]	O
VFA's in effluent	Va [mg.l^{-1}]	O
Gas production rate	Q [ml.min^{-1}]	O
Methane production rate	$Qch4$ [ml.min^{-1}]	O
CO$_2$ production rate	$Qco2$ [ml.min^{-1}]	O
CO$_2$ Volume produced	$gasCO2$ [ml]	O
pH	pH	O
Bicarbonate alkalinity	BA [mgCaCO$_3$.l^{-1}]	O
CO$_2$ partial pressure	$Pco2$ [atmos]	O

The model inputs

The dilution rate $D=F/V$, is a quotient of the flow rate to the reactor (F [m^3.d^{-1}]), and the volume of the liquid phase, into which it is diluted (V [m^3]). The Sodium Bicarbonate (B_{in}) input to the system is assumed to enter through the feed tank (which includes the transportation dynamics of the hydraulic regime). Similarly, the substrate feed (Sin) is assumed to enter via a feed tank and the model supplies the possibility to take account of pre-acidification in this storage tank, by applying an extra supply of VFAs as an input (called Va_{in} in the model). The liquid and gas phase volumes (V and Vg respectively), define the reactor size and the hydraulic regime as a consequence. The only supplement to this is the parameter δ in Equation 3.3.12, which is able to give a mechanism by which account can be take of retained solids for durations that exceed the HRT. The model is also able to simulate shock loading (spiked directly into the reactor without considering the transportation dynamics) from acetic acid and sodium acetate and/or sodium hydroxide.

The model outputs

The outputs allow key process parameters to be monitored during simulation. These include the concentrations of acidogens and methanogens, which are assumed to be the only two trophic groups. Substrates in the form of primary organic feed (S) and possibly acetic acid (*acetic acid*), as well as secondary product from the acidogens (Va, assumed to be totally acetic acid), can be

monitored. Of particular importance to this work is the effluent bicarbonate alkalinity (BA) which is the measured variable in the control strategy and pH and gas production parameters, which are of interest in assessing the operation of the system.

Model performance verification

A major problem, acknowledged by Marsili-Libelli and Beni (1996), is that the model is very sensitive to initial conditions. They solved the problem of selecting initial conditions (so that the model could be parameterised), by exploring the steady state performance of the model. As the initial conditions were not published, the only course of action open to the author was to take the initial conditions from the steady state plots and to use the parameter values published in Marsili-Libelli and Beni (1996). The model could be thought of as 'almost' an optimal process as the fluidised bed reactor was working well, at a high loading rate at the time of the data capture (baseline OLR of 9.5 $kg.COD.m^{-3}.d^{-1}$ and overloads reaching 27 $kg.COD.m^{-3}.d^{-1}$). The purpose to which the model would be applied would be to design a control strategy able to take a similar but different reactor (EGSB as opposed to a fluidised bed reactor) from start-up to relatively high loading rate. The expectation was that there would be variations in the model performance, particularly due to time variance. The initial conditions will take account of the differences to some extent, such as the lower populations of active bacteria, though accurately determining the true active biomass concentrations would be almost impossible practically. The activity and acclimatisation of the bacteria are not considered other than through identified parameters such as yield coefficients in the model, nor are populations of bacteria or products other than those presented.

It is also worth considering the time variation, about which little is known as it may involve imponderables such as toxic shocks which have not been detected or perhaps variations in the hydraulic characteristics of the reactor over long time periods, due to silting or channelling perhaps. Also drift in the demography of the bacterial populations through selection or de-selection on the basis of the environment may occur.

Verification of the implemented lumped-parameter model

In order to be satisfied that the model has been replicated, there needed to be a reasonable comparison between the model results published by Marsili-Libelli and Beni (1996) and those obtained by the author. As stated, the initial conditions of the model are not explicit in the paper and for that matter nor are the operating conditions. However the paper does give some information from which to estimate the values. Table 3.3.5 shows the parameter values obtained

from Marsili-Libelli and Beni (1996), as well as others not given in that paper and Table 3.3.6 shows the initial and loading conditions used in the verification simulations.

Table 3.3.5 Model parameter values (after Marsili-Libelli and Beni (1996))

Symbol		Value	Units	Purpose
Kinetic constants				
μ_{amax}	L[a]	0.5033	h^{-1}	Acidogenic bacteria maximum growth rate
K_{sa}	C	238.1±3.7	$mg.l^{-1}$	Acidogenic bacteria half-velocity
k_{da}	C	0.03104±0.000484057	h^{-1}	Acidogenic bacteria decay rate
μ_{mmax}	C	0.00227±9.6834x10^{-6}	h^{-1}	Methanogenic bacteria maximum growth rate
K_{sm}	C	0.01453±0.000226874	$mg.l^{-1}$	Methanogenic bacteria half-velocity
k_{dm}	L	0.0008	h^{-1}	Methanogenic bacteria decay rate
K_{im}	C	35.47±0.4923	$mg.l^{-1}$	Methanogenic bacteria inhibition concentration
Yield coefficients				
y_{sa}	L	0.688		Substrate → acidogenic bacteria
y_{vfa}	L	0.427		Substrate → acetic acid
y_{co2a}	C	0.5±0.00704515		Substrate → CO_2
y_{sm}	L	3.2702		Acetic acid → methanogenic bacteria
				(Marsili-Libelli and Beni (1996) writes *acidogenic bacteria* it is believed, in error)
y_{ch4}	L	20.7321		Acetic acid → methane
y_{co2m}	C	5.174±0.4923		Acetic acid → CO_2
Physico-chemical constants and reactor design parameters				
K_w	L	1×10^{-14}		Water dissociation constant
C_{co2}	L	44 000		mole → $mg.l^{-1}$ conversion constant for CO_2
C_{ch4}	L	16 000		mole → $mg.l^{-1}$ conversion constant for CH_4
P_t	E	1	atmos	Total pressure in gas phase
V	E	10	l	Liquid phase volume
V_g	E	2.5	l	Gas phase volume
F	E	0.48	$l. h^{-1}$	Liquid flow rate
δ	E	0.01666		Liquid/solid dilution rate ratio
K_la	C	6.328±0.100045	h^{-1}	CO_2 mass transfer rate coefficient

[a] C=calibrated; E=experimental; L=literature

Parameters and constants required but not included in Marsili-Libelli and Beni (1996)				
Kh	L	1080	atmos/mol fraction	Henry's constant
Kh	L	2100	atmos/mol fraction	Henry's constant – alternative form Tchobanoglous and Burton (1991) used in Figure 3.3.5
Ka	L	1.85e-5		Acetic acid (CH_3COOH) dissociation const.
Kw	L	1e-14		Water dissociation constant
Kc	L	5e-7		H_2CO_3 (bicarbonate) dissociation constant

Table 3.3.6 Initial and loading conditions for model based on Marsili-Libelli and Beni (1996)

D	L[a]	0.069 d^{-1} Dilution rate
Sin	L	Background of 4468 mg $COD.l^{-1}$ with 8 hr initial shock of 12470 mg $COD.l^{-1}$
Xa	ES	1500 mg. l^{-1}
PCO2	L	23×10^{-2} atmos
QCH4	ES	0.7 $l.min^{-1}$
pH	ES	7
BAout	ES	1700 $mgCaCO_3 l^{-1}$
Va	ES	100 mg. l^{-1}
Sodium acetate and/or NaOH added		0
Pt	L	1 atmos (Gas Phase Pressure)
Vg	L	2.5 l (Gas Phase Volume)
BA	ES	1700 $mgCaCO_3 l^{-1}$ (Marsili-Libelli and Beni (1996) show steady state plot against D to be under 800 $mgCaCO_3 l^{-1}$ continually)
Xm	ES	1000 mg. l^{-1}
Qco2	ES	0.2 $l.min^{-1}$
Q	ES	0.9 $l.min^{-1}$ (sum of *Qco2* and *Qch4*)
H+	L	5e-8 in fact equiv. to pH 7.3
C	ES	300 mg. l^{-1}
VFA's		0
Acetic acid added		0

[a] L = Literature; ES = Estimate
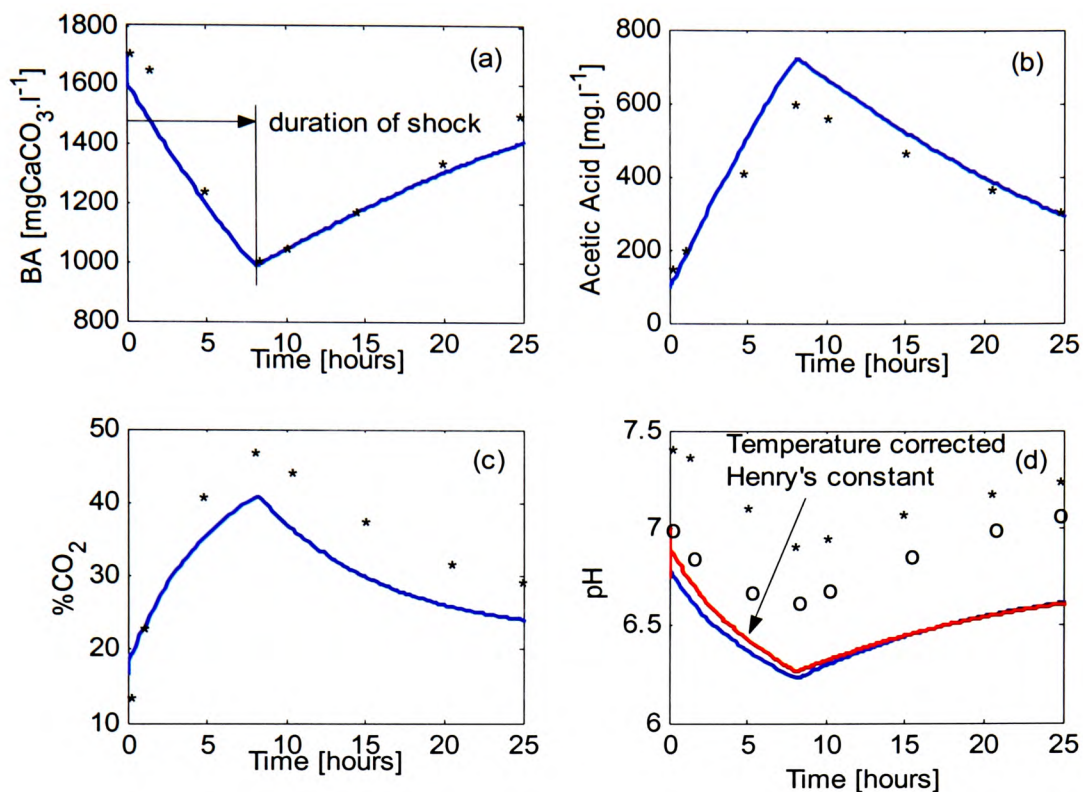
Figure 3.3.5 Verification results of the model derived from Marsili-Libelli and Beni (1996).

Figure 3.3.5 shows the results of the verification simulation using florence_model_verification.mdl, with initial and loading conditions as stated in Table 3.3.6 and parameter values as indicated in Table 3.3.5. The loading conditions represent 'Experiment 2' in the paper of Marsili-Libelli and Beni (1996), for which they plot their model performance for BA, Acetic acid, $\%CO_2$ and pH, as in Figure 3.3.5. The aim of the verification was to show that the model coded by the author was similar to that published by Marsili-Libelli and Beni (1996). This comparison can only be done using the published data and thus is taken directly from the Figure 9 of Marsili-Libelli and Beni (1996), and key values, reproduced as faithfully as possible, (indicated by asterisks '*') have been included in Figure 3.3.5. The validity, in all cases is approximately 5% or better, of the estimated full variation (Figure 3.3.5), which was thought to be sufficiently accurate, given the lack of information regarding initial conditions. With regard to all the parameters, Marsili-Libelli and Beni (1996) noted the sensitivity of their model to these initial conditions but did not publish these values. Furthermore, they did not publish the values they used for dissociation constants (of bicarbonate and acetic acid), or the integration method used. While these may not be expected to yield large discrepancies in the simulation results, it is

possible that, cumulatively, they could account for the differences. It is felt that the pH simulation results of Marsili-Libelli and Beni (1996) were high, and this is supported by comparison to the data against which they were measured in their paper. In comparing the simulation of Figure 3.3.5 (d), with this 'real' data (indicated by 'o'), the model used by the author shows significantly better correlation. The indicated plot in Figure 3.3.5 (d) is a further improvement which was obtained by using temperature corrected values for the Henry's constant of CO_2 from Tchobanoglous and Burton (1991). The important factor is that the model herein is thought to be a reasonable representation of the AD process from which it was parameterised.

3.4 DEVELOPMENT OF A CONTROL STRATEGY

The development of a strategy for the control of the AD process depends greatly on the ambitions of the project. There would be significant differences between control systems which had, for example, markedly different designs of reactor as their focus of attention. The AD process is essentially a multivariate non-linear system when viewed as a lumped parameter model and the definition of its state would require several parameters to be measured or deduced from other measurements. The system could then be treated as a MIMO (multi-input, multi-output), state space process, and appropriate control strategies developed to suit. State space is a matrix representation of the coupled differential equations written in such a manner that a notional 'state' is defined for the system. The practical applications of such systems are rare, other than in industries that have a tradition of high levels of instrumentation. The possibility of a control system finding full-scale application is greatly enhanced by minimising the number of measuring instruments required and increasing the transparency of its functionality. Once more invoking the principle of parsimony, the appeal of SISO (single-input, single-output) control systems is therefore high, provided the performance obtained from the controller is sufficient.

The development that follows was informed by the desire to use a single measuring instrument (or measured variable) and to use this information in situations which might otherwise make the AD process unstable. Furthermore, this should be possible with the minimum prior knowledge of the reactor and its content. The operator would wish to have an instrument, (instrumentation and control system) which could be applied to the process, without the need for extensive modelling or data collection and analysis.

3.4.1 Choosing an available strategy for control

The following is not intended to be an exhaustive view of control strategies, which could have application in the control of AD. This would be a prohibitively large treatise. Instead, it is hoped that the presentation of important adaptive schemes will lead the reader into the techniques used in this study. This section starts by establishing broadly, the requirements which were considered during the development of the control strategy which was eventually employed. It then briefly examines a number of candidate strategies before detailing the development of the strategy used.

Requirements which inform the development of the control strategy

The control strategy was to be developed by simulation and computational techniques, which are considered to be the only viable possibility in view of the slow nature of the process dynamics and the difficulty in operating the process.

The control actions to maintain stable operation of the AD process are somewhat limited. It is possible to:

1. Reduce the organic loading rate (OLR) in response to a tendency of the reactor to sour, which would allow the trophic groups which use VFAs as substrate to reduce VFA levels and convert the heavier species to acetate. The reduced loading will also allow the hydrogen consuming acetogenic bacteria to reduce the dissolved hydrogen to levels, which are not inhibiting to the methanogenic bacteria.

2. Dose the reactor with an alkaline flow, which would increase the buffering capacity against the build up of VFAs, thus stopping those bacteria with pH sensitivity being inhibited in this way.

3. Increase the bacteria available to deal with the excessive products from various shock loadings or stressed operation. This is likely be of little benefit, as the bacteria will need to be farmed specifically for this purpose and may as well be in use continually.

4. Use hydrogen stripping by sparging or other techniques, but this would not increase the metabolism of the methanogens beyond their potential and hence may still allow the VFA build up to progress.

5. Increasing HRT and/or SRT, which is similar in consequence to changing the OLR, however in this case extra time is available for hydrolysis, and the metabolising of VFAs etc.

Of the above control actions, the most appropriate were considered to be the first two. It is conceivable that the ORL can be altered in order to protect the eco-system in the reactor by diverting the remaining waste stream to a buffering tank. Naturally this could not be done indefinitely, but the respite provided may be sufficient to avoid damage to the bacterial consortium. In any event, maintaining the viability of the bacteria would be preferable to restarting with a new inoculate when the reactor totally fails. Maintaining an alkalinity-buffering margin is also a practical proposition, though the cost of adding say, calcium carbonate or sodium bicarbonate may give pause for thought. It was decided that both systems would be considered and appropriate control strategies designed.

As discussed above, the SISO control philosophy was considered to be desirable and BA was selected to be the control variable on the basis of the information content it represents with respect to reactor stability. The BA was measured using the instrument developed by Guwy *et al.* (1994), because of its admirable record on reliability in previous experimental work.

It is normal to define a specification to which the implemented control is expected to conform. In this treatise, the response of the system to disturbances was defined as a target time evolution of the measured variable (BA), which then became an embedded element of the control strategy. The selection of this time response was made heuristically, on the basis of previous experience of the fluidised bed reactor described in Section 3.1, when subjected to overload conditions. The time constants derived from these data were estimated and initially a first order reference model which was thought to be achievable was defined, as shown below in Figure 3.4.1. This proved to be a very tight constraint which led to severe control actions being applied, so the reference model was relaxed to the second order model shown in Figure 3.4.1.
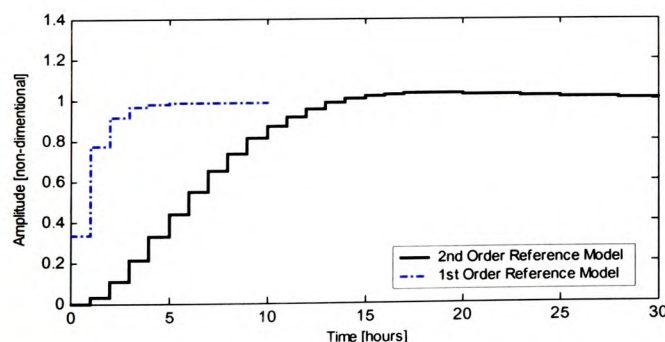
Figure 3.4.1 Reference models for target system performance showing initial first order model and the selected second order model.

The associated transfer functions are:

First order reference model

$$\frac{BA_{ref}}{BA} = \frac{0.33(z+1)}{(z-0.33)}$$

(3.4.1)

Second order reference model

$$\frac{BA_{ref}}{BA} = \frac{0.03059z + 0.02677}{z^2 - 1.613z + 0.6703}$$

(3.4.2)

No further specification was defined beyond defining the reference model, accepting that the reference model was not likely to be achieved accurately, but would form the basis of the motivation to adapt the control and, as such, be used in performance optimisation, which will be discussed in Section 3.4.2. The convergence criteria associated with the optimisation and applied in a least squares sense to the reference model defined the required performance of the control system and can be thought of as the control specification. However the optimisation process was iterative in its execution which implies an iterative and flexible approach to specifying the controller performance. It was felt that this philosophical approach was justified in the interest of trying to achieve the highest performance in the given circumstances.

Adaptive control vs other techniques

The preceding discussions have highlighted the fact that the AD process has non-linear and to some extent time varying dynamics. This may preclude the use of standard linear control techniques because the tuning of such controllers will only be relevant (or optimal) for the operating conditions for which the controller is designed. Should the process characteristics alter with time (or any other parameter), the controller will not be optimally tuned. This may or may not cause the control to fail depending on how far the system has diverged from its original dynamics. In many situations the linear controller will cope with the variance, treating it as disturbances, and perhaps giving acceptable performance. It is also possible that the controller can be re-tuned by human intervention as necessary, though this would seem an undesirable modus operandi.

In the case of AD, the justifications for using a more complicated control strategy are:

- Plant components may degrade or malfunction causing the plant characteristics to change over time. Silting, clogging and other physical processes may be apparent, as is the case in most process plant. Prolonged stress or toxicity in the feed amongst other reasons may cause changes in the kinetic rates of the bacterial groups.

- The plant may be subject to disturbances, which will also be variable over time, such as the composition of the waste stream due to upstream changes such as new industrial processes or sewer system alterations.

- The non-linear characteristics of the anaerobic biological process itself, which may cause changing requirements and responses at differing operating or initial loading conditions.

- Plant modifications can have marked effects on the AD process, even though they may be modest, like the changing of a valve or the alteration of a recirculatory flow. Variations in transport delays can also have a significant effect.

There is significant difficulty in defining adaptive control, as adaption is the process of adjustment to changing circumstances, which is essentially the purpose of normal closed loop control. However, without becoming involved in such semantic debate, it is the intention of the author to consider adaptive control to constitute systems which are able to improve their performance over what would be possible with simple closed loop control. Adaptive control could then be considered a suitable control strategy to address the points listed above. There are arguably three fundamental approaches to adaptive control:

- Gain scheduling control
- Self-tuning control
- Model reference control

Gain scheduling control

Gain scheduling (Åström and Wittenmark (1989)), can be thought of as the piecewise linearization of a process for the purpose of applying a linear control strategy. It is often the case that parameters within a system will vary in response to variations of some other parameter. An example of this is, (and indeed, the original application impetus for gain scheduling control) the variation of aerodynamic properties of the atmosphere with respect to altitude, which is of particular concern to control systems in aircraft. In the case of AD, it would be possible to make an analogue between the aircraft altitude and the reactor temperature, and the forces generated by the aircraft control surfaces and the metabolic rates of the bacterial consortium. There are however more appropriate solutions in the case of AD as the relationship between temperature and metabolism have been determined empirically and are well known. The main benefit in this type of adaption is the speed at which the processing can be performed is very high, which is crucial for systems which experience rapid changes in circumstances (e.g. an aircraft in vertical, supersonic flight). The disadvantage lies in the need to characterise the system at all the operating

conditions, which are likely to be encountered. The gain-scheduling element of the system is in fact an open loop arrangement, with all the intrinsic disadvantages which follow from this.

Self-tuning control strategy

Self-tuning control (Wellstead and Zarrop (1991)), was initially used in the digital control of industrial chemical processes which employed PID controllers. The typical empirical methods for tuning these controllers (e.g. Zeigler-Nichols methods) are often used even in complex plants. However with several hundred individual control loops the effort can become prohibitive, particularly when system changes occur in areas such as dead-time, non-linearities, and variation of plant gain with set-point and load conditions. Furthermore, the economic and environmental imperative to reduce energy consumption has also motivated the use of controllers that can retune automatically to ensure the process is maintained at a high state of efficiency.

The block diagram for a typical self-tuning controller is shown in Figure 3.4.2. The inner loop behaves like a typical feedback control loop, and outside this there is another loop, which acts to optimise the inner loop controller parameters. The 'self-tuner' needs to perform two tasks:

1. It estimates the plant dynamics.
2. It uses this estimate to determine appropriate values for the controller parameters.
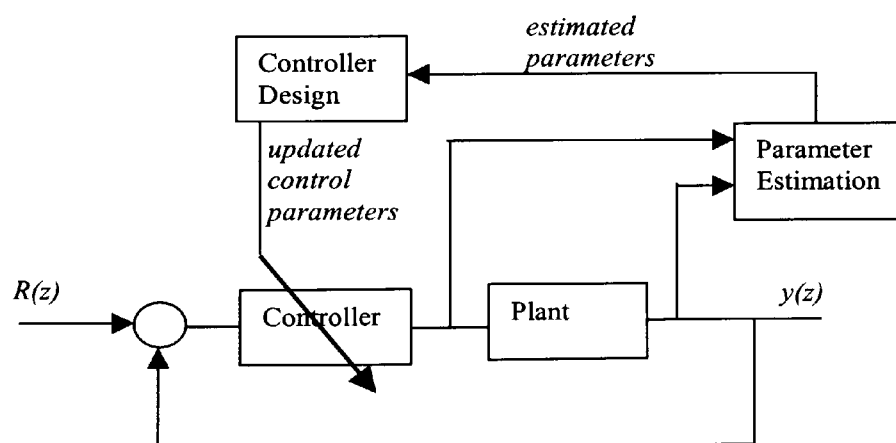
Figure 3.4.2 Block diagram of a typical self-tuning adaptive control system

The parameter estimation is normally conducted on the basis of a known or assumed model structure using normal recursive identification techniques as detailed in for example, Ljung (1987) or Wellstead and Zarrop (1991). The controller design then proceeds in an automated sense using techniques such as pole placement or minimum variance. The self-tuning can and is often done perpetually and at each sample interval, thus maintaining an optimal controller. There is a

requirement of persistent excitation in order that the identification procedure can be relied upon to deliver acceptable estimates of the plant model parameters.

Model reference adaptive control (MRAC) strategy

MRAC relies on the generation of a so called model error (e_m), which is the difference between the process output and the output from a reference model (y_m), where the reference model defines the desired behaviour of the process when under control. If the process output matches the reference model output, there is no model error and perfect control is assumed at that time instant. In the case where a model error exists, an adaption mechanism is used to alter the controller parameters in such a way as to drive the model error to zero. Numerous adaption mechanisms exist, and a discussion of the approach adopted is presented in this section. A stated advantage of this technique is that the primary feedback loop (if indeed one exists), remains intact and if the controller is stable for all allowed controller values, then the system will still be in control even if the adaptive loop fails in some way. However this was not the case in the arrangement that was used which is described below. The fundamental assumption behind the method is that the adaption mechanism can force the system to behave in the manner specified by the reference model.
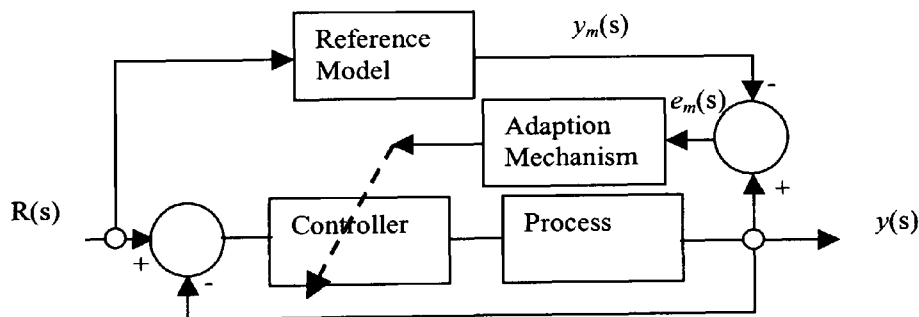
Figure 3.4.3 Typical scheme for Model Reference adaptive Control (MRAC)

Controller architecture and adaption mechanism used for MRAC

The method by which the controller parameter vector (θ) is adjusted is termed the adaption mechanism. The parameter vector can be considered to define an n-dimensional hyperspace with each element representing a dimension, which is plotted in turn against the model error (e_m). The problem then becomes one of minimising the model error with respect to the n parameters, which is essentially an optimisation problem (in which all the methodologies of this discipline could apply). There are several alternative methods of adjusting the parameter vector such that the model error is minimised. The approach taken was a development of the *normalised MIT*

(Massachusetts Institute of Technology) *adaption rule* as discussed by Åström and Wittenmark (1989). It should be noted that the stability of the system is not guaranteed. The original MIT rule is shown in Equation 3.4.3.

$$\frac{d\theta}{dt} = -\gamma e_m \frac{\partial e_m}{\partial \theta} \qquad (3.4.3)$$

where the partial derivatives of model error with respect to the parameter vector are known as the *sensitivity vectors*. The adjustment rate is determined by a constant (γ).

The MIT rule assumes that the controller parameters change more slowly than the system parameters and that to reduce the $(e_m)^2$ in the hyperspace of controller parameters, it would be logical to change the parameters in the direction of negative gradient of e_m. The loss function is defined as:

$$J(\theta) = \frac{1}{2}e_m^2 \qquad (3.4.4)$$

So to reduce J we need to alter the parameters in the direction of negative slope.

$$-\frac{\partial J}{\partial \theta} = -e_m \frac{\partial e_m}{\partial \theta} \,.$$

It can be stated that

$$-\frac{d\theta}{dt} = -\gamma \frac{\partial J}{\partial \theta} = -\gamma e_m \frac{\partial e_m}{\partial \theta} \qquad (3.4.5)$$

The implementation of the adaption rule in Equation 3.4.5, in the typical MRAC arrangement of Figure 3.4.3 is shown in Figure 3.4.4, in what as known as the *error model*.
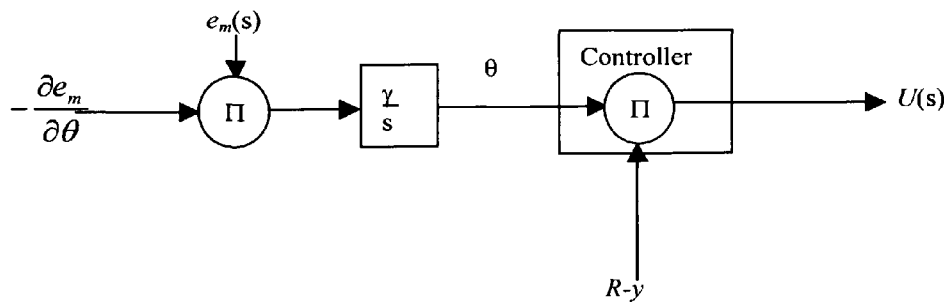
Figure 3.4.4 Schematic representation of the typical MRAC error model with a Proportional controller

Åström and Wittenmark (1989) discussed the application of the MIT rule to a Proportional controller (or feed-forward gain, K) and this is paraphrased for continuity here. Figure 3.4.4 shows the control effort (U) generated from the model error (e_m), but θ in this case is multiplied by the difference between the reference signal and the process output $(R\text{-}y)$ to produce U. It is

possible to arrange the system as shown in Figure 3.4.5, which can be seen to be equivalent to the system shown in Figure 3.4.6
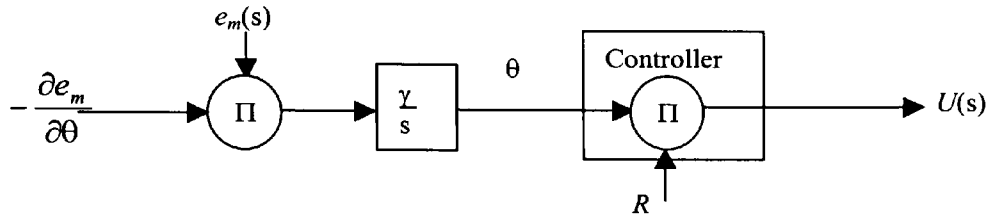
Figure 3.4.5 Schematic representation of an alternative error model for MRAC
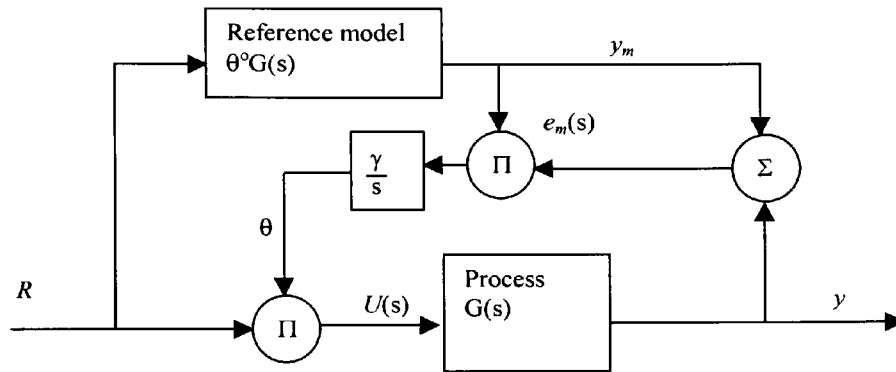
Figure 3.4.6 Block representation of an MRAC adaption of a feed-forward gain based on the MIT rule.

(after *Åström and Wittenmark (1989)*)

Assuming that the process model is known and it is possible to determine the reference model such that θ^o is a constant parameter vector from its structure, the model error is therefore

$$e_m = y - y_m = RKG(s) - \theta^o G(s)R$$

$$e_m = G(s)(K - \theta^o)R$$

Also

$$\frac{\partial e_m}{\partial K} = G(s)R = \frac{y_m}{\theta^o} \qquad (3.4.6)$$

From the MIT rule,

$$\frac{d\theta}{dt} = -\gamma e_m \frac{\partial e_m}{\partial \theta}$$

Which in this particular case gives...

$$\frac{dK}{dt} = -\gamma e_m \frac{\partial e_m}{\partial K}$$

And from equation 3.4.6

$$\frac{dK}{dt} = -\gamma e_m \frac{y_m}{\theta^o}$$

Lumping the constants together in γ...

$$\frac{dK}{dt} = -\gamma e_m y_m \tag{3.4.7}$$

In this implementation of the MIT rule, it is possible for the adaption mechanism to perform adequately at a particular reference signal (R) and be unstable or with adaption being too slow, at another. The adaption rate, in other words, is dependent on the reference signal. In this work the signal has been normalised according to Equation 3.4.8.

$$\frac{d\theta}{dt} = -\gamma \left(\frac{e_m \dfrac{\partial e_m}{\partial \theta}}{\alpha + \left(\dfrac{\partial e_m}{\partial \theta}\right)^T \left(\dfrac{\partial e_m}{\partial \theta}\right)} \right) \tag{3.4.8}$$

where $\alpha > 0$ to avoid division by zero.

From Equation 3.4.6, this reduces to...

$$\frac{d\theta}{dt} = -\gamma \left(\frac{e_m y_m}{\alpha + y_m^2} \right) \tag{3.4.9}$$

The need for normalisation of the MIT adaption mechanism

To illustrate the possibility of instability, a discretised system has been created in MatLAB/Simulink™, showing the system without normalisation (Figure 3.4.7 and Appendix A – mitdig.mdl) and with normalisation (Figure 3.4.8 and Appendix A – modmit.mdl). The reference signal is a square wave of unit amplitude initially and the time evolution of the output is shown in Figure 3.4.9, and a reference input of five times this to demonstrate the onset of instability, shown in Figure 3.4.10. Finally, Figure 3.4.11 shows the system response where $R=5$ and when normalised MIT rule is used.
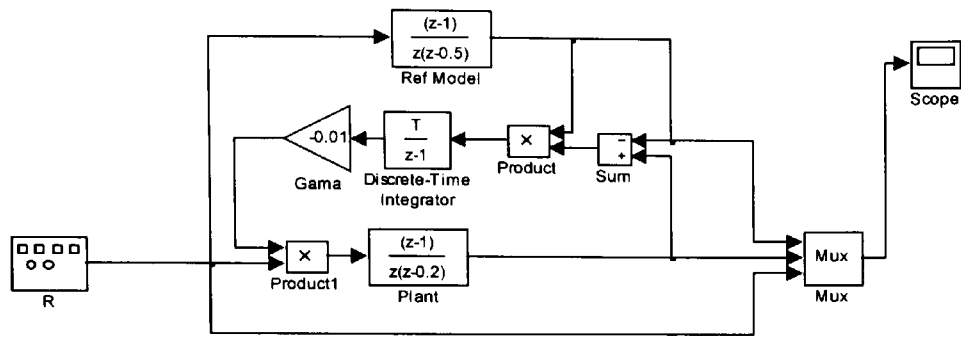
Figure 3.4.7 Illustrative system without normalisation (Simulink™ model)
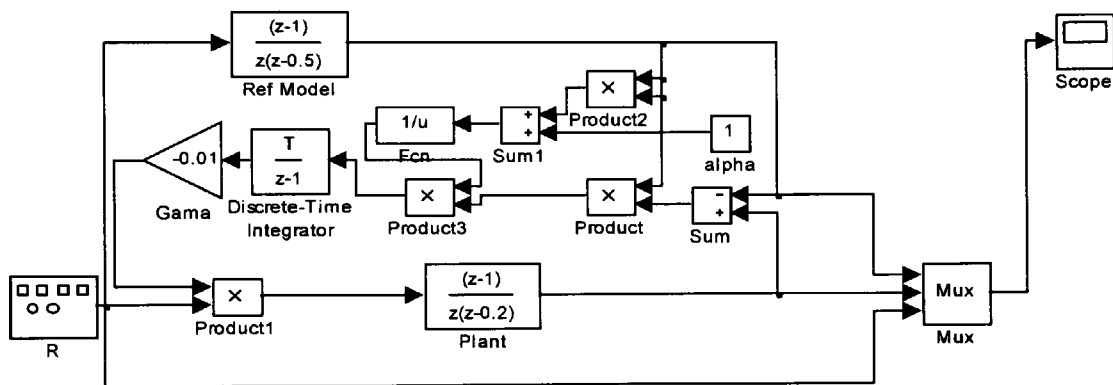
Figure 3.4.8 Illustrative system with normalisation (Simulink™ model)
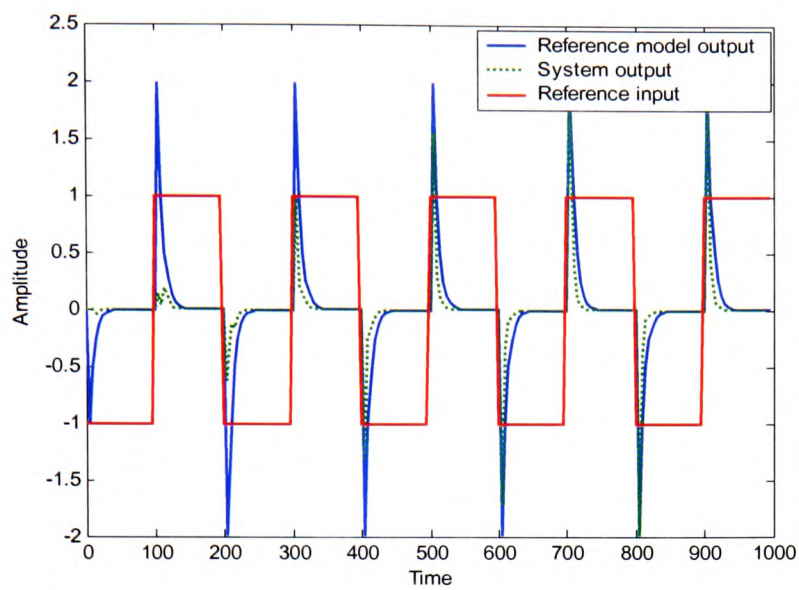
Figure 3.4.9 Illustrative system without normalisation R=1
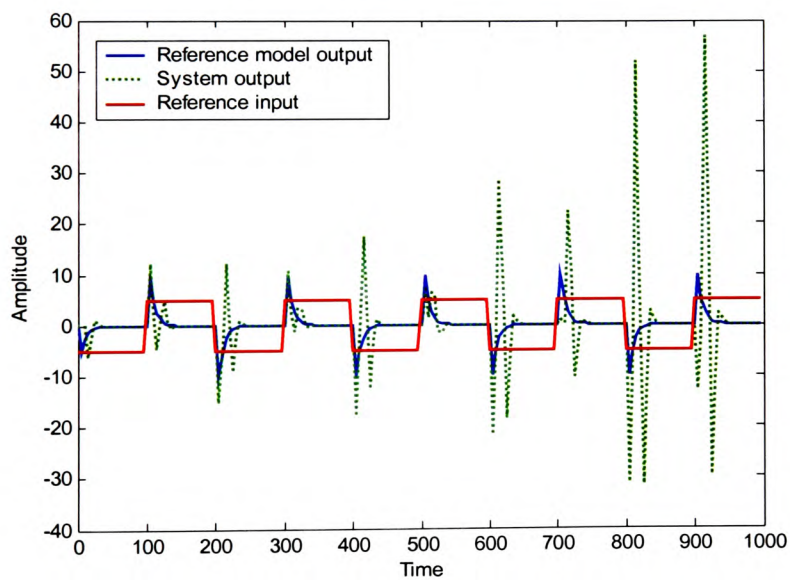
Figure 3.4.10 Illustrative system without normalisation R=5
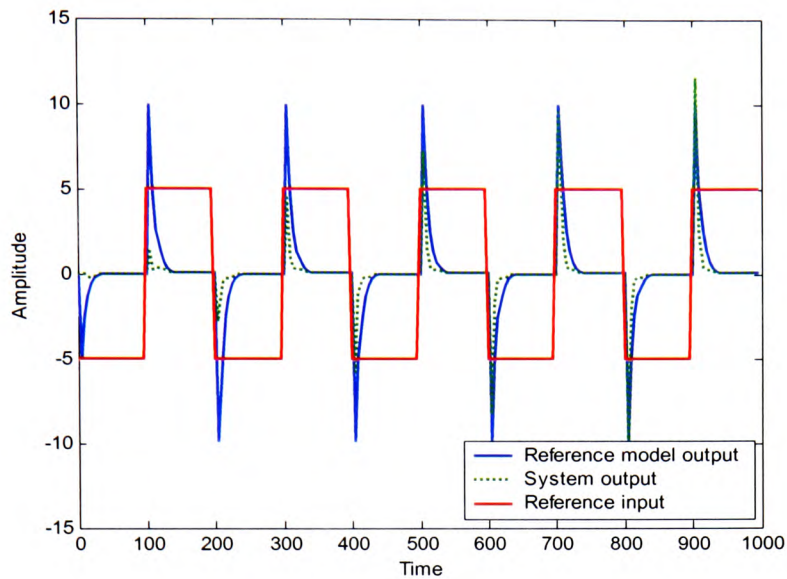
Figure 3.4.11 Illustrative system with normalisation R=5

3.4.2 Development of the control strategy – Feed-forward gain

The reactor was started up as described in Section 3.2, where four *Start-up* experiments are outlined. Each of the control strategies adopted will be presented here, although the results will be considered elsewhere in Chapter 4. Prior to the first start-up experiment (*Start-up 1*), some preliminary work was conducted in order to establish the viability of the control strategy and these were reported in Premier *et al.* (2000); Premier *et al.* (2001), which are included in Appendix B.

Initially, the controller architecture was that of a normalised MIT rule acting upon a feed-forward gain, as illustrated in Figure 3.4.12 (and Appendix A – modmit2.mdl). The reactor model was grossly simplified in the initial development, by using a second order model with a natural frequency of 16.67×10^{-3} rad.s^{-1} and an over-damped, damping ratio of 1.5. This was converted to discrete time using the Tustin transformation. The reference model was initially taken to be first order with a time constant of 1.5 hours and was discretised in the same way. Bandwidth-limited white noise was added to the measured variable in recognition of the measurement noise that was expected from the BA sensor in the experimental arrangement.
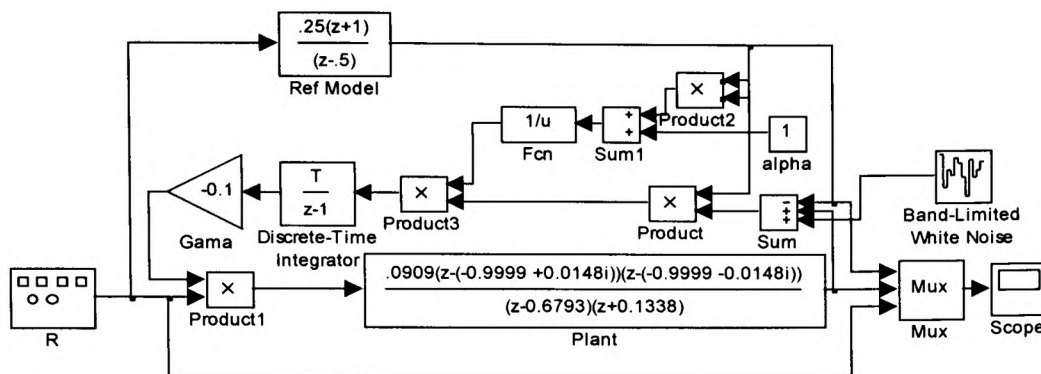
Figure 3.4.12 Initial Simulink™ development model for first experiment control strategy

The subsequent simulations are shown in Figure 3.4.13, both with and without the bandwidth-limited white noise.
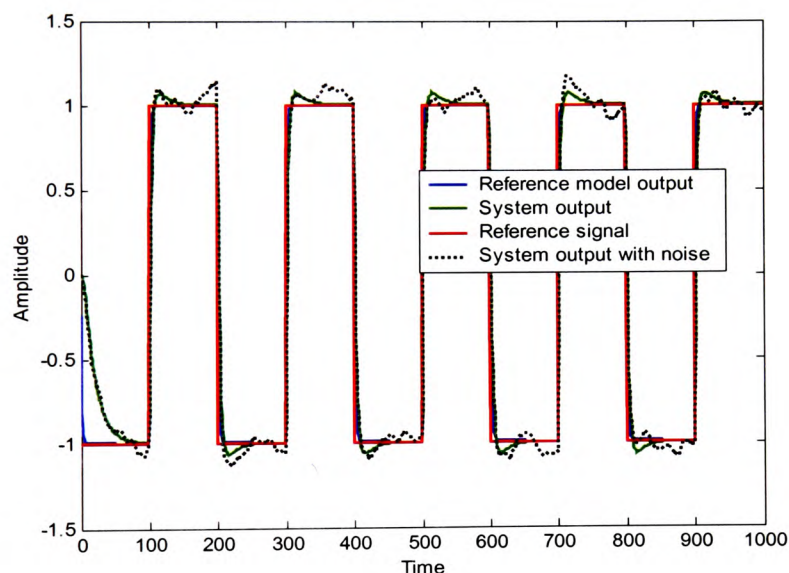
Figure 3.4.13 Simulation showing the response of the first control strategy, with and without band limited white noise (of power of 10% of input amplitude)

There is a markedly reduced deviation between the reference model output and the system output after t=100 hours, where the adaption has settled. It can be seen however that the noise has a significant effect, even at a power level of 5% of the step size on the reference input.

As discussed in Section 3.2, the control system was implemented in MatLAB/Simulink™ and run on a personal computer. LabVIEW™ effected the Input/Output and communication between the

applications was conducted using DDE. The control strategy required testing to ensure that any asynchronous behaviour caused by the DDE did not introduce inordinate delays and by so doing affect the control strategy. This was achieved by implementing a model in LabVIEW™, the parameters of which could be altered at will to simulate time variation in the reactor system. A more demanding reference model was at this stage also employed, to improve the response of the control system. In this case, a first order model was used, yielding a discrete time model of

$\dfrac{y_m}{R} = \dfrac{0.1429(z+1)}{z - 0.7143}$. The LabVIEW™ Virtual Instrument (VI) included two models. The first would be used to settle the adaptive controller prior to switching to the second model, which would represent (nominally), the AD reactor. Suitable I/O, to include the reactor hardware in the control loop would then replace the 2nd LabVIEW™ model. The complete VI (ddemrac_4.vi) is included in Appendix A along with the MatLAB/Simulink™ model used in its control (modmit6.mdl). The response of the complete system, including the DDE communications, is shown in Figure 3.4.14. The signals would require inversion to effect a reduction in OLR at a time when BA was below the set point and vice versa.
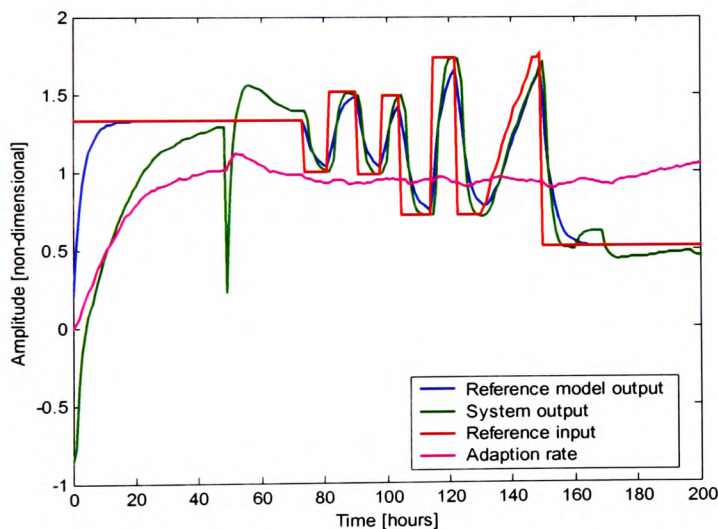
Figure 3.4.14 Simulation including DDE communications between MatLAB™ and LabVIEW™

Figure 3.4.14 shows the initialisation using the first model, between 0 and 50 hours, when the controller is switched to the second model (simulation of the AD process). Beyond this, a series of steps and a ramp are applied to the reference signal. Beyond 150 hours, the second model

parameters are altered in steps of roughly 10% of the parameter value, in order to demonstrate adaption to time variation in the AD process.

Development of the control strategy – 3-term, Fast Adaption Trajectory (FAT)

Consideration of the results from the MIT feed-forward control strategy indicated that the adaption rate was not sufficiently high to preserve the system (biological consortium) from periodic damage. Increasing the value of γ would cause the integration function of the adaption mechanism, to 'wind-up' rapidly. This would lead to intrinsically oscillatory (in the extreme, unstable) behaviour. Heuristically it was evident that a rapid error dependent and proportional adjustment was desirable. Derivative action may also prove useful for the same reason, however the slow integral action was still required to 'trim' the adaption rate. A 3-term (Proportional + Integral + Derivative) adaption mechanism, as opposed to a 3-term controller, was employed along side the feed-forward gain as in the previous strategy. This strategy will, for the sake of convenience, be called the Fast Adaption Trajectory (FAT) controller henceforth. The MatLAB/Simulink™ implementation of this strategy is shown in Figure 3.4.15. (and Appendix A - mrac_ugsb_startup_3).
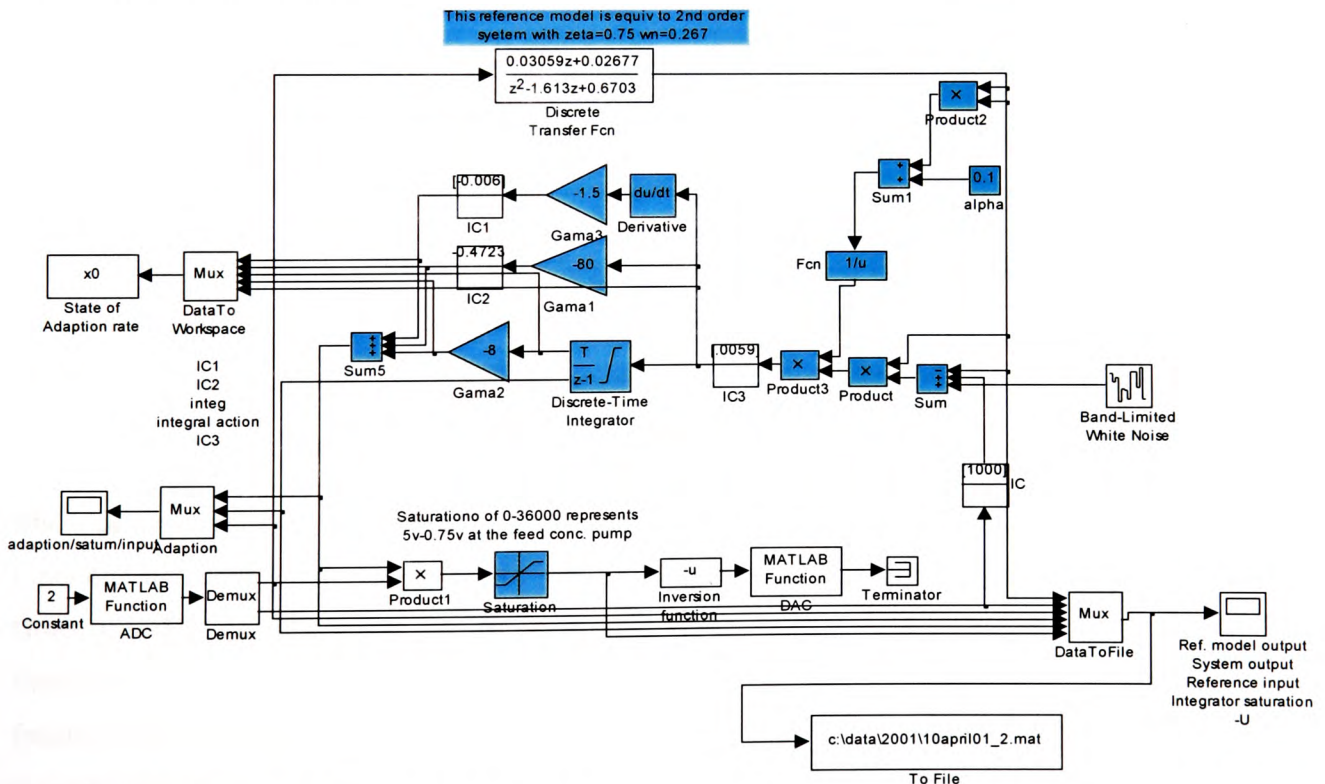
Figure 3.4.15 Simulink™ model of Fast Adaption Trajectory (FAT) controller

The values of three parameters in the adaption mechanism of the FAT controller are critical to the stability and performance of the control strategy. Given that start-up and commissioning was a key control objective of the research, the controller would need to be parameterised on the basis of limited knowledge as discussed in Section 2.4. The information available (particularly in the commissioning phase) is limited to a model in which one could have only limited confidence. Such a model would be one which has for example been parameterised using data from a different reactor or perhaps operating on different waste streams. The model described in Section 3.3.2 (Marsili-Libelli and Beni (1996)), would be a possible candidate. Parameterisation of the FAT controller could then proceed by using non-linear numerical optimisation techniques as described below in Section 3.4.3.

3.4.3 Optimisation of the Fast Adaption Trajectory (FAT) controller

Optimisation, in the sense used herein, is a synthesis process, which generally seeks to minimise or maximise a cost function (or objective function), which may be subject to constraints and convergence criteria. It is essentially an armoury of numerical techniques, each having advantages or limitations and often arranged as a mathematical toolbox, as is the case with that used in the current study.

The adaption mechanisms used in the control scheme for the experiments were optimised using a non-linear least squares optimisation routine:

$$\min_{x \in \Re^n} f(x) = \frac{1}{2} \sum_i F_i(x)^2 \qquad \text{3.4.10}$$

which is able to deal with multi-objective functions, as is the case in time series problems such as that in question. In control type problems, the output (in general a vector), $y(x,t)$ is required to mimic some trajectory, $\phi(t)$. The function that is to be minimised then becomes:

$$\min_{x \in \Re^n} f(x) = \frac{1}{2} \sum_{i=1}^{m} (\bar{y}(x,t_i) - \bar{\phi}(t_i))^2 \qquad \text{3.4.11}$$

The optimisation of the 3-term FAT controller strategy was performed numerically using functions available in the Optimisation toolbox supplied by The Mathworks Inc. (Branch and Grace (1996)). The problem was as suggested above, essentially a non-linear multi-objective function, which was modelled in Simulink™. The aim of the optimisation was to minimise a cost function for all time instances over a fixed period of time, each time instant representing a separate objective function.

Two optimisation functions were used, the first being leastsq from MatLAB™ 5 and the second was lsqnonlin from MatLAB™ 6, the second having marginal improvements to the algorithm over the first. Both solve problems of the form:

$$\min_{x \in \mathfrak{R}^n} f(x) = \frac{1}{2}\|F(x)\|_2^2 = \frac{1}{2}\sum_i F_i(x)^2 \qquad 3.4.12$$

Here the function can be a Simulink™ model as indeed is the case in this work. The non-linear least squares algorithm used was the Levenberg-Marquardt method which uses a search direction governed by the solution of a linear set of equations:

$$(J(x_k)^T J(x_k) + \lambda_k I)d_k = -J(x_k)F(x_k) \qquad 3.4.13$$

As described in Branch and Grace (1996), where $F(x_k)$ represents the residuals, $J(x_k)$, its Jacobian and λ_k controls the magnitude and direction of d_k, the search direction. The value of λ_k in the MatLAB™ implementation is determined interatively by estimating the non-linearity of the objective function.

Convergence criteria

Various options are available in the optimisation functions, but the most important of these are the convergence criteria. If the convergence criteria are constrained too tightly, it is possible that the solution will not converge within the limit of iterations set. The default setting, (which is a measure of the precision required) of the objective function for the optimisation routines used was 1×10^{-4}. Similarly, the precision required of the variables (in our case controller parameters), was also 1×10^{-4}, but both these constraints often need to be relaxed or tightened depending on the circumstances of the optimisation.

Cost functions for optimisation

A series of optimisations were performed in an iterative manner to try to improve the controller performance. In all cases the model of Marsili-Libelli and Beni (1996), developed in Section 3.3.2, was used to simulate the AD reactor. Table 3.4.1 indicates the cost functions used in the optimisation runs and the comments describe key criteria used. In all cases, the reference signal was varied in steps, as is evident in Figure 3.4.16 and 3.4.19. The parameter vector shows the resulting values of proportional (Kp), integral (Ki) and derivative (Kd) actions in the adaption mechanism. The shaded optimisation runs were not used in experimental work and are included here to show the iterative steps used in arriving at the parameterised controllers. These were used later in the experiments identified as *Start-up 1* (controller defined in g)), *Start-up 2* and *Start-up 3* (controller defined in i)) and *Start-up 4* (controller defined in k)).

Table 3.4.1 Numerical optimisation of controller parameters

Cost function	Parameter vector $[Kp, Ki, Kd]^T$	Comments
a $\quad f = 0.01(2 - \dot{X}_m) + e_m$	-76.0098 -0.1462 -2.6150	**Not used – OLR actuation** • Using leastsq function • Using trackflorPID.m (Appendix A) • Termination criteria [0.1x10^{-3} 0.1x10^{-3}] • Start time – 0 hrs Stop time – 600 hrs • First order reference model
b $\quad f = 0.1(2 - \dot{X}_m) + e_m$	-45.3763 -4.6393 -0.5767	**Not used – OLR actuation** • Using leastsq function • Using trackflorPID.m (Appendix A) • Termination criteria [0.1x10^{-3} 0.1x10^{-3}] • Start time – 0 hrs Stop time – 300 hrs • Max number of iterations exceeded • First order reference model
c $\quad f = 0.1(2 - \dot{X}_m) + e_m$	-10.2738 -9.6089 -0.4989	**Not used – OLR actuation** • Using leastsq function • Using trackflorPIDb.m (Appendix A) • Termination criteria [0.1x10^{-3} 0.1x10^{-3}] • Start time – 100 hrs Stop time – 300 hrs • First order reference model
d $\quad f = 0.1(2 - \dot{X}_m) + e_m$	-61.8821 -4.2291 -2.3905	**Not used – OLR actuation** • Using leastsq function • Using trackflorPIDb.m (Appendix A) • Termination criteria [1 1] • Start time – 100 hrs Stop time – 300 hrs • First order reference model
e $\quad f = 0.1(2 - \dot{X}_m) + e_m$	-57.1624 -4.3402 -2.2981	**Not used – OLR actuation** • Using leastsq function • Using trackflorPIDb.m (Appendix A) • Termination criteria [10 10] • Start time – 100 hrs Stop time – 120 hrs • Max number of iterations exceeded • First order reference model
f $\quad f = 0.1(2 - \dot{X}_m) + \|e_m\| + 0.001\|\dot{U}\|$	-86.1688 -7.9323 -1.7557	**Not used – OLR actuation** • Using leastsq function • Using trackflorPID2nd.m (Appendix A) • Termination criteria [1 1] • Start time – 100 hrs Stop time – 200 hrs • Max number of iterations exceeded • 2nd order reference model
g $\quad f = 0.1(2 - \dot{X}_m) + \|e_m\| + 0.001\|\dot{U}\|$	-80.3543 -7.9973 -1.5604	*Start-up 1* – OLR actuation • Using leastsq function • Using trackflorPID2nd.m (Appendix A) • Termination criteria [1000 1000] • Start time – 100 hrs Stop time – 200 hrs • Max number of iterations exceeded • 2nd order reference model • Implementation Software (Appendix A) mrac_ugsb_startup_3.mdl and mrac_3.vi
h $\quad f = 0.1(2 - \dot{X}_m) + \|e_m\| + 0.001\|\dot{U}\|$	-20.0 -3.8445 -2.3049	**Not used – OLR actuation** • Using lsqnonlin function • Using track2florPID2nd.m (Appendix A) • Termination criteria [0.1x10^{-3} 0.1] • parameter limits [-20 -10 -10] • Start time – 100 hrs Stop time – 200 hrs • Max number of iterations exceeded • 2nd order reference model • Transport and sampling delays in BA measurement included.

Table 3.4.1 Numerical optimisation of controller parameters... continued

	Cost function	Parameter vector $[Kp,Ki,Kd]^T$	Comments
i	$f = 0.1(2 - \dot{X}_m) + \lvert e_m \rvert + 0.001\lvert \dot{U} \rvert$	-27.1952 -5.0322 -2.6103	**Start-up 2 and 3 – OLR actuation** • Using lsqnonlin function • Using track2florPID2nd.m (Appendix A) • Termination criteria [0.1x10⁻³ 0.1] • parameter limits [-30 –10 –10] • Start time – 100 hrs Stop time – 200 hrs • Max number of iterations exceeded • 2nd order reference model • Transport and sampling delays in BA measurement included • Implementation Software (Appendix A) mrac_ugsb_startup_4.mdl and mrac_4.vi mrac_ugsb_startup_5.mdl and mrac_5.vi
j	$f = 0.1(2 - \dot{X}_m) + \lvert e_m \rvert + 0.001\lvert \dot{U} \rvert$	-13.6498 -0.8804 -0.2077	**Not used – BA dosing actuation** • Using lsqnonlin function • Using track2florPID2nd.m (Appendix A) • Termination criteria [0.1x10⁻³ 0.1] • parameter limits [-20 –10 –10] • Start time – 120 hrs Stop time – 200 hrs • Max number of iterations exceeded • 2nd order reference model • Transport and sampling delays in BA measurement included.
k	$f = 0.1(2 - \dot{X}_m) + \lvert e_m \rvert + 0.001\lvert \dot{U} \rvert$	-11.8812 -1.2157 -0.1867	**Start-up 4 – BA dosing actuation** • Using lsqnonlin function • Using track2florPID2nd.m (Appendix A) • Termination criteria [0.1x10⁻³ 0.1] • parameter limits [-20 –10 –10] • Start time – 40 hrs Stop time – 200 hrs • Max number of iterations exceeded • 2nd order reference model • Transport and sampling delays in BA measurement included. • Implementation Software (Appendix A) mrac_ugsb_startup_6.mdl and mrac_6.vi

Controller optimisation for OLR actuation

The optimisation iterations that were applied experimentally and are highlighted and summarised in Table 3.4.1 will be considered in this section. It was necessary to investigate the predicted performance and to assess if it would be acceptable in practical terms. The file florence_Simules_Sin_PID_2nd.mdl, included in Appendix A, was used to simulate control strategy (*g*) of Table 3.4.1 and this is associated with *Experiment 1* presented in Sections 3.1 and 4.3. The simulation used the same model as was used in optimising the controller. Figure 3.4.16 shows the first and last iterations in the optimisation process, where the initial values of the adaption mechanism parameters were Kp=-10; Ki=-1.0; Kd=-0.1 and the converged resultant values were Kp=-80.3543; Ki=-7.9973; Kd=-1.5604.
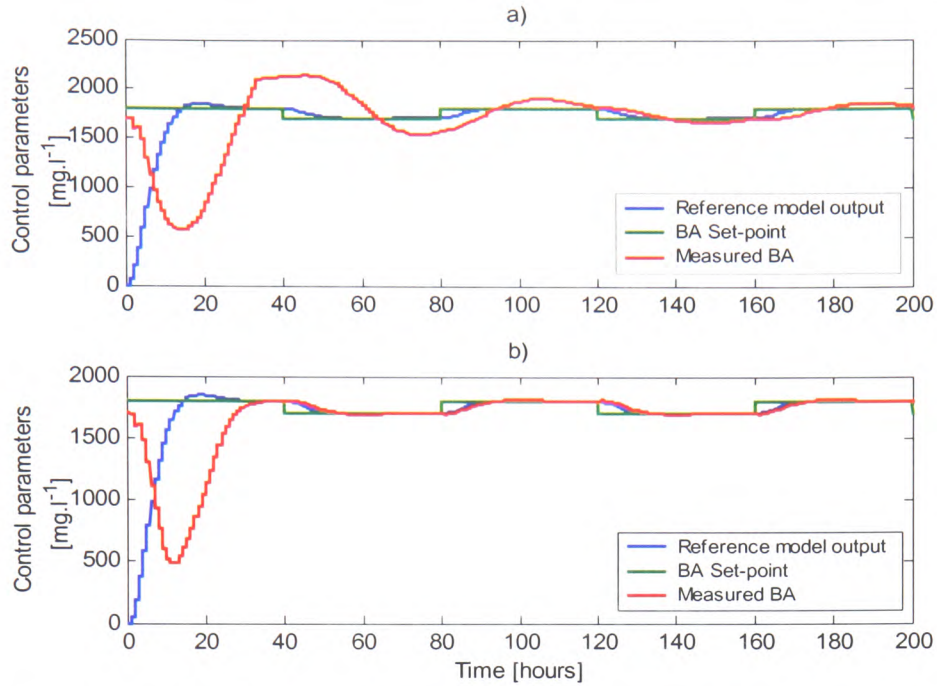
Figure 3.4.16 Simulation of the controller response at starting:

a)   [Kp=-10.0;Ki=-1.0;Kd=-0.1] and converged conditions,

b)   [Kp=-80.3543;Ki=-7.9973;Kd=-1.5604], of optimisation
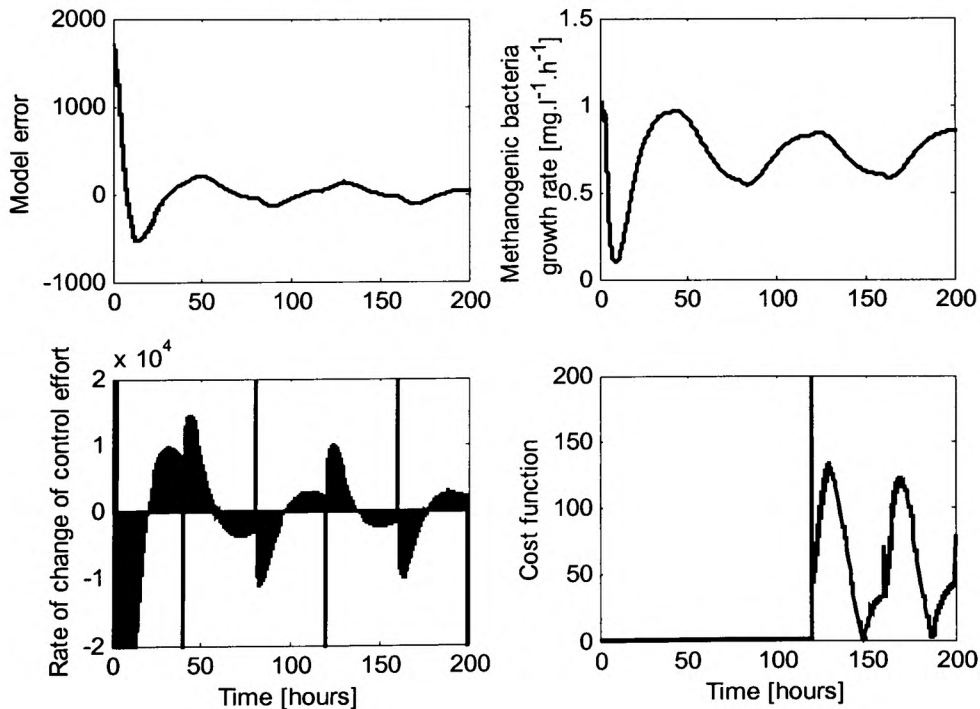
Figure 3.4.17 Optimisation parameters for starting conditions (first iteration) with   [Kp=-10.0;Ki=-1.0;Kd=-0.1]

It can be seen that the optimisation procedure has tended to eliminate the model error to a large extent and that the measured value of BA follows the reference model output closely. This is confirmed in Figures 3.5.17 and 3.4.18, which show the model error reduces from the first to the last iteration, while the growth rate of the methanogenic bacteria and the rate of change of the control effort are increased and reduced respectively, when looking over the entire time series. These three parameters form part of the cost function detailed in Table 3.4.1 (*g*), and it is evident from Figures 3.5.17 and 3.4.18 that the cost function has also reduced.
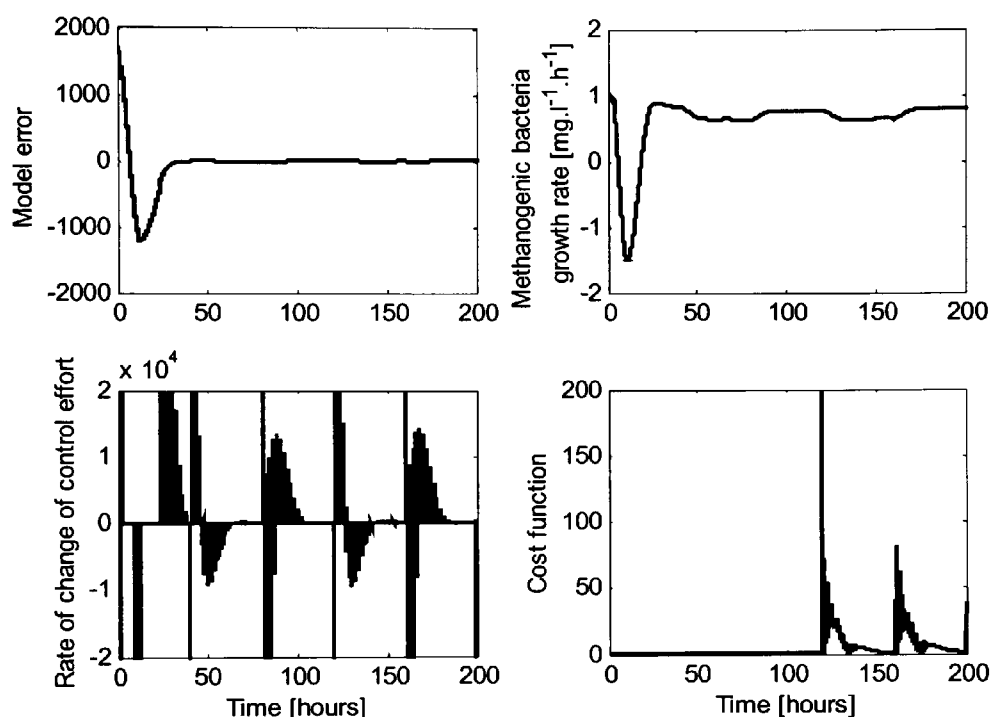
Figure 3.4.18 Optimisation parameters for convergence conditions (final iteration) with [Kp=-80.3543;Ki=-7.9973;Kd=-1.5604]

The experimental results forced a reappraisal of the model used in optimisation (*g*). A unit sample delay caused by the communication between MatLAB™ and LabVIEW™ was included, as was a first order model of the settling device described in Section 3.1, for removing particulate in the flow between the reactor and the BA monitor. Similar optimisations to (*g*) were conducted and are summarised in Table 3.4.1 (*h* and *i*). The effects described above are typical, as can be seen from Figures 3.4.19 to 3.4.22, though the detail alters depending on the model and the time at which the optimisation was invoked. The controller response for optimisation (*i*) has not been included as it differed little from that of optimisation (*h*) shown in Figure 3.4.19.
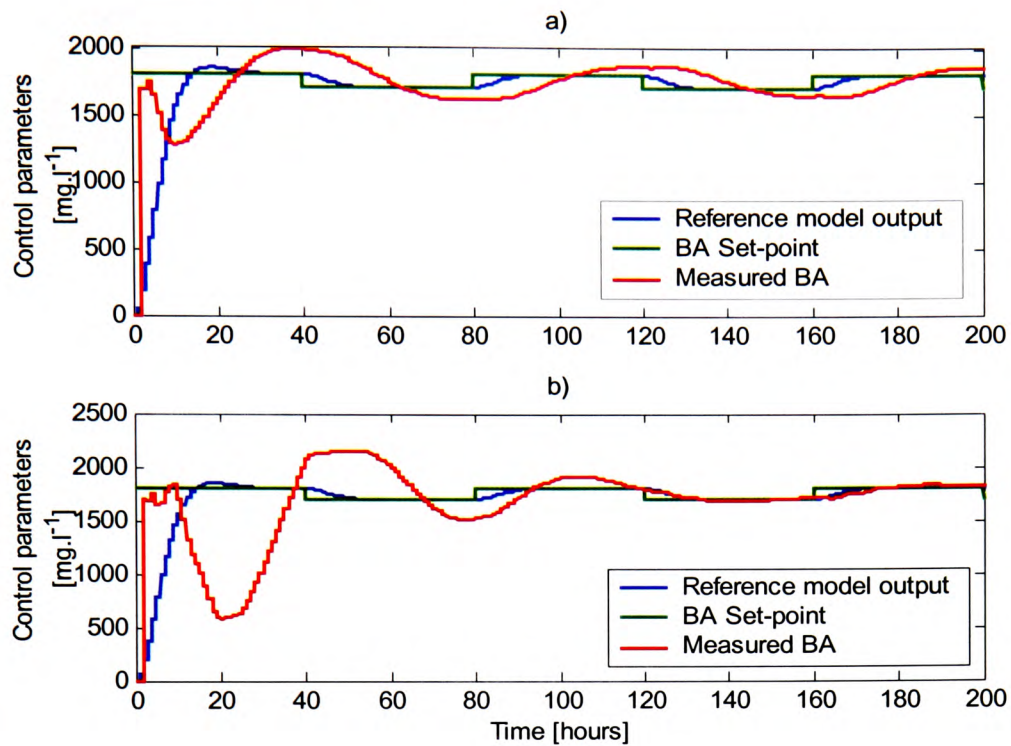
Figure 3.4.19 Simulation of the controller response at starting.

a) [Kp=-10.0;Ki=-1.0;Kd=-0.1] and converged conditions,
b) [Kp=-20;Ki=-3.8445;Kd=-2.3049]
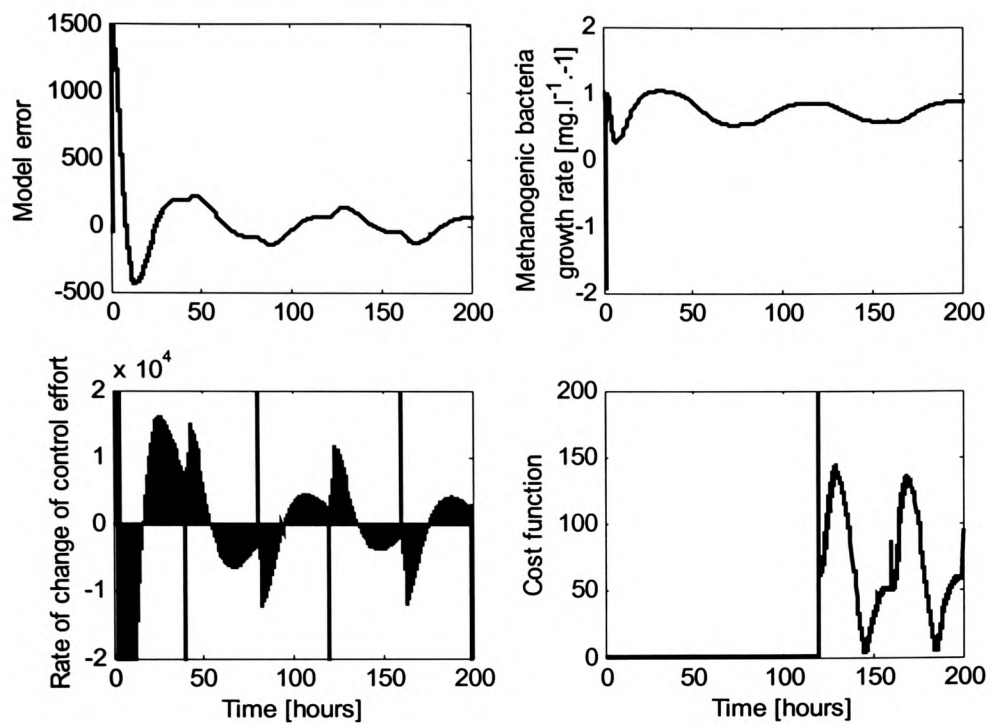
Figure 3.4.20 Parameters for Optimisation (*h*) starting conditions (first iteration) with [Kp=-10.0;Ki=-1.0;Kd=-0.1]
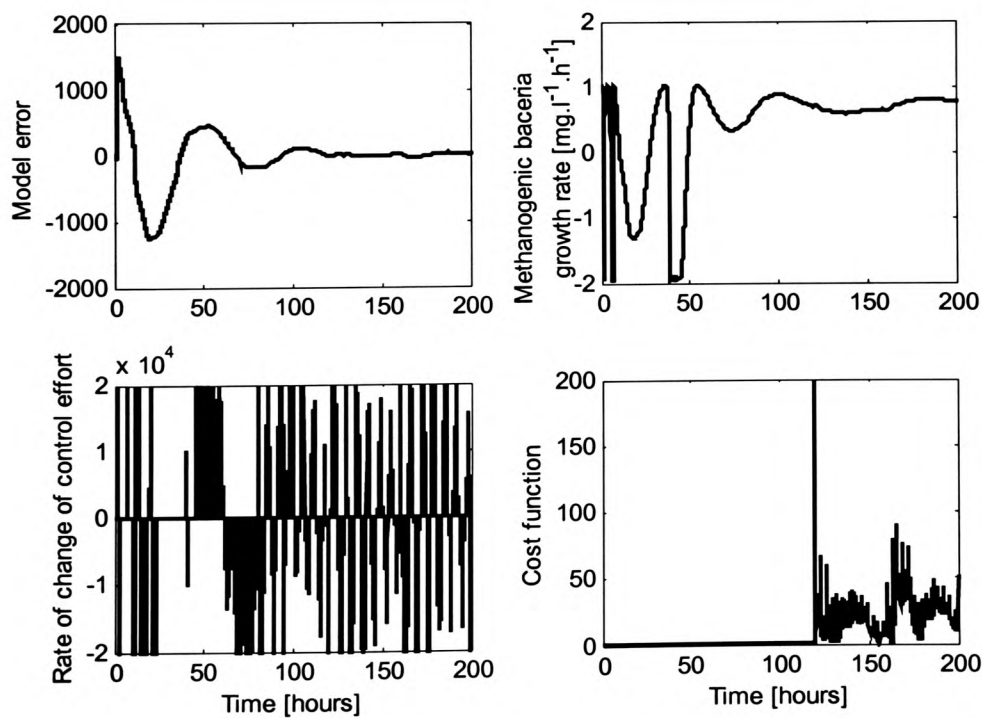
Figure 3.4.21 Parameters for Optimisation (*h*) convergence conditions (last iteration) with [Kp=-20;Ki=-3.8445;Kd=-2.3049]
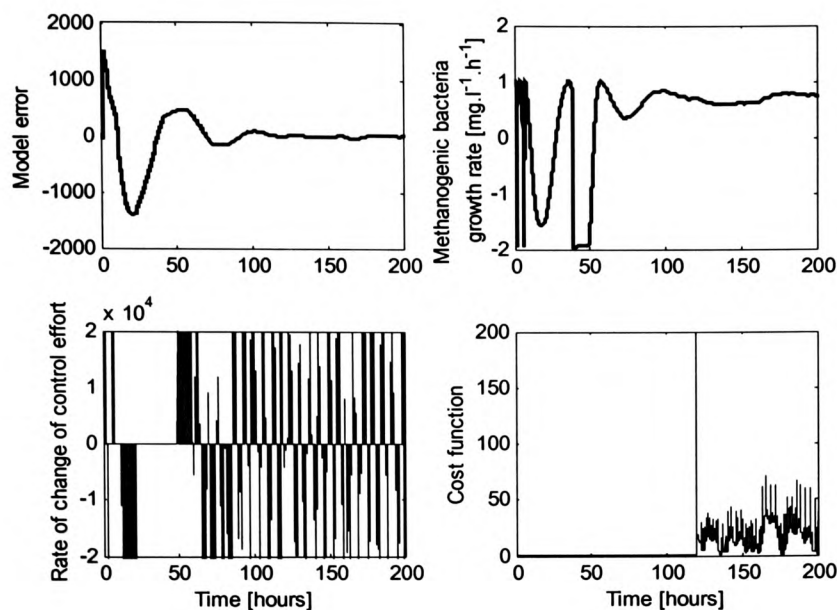
Figure 3.4.22 Parameters for Optimisation (*i*) convergence conditions (last iteration) with [Kp=-27.1952;Ki=-5.0322;Kd=-2.6103]

Optimisation (*i*), was used in Experiments *2* and *3* as the convergence parameters were not limited in the optimisation procedure as was the case in (*h*). Simulations were conducted to determine the long-term behaviour of the system with these adaption parameters. In Figure 3.4.23 (optimisation (*h*)) it can be seen that the bacterial growth did not adversely affect the response of the system, even when Gaussian white noise was added to the measured variable at a variance that one might expect experimentally. The noise variance was 500 mg.l^{-1} CaCO$_3$ equiv. at a sample rate of 1 hour. The BA set point was varied in a series of random steps according to a Gaussian distribution of variance 500 mg.l^{-1} CaCO$_3$ equiv., added to a base line of 1700 mg.l^{-1} CaCO$_3$ equiv., at a sample time of 10 hours. Figure 3.4.23 b) shows that the measured BA under the simulation conditions varies roughly ±100 mg.l^{-1} CaCO$_3$ equiv.
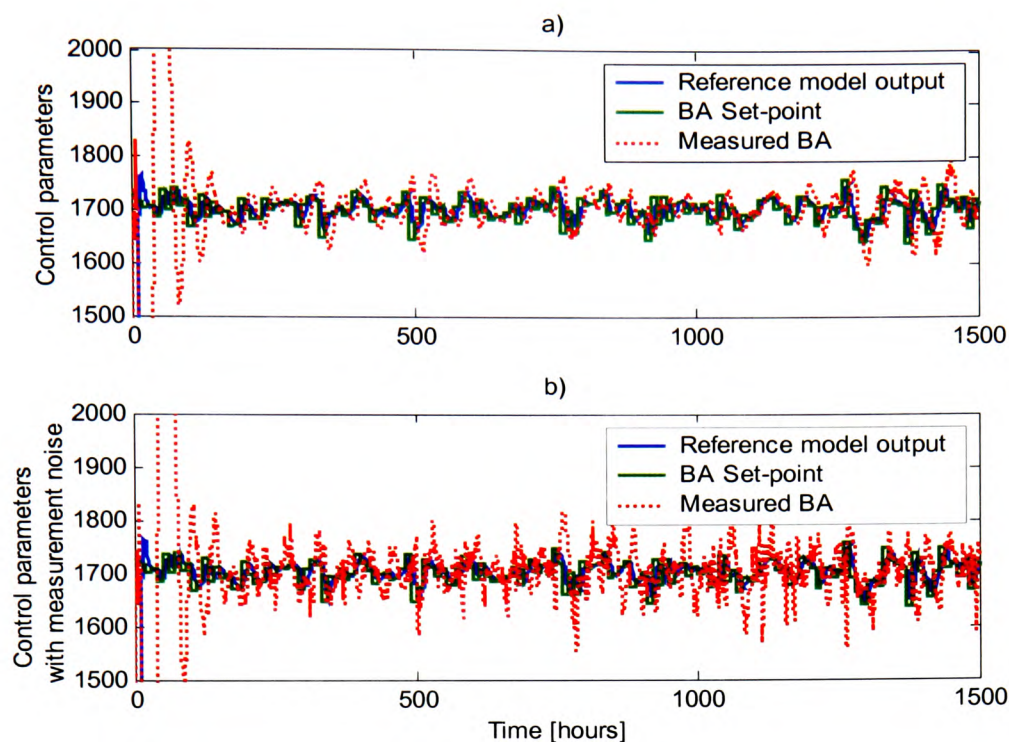
Figure 3.4.23 Simulation of controller response for optimisation (*h*).

a) without measurement noise,
b) with measurement noise of variance 500 mg.l^{-1} CaCO$_3$ equiv.

Closer inspection of the data generated from optimisation (*h*), (Figure 3.4.24) shows the effect of random noise on the measured BA signal. The true nature of the noise on the BA monitor is however likely to be coloured, and will include drift as a significant component. One of the main causes of the drift is the gradual deterioration of pumping efficiency of the peristaltic pumps used in the BA monitor.
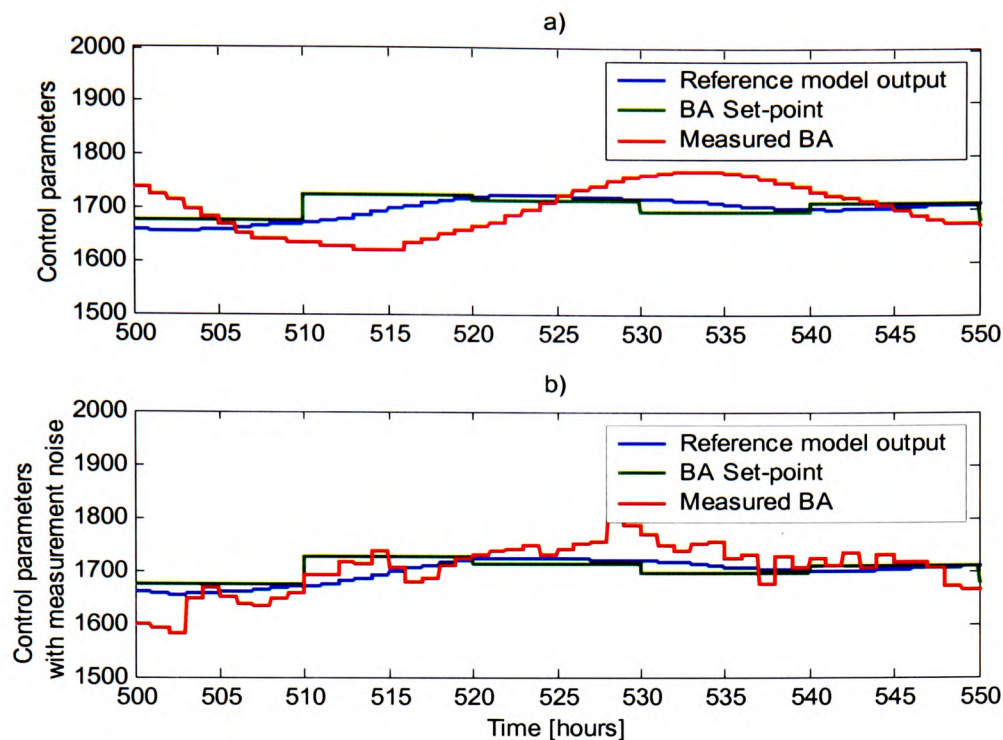
Figure 3.4.24 Simulation (zoom in on Figure 3.4.23) of controller response.

a)   without measurement noise,
b)   with measurement noise of variance 500 mg.l^{-1} CaCO$_3$ equiv.
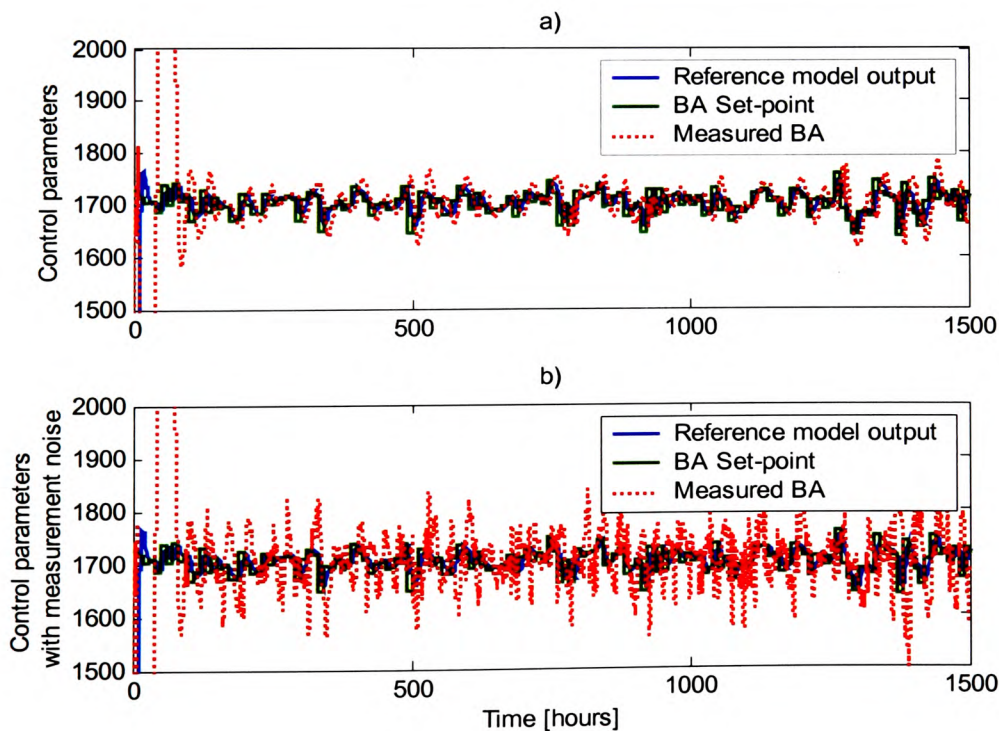
Figure 3.4.25 Simulation of controller response for optimisation (*i*).

a)   without measurement noise,
b)   with measurement noise of variance 500 mg.l^{-1} CaCO$_3$ equiv.

A similar analysis can be undertaken with reference to optimisation (*i*), with the long-term time evolution of the data shown in Figure 3.4.25, using the same simulation conditions as Figure 3.4.23, with the exemption of the adaption parameters. A comparison of these two figures shows similar behaviour. Furthermore, a comparison between the enlarged portion of data in Figure 3.4.24 and the corresponding enlargement for optimisation (*i*) in Figure 3.4.26, show only a slight deterioration with respect to the noisy signal, while showing a marginal improvement where noise is not included.
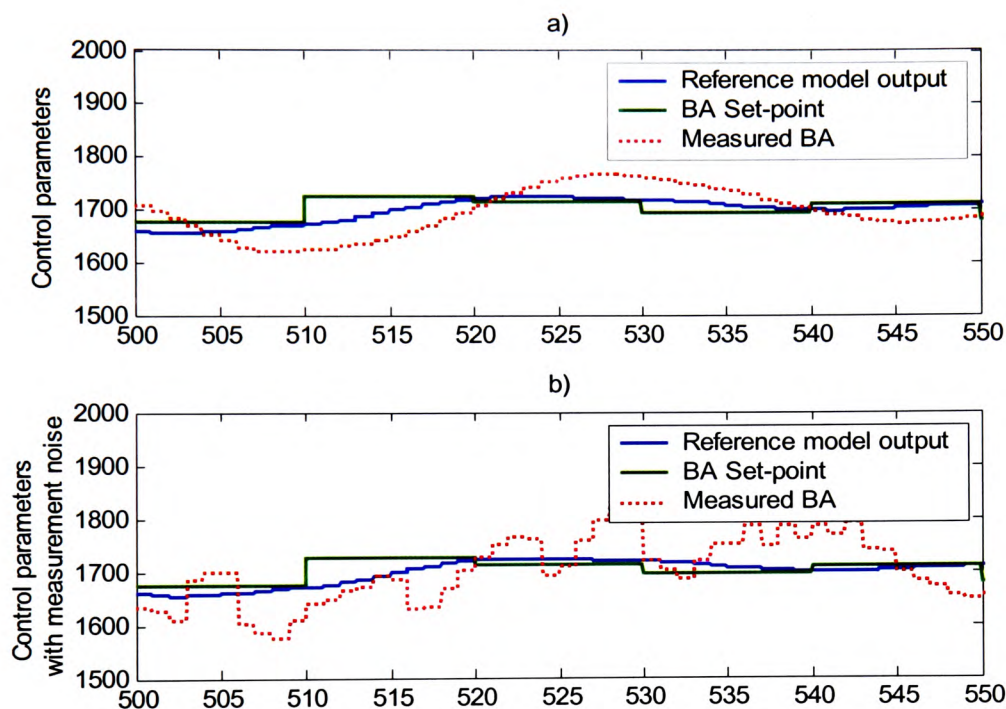
Figure 3.4.26 Simulation (zoom in on Figure 3.4.25) of controller response.
a) **without measurement noise,**
b) **with measurement noise of variance 500 mg.l^{-1} CaCO$_3$ equiv.**

Care should be taken to maintain reasonably sedate variations in control effort. Figure 3.4.27 shows by simulation, the resulting control effort from three different adaption mechanism parameter vectors, which in turn resulting from three optimisation procedures (Table 3.4.1, *g*, *h* and *i*). The first (Figure 3.4.27a) represents the optimisation (*g*) conducted without consideration of the unit delay and BA monitor model in the feedback path, and was used to control the system for a considerable period and will be detailed elsewhere (Chapter 4). The second and third plots, (Figure 3.4.27 b and c) which correspond to subsequent optimisations (*h* and *i*), included the delay and the BA monitor model. The only difference between them is that in Figure 3.4.27 a, the Kp

value was limited to 20 while it was not in Figure 3.4.27b. The steadily rising trend in all cases reflects the increased microbial population brought about by growth.
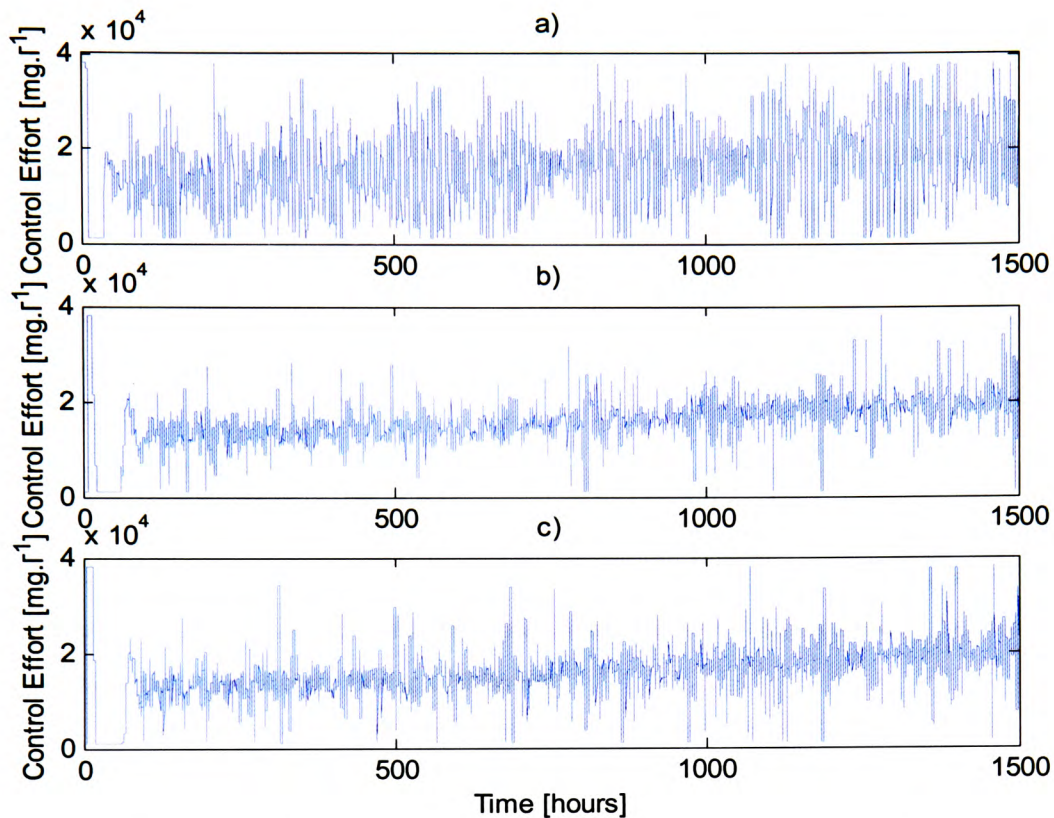
Figure 3.4.27 Comparison of control effort by simulation with sensor noise.

a)   [Kp=-80.3543;Ki=-7.9973;Kd=-1.5604]
b)   [Kp=-20.0;Ki=-3.8445;Kd=-2.3050]
c)   [Kp=-27.1952;Ki=-5.0322;Kd=-2.6103]

Controller optimisation for BA dosing actuation

Previous optimisations have used the OLR as the control action and the experimental work is reported in Chapter 4. Although the reliability of the BA monitor was a significant problem, some success was noted. The indications were that the control action was causal in adjusting the BA in the reactor, but that it was not overly accurate in maintaining the set point.

The use of an alternative control action, namely the dosing of BA, would be of considerable interest, to see if the resulting control would show improvement. This would require the controller to be re-parameterised and this was undertaken in the same way as the optimised parameters were determined above for the OLR actuated system, (which included using the same cost function). The parameter values and optimisation conditions are summarised in Table 3.4.1 (*j* and *k*).

The significant differences between the two actuation modes were that the control action in BA dosing would need to be inverted compared to that of the OLR actuation. This is because an increase in OLR would tend to reduce the measured BA while an increase in BA dosing would tend to increase the measured BA. This is shown in the Simulink™ model Florence_Optim4_BA_PID_2nd.mdl, in Appendix A. The control effort (BA dosing) was limited to the range 0 to 3000 mg.l^{-1} CaCO$_3$ equiv. and the S_{in} was set to 7000 mgCOD.l^{-1}. This loading rate is dependant on the initial conditions in the model, particularly the concentrations of the bacterial groups. For example, an S_{in} of 15000 mgCOD.l^{-1} made the system unstable to the point of catastrophic failure, (at least as far as the simulation was concerned). As the biomass increases, so higher loading rates are possible.

Optimisation (j) yielded parameter values, which were then investigated by simulation in model florence_simul_cont_BA_PID_2nd.mdl, which is in Appendix A. Figure 3.4.28 shows the control effort for differing conditions of additive Gaussian noise on the measured BA (with sample time of 1 hour). This optimisation was conducted with the threshold (before which the cost function was not minimised), being 120 hours.
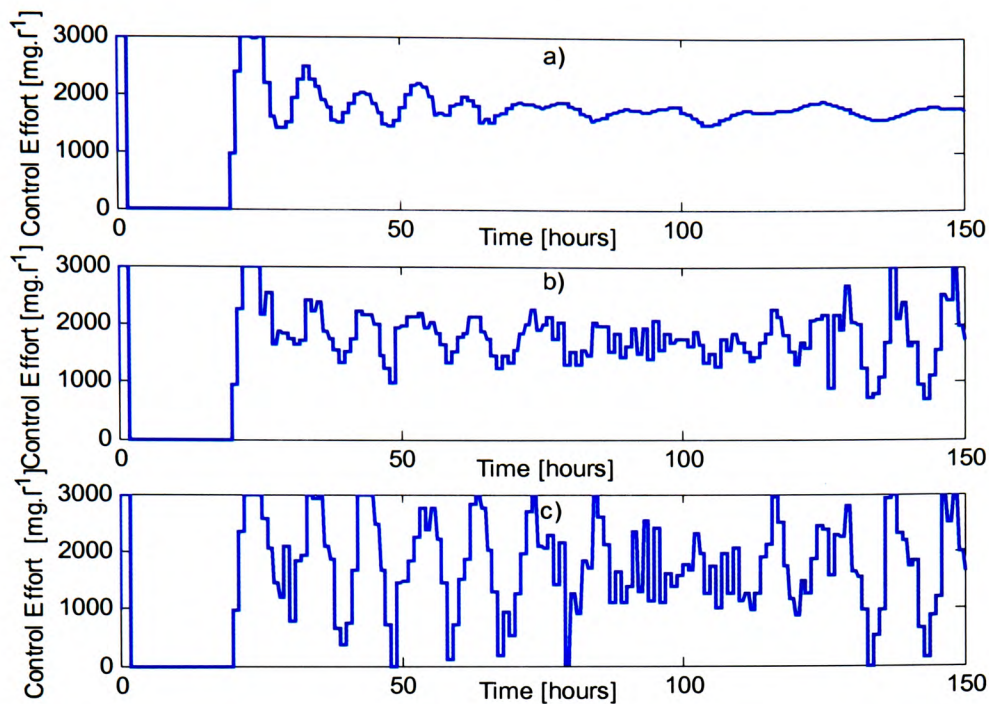
Figure 3.4.28 Comparison of control effort by simulation with sensor noise (ranging from variance 0 to 500 mg.l^{-1} CaCO$_3$ equiv.).

a) variance 0
b) variance 100
c) variance 500

The control effort was seen to react in a 'stiff' manner as a result of optimisation (j), tending to oscillate. The threshold was then altered to include earlier data in the same simulation/optimisation, by positioning it at 40 hours, according to optimisation (k). The effect was to reduce the 'stiffness'. The figures below show the optimisation parameters using initial conditions (Figures 3.4.29), and after convergence in two cases (j and k), (shown in Figure 3.4.30 and Figure 3.4.31 respectively). In both optimisations, the simulation had a time span of 200 hours but the optimisation threshold was set at 120 hrs for Figure 3.4.30 and 40 hrs for that shown in Figure 3.4.31. Appendix A contains the model (Florence_optim4_BA_PID_2nd.mdl), used in the optimisation.
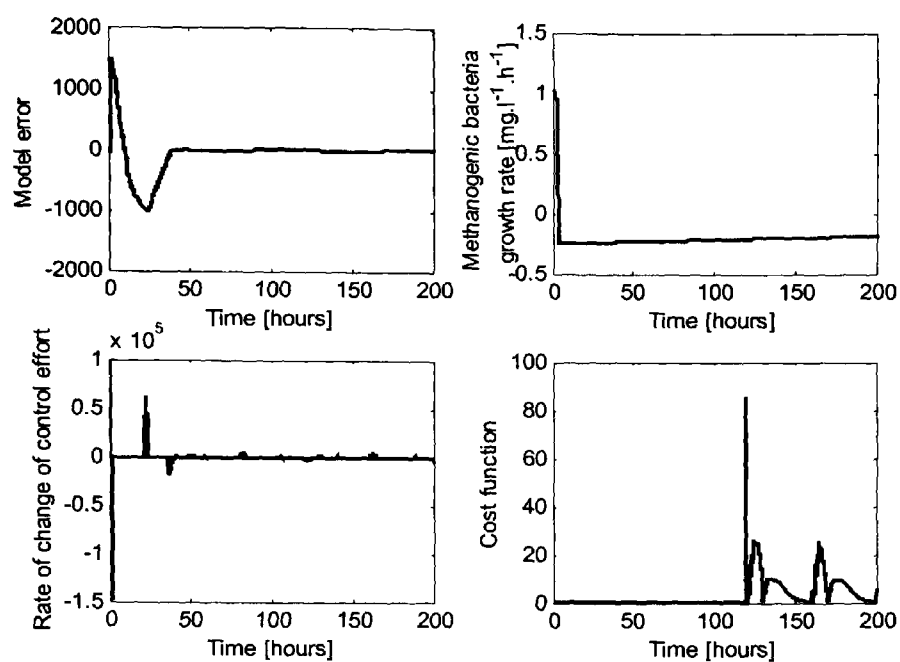
Figure 3.4.29 Optimisation parameters for starting conditions (first iteration) with [Kp=-10.0;Ki=-1.0;Kd=-0.1]
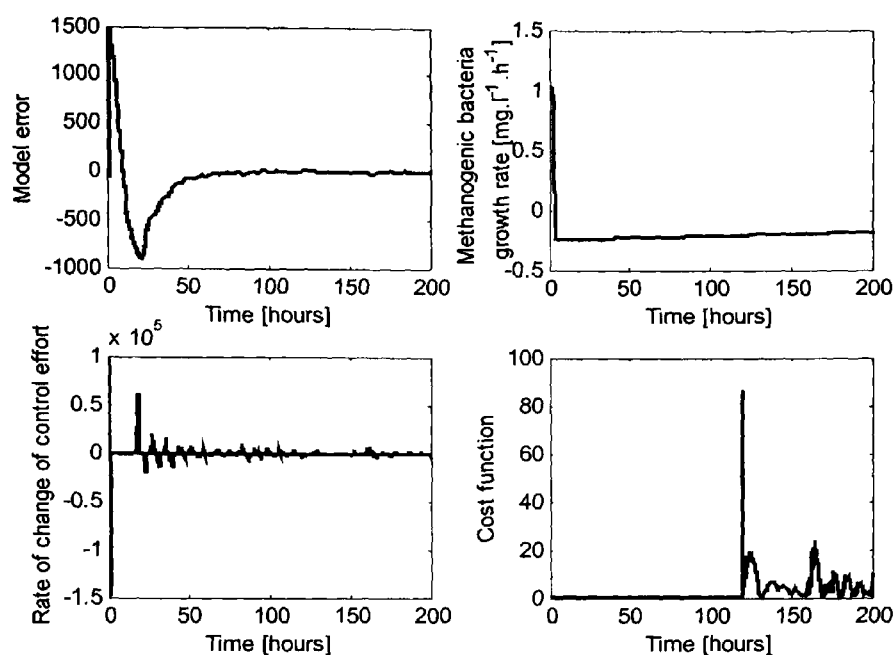
Figure 3.4.30 Optimisation parameters for optimisation (j) convergence conditions (last iteration) with [Kp=-13.6498;Ki=-0.8804;Kd=-0.2077]
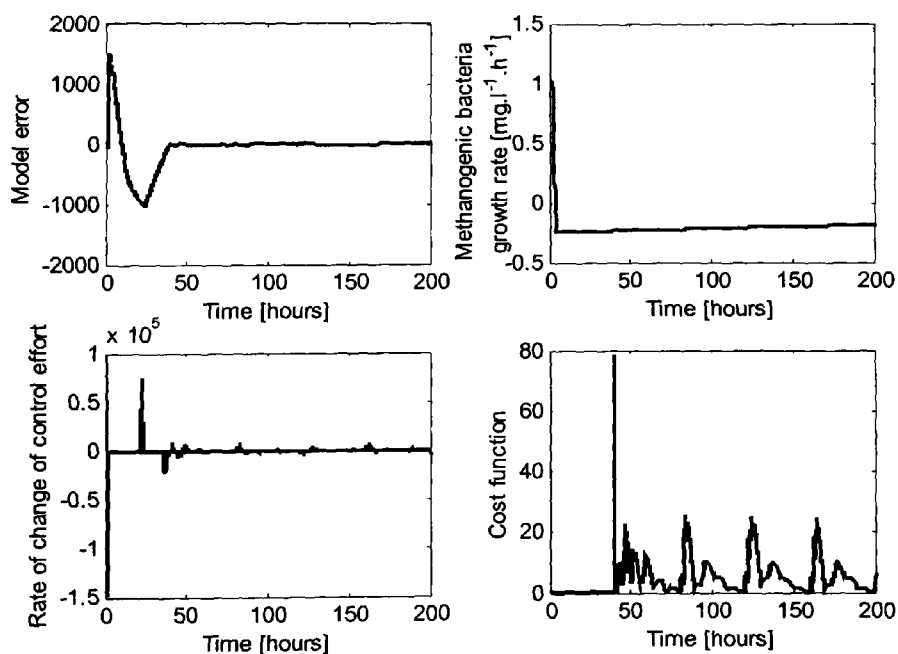
Figure 3.4.31 Optimisation parameters for optimisation (k) convergence conditions (last iteration) with [Kp=-11.8812;Ki=-1.2157;Kd=-0.1876]
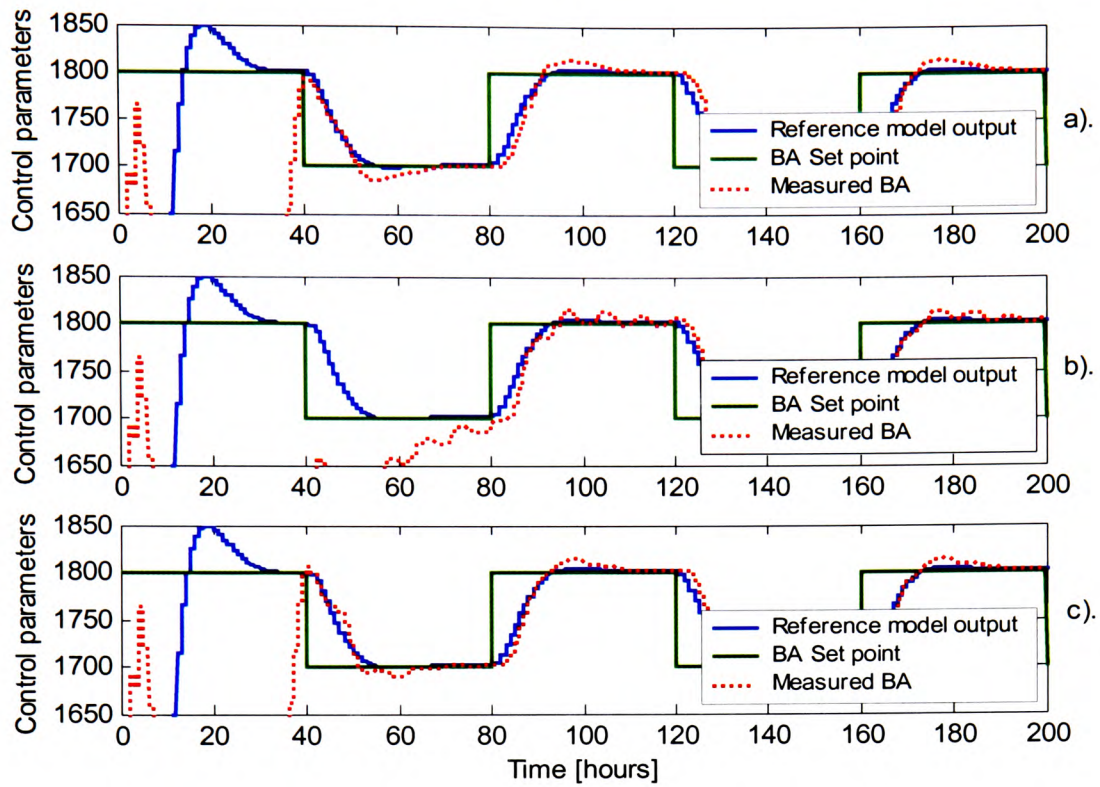
Figure 3.4.32 Simulation of controller response:

a)   with [Kp=-10;Ki=-1;Kd=-0.1]
b)   with [Kp=-13.6498;Ki=-0.8804;Kd=-0.2077]
c)   with [Kp=-11.8812;Ki=-1.2157;Kd=-0.1876]

Figure 3.4.32 shows the responses of the system to the initial conditions and optimisation (*j* and *k*)

parameters, where it can be seen that the oscillatory behaviour derived from optimisation (*j*),

Figure 3.4.32 b, has been significantly reduced through optimisation (*k*), Figure 3.4.32 c. In so

doing there has been little, if any loss in expected performance from the system.

4.0 RESULTS AND DISCUSSION

The following is an analysis of the results obtained from the techniques and tasks presented in Chapter 3. The order of presentation will follow the Tasks as presented in Table 3.1, and seeks to make clear to the reader:

- The identification and performance of SISO black box models representing BA, % CO_2 in the biogas, biogas production rate and TOC – Task 1 in Section 4.1.1

- The comparative performance of SISO, MIMO and neural network based black box models of ARX structure representing BA, % CO_2 in the biogas and biogas production rate – Task 2 in Section 4.1.2

- A simulation study of the performance of two-population lumped-parameter deterministic models – Task 3 in Section 4.2

- Model reference adaptive controlled reactor start-up performance, (using the system designed and detailed in Section 3.4) – Task 4 in Section 4.3

4.1 IDENTIFICATION OF BLACK BOX MODELS (TASKS 1 & 2)

The simplicity of the black box modelling approach was at once its strength, and a major influence in the consideration of such models, and its weakness, in so far as the integrity of the results obtained were difficult to judge. The nature of this methodology meant that the underlying reason for accuracy or its absence was largely imponderable, particularly in the case of the connectionist approach using neural networks. The 'blackness' of the model made the prospect of incremental improvement difficult to achieve and the process became one of 'informed trial and error'.

The ARX model structure was selected on the basis of a brief study of the behaviour of a number of linear SISO black box models (such as the AR, ARMAX, OE and Box Jenkins). The iterative procedure indicated that the linear ARX model's performance was for the most part superior to the alternatives. As suggested by many authors (including Bishop (1995)), Occam's Razor, which paraphrased affirms that the simplest adequate solution is the best, was employed and the ARX structure was extrapolated to include the MIMO and Neural Network models in Task 2.

4.1.1 Identification and performance of the SISO black box approach (Task 1)

The parameter estimation for the respective models was performed using the data shown in Figures 4.1.1 and 4.1.2, which presents gas production rate and % CO_2, and BA and TOC respectively, varying with organic load (represented by the feed pump voltage). Figure 4.1.3 shows the parameter estimation data after filtering and normalisation.
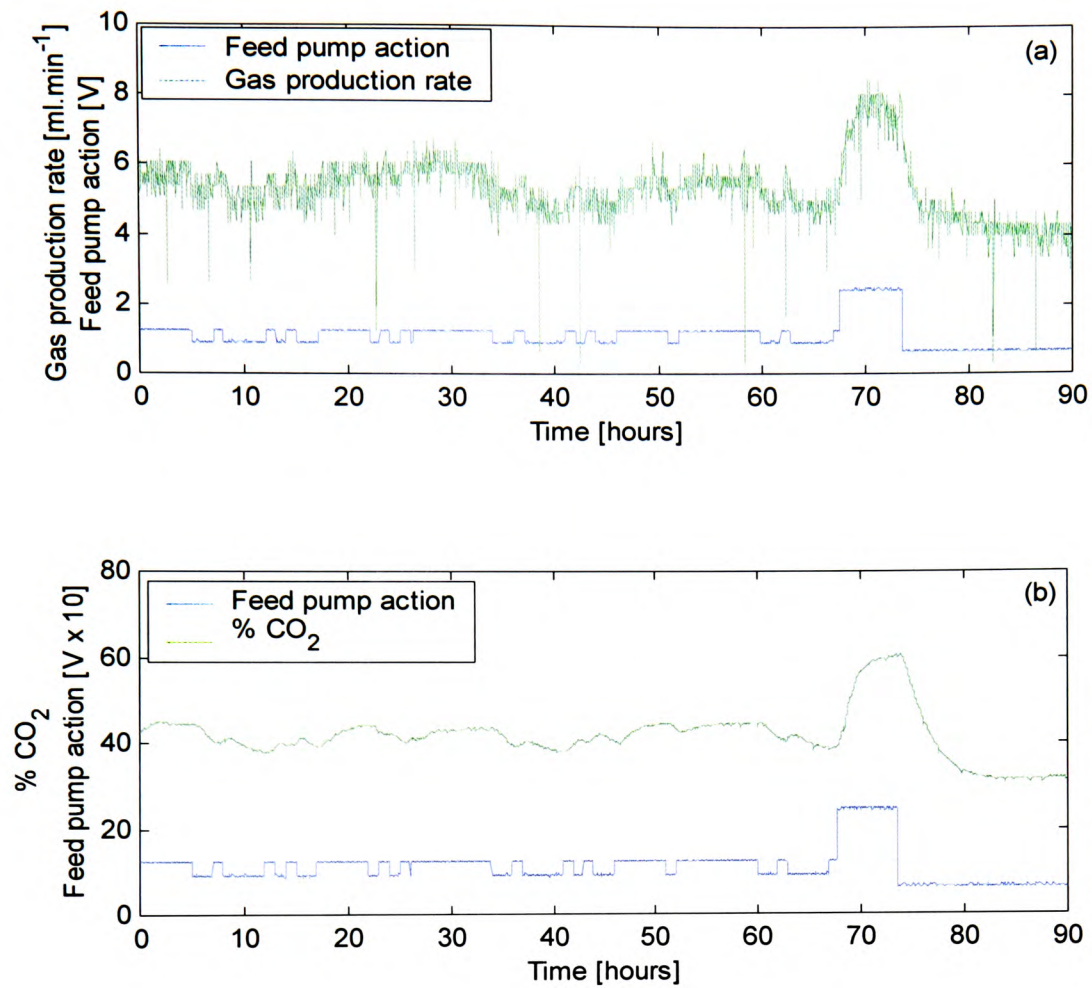
Figure 4.1.1 SISO black box modelling (Task 1), data for parameter estimation: (a) Gas production rate, (b) %CO₂
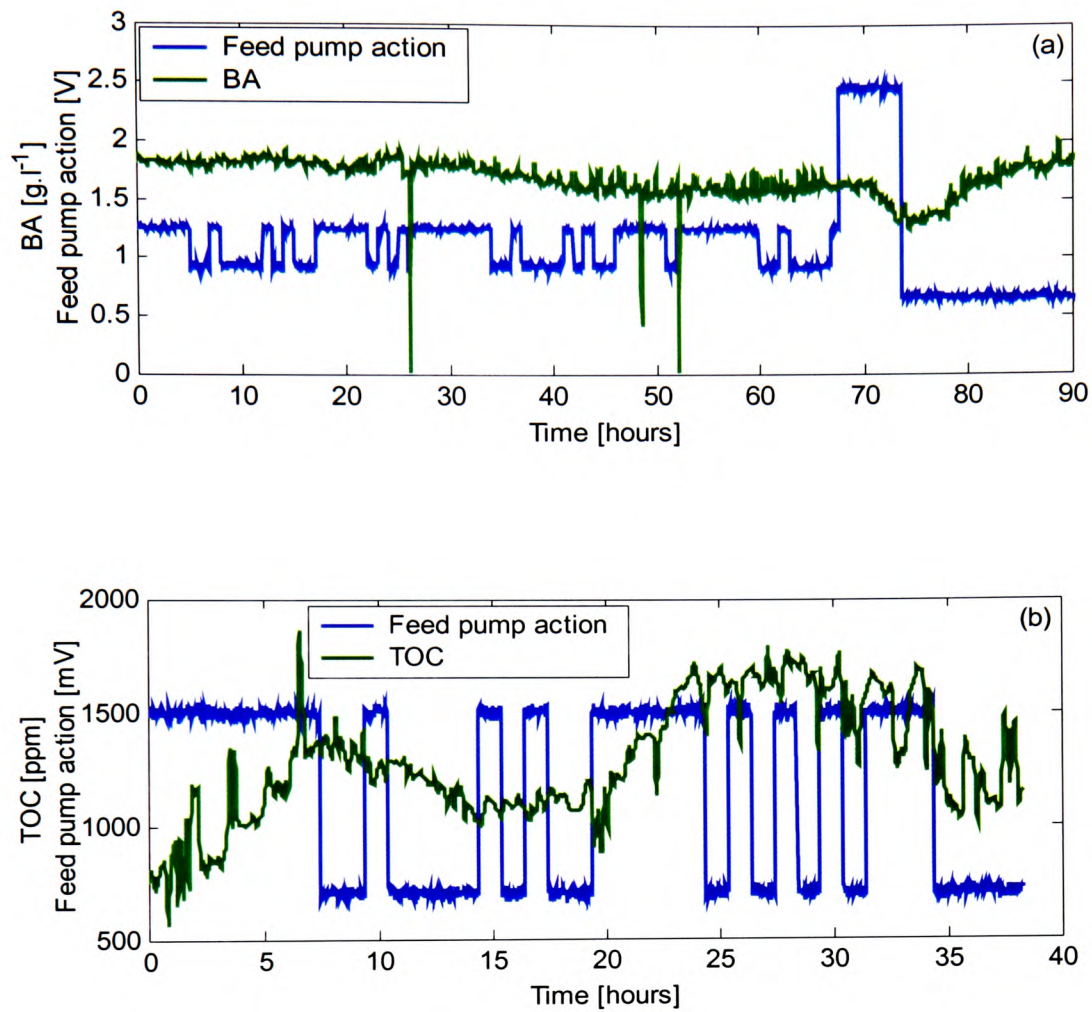
Figure 4.1.2 SISO black box modelling (Task 1), data for parameter estimation: (a) BA, (b) TOC
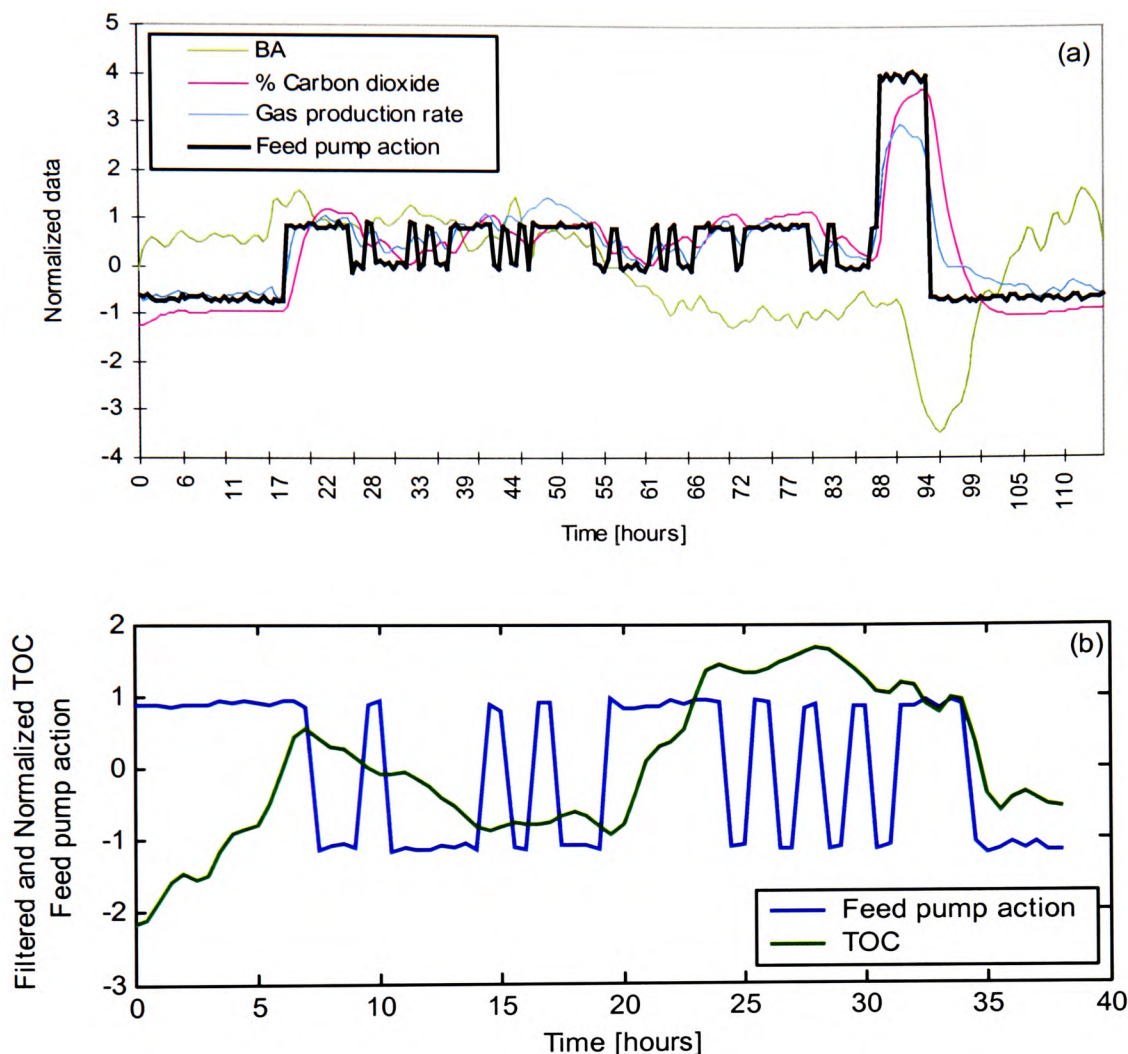
Figure 4.1.3 SISO black box modelling (Task 1), Filtered and normalised data for parameter estimation: (a) Gas production rate, %CO$_2$ and BA and (b) TOC

There would be little chance of extracting a comprehensive model for the process with such excitation, as there is a need to excite all the modes of the system. The disturbance which would yield sufficiently information rich data is known as *persistently exciting* and is essentially the only way to experimentally search the entire state space. This would require exhaustive testing and would include running the digester to failure. Not withstanding the limitations of the models derived from this lack of complete modal excitation, it was possible to make significant predictions of BA, % CO$_2$, gas production rate and TOC using independent (SISO) ARX black box models. All the models consisted of only second or third order

polynomials, with a single sample period delay between the input (loading rate) and the output (the relevant parameter e.g. BA). These are shown in Table 4.1, which includes:

- the mean and standard deviations used in normalising the data prior to the identification step

- the transfer functions and their polynomial coefficients and associated standard deviations (innovations variance)

- measures of quality of fit, namely the *Loss Function* which in the case of SISO systems, is the sample mean of the prediction errors and Akaike's Final Prediction Error (*FPE*) criterion (Equation 4.1.1).

$$FPE = \frac{1 + n/N}{1 - n/N} \times V$$

4.1.1

Where n is the number of estimated parameters, N is the length of the data time series and V is the quadratic fit loss function for the structure under consideration.

Table 4.1 ARX SISO models identified from data

Parameter	Normalisation parameters	Polynomial coefficients		Fit	Transfer function (with Feed pump action as input)
	Mean	B Coeff.	A Coeff.	Loss Fcn	
	SD	SD	SD	Akaike's FPE	
BA	1.7064	-0.0133 -0.0152	1.0000 -2.3277 2.1645 -0.8256	0.0079056	$\dfrac{-0.01333z - 0.01519}{z^3 - 2.328z^2 + 2.1645z - 08256}$
	0.1150	0.0123 0.0125	0.0333 0.0622 0.0344	0.0081459	
%CO₂	37.7881	0.0936 0.0092	1.0000 1.4833 0.5817	0.0014063	$\dfrac{0.0936z + 0.009214}{z^2 - 1.483z + 0.5817}$
	6.1471	0.0054 0.0075	0.0321 0.0270	0.0014404	
Gas production rate	46.1756	0.0336 0.0260	1.0000 1.7711 0.7901	0.014469	$\dfrac{-0.03362z - 0.02596}{z(z^2 - 1.771z + 0.7901)}$
	10.9628	0.0185 0.0194	0.0398 0.0430	0.014819	
TOC	1.2790×10^3	0.0309 -0.0178 0.0177	1.0000 -1.5554 0.5990	0.021109	$\dfrac{-0.03087z^2 - 0.0178z + 0.01769}{z(z^2 - 1.555z + 0.599)}$
	0.2468×10^3	0.0227 0.0249 0.0216	0.0995 0.0968	0.02404	

The model validation was performed using data (Figure 4.1.4) unrelated to the parameterisation date, either temporally or in terms of levels or nature of the excitation, as summarised in Table 3.3.2. Figure 4.1.4 (b) also shows the effect of filtering the TOC data, which was somewhat similar to all the other data streams.
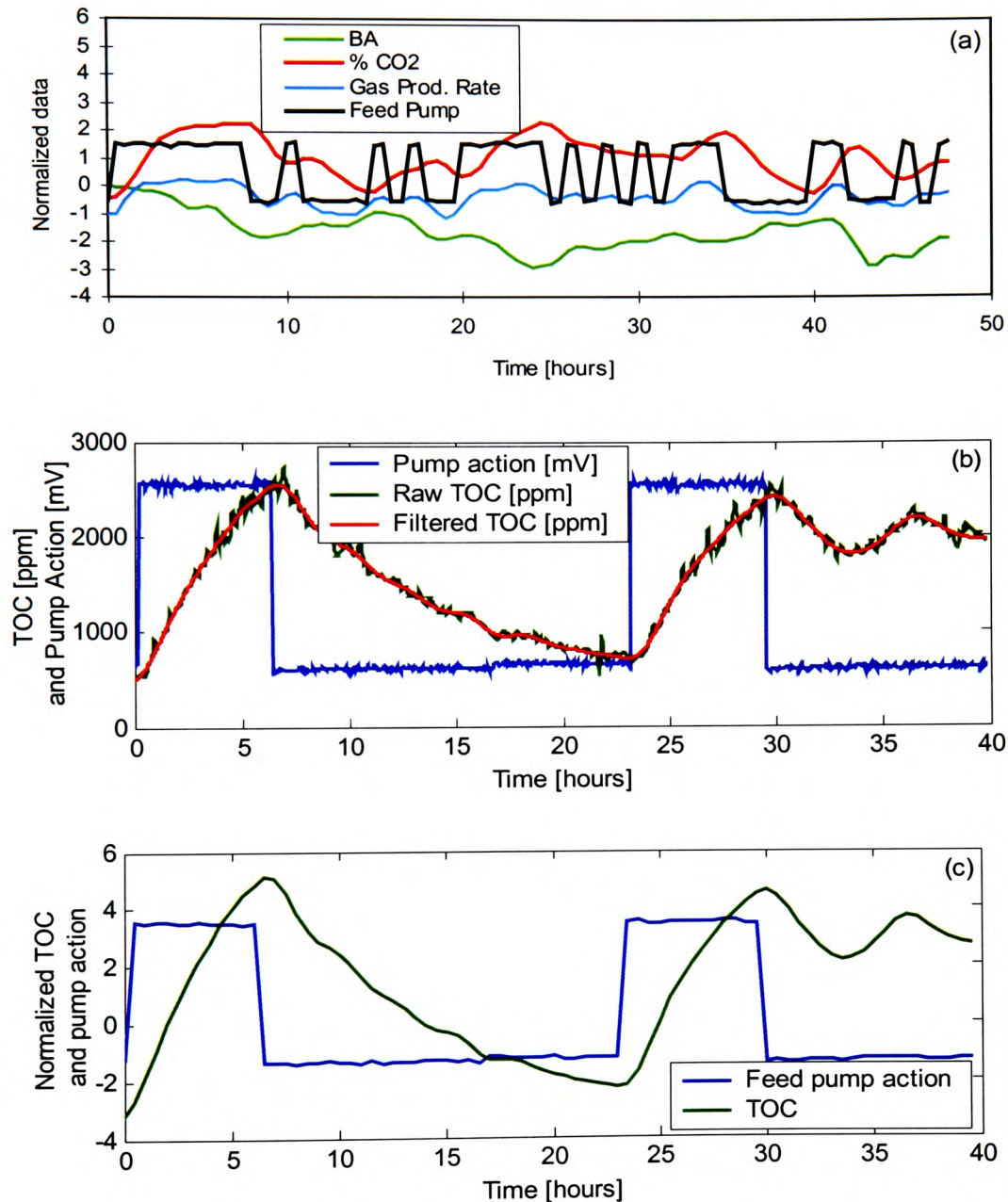
Figure4.1.4 Validation date for: (a) BA, %CO_2, and gas production rate and (b & c) TOC for the SISO ARX models, raw and normalised data respectively.
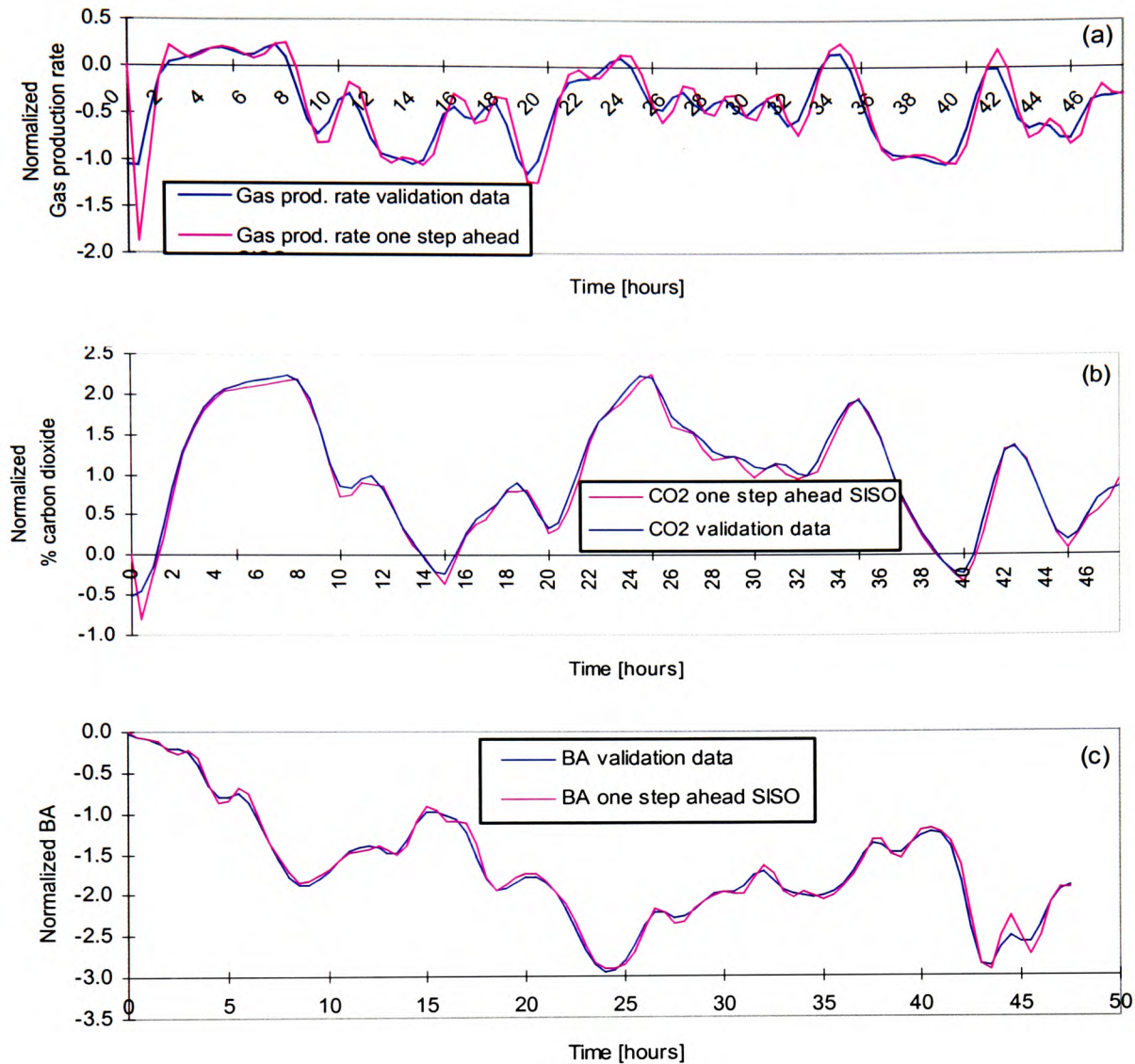
Figure 4.1.5 SISO black box modelling (Task 1), validation of (a) Gas production rate, (b) %CO$_2$ and (c) BA models, showing predictions 30 minutes ahead.

The predictions of the %CO$_2$, gas production rate and the BA models are shown in Figure 4.1.5. This indicates that it was possible to predict with a relatively high degree of accuracy the future value (30 minutes, one step ahead) when subjected to loads comparable though different to those used in the parameter estimation. This was despite the fact that the models were essentially structurally simple (ARX) and assumed to be totally uncoupled. Similarly in Figure 4.1.6, predictions of TOC using step changes greater than those used in the parameter estimation data and show again a relatively high degree of accuracy. When the models for the other parameters, BA and gas production rate, where similarly tested with the large step change (Figure 4.1.7),

similarly accurate predictions were obtained. In validation, no attempt was made to match initial conditions, but instead, account should be taken of this when assessing the predictions.

The horizon over which predictions are made (30 minutes) is considered to be ample in terms of time required to execute recursive parameter estimation for such linear models with a view to their use in a MRAC scheme similar to that proposed by Emmanouilides and Petrou (1997). However, consideration is given here to using a linear model as the reference model instead of a neural network as these have inherent problems of initial training and subsequent recursive parameter (weights and biases) estimation. It was found that looking more than one step ahead leads to a progressive deterioration in accuracy of prediction when using the above black box models.

The validation data sets were chosen to force the models to predict at operating conditions which were not used in the parameter estimation, which would, if non-linearity were significant, cause the model to deviate in its predictions. The non-linear nature of the process was found to have little effect over the operating conditions investigated. Also, when considering the variation of the process with time, separating the parameterisation data from the validation data (1-2 months) was not sufficient to cause the models to predict badly. It thus appears that simple, linear, independent black box models of gas production rate, $\%CO_2$, BA and TOC are able to represent the AD process under the conditions tested with an accuracy which may be sufficient as the basis for process controller design. It should be noted however that the models were dependant on very recent online data of both the feed pump action and the corresponding measured variable (BA, $\%CO_2$ etc.), in order to achieve the accuracy described. The prospect of predictions over very large time horizons, using only past predictions to replace real data would not yield similar accuracy and is discussed further in Section 4.1.2.
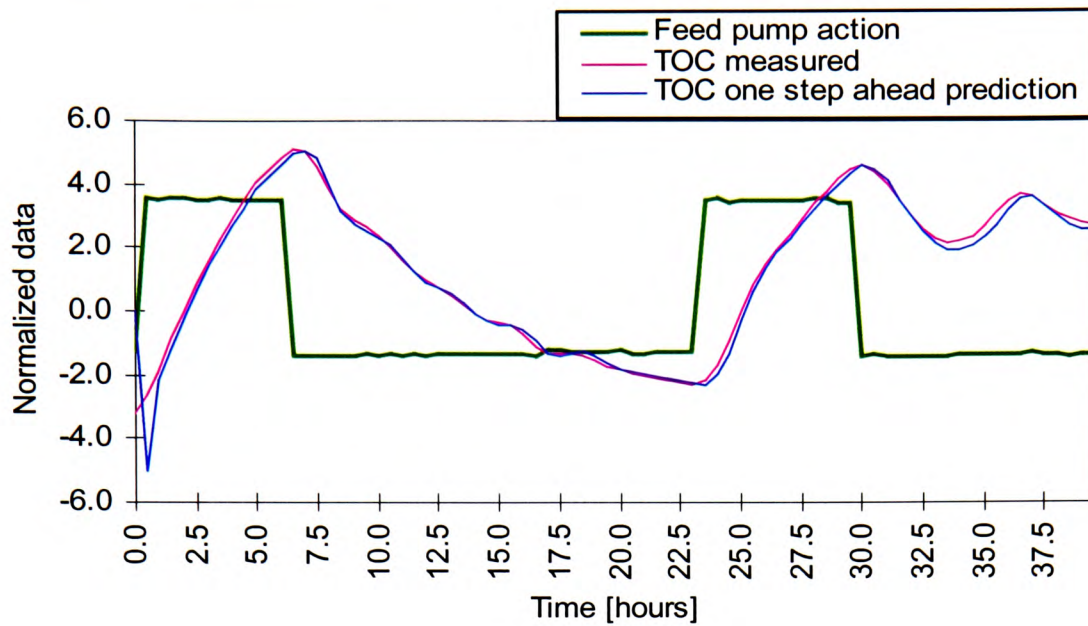
Figure 4.1.6 SISO black box modelling (Task 1) validation of TOC model, showing predictions 30 minutes ahead.
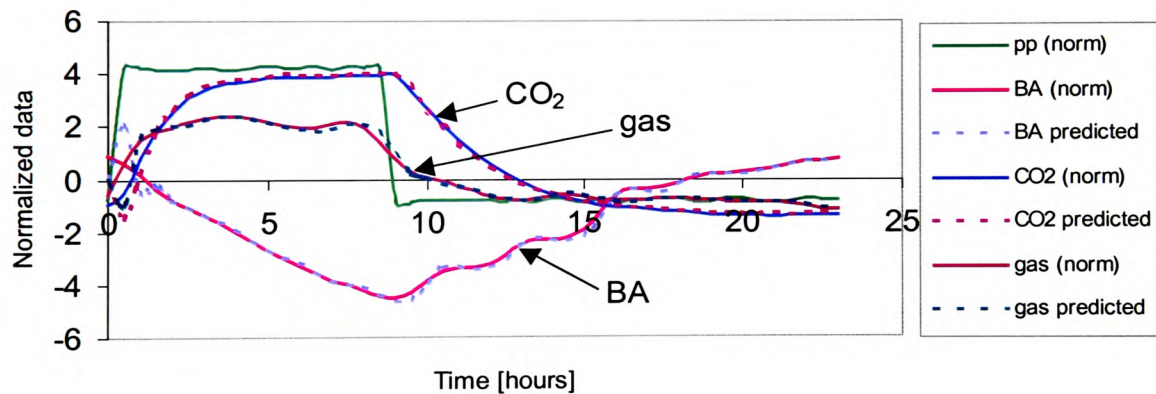
Figure 4.1.7 SISO black box modelling (Task 1), validation of gas production rate, BA and %CO_2 models, showing predictions 30 minutes ahead.

4.1.2 The comparative performance of SISO, MIMO and Neural Network black box models of ARX structure (Task2)

This work is seen as a continuation of Task 1, where the analysis looked at four key parameters (Gas production rate, %CO_2, BA and TOC), using SISO ARX models. Task 2 seeks to investigate different models applied to all but the TOC parameters. The justification for this is that TOC was

not of primary concern in the control study and its measurement on-line caused difficulties. The question posed by the author was... would the adoption of increased complication in the ARX models by way of coupling the parameters or the introduction of non-linearity, improve their ability to predict reactor parameters over different time horizons?

The choice of say, second order functions in the delay operator (z^{-1}) means that the models have a regression vector looking back over two samples, which at a sampling time of 30 minutes, will include data collected over an hour. Increasing the order of the models excessively would be likely to lead to lower normalised sum of squared errors (NSSE's), or error function, but would to an increasing extent cause over fitting to the data and hence the model would not represent the underlying dynamics of the process. The dimensionality of the neural network model is also dependent on the size of the parameter vector (i.e. the number of weights and biases) so is not directly comparable with the linear models, although significant similarity exists, as shown in Equation (3.3.8). The technique employed by Norgaard (1995) to determine the length of the regression vector, was to calculate the index of He and Asada (1993) and to look for a knee point in the index, beyond which, increasing the regression vector would have little effect. More weight was given to the insight obtained by investigating the responses of the process to a step input, which on a heuristic level appeared similar to over damped second or third order systems.

The sampling time of 30 minutes is considered to be relatively short, however a compromise was sought between that suggested by the process dynamics and that suggested by the dynamics of the slowest instrumentation (bicarbonate alkalinity monitor of Guwy et al. (1994)).

The time varying characteristics of the fluidised bed reactor are not known, so the time lapse between the data sets for training and validation were a matter of judgement. It is of course possible that the data selected, was not separated sufficiently in time to account for microbial population changes, or that the populations were by chance similar in their dynamics for both sets of data. The time variance was assumed to be unpredictable, though dependent on the reactor's operating history (loading, environmental and inhibitory episodes). Variations over time in parameters such as biomass yield or endogenous decay coefficients, were assumed to be small and as such could be treated as system disturbances. Furthermore, it was assumed that the loading regime, which extended over approximately 3 months, was sufficiently varied so as not to favour the development of specialised (and perhaps fragile) consortia of microbial populations. Figures 4.1.8 to 4.1.10 show the BA, %CO_2 and gas production rate, one-step-ahead predictions, (for the three alternative ARX models investigated), compared to the measured validation data set. It

would be possible to compare the model predictions to the parameter estimation/training data, however one would expect a good fit in this case as the objective is to minimise the sum of the errors squared. The validation set is of key significance, as it indicates the ability of the model to generalise, (or represent an 'unseen' data set). The validation data and the corresponding predictions seem at first sight to be very close to each other, which is often the case with one step ahead prediction where the step size is of relatively short duration. It is difficult to assess the performance of the model by looking at such plots and statistical techniques are normally employed. Figures 4.1.8 to 4.1.10 do indicate however, the excellent predictions achievable with short temporal prediction horizons.

Non-linear (Neural Network) ARX Model for Bicarbonate Alkalinity—The neural network regressors were chosen to be the same as those used for the linear ARX model, these being 2 previous inputs, 2 previous outputs and a single delay. The architecture of the network was initially a fully connected feed-forward network, with one hidden layer of 10 hyperbolic tangent activation function neurones and an output layer of one linear activation function neurones.

The predictions obtained from this model, (when considering the auto-correlation of residuals and cross-correlation of the input to the residuals, which are explained below) were poor. The auto-correlation, in particular, remained consistently outside the 95% confidence band, implying that the model was over-fitting the data. The solution proposed by Norgaard (1995) is to reduce the dimensionality of the network by applying an OBS (Optimal Brain Surgeon) algorithm, which is used to 'prune' the weights to the point where near-optimal results are obtained. This involves retraining (for a limited number of epochs) the network, as its structure is altered by removing a single weight at a time, and keeping track of test errors, to see at which point they are minimised. In so doing, the predictive performance of the neural model was improved significantly, and the results are shown in Figure 4.1.8 to 4.1.10. The model structure was reduced to eight weights in total for the bicarbonate alkalinity neural model.

Non-linear (Neural Network) ARX model for % CO_2 and gas production rate—A similar procedure was followed for these data streams, with similar results, although in both cases, the number of weights left after pruning was almost double that of the bicarbonate alkalinity.
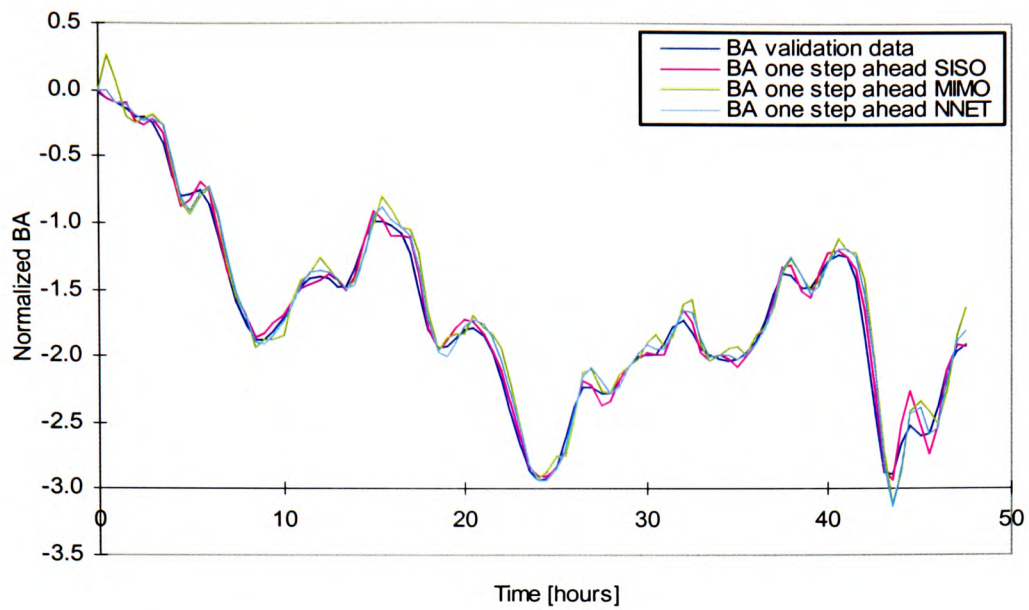
Figure 4.1.8 Bicarbonate alkalinity predictions for ARX models.
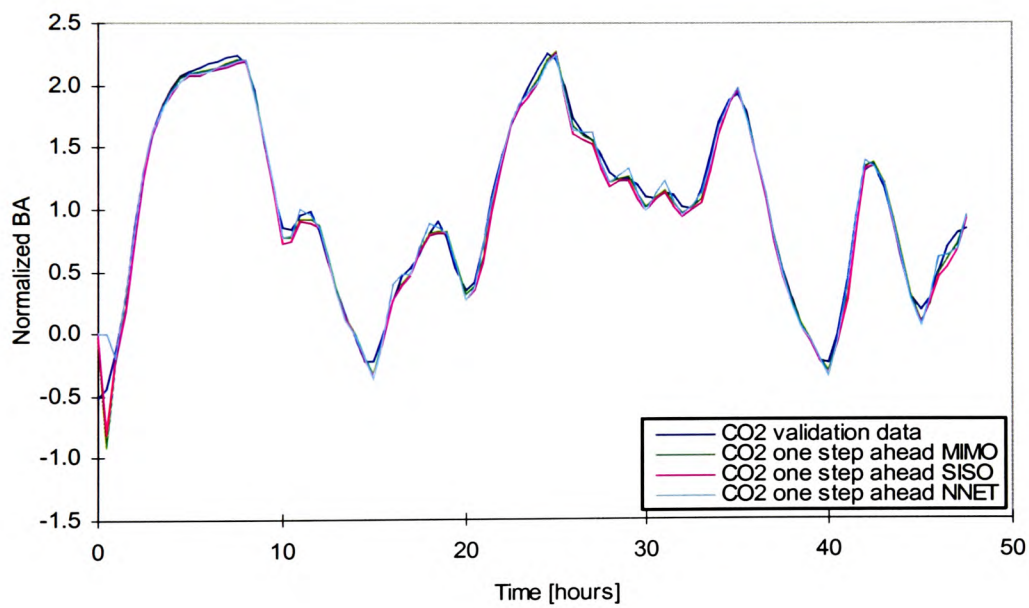
Figure 4.1.9 %CO$_2$ predictions for ARX models.
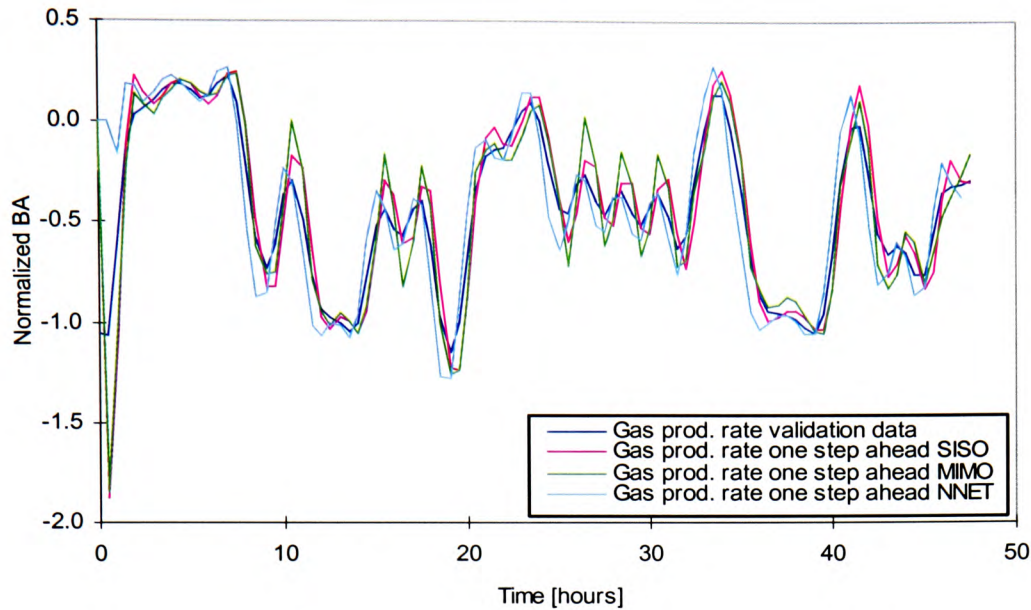
Figure 4.1.10 Gas production rate predictions for ARX Models.

Correlation analysis

For the purposes of comparison, it is necessary to consider measures of performance from one model structure to another. Investigations of non-linear ARMAX (Auto Regressive with Moving Average and eXogenous input) model performance, using synthesised and experimental data, were conducted by Chen *et al.* (1990), who applied a number of statistical tests which were based on correlation analysis and the Chi-squared tests. It is common in system identification to consider the correlation analysis as the primary measure of model performance in particular the auto-correlation of the residuals (errors between predictions and real validation data), and the cross-correlation of the input (feed pump action) and the residuals.

The auto-correlation function of the residuals should ideally resemble an impulse. This would indicate that the residuals are 'white', i.e. no correlation exists between the residuals and any time shifted replica of the series. There should also be, according to Chen *et al.* (1990), no correlation between the residuals and any linear or non-linear combinations of past inputs and outputs.

If the identification of an ARX model were successful then one would expect the residuals to be unpredictable. The predictability and hence deviation from optimum can be assessed by using correlation analysis. Specifically the auto-correlation of the residuals should exhibit correlation only when the time series are not time shifted (one to the other). Similarly, in cross correlating, no correlation should exist between the residuals and the systems input signal (feed pump action).

If the correlation functions are within a confidence interval of 95% of the conditions mentioned, then it is reasonable to accept the model as a fair representation of the system.

A comparison of the predictions produced by the models was performed, by analysing the residuals. The results for bicarbonate alkalinity, $\%CO_2$ and gas production rate, are presented in Figures 4.1.11 to 4.1.13 respectively. It can be seen from these figures that the SISO ARX model fails to achieve the 95% confidence criteria for $\%CO_2$, although it gives adequate results for the BA and gas production rate. Comparing the MIMO ARX to the neural network ARX model, it would seem that the former is able to represent the system with inferior accuracy in the case of BA and better accuracy for $\%CO_2$ and gas production rate. While it may be possible that the neural network could be improved by optimising the training process and network structure iteratively, the same can be said for all the models. It is not clear to what extent the models are optimised, which is usually the case in identification.

The underlying biochemical processes point to there being significant coupling in the data streams measured. It is perhaps not surprising therefore that the MIMO and neural network models which both include cross coupling, out perform the linear SISO model overall, with the $\%CO_2$ for the latter being significantly outside the confidence limits.

It is worth restating, (in order to highlight the increased computational effort), that in order to obtain the performance presented here, when using the neural network ARX model, a pruning algorithm was employed. This reduced the number of weights and biases so that the model did not over fit the data. Prior to its use the results from the correlation analysis were consistently outside the 95% confidence limits.
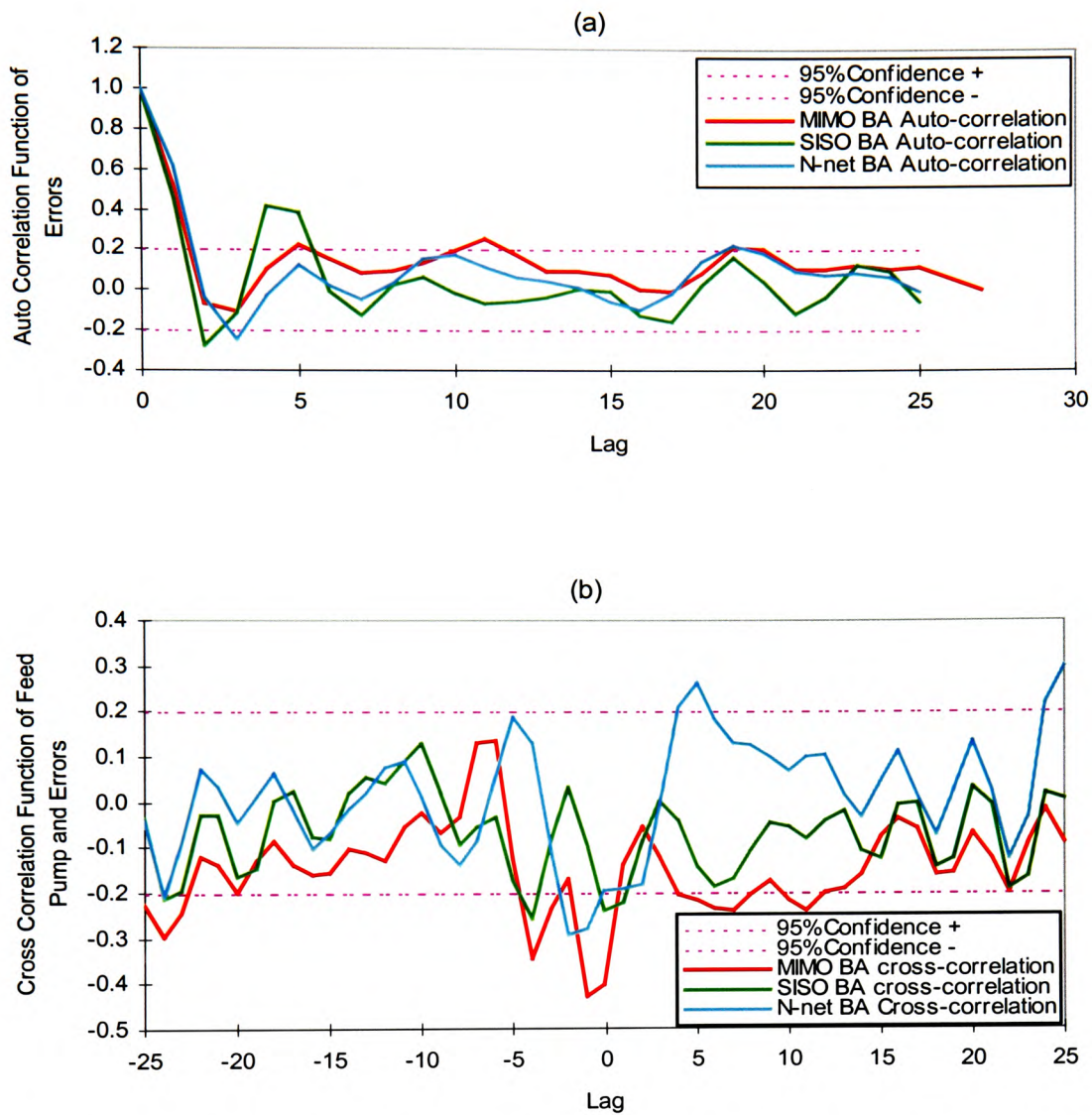
Figure 4.1.11 Correlation Analysis for Bicarbonate alkalinity using non-linear, MIMO and SISO ARX models.

(a) Auto-correlation of residuals from prediction of validation data.
(b) Cross-correlation of feed pump action to the residuals from prediction of validation data.
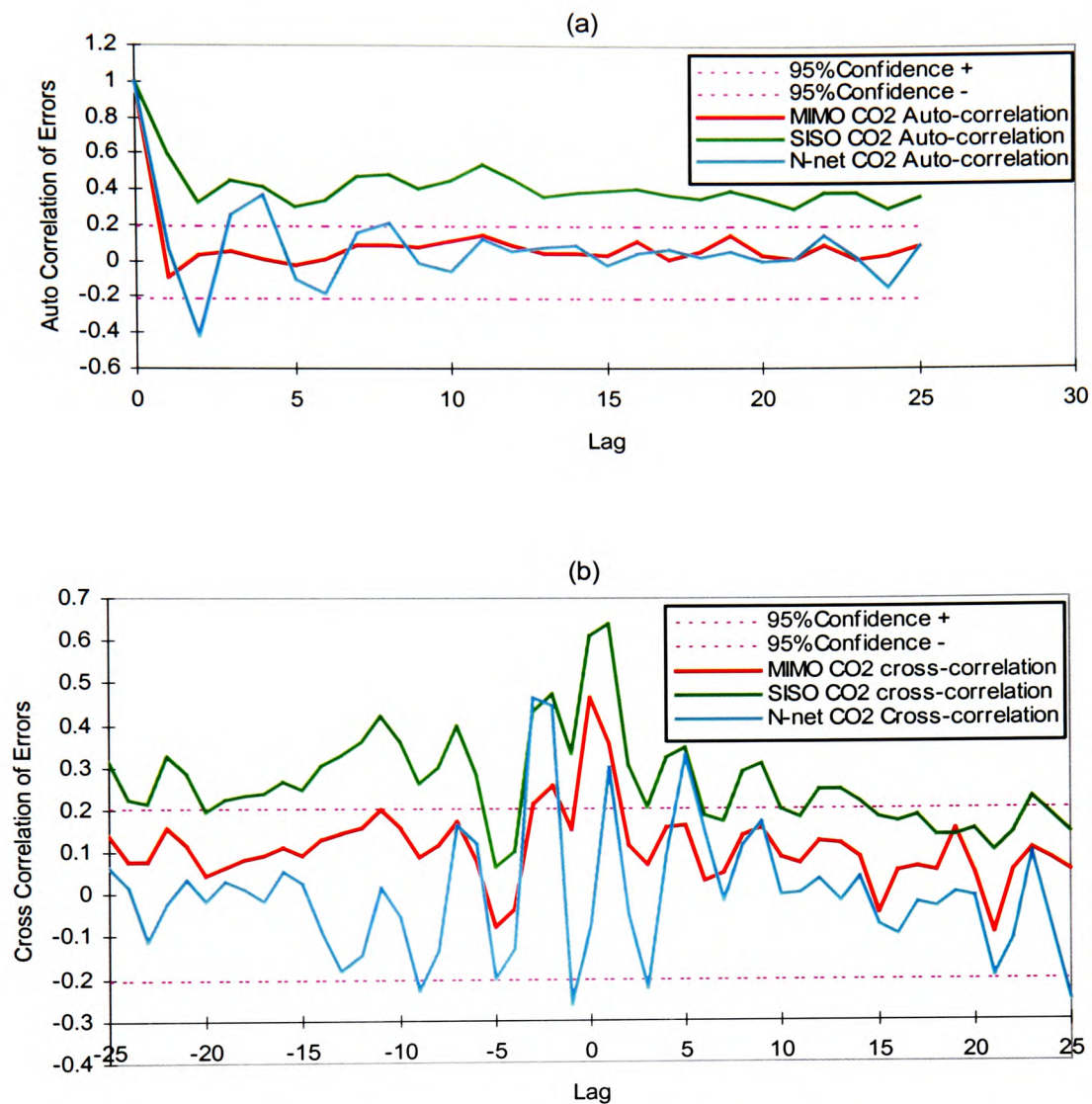
Figure 4.1.12 Correlation Analysis for % CO$_2$ using non-linear, MIMO and SISO ARX models.

(a) Auto-correlation of residuals from prediction of validation data.
(b) Cross-correlation of feed pump action to the residuals from prediction of validation data.
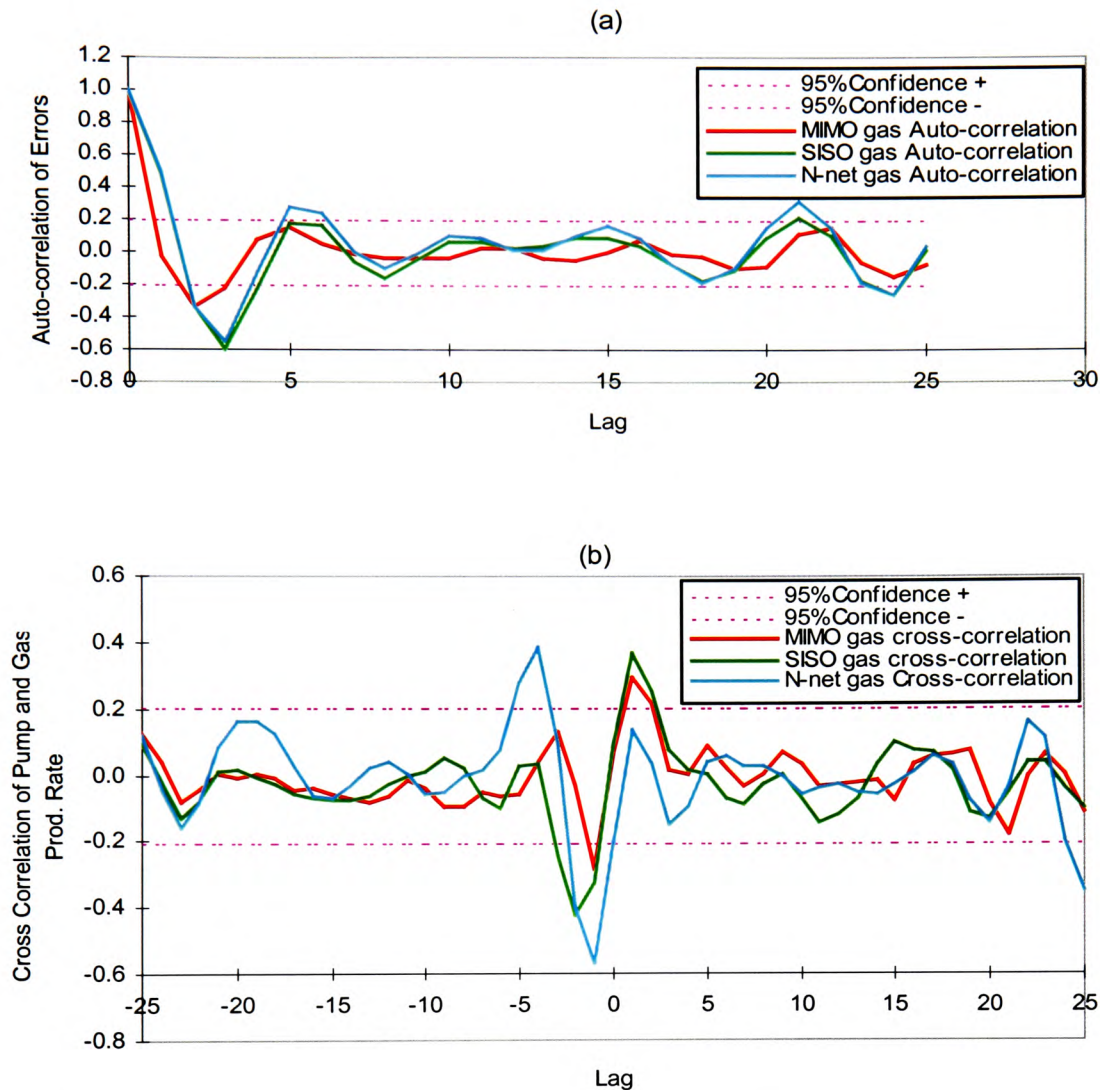
Figure 4.1.13 Correlation Analysis for Gas Production Rate using non-linear, MIMO and SISO ARX models.

(a) Auto-correlation of residuals from prediction of validation data.
(b) Cross-correlation of feed pump action to the residuals from prediction of validation data.

Given that the MIMO model is generally less complicated than the non-linear neural model, while producing comparable predictions, its use should be considered with some favour. To investigate the behaviour of the MIMO model, it is useful to consider its performance in predicting over a long period of time. Figure 4.1.14 presents a pure simulation using the MIMO ARX model, which uses only initial (input and output) data as starting conditions and from then on uses the predicted data and the input (feed pump action) in order to predict subsequent steps ahead. If the MIMO model were a perfect representation of the data generating mechanism of the anaerobic process, then the predicted response would be coincident with the validation data. It is unlikely that this

would be achieved as the model is LTI and is attempting to represent a non-linear process. It is only feasible with the one step ahead prediction because this technique is essentially a piece wise linearization of the process dynamics by continually using the most recent measurements in making a prediction a short step in time ahead. Having accepted the limitations of a pure simulation, the general behaviour (rather than the absolute values) indicate that the model is at least similar dynamically to the anaerobic process under consideration. The least accurate predictions are those for bicarbonate alkalinity (Figure 4.1.14 (a)) which indicates significant deviation after about 15 hours. It is possible that the prevailing bacterial stress levels of the validation data set were higher than those produced by the parameter estimation data set. This fact is supported in part by the bicarbonate alkalinity time series of the parameter estimation data set reacting after a delay of circa 5 hours, (which is most visible after the final over load at 90 hours on Figure 4.1.3 (a)). The response of the bicarbonate alkalinity to the end of the over load is much quicker, with a delay of less than 1 hour. The implication is that the biological system is able to cope with the increased loading rate for about 5 hours before the bicarbonate alkalinity starts to reduce. In the case of the validation data set however, the bicarbonate alkalinity begins to reduce more rapidly, indicating that the system is less able to generate bicarbonate alkalinity. The delay, (which may vary within each data set) is therefore built into the ARX models through the parameter estimation data and is an example of the time variance of the system.
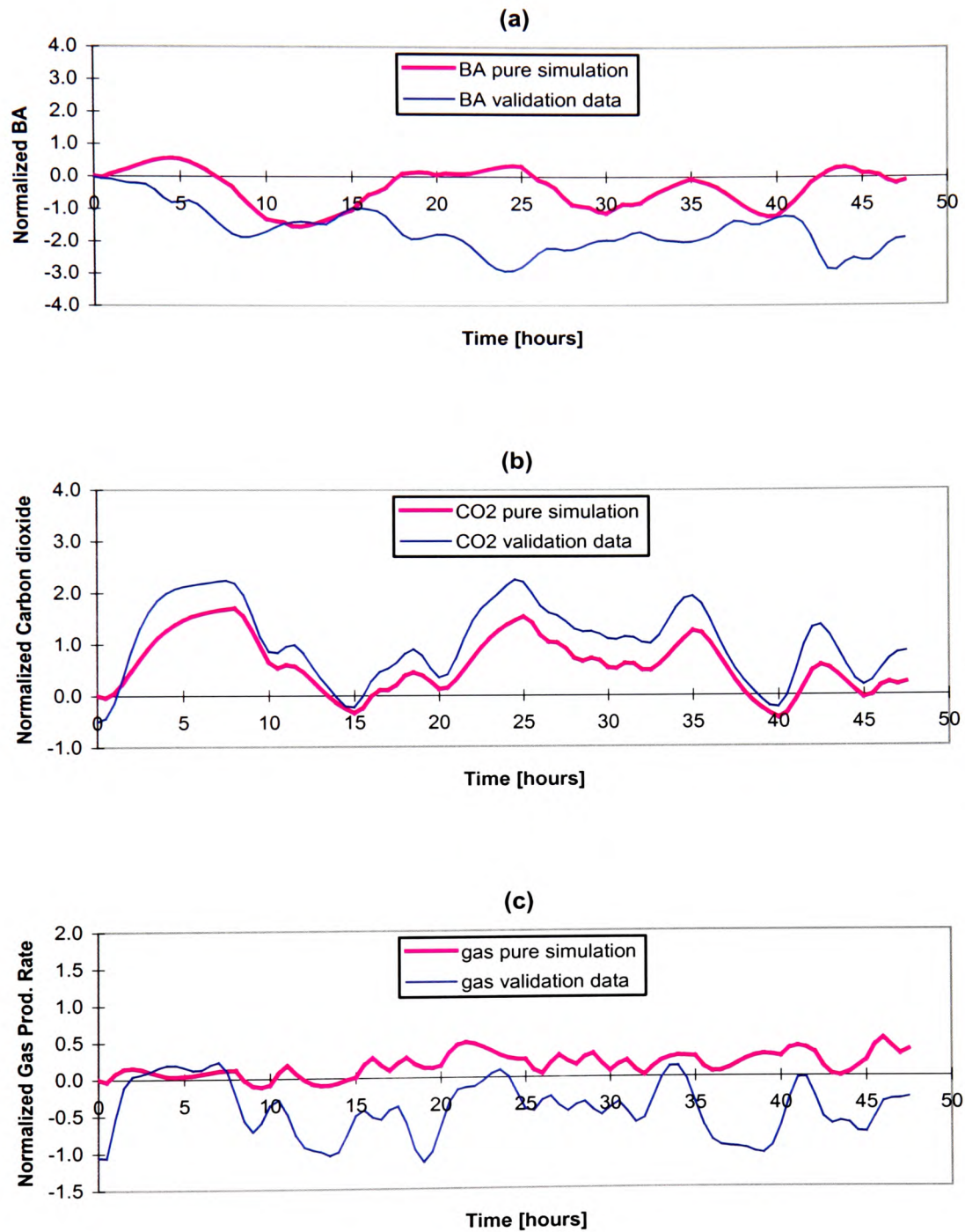
Figure 4.1.14 Comparison of validation data with predictions from a pure simulation, using the MIMO ARX model.

(a) **Bicarbonate alkalinity**
(b) **%CO$_2$**
(c) **Gas production rate**

The ARX model structure pre-supposes that the noise is filtered when passing through the system, by a transfer function, which has the same poles as the ARX model. If this assumption is not valid, the resulting model accuracy is deleteriously affected. There is no simple means known to the author for determining the consequence of the noise filtering, other than observing the performance of the model that results and determining if the model is 'good enough'.

Of the three ARX models that have been presented, all were parameterised and validated using the same data and in an attempt to make the resulting models comparable, the regression vectors (past data samples) were the same for all the models and all the data streams. While it is not claimed that the models were in any sense optimal, the approach of maintaining constant those parts of the identification procedure which were common to all models, has produced results which may form the basis of a selection procedure with respect to the three model structures used.

It can be seen that the performance of the MIMO model was superior to that of the SISO and comparable with the Neural Network approach when considering the 95% confidence intervals on the correlation analysis of the residuals. Overall, the neural network had higher performance than the linear models, however the added complexity of the neural network model and associated identification process is not considered to warrant its adoption, unless the accuracy of the model is a paramount factor. If recursive identification is to be performed, where the neural model would require repeated retraining, it is likely that the improvement in performance indicated by the results, may lead to the computing overheads becoming a significant mitigating consideration. Not only would the training of the network require a considerable number of presentations of the data (epochs), but a large amount of training data would be needed to ensure adequate training. There are in contrast, well established recursive identification algorithms used in linear black box techniques which require very little historical data to be stored and are fast in their execution, (Soderstrom and Stoica (1989)). There are however training techniques which significantly increase the speed of training neural networks, such as that proposed by Venugopal and Pandya (1992), and provided the sampling time is similar to that chosen in this work, processing time should not be a significant problem with modern computers.

The key issue in deciding to adopt a black box approach to the representation of the AD process during the controller design task is that the pure simulation performance of the ARX model, regardless of detail, is poor. Significant deviations are evident after a relatively small period of time. The design of a control strategy and its subsequent optimisation depend on a representative model, which the ARX models (at least in pure simulation) are not thought to be. In a situation

where the model is employed in on-line identification, then the ARX structure does appear to be useful and judging by the above comparison, any of the model structures could give useful performance.

4.2 A SIMULATION STUDY USING DETERMINISTIC MODELS (TASK 3)

The behaviour of the BA and other parameters within the AD process while the system is under control is not totally intuitive. The complex interactions (or couplings) between the differential and algebraic equations make it difficult to foresee the long-term behaviour of the process. It was considered necessary to run simulations, which would consider key parameters over a period of about 2 months.

- The first simulation sought to investigate a relatively relaxed control strategy which, as a consequence, demonstrates a notional lower limit of likely behaviour, which could then be compared to the more aggressive control derived from the numerical optimisation procedures used.

- So the second simulation looked at the most severe controller generated during the optimisation procedure.

- The third simulation sought to explain the reason for oscillatory behaviour in the experimental work and verify that unmodelled dynamics and transmission delays in the software communications caused this behaviour.

4.2.1 Effects of a relatively relaxed control strategy on the AD process

The simulation that was considered in this section was conducted using the model shown in Figure 4.2.1, which is included in Appendix A as a Simulink™ model (ControlSimulationModel_1.mdl). The control strategy was based on the MRAC architecture, which was the focus of this thesis, but used a heuristically parameterised P+I adaption mechanism and a reference model, which was undemanding and corresponded to an equivalent first order dynamic with a 5-hour time constant. The parameter vector for proportional and integral action respectively was [-10.0 -1.0]. The controller set point was placed at 1700 mg.l^{-1}CaCO$_3$ equiv., to which was added a Gaussian disturbance with zero mean and a variance of 500 mg.l^{-1}CaCO$_3$ equiv. at a sample time of 10 hours (i.e. this random disturbance changing every tenth hourly sample). The initial conditions of the concentrations of the bacterial populations in particular were considered. This set of simulations showed that the initial conditions, with respect to the concentrations of acidogens and methanogens, had a critical effect on the steady state concentrations of the same and on the time taken to achieve this, as might be expected.

Figure 4.2.1 Simulation of an MRAC controller using P+I adaption mechanism to investigate the behaviour of the BA when feed rate actuation is in use.

Figure 4.2.2. shows the consequences of altering the initial bacterial population concentrations, when under the control of the regime described by Figure 4.2.1. The variations in concentration are relevant to the inoculum in particular, which can conceivably have very variable and often unpredictable concentrations of acidogens (Xa) and methanogens (Xm) depending on the history and source of the sample used as an inoculum. The four plots in Figure 4.2.2 all depict the same parameters (reference model output, BA set point including the Gaussian disturbance and the (would be) measured BA). It can be seen that with starting conditions of Xa=1500 mg.l^{-1}and Xm=1500 mg.l^{-1} (Figure 4.2.2 a)), the BA begins to saturate after 1000 hours because the maximum feeding rate (Sin) is reached. At this point the controller adaption would continue to 'wind down', as is evident from Figure 4.2.3 and some mechanism such as a limit on the adaption rate would be necessary to avoid this situation. Figure 4.2.3 also shows that the biomass concentrations saturate when their respective substrates are depleted due to the limited control action (loading rate). Lower initial bacterial concentrations such as in Figure 4.2.2 b), lead to slow growth rates, particularly for the methanogenic bacteria, with slow increases in control effort and hence feeding (Sin), as can be seen from Figure 4.2.4. If the concentration of methanogens is comparatively low as in Figure 4.2.2 c), the feed rate evidenced by the control effort, increases at a low rate (Figure 4.2.5), with the methanogen concentration being the limiting factor once more. If the converse is true, with high concentration of methanogens compared to acidogens, then the saturation of the control effort, feeding and BA in the reactor, occurs rapidly, (Figures 4.2.2. d) and 4.2.6). Determination of the relative, active proportions of the bacterial groups and their absolute concentrations is difficult and seldom done industrially, though measures are possible, such as the Biological Methanogenic Potential (BMP) where the specific production of methane is measured. As this is unlikely to be known in industry, it was not considered in this work. Figure 4.2.6 shows a rapid and somewhat spurious increase in all parameters but the adaption rate and volatile acids, which do the reverse. This is thought to be caused by mathematical instability in the model and cannot be ascribed to any biochemical phenomenon.
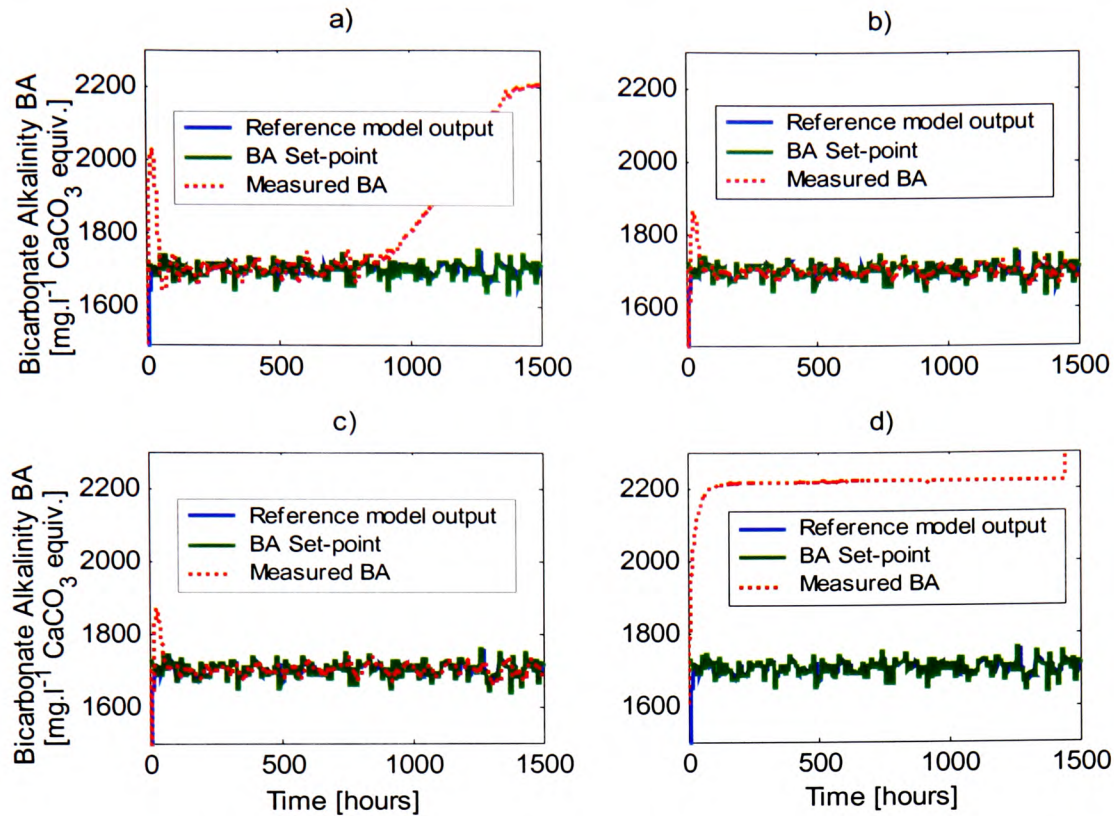
Figure 4.2.2 Simulation with P+I adaption mechanism showing the effect of altering bacterial concentrations on Reference model output, Set-point and Measured BA.

a) Initial conditions, Kp=-10, Ki=-1; Xa=Xm=1500 mg.l^{-1}
b) As a) but Xa=500 mg.l^{-1} and Xm=100 mg.l^{-1}
c) As a) but Xa=2000 mg.l^{-1} and Xm=100 mg.l^{-1}
d) As a) but Xa=200 mg.l^{-1} and Xm= 3000 mg.l^{-1}
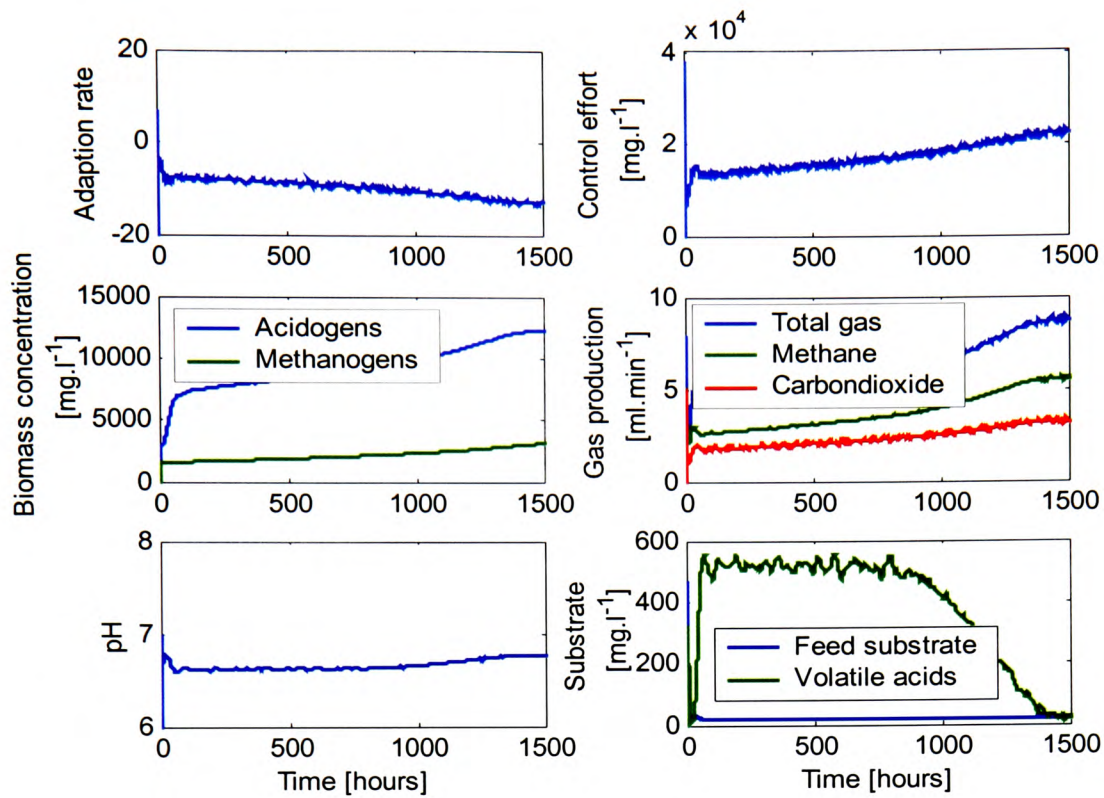
Figure 4.2.3 Variations in associated parameters for Figure 4.2.2 a)
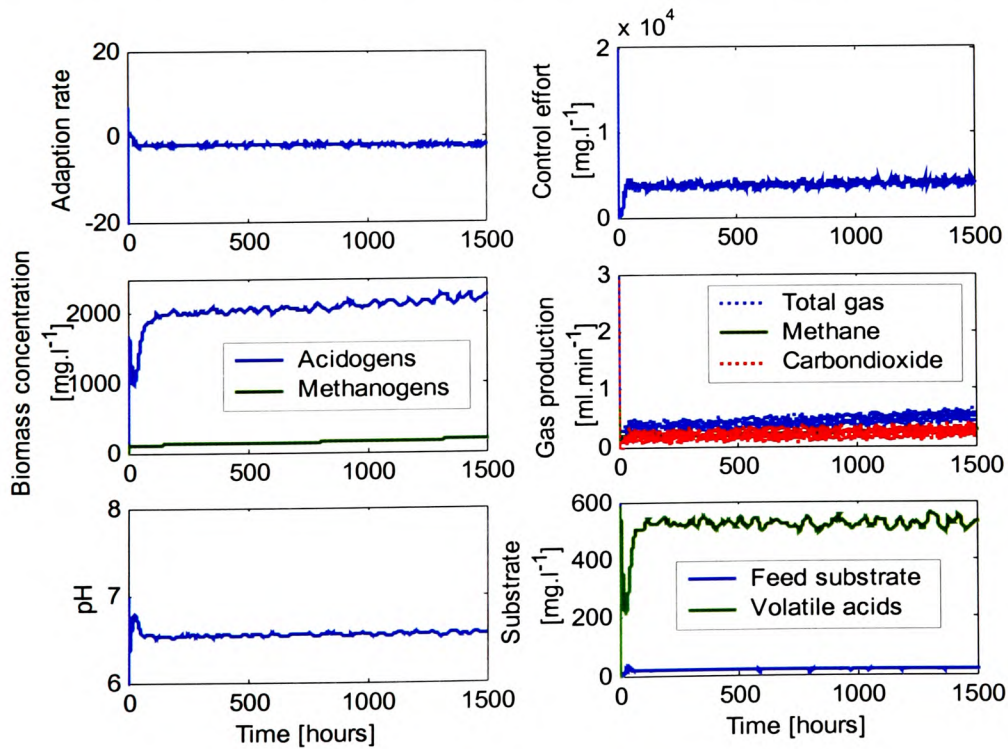
Figure 4.2.4 Variations in associated parameters for Figure 4.2.2 b)
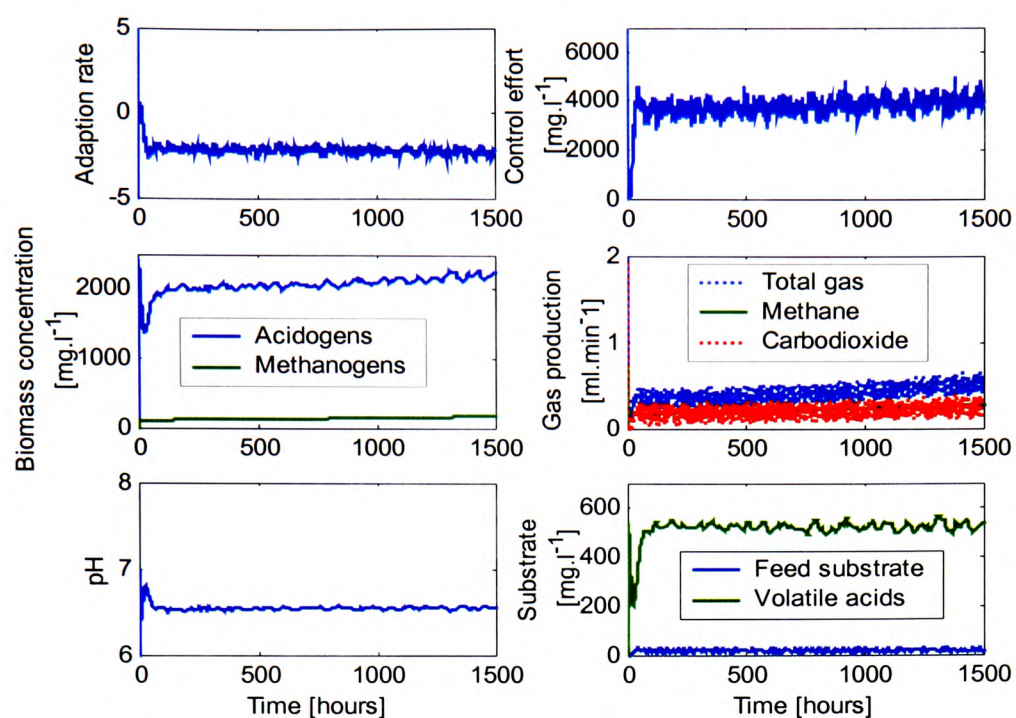
Figure 4.2.5 Variations in associated parameters for Figure 4.2.2 c)
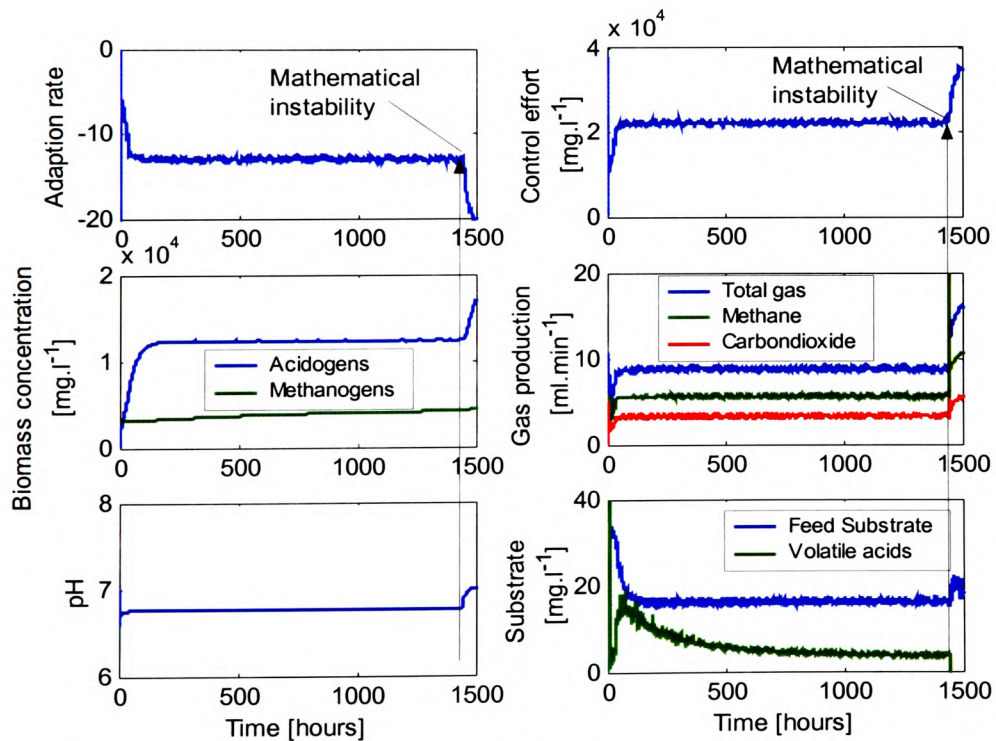
Figure 4.2.6 Variations in associated parameters for Figure 4.2.2 d)
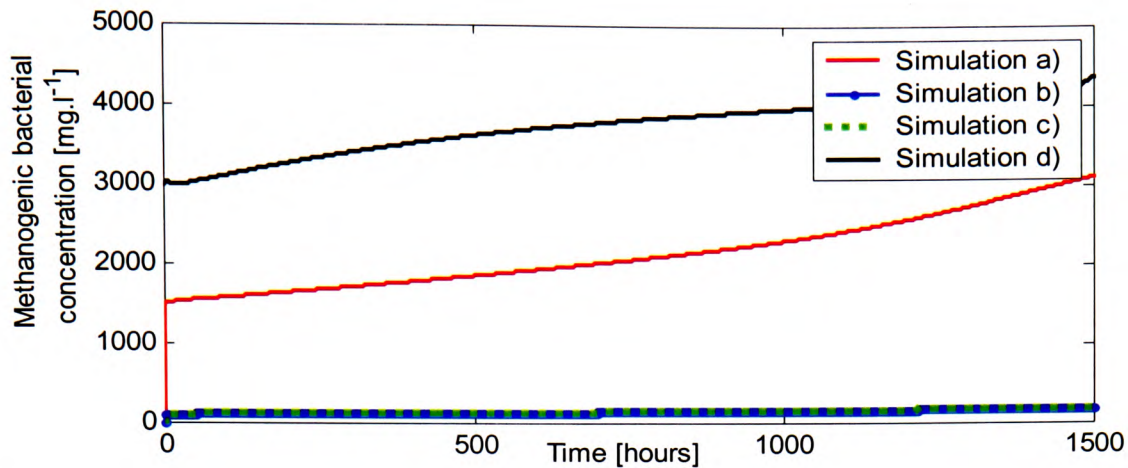
Figure 4.2.7 Methanogenic bacterial concentration for the simulations of Figure 4.2.2 a) to d)

Figure 4.2.7 considers the concentration of methanogenic bacteria, as they have been shown to be the limiting population which govern the rate of increase of the control action and hence the feeding rate. The populations of these bacteria depend greatly on the initial concentration (over the time scales observed) and the simulation of Figure 4.2.2 d) indicates the highest final concentration even if the excess due to mathematical instability is removed. Simulation a) by contrast has the highest rate of increase at the end of the trajectory, but has a magnitude of the order of 100 mg.l^{-1}. below simulation d). The steady state concentrations will probably tend to converge in these simulations, though the time required to do so may be many months in the worst cases. It is therefore obvious that the highest population of methanogenic bacteria should be present at start-up in order that it should be rapid. However the simulation gives an indication of how long it could take before a 'full' population is established.

4.2.2 Comparison of two control strategies of differing structure and specification, on the AD process

If one compares the relaxed model of Figure 4.2.2 with the most aggressive parameterised model generated by the optimisation procedures described in Section 3.4.3, and shown in Figure 4.2.8, (ControlSimulationModel_2.mdl in Appendix A), it can be seen that the resulting performance has dramatically altered. This is true even though the simulation conditions have remained the same. Whereas previously, the 'Measured BA' saturated under conditions a) and c), saturation only occurs under conditions d), and then only after 1300 hours of operation, as can be seen in Figure 4.2.9 The associated parameters are plotted in Figure 4.2.10 and can be compared to the corresponding results plotted in Figure 4.2.3, where the most significant difference exists. This comparison indicates that the variations in adaption rate and control effort have greater amplitude, which is to be expected with the significantly higher adaption gains involved. The terminal biomass concentrations are similar for both trophic groups, though the aggressive control has allowed marginally less biomass to grow. The gas production too is slightly reduced, however, the pH and substrate levels have been maintained virtually constant. The interesting fact is that aggressive control action has not developed the reactor ecosystem more rapidly than the less aggressive control, though the control of BA has been maintained over a wider range of initial biomass concentrations, giving a more predictable performance.

Maintaining stability of the volatile acids in the reactor by adjusting the feed rate is intuitively a sensible means of maintaining the maximum feed rate to the reactor at all times. The ability of the methanogenic bacteria to cope with the VFAs produced by the acidogens is determined by the population and metabolic health of the methanogens which, it is suggested, is maximised by a stable and optimally bounded environment. This is not clearly evident from the simulations above, primarily because both controllers maintain reasonable control of the environment. If anything, the aggressive control causes continual fluctuations which are not present in the P+I adaption mechanism controller and which may be the cause of the slight retardation of the development of the biocultures.
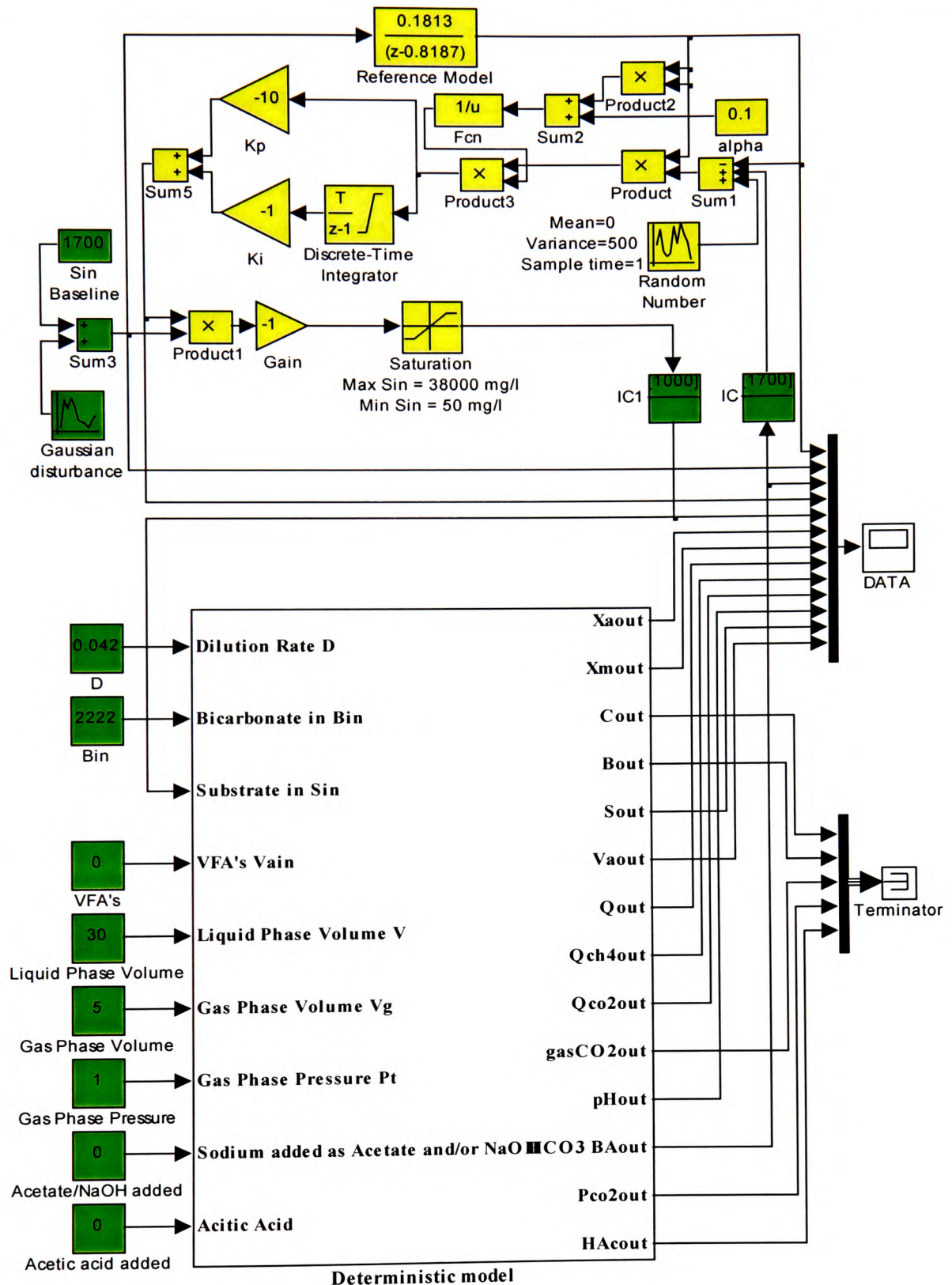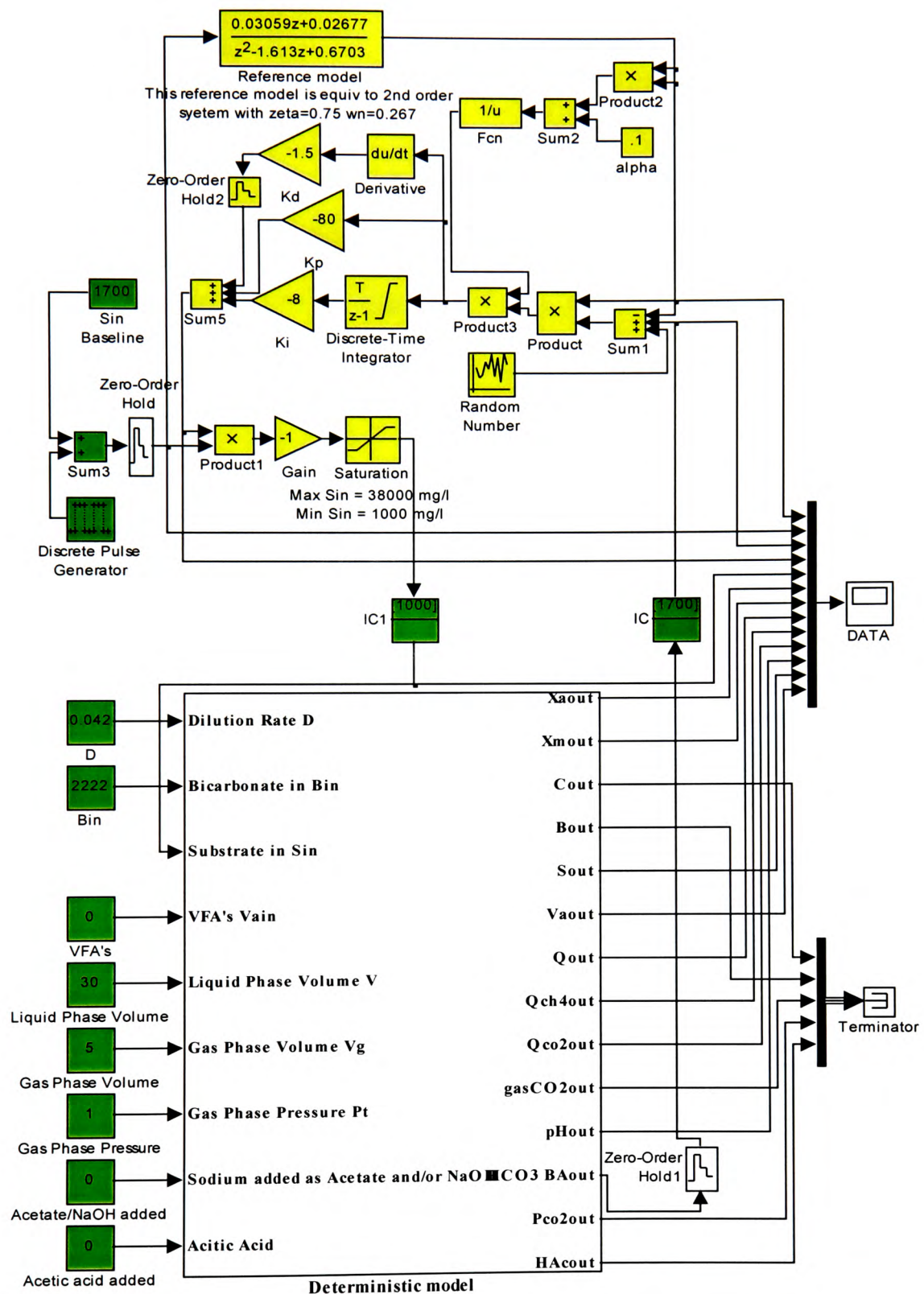
Figure 4.2.8 Simulation of an MRAC controller using P+I+D adaption mechanism to investigate the behaviour of the BA when feed rate actuation is in use.
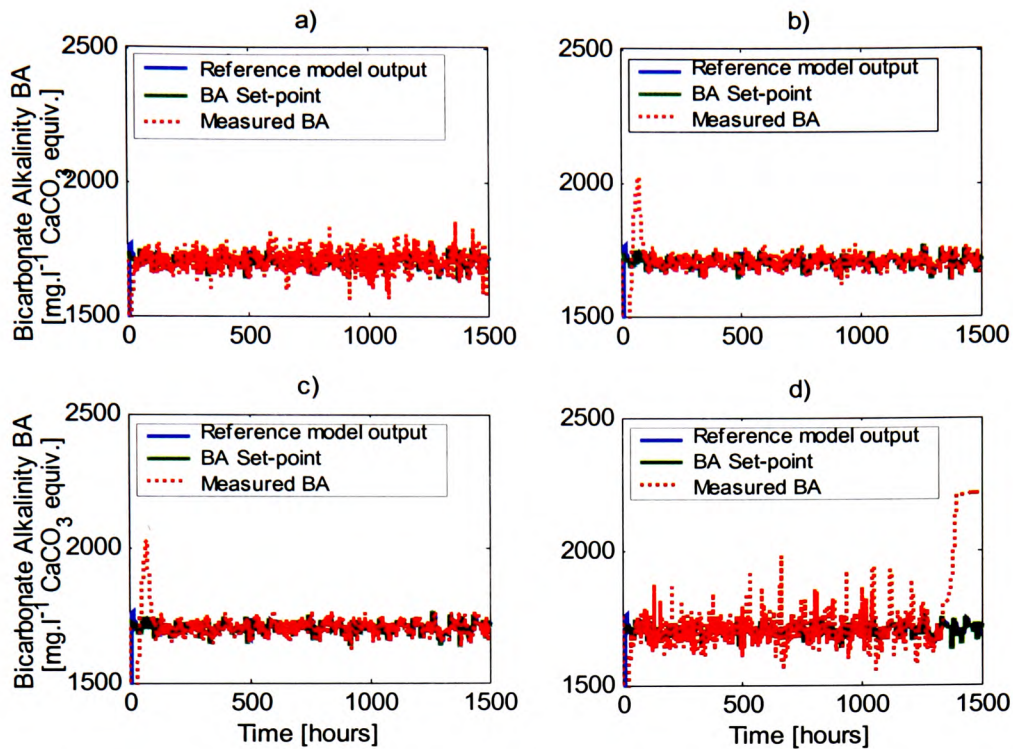
Figure 4.2.9 Simulation with P+I+D adaption mechanism showing the effect of altering bacterial concentrations on Reference model output, Set-point and Measured BA simulation experiments.

a) Initial conditions, Kp=-80, Ki=-8, Kd=-1.5; Xa=Xm=1500 mg.l^{-1}CaCO$_3$ equiv.
b) As a) but Xa=500 mg.l^{-1}CaCO$_3$ equiv. and Xm=100 mg.l^{-1}CaCO$_3$ equiv.
c) As a) but Xa=2000 mg.l^{-1}CaCO$_3$ equiv. and Xm=100 mg.l^{-1}CaCO$_3$ equiv.
d)   As a) but Xa=200 mg.l^{-1}CaCO$_3$ equiv. and Xm= 3000 mg.l^{-1}CaCO$_3$ equiv.
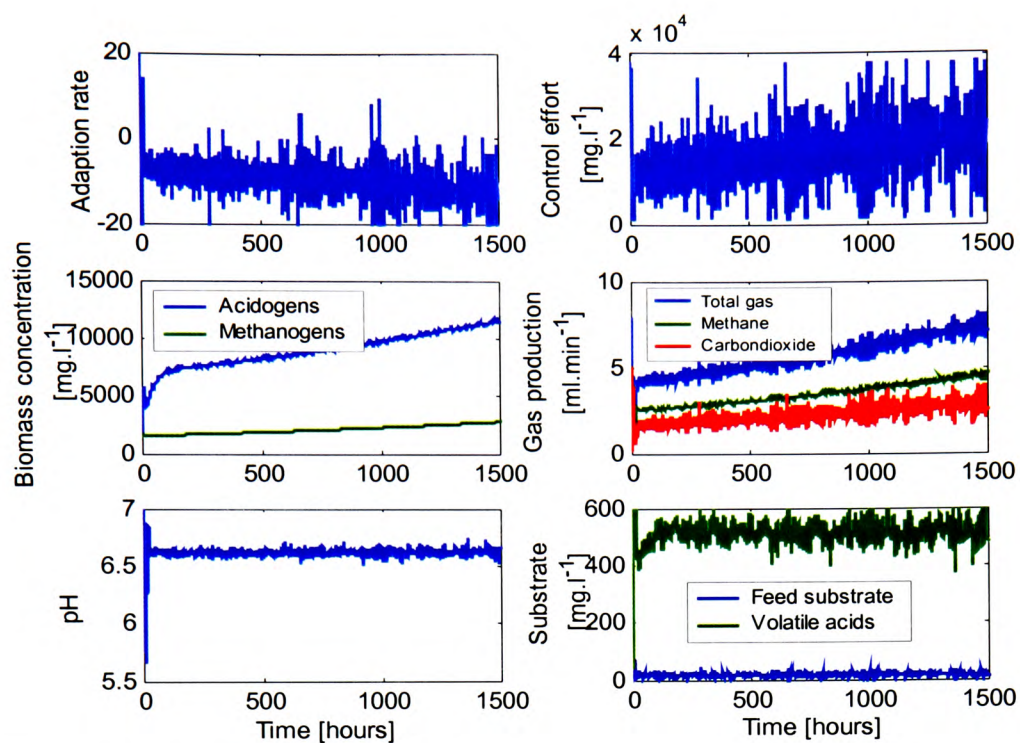
Figure 4.2.10 Variations in associated parameters for Figure 4.2.9 a)

4.2.3 A simulation investigation of the oscillatory behaviour evident in the laboratory experimentation

The experimental work described in Section 3.2, which was conducted on a laboratory scale EGSB reactor, showed oscillatory behaviour (and the data is presented later in Section 4.3, where the oscillations are evident in Figures 4.3.1 to 4.3.4 which show results from the first start-up experiment). The reason for this behaviour needed to be explained and reproduced in simulation as, in fact, the optimisation process indicated that the performance should be somewhat different to that in evidence. The behaviour may have been the result of unmodelled characteristics of the reactor, its seed and operating parameters, but if the behaviour could be simulated by an altered model which had justifiable amendments in place, then confidence could be built in respect of the reasons for the oscillation. The model used in the optimisation of the process was that shown in Figure 4.2.8. The resulting adaption parameter gains were somewhat higher than anticipated at [-80 -8 -1.5] for the proportional, integral and derivative gains respectively. Oscillatory behaviour could be expected in a situation where transport or other delays were not considered and should have been. A series of simulations were conducted in order to test this hypothesis using the model of Figure 4.2.8. Firstly, a model was set up as follows:

a) For 150 hour at 1 hour sample time, with a set point of 1700 mg.l^{-1} CaCO$_3$ equiv. disturbed with a discrete pulse generator signal with an amplitude of 100 mg.l^{-1} CaCO$_3$ equiv., a period of 80 hours and a pulse width of 40 hours.

b) As a) but with added measurement Gaussian noise with a mean of zero and variance of 500 mg.l^{-1} CaCO$_3$ equiv. and updated every sample

c) As a) with a unit delay representing communication delay between the software applications, in the BA feedback path and measurement noise as in b)

d) As c) but with a 1st order transfer function with a time constant of 0.1875 hours, in the BA feedback path, (i.e. a 4 time constant delay of 45 minutes). The model simulation was used to investigate the effect of placing a model of the BA monitor and settler into the feedback path and the addition of perceived noise and a delay in the control action propagated through the Analogue to Digital/Digital to Analogue conversion (ADDA) scheme. The DDE approach and the control algorithm induced a sample delay, which was not accounted for in the original optimisation model based on ControlSimulationModel_2.mdl, Appendix A. This model, augmented with all noise and delay elements is included in Appendix A as ControlSimulationModel_3.mdl.
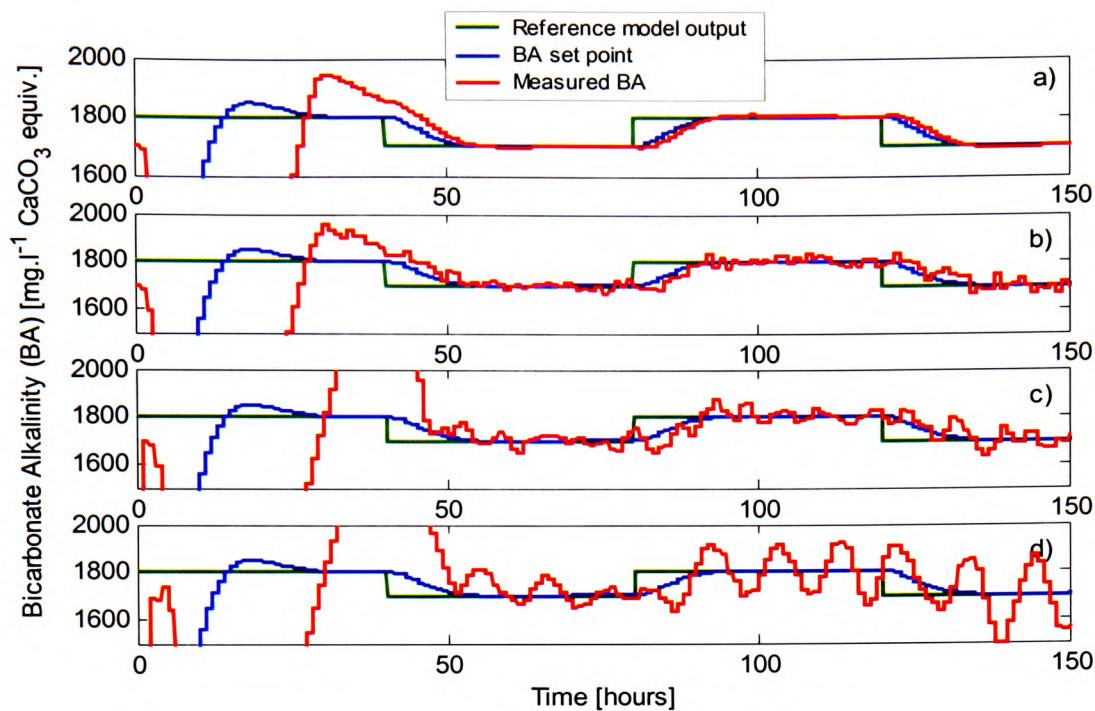
Figure 4.2.11 Control Simulation showing BA set-point, reference model output and measured BA. Controller gains [Kp= -80.0; Ki= -8.0; Kd= -1.5]

a) Set-point of 1700 mg.l^{-1} CaCO$_3$ equiv. and an additive pulse disturbance of amplitude 100 mg.l^{-1} CaCO$_3$ equiv.
b) As a) with added noise of variance 500 mg.l^{-1} CaCO$_3$ equiv. on measured BA
c) As b) with unit delay on measured BA
d) As c) with added 1st order model for BA monitor (τ=0.1875 hrs)

Figure 4.2.11 shows the progressive inclusion of noise, communication delay and instrumentation dynamics from a) to d). The consequence is that the 'Measured BA' becomes progressively more prone to error from the reference model output, which is the intended behaviour. In Figure 4.2.11 c) and d), the deviation is seen to be oscillatory and dependent on the delay. The latter corresponds quite well to the situation observed in the real data of, for example Figure 4.3.3 (between 1300 and 1400 hours) which is also somewhat oscillatory and thus supports the hypothesis that the modelling was too ambitious in attempting to ignore the effects of sensor dynamics. Furthermore, it can be seen from Figure 4.2.12 to 4.2.15 that the control action becomes progressively more oscillatory in character till in Figure 4.2.15 it resembles quite closely the experimental behaviour shown in Figure 4.3.3. The other parameters (namely biomass concentrations, gas production rates and pH, also respond to the increased measured BA delay in an oscillatory manner.
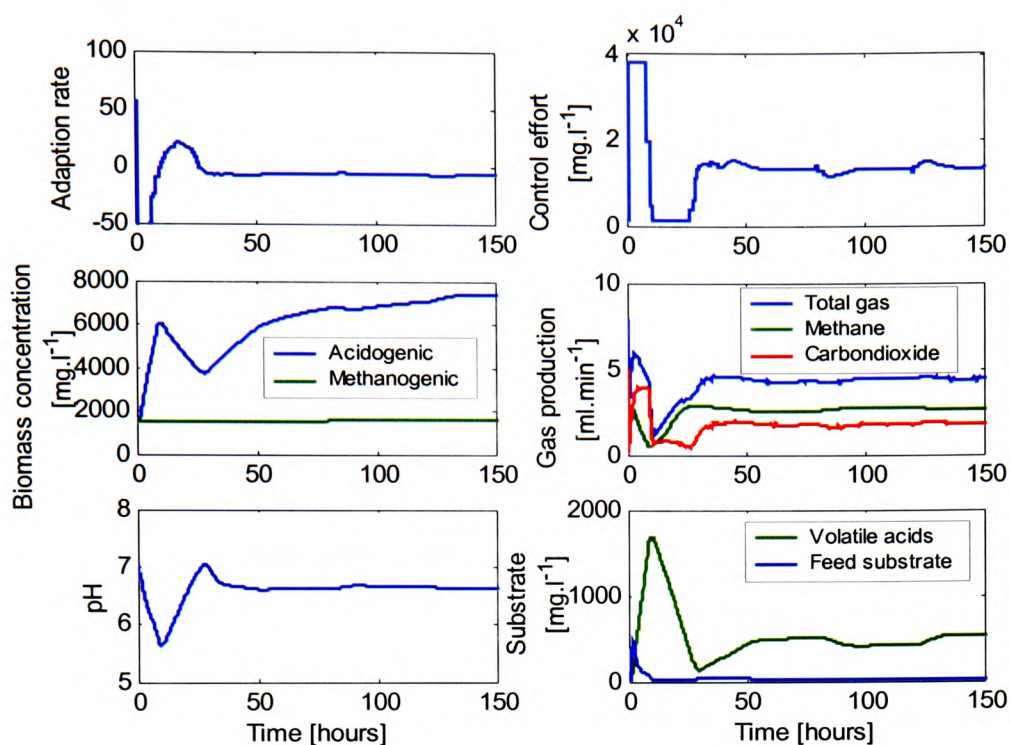
Figure 4.2.12 Variations in associated parameters for Figure 4.2.11 a)
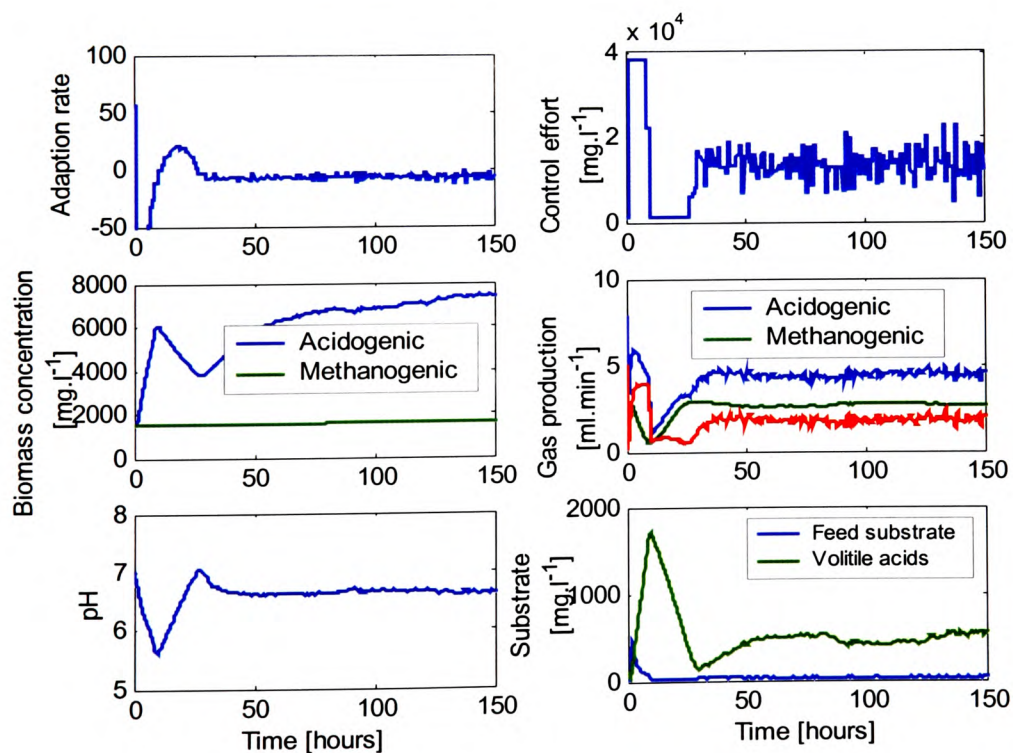
Figure 4.2.13 Variations in associated parameters for Figure 4.2.11 b)
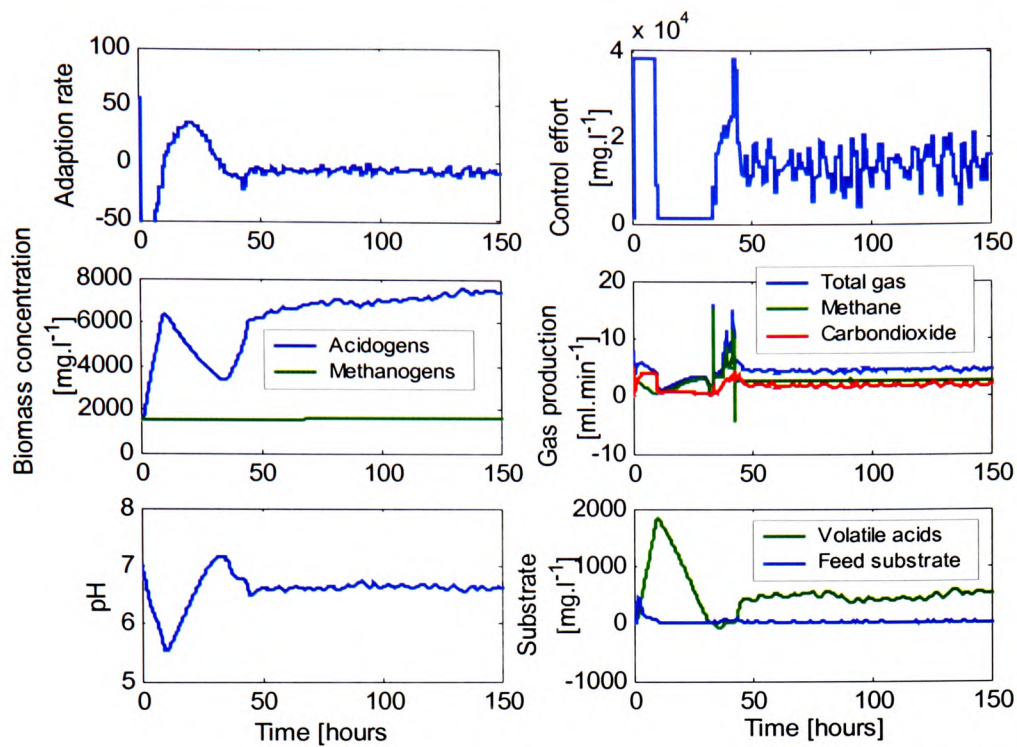
Figure 4.2.14 Variations in associated parameters for Figure 4.2.11 c)
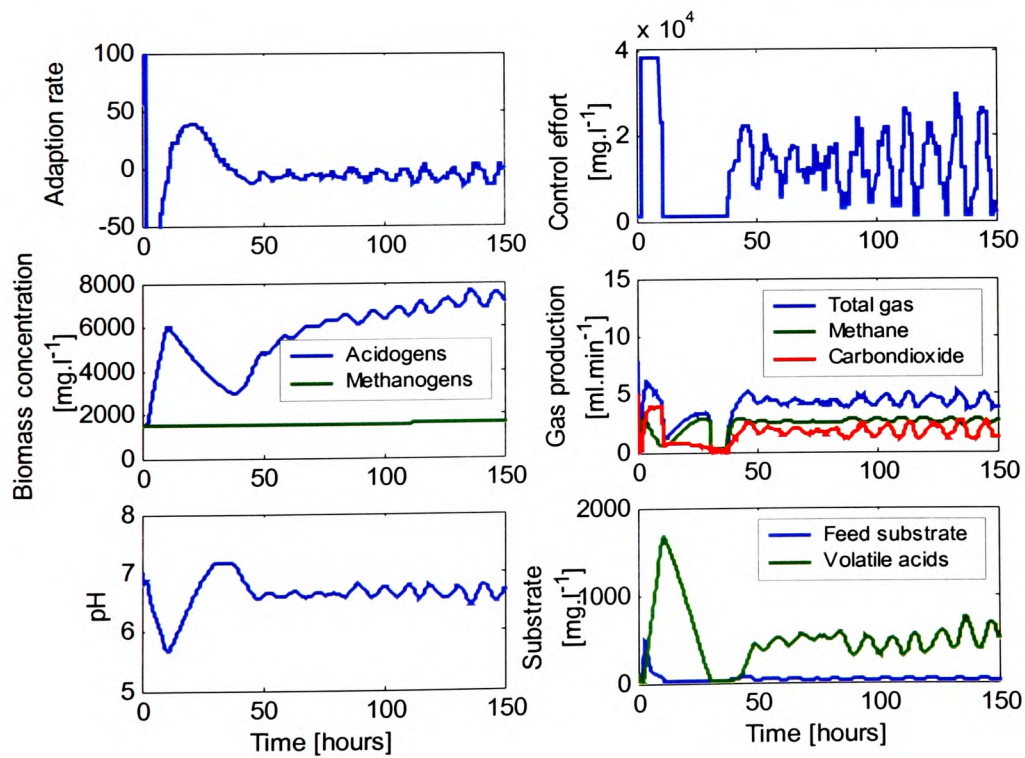
Figure 4.2.15 Variations in associated parameters for Figure 4.2.11 d)

It can be seen from Figure 4.2.16 that the limiting parameter of methanogenic bacterial concentration is retarded slightly by the degraded control action due to instrumentation delays, at least up to 150 hours of lapsed time (6.25 days). As the model does not include other trophic groups which are known to exist in the AD process, such as hydrogenotrophic methanogens, or the inhibitions so derived from hydrogen or other parameters such as pH, one might expect the variation to be increased slightly in reality. The increased physical effects of CO_2 liberation variations are also not considered, but could have deleterious consequences on the granules and may increase selective washout dependant on the morphology of the bacterial species.
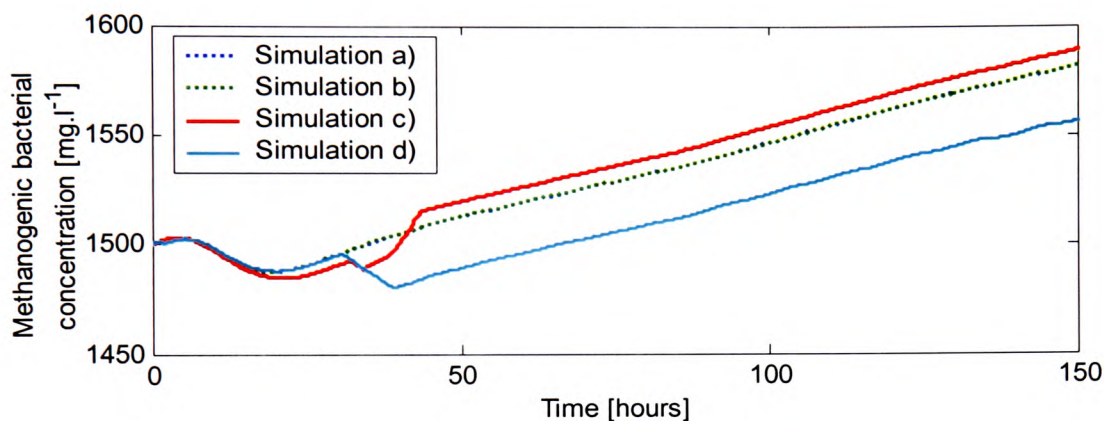
Figure 4.2.16 Methanogenic bacterial concentration for simulations a)-d)

4.2.4 Simulation study to assertain the effect of discrepancies in the OLR actuated control implementation

Start-up 1,2 and 3 experiments were conducted on the basis of variations in OLR as a means to affect control. The FAT controller was parameterised according to the details presented in Table 3.4.1 and *Start-up 1* had significantly higher parameter gains then *Start-up,2 and 3* which had the same parameter gains

A discrepancy was discovered in the implementation of the control system associated with the OLR actuated experiments. The parameterisation/optimisation and subsequent simulations were done with the substrate supplied to the reactor model (*Sin*) defined in [mg.COD.l^{-1}], which is evident from a dimensional analysis of the model, while the implementation in the lab scale experimentation assumed *Sin* represented OLR with associated units, [kg.COD.m^{-3}.d^{-1}]. In other words, the units were inconsistent. The effect of this discrepancy was to include a gain of 5.943 m^3.d.l^{-1} [(mg.COD.l^{-1}).(mg.COD.m^{-3}.d^{-1})$^{-1}$] between the control and monitoring computers.

Comparison of predicted performances between the system as implemented and the optimisation model

The expected performance of the optimised control systems is compared here, with the simulated performance when the extra gain (5.943) derived from the discrepancy of dimensions incorporated during the control system implementation described above.

Each of the Start-up experiments (*Start-up 1,2 and 3*), were simulated using the control simulation model in Simulink™ ControlSimulationModel_2_Discr.mdl (Appendix A). In this model, the control effort signal connected to *Sin* has a gain of 5.943 associated with it, which takes account of the implementation discrepancy. With this gain replaced by unity, the system does not account for the discrepancy and represents the system as implemented. Simulations were conducted for each affected Start-up experiment and are presented as time evolutions of the system response below.

Start-up 1
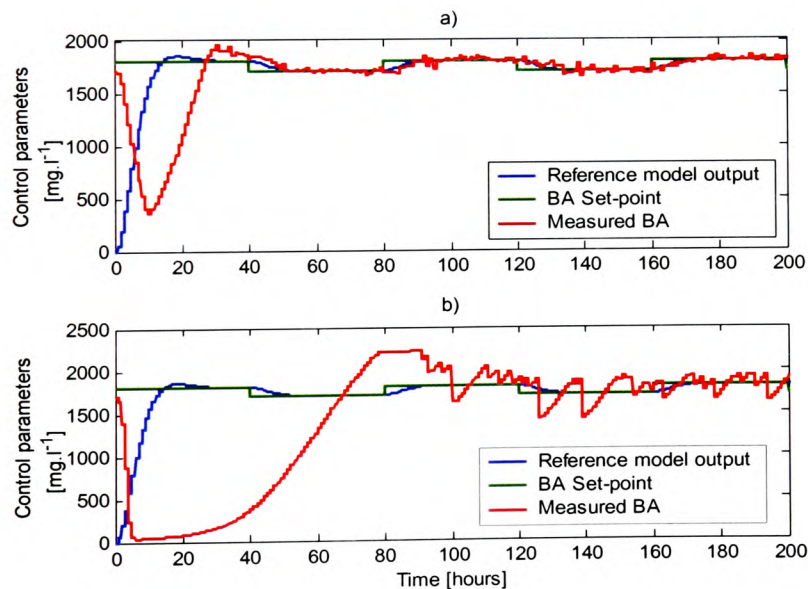
Figure 4.2.17 Comparison of performance from controller used in *Start-up 1*

(Optimisation g) from Table 3.4.1 with parameter vector [-80.0000 -8.0000 -1.5000]) – Pulsed set-point and sensor noise variance 500 mg.l^{-1} CaCO$_3$ equiv.
a)   expected performance without correction of the control effort gain discrepancy
b)   expected performance with correction of the control effort gain error

Figure 4.2.17 indicates that the increased gain would result in a more erratic behaviour from the control system, which is comparable with the experimental performance observed in Figures 4.3.8 to 4.3.12.

Figure 4.2.18 shows a similar comparison to Figure 4.2.17 with the exception that the set-point is held constant at 1700 mg.l^{-1} CaCO$_3$ equiv. Again the response is similar and hence for other Start-up comparisons only the pulsed situation will be considered.
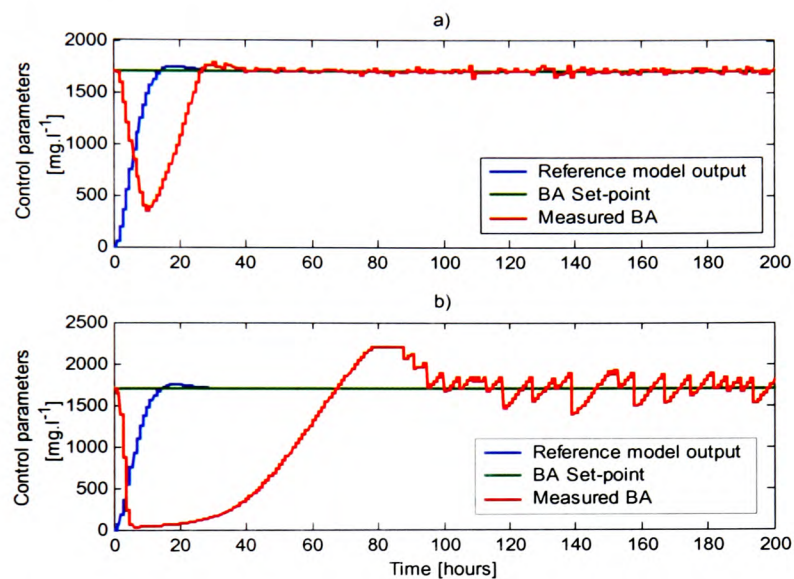
Figure 4.2.18 Comparison of performance from controller used in *Start-up 1*

(Optimisation g) from Table 3.4.1 with parameter vector [-80.0000 –8.0000 –1.5000]) – Sensor noise variance 500 mg.l^{-1} CaCO$_3$ equiv.
a) expected performance without correction of the control effort gain error
b) expected performance with correction of the control effort gain error

Start-up 2 and 3
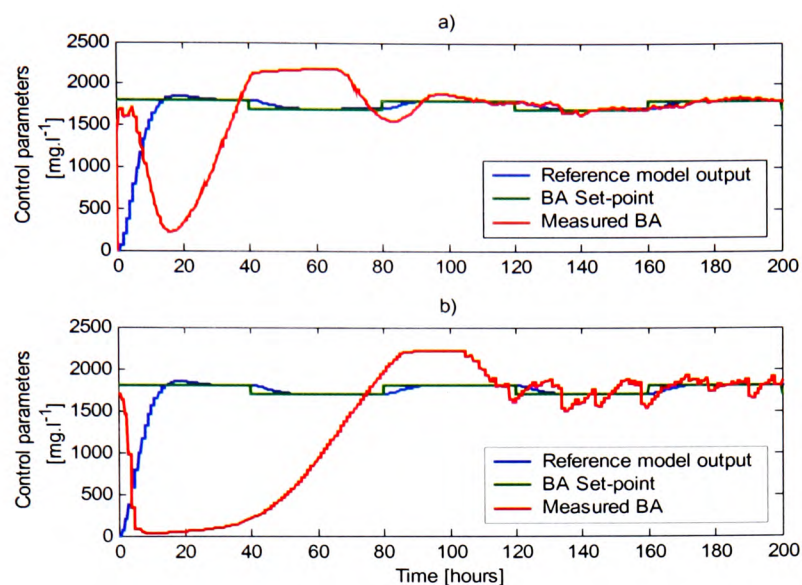
Figure 4.2.19 Comparison of performance from controller used in *Start-up 2 an 3*

(Optimisation i) from Table 3.4.1 with parameter vector [-27.1952 –5.0322–2.6103]) – Pulsed set-point and sensor noise variance 500 mg.l^{-1} CaCO$_3$ equiv.
a)   expected performance without correction of the control effort gain error
b)   expected performance with correction of the control effort gain error

It can be seen that even in the case where the adaption gains were reduced (Figure 4.2.19), the response was similar and somewhat erratic though to some degree periodic.

4.3 MODEL REFERENCE ADAPTIVE CONTROLLED REACTOR START-UP EXPERIMENTATION (TASK 4)

The fundamental question, which this work makes initial strides to answer, is:

Would it be possible to design a generic adaptive controller for a variety of anaerobic digesters?
More specifically, could the MRAC structure, a single measured variable and little prior knowledge of the reactor to be controlled, act as constraints on the design process, yet still yield a transferable generic controller for use in anaerobic digester commissioning, start-up and operation? The work in this thesis has not considered the transferability of such a controller, between a representative sample of specific anaerobic reactors, but has considered a design process, which may be fruitful in the final objective. The single measured variable implies that the cost of instrumentation is minimised. It is believed that the BA monitor used in the experimentation could be produced at a relatively low cost, (circa £5000 Sterling, in 2002, depending on sales of the instrument), even though significant development work would be required to improve reliability. Scale-up of the monitor, which would allow higher flow rates through the monitor, would increase the tube diameters throughout the measurement system and this would reduce its susceptibility to blockages.

At the commissioning stage of an anaerobic digester, the commissioner or operator would have little knowledge of the behaviour of the system other than the design information and any comparable, previously commissioned system from which experience may have been gained. The start-up and subsequent operation of the reactor could therefore require considerable expertise, which would have a cost associated with it. A control system, which would start-up the reactor at a sub-optimal but reasonable rate with minimal effort from specialist operators, should be a useful device. As each reactor has different operating conditions, feed and seed characteristics, one would in general expect variations in the operating regimes. Designing a control system would normally involve the characterisation of the reactor (i.e. modelling), from which a bespoke control strategy can be developed. The advantage of a generic controller, which could be placed directly into a system without any design effort, should be clear. The cost of model development at the commissioning stage in any case could be significant, particularly if experimentation is necessary in order to parameterise (or calibrate) the model. The first stage in testing the feasibility of such a system has been to design the controller on the basis of a particular reactor system and to test its ability to control a reactor of different design and operating characteristics. This section considers just such an approach. The optimised FAT controllers developed in Section 3.4 and summarised in Table 3.4.1 were used in four start-up experiments. The model used in the development of

these controllers was derived from a fluidised bed reactor as described in Chapter 3.0 which was fed a simulated yeast waste. Whereas the experiments to study the performance of the same controllers were performed using an EGSB reactor fed with a sucrose solution. While this is not an exhaustive investigation as to the transferability of the control strategy, it does allow some conclusions to be drawn and further work to be identified.

The experimentation to test the control strategy and the specific optimised controllers were split into four start-up experiments. Start-up can be considered as a significant and protracted period of over load conditions, governed primarily by the rate at which the bacterial consortium is able to grow, and hence consume a continually increasing feed rate. By considering start-up, the experiments are considering a severe loading regime and extrapolating to generalise the controller performance at steady state or under conditions of hydraulic, organic or toxic shock, is at the very least, ponderable. Explicit experimentation considering hydraulic and organic over loads are currently the subject of a separate Ph.D. study at the University of Glamorgan. The start-up experiments indicating the FAT controller adaption parameters [Kp Ki Kd] and the actuation which constituted the causal action by which the system was controlled (briefly summarised) were as follows:

Start-up 1

Experiment run over 73 days from 26th March 2001 to 8th June 2001; Actuation – OLR; Adaption parameters – [-80 –1.5 –8.0]; Seed - granules taken from a UASB reactor at Davidson's Paper Mill (Aberdeen, Scotland).

Start-up 2

Experiment run over 22 days from 16th July 2001 to 9th August 2001; Actuation – OLR; Adaption parameters – [-27.1952 –5.0322 –2.6103]; Seed – continued from *Start-up 1*

Start-up 3

Experiment run over 47 days from 25th October 2001 to 13th December 2001; Actuation – OLR; Adaption parameters – [-27.1952 –5.0322 –2.6103]; Seed- from a UASB reactor used to treat molasses waste from a citric acid producing plant at Tate and Lyle Citric Acid, Selby, N. Yorkshire

Start-up 4

Experiment run over 70 days from 26th February 2002 to 9th May 2002; Actuation – BA dosing; Adaption parameters - [-11.8812 -1.2157 -0.1867]; Seed- from a UASB reactor used to treat molasses waste from a citric acid producing plant at Tate and Lyle Citric Acid, Selby, N. Yorkshire.

In order to have a clear indication of the performance of the control strategy and the associated controller parameters, it would be necessary to have uninterrupted data which was not perturbed by unforeseen events. The existence of such aberrations is not particularly rare as can be seen from Steyer *et al.* (2002), who, perhaps not to the same extent, experienced comparable incidents during the typical weeklong data set they presented. Failure free operation was not achieved during the experiments reported here and it is therefore necessary to detail what proved to be frequent aberrations. Furthermore, the control system employed is adaptive and depends to a significant extent on historical data so that a summary view is required in order to make sense of the controller performance. Presenting the entire time series for the four experiments, indicating the occurrence of critical events should help the reader in this respect. The data is presented in six graphs a) to f) showing $\%CO_2$, pH, measured and set point BA, temperature, OLR (or BA dosed) and gas production rate respectively. Labelled vertical lines (indicating time instants) mark critical episodes, which are briefly explained in the associated tables.

4.3.1 A summary of the data from the optimised (FAT) controller experimentation

Start-up 1

Figure 4.3.1 shows the data collected by the data logging system in the first 20 days of *Start-up 1* and is followed by Table 4.3.1 explaining the aberrations marked on Figure 4.3.1. Similarly, Figures 4.3.2.to 4.3.4, show consecutive 20-day periods of data or in the latter instance, to the end of the data. Associated Tables 4.3.2 to 4.3.4 follow these figures, indicating the perturbations.

Figure 4.3.1 *Start-up 1* **Performance of the optimised FAT controller over the first 20 days**

a) %CO₂, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

Table 4.3.1 *Start-up 1* **Perturbations during the First 20 days of 1st optimised start-up experiment**

A.	The BA monitor had a susceptibility to becoming blocked by particulate at the outlet to a U tube, which maintained the liquid level in its acidification chamber. Sediments would accumulate in the U tube and carry over to and block the small orifice, which formed its outlet. This had a direct influence on the gas flow measured and consequently, the BA measured. The peristaltic pumps were also prone to blockages and the position of the tube relative to the rollers needed to be moved frequently, which affected the associated flow rates and again the BA reading. The data shows a slight rise at this point, when the peristaltic tubes were moved and the U tube cleared of debris.
B.	At this point in the data, the antifoam supply tube in the BA monitor became blocked and hence changed the flow through the monitor and consequently caused a drop in measured BA
C.	The U tube in the BA monitor became blocked, thus causing a sudden rise in the measure BA.
D.	Guwy *et al.* (1994) describes the BA monitor in which acid is supplied to the acidification chamber of the BA monitor in order to evolve all the bicarbonate as CO_2 gas. The acid is supplied via a peristaltic pump and is connected to the suction is a centrifugal pump which acts as a mixer on the acidification chamber. The connection of the acid pipe to the pump suction became loose and the subsequent spillage (during a Sunday when the laboratory was not continually manned) cased the power to trip with a loss of instrumentation and ancillary equipment, though data logging continued. The problem persisted and after restoring power, air was pumped into the BA monitor from the pipe failure point, causing false high readings on the BA monitor. This caused the feed to increase to its maximum of 38 kg COD $m^{-3}d^{-1}$. After this the monitor was stopped and a static BA reading supplied to the control in its place, while the feeding was suspended and BA was dosed into the reactor to stabilise it.
E.	Control was restored towards the evening of the 8th day
F.	The acid pipe became disconnected once more with a rapid drop in BA ensuing.
G.	A rapid rise in the BA data was observed to have occurred while the reactor was not being observed and was thought to be due to a blockage in the BA monitor U tube.
H.	The sudden increase in BA is due to the unblocking of the antifoam line.
I.	The BA monitor was erratic over night. This behaviour was probably due to blockages in the U tube.
J.	The feed pump (peristaltic) stopped pumping when the tube became flattened and simultaneously, air was pumped into the BA monitor through the connection between the acid supply pipe and the mixing system on the acidification chamber.
K.	Further acid line problems lead to the restarting of the controller, with the minimum OLR threshold removed. Over night the liquid level in the reactor dropped to the point where the recycle line was pumping biogas and causing considerable disturbance to the sludge bed. The reactor was filled with a BA solution of 2222 mg $l^{-1}CaCO_3$ equiv., the BA monitor was recalibrated and the control was restarted. Initially the BA set point was 2000 mg $l^{-1}CaCO_3$ equiv. and reduced in steps to 1700 mg $l^{-1}CaCO_3$ equiv. by 342 hours into the experiment.
L.	The feed pump failed as in J, with similar consequences.

The duration of *Start-up 1* was approximately 75 day (1800 hours), which would normally be considered ample for starting an EGSB reactor, for example the 35 days start-up reported by Borja *et al.* (1995), is by no means exceptional. The measured BA and OLR in Figures 4.3.1 to 4.3.4 show a tendency to behave in a very 'stiff' manner, with large changes (spikes) in the control effort evidenced (by simple zero order relationship), with the OLR signal. Initially (say over the first 100 hours), these spikes are infrequent, but by 600 hours, the frequency has markedly increased. The frequency and amplitude of the OLR spikes continues to increase to 1550 hours, but is retarded and often reversed by system failures, which are predominantly due to the BA monitor's unreliability. It is fair to say that the behaviour of the control system over *Start-up 1*

was not well correlated to the expected behaviour indicated by the simulation of the optimised controller as indicated by Figure 4.2.1 a) and b). The control effort shown in Figure 4.2.13 is comparatively subdued compared to the control effort seen in *Start-up 1*, even with the simulated Gaussian measurement noise, previously described. The adaption gains are necessarily high in order that the optimisation procedure should deliver close following to the reference model of the MRAC scheme. This however has the effect of making the system highly sensitive to the unmodelled dynamics and transport (or other) delays. At the time of running the experiment, the systems behaviour was suspected to be attributable to such dynamics and delays, and the simulation study of Section 4.2 lent support to this hypothesis. Subsequent controller parameterisations took account of the delayed measurement signal and showed some improvement in the dynamic behaviour of the control system. Never the less, the 'on-off' behaviour of *Start-up 1* serves to illustrate the likely problems which may arise in trying to apply a generic control system to a variety of anaerobic digesters. High gains will produce rapid adaption but delays on the measured variable will lead to overshoot and a tendency toward marginal stability or possibly instability. It is conceivable that the control effort could be used to indicate the existence of unmodelled dynamics, and appropriate adjustments to the adaption mechanism could be made. The result of this feeding pattern is to prolong or slow down the start-up phase and in the case of a highly digestible waste such as sucrose, the conversion of the
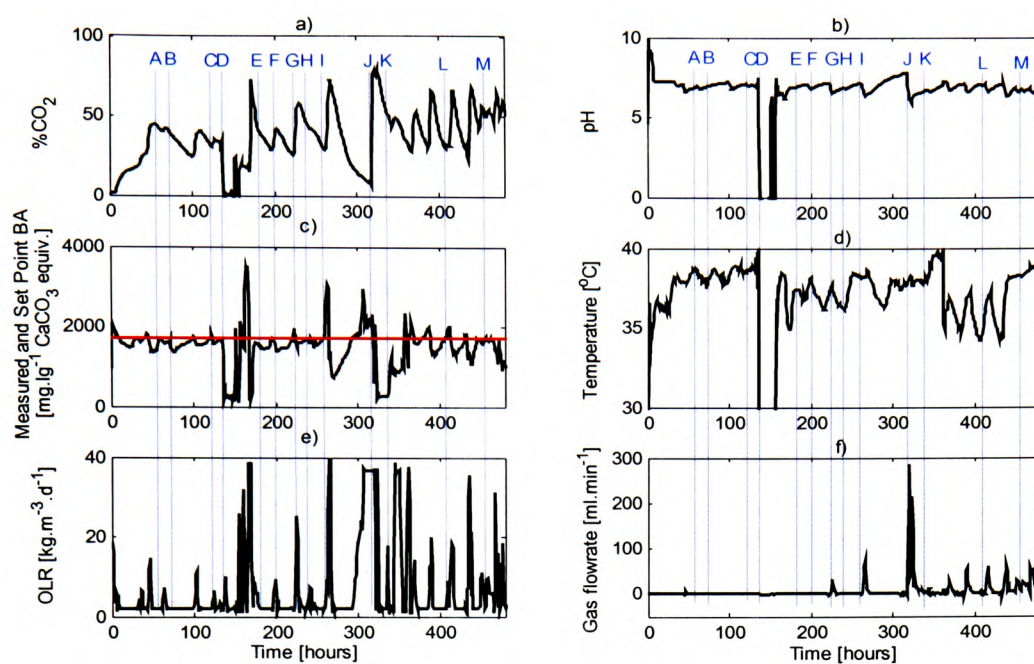
Figure 4.3.2 *Start-up 1* **Performance of the optimised FAT controller over days 21-40**

a) %CO₂, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

Table 4.3.2 *Start-up 1* **Perturbations during days 21-40 of 1ˢᵗ optimised start-up experiment**

A.	Antifoam stopped pumping, which lead to foam building up and obstructing the solenoid valve, which was stripped and cleaned prior to re-commissioning.
B.	Feed concentrate line became blocked due to a blockage caused by bacterial growth further upstream. The blockages were cleared and were followed by a slight drop in pH.
C.	At this point, the U tube in the BA monitor was cleared and the peristaltic tubing for the acid supply in the BA monitor was changed, leading to a short lived increase in the measured BA. This was followed by the antifoam tube blocking and the saturation chamber overflowing, which lead to the acidification chamber foaming. This was all put right, by which time the BA read approximately 900 mg l⁻¹ CaCO₃ equiv., then rising once more to over 1700 mg l⁻¹ CaCO₃ equiv.
D.	BA monitor U tube blocked, leading to liquid in the solenoid. This was put right and the BA monitor re-calibrated with a 2000 mg l⁻¹ CaCO₃ equiv. standard.
E.	It was noted that the U tube was blocking (probably) with bacterial matter, with a remarkably regular frequency and that on occasions the control system samples at the extreme of the aberration. The software based Butterworth filter was increased to 5ᵗʰ order from 2ⁿᵈ order, to try to reduce the out-layer's effects, with some success. At this point, the gas pressure in the headspace had risen sufficiently to drop the liquid level and cause biogas to be re-circulated in the reactor. The reactor was filled with tap water.
F.	The antifoam system in the BA monitor had blocked and caused foaming in the acidification chamber and hence, the solenoid to be flooded. The solenoid was stripped and cleaned. The outlet of the U tube was replaced by a small bore stainless steel tube (in place of the original copper tube). The BA monitor was re-calibrated.

G.	The antifoam pump developed a fault and pumped air into the BA monitor, causing the BA reading to jump up to 2340 mg l^{-1} $CaCO_3$ equiv. This reading dropped rapidly once the fault was repaired, and the spike of feed made the system gas significantly, with $\%CO_2$ rising to 61%, indicating the BA was being converted to CO_2. Bacteria began to carry over to the BA monitor and some difficulty was experienced trying to maintain the liquid level in the reactor. The BA monitor blocked causing the solenoid to flood. Corrective action was taken and the system began to stabilise.
H.	Re-calibrated BA monitor.

substrate to volatile acids by the acidogenic bacteria would be very fast. Large spikes in the OLR will lead to similar surges in VFAs and in the presence of bicarbonate, will evolve CO_2 at increased rates, reduce buffering and pH. This could disrupt the bacterial flocs or granules at the same time as placing the methanogenic bacteria under some stress. Sucrose, though highly digestible, may paradoxically be a difficult substrate for control purposes, because of this susceptibility to favour some trophic groups over others.

There is a discernible trend, showing that the OLR and (by implication) the active microbial populations increase, as does the gas flow rate over the duration of *Start-up 1*, even though the control action is less than optimal and the measured BA gives false readings, (often with disturbing regularity). The control and the adaption of the control action are highly dependent on accurate and reliable periodic measurements of BA in order that appropriate actions can be taken. Given that BA sensor failure, blockages and recalibrations caused major perturbations to the measured BA, it is arguably an indication of the robustness of the method, that the system was able to maintain a living reactor over the period of *Start-up 1*.

Figure 4.3.3 *Start-up 1* Performance of the optimised FAT controller over days 41-60

a) %CO_2, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

Table 4.3.3 *Start-up 1* Perturbations during days 41-60 of 1st optimised start-up experiment

A.	BA monitor failed as U tube became blocked. Reactor was recovered by pumping 5 l of 30000 mg l^{-1} $CaCO_3$ equiv. solution to the reactor, and running on manual until stability was restored. It was noted that a significant amount of granules had been washed out. A small settling chamber was placed between the reactor and the BA monitor, to try to remove the fine particulate which was frequently causing the BA monitor to become blocked at the U tube outlet.
B.	Back to normal operation.
C.	Liquid level dropped to the point that gas was recirculating, causing bacteria to block the BA monitor. Recovery achieved by pumping 5 l of 30000 mg l^{-1} $CaCO_3$ equiv. solution to the reactor and running manually until stability was restored.
D.	Back to normal operation.
E.	Antifoam pump system in BA monitor blocked.
F.	Antifoam blocked.
G.	A larger tube (grey-grey replacing orange-white) was employed while increasing the dilution of the antifoam to maintain flow rate of antifoam to the system. BA monitor recalibrated on a single standard solution.
H.	Unblocked tubing, which had become clogged with biological growth. Beyond this point, the in-line settler between the reactor and the BA monitor was periodically drained of the settled biomass and the tubing in the BA monitor was cleared. These actions caused the measured BA to drop between approximately 200 to 700 mg l^{-1} $CaCO_3$ equiv.

Figure 4.3.4 *Start-up 1* **Performance of the optimised FAT controller over days 61-75**

a) %CO$_2$, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

Table 4.3.4 *Start-up 1* **Perturbations during days 61-75 of 1st optimised start-up experiment**

A.	Control computer crashed so the system was put onto manual operation for approximately 6 hours, after which the controller was restarted.
B.	CO$_2$ Supply used to saturate sample in the BA monitor was found to be empty. The cylinder was replaced.
C.	BA monitor recalibrated.
D.	Antifoam became blocked causing foaming in the acidification chamber and consequently liquid to enter the solenoid valve. The valve was stripped and cleaned.
E.	Replaced peristaltic tubing (green-green) between saturation and acidification chambers.
F.	Antifoam supply system blocked.
G.	Controller stopped and the experiment was terminated.

Start-up 2

Figure 4.3.5 shows the complete time series for *Start-up 2*, which took account of the instrumentation delays at the point of optimising the adaption mechanism parameters. The resulting proportional and derivative gains were significantly reduced, meaning that the near instantaneous response of the adaption mechanism was also reduced. The integral gain was in fact increased, which means that persistent deviation from the reference model trajectory are 'integrated out' more rapidly than previously.

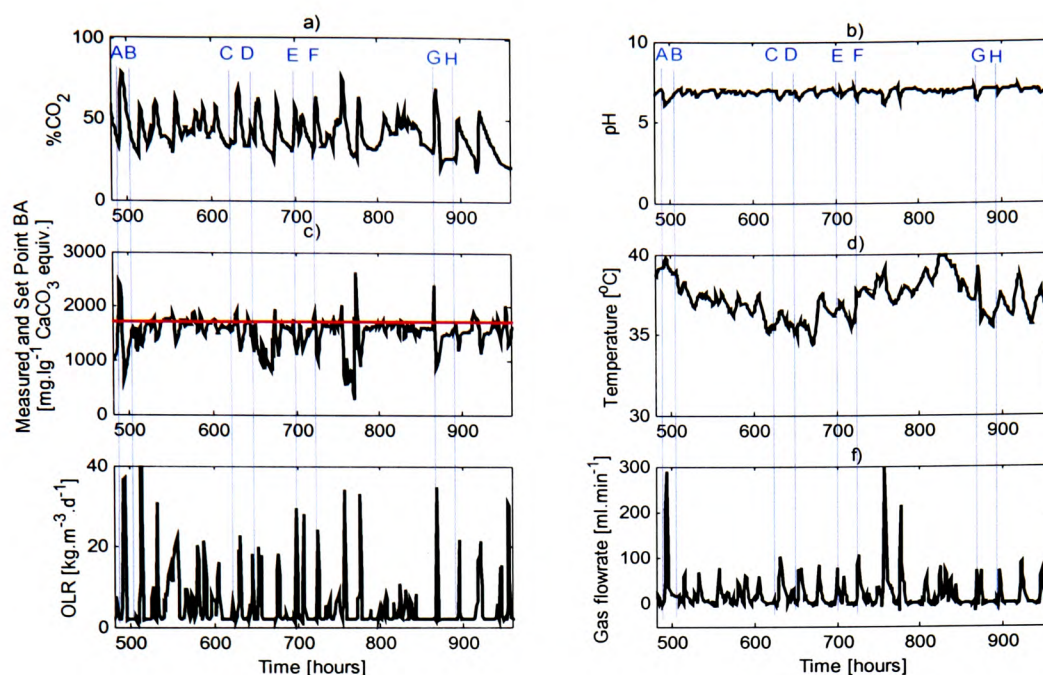**Figure 4.3.5 *Start-up 2* Performance of the optimised FAT controller**

a) %CO₂, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

Table 4.3.5 *Start-up 2* Perturbations: 2ⁿᵈ optimised start-up experiment
A.   At start-up, the settled volume of biomass was approximately half of the original seed volume, although the characteristics of the sludge would be different.
B.   Control computer crashed and was restarted. CO_2 meter recalibrated.
C.   BA monitor recalibrated.
D.   Settler emptied hence saturation chamber emptied and air was pumped into the acidification chamber of the BA monitor causing a false high reading and a high OLR. The pH dropped significantly so that a high rate of BA dosing was necessary to recover the reactor.
E.   Cleared tubing in the BA monitor of bacterial growth.
F.   Similar failure to D and cleared tubing in the BA monitor of bacterial growth.
G.   Similar failure to D.
H.   Similar failure to D. Settler lowered to try to overcome the problem.
I.   BA dosing pump stopped pumping.
J.   BA solution tank became soured, BA dosing stopped and pH dropped dramatically. Dosed with 15000 mg l⁻¹ $CaCO_3$ equiv. at maximum pumping rate, to recover the reactor. The reactor was run in recovery mode till K.
K.   Back to normal automatic operation.
L.   Experiment terminated as biomass washout had become a serious concern. The biomass volume at the end of the experiment had reached approximately 25% of the original seed volume.

The set point in *Start-up 2* remained persistently above the measured BA. It is believed that this occurred because the microbial population was heavily unbalanced toward the acidogenic stage, by the repeated and dramatic perturbations experienced through *Start-up 1*. The effect of the

integral parameter in the adaption mechanism was not allowed to develop because of further perturbations and the OLR variations are primarily the result of derivative and proportional actions from the adaption mechanism.

Start-up 3

As mentioned in Table 4.3.5 point L., the washout of bacteria in *Start-up 2* was significant and left only 25% of the original seed volume by the end. The reactor was seeded anew, with granules from Tate and Lyle Citric Acid, Selby, N. Yorkshire, as described in Section 3.2. Initially (around 200 hours), the system seemed to cope reasonably well, however further perturbations from the BA monitor caused the measured BA to be less than the set point until a major interruption occurs between 400 and 800 hours. Again the microbial population was thought to be reduced and arguably stressed. In periods where control was relatively uninterrupted (170 to 210 hours), the control action appeared to be far less aggressive than *Start-up 1*. The consequence of the persistent perturbations was to make it difficult to assess the performance of the control strategy. If the reliability of the BA monitor was part of the investigation, then it would become very difficult to justify using control in the face of such an unpredictable sensor.
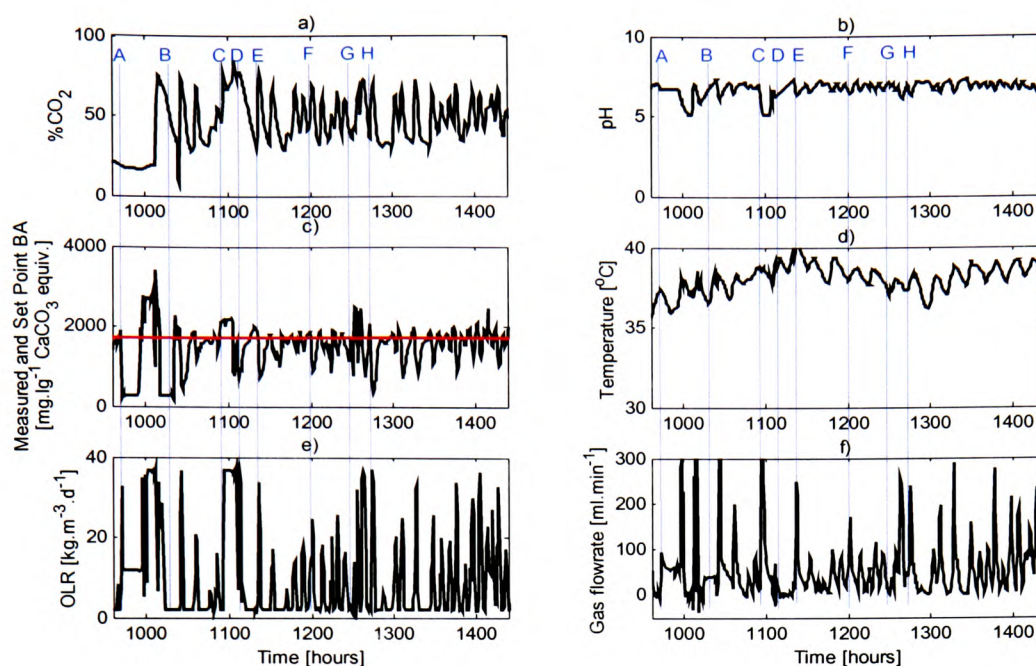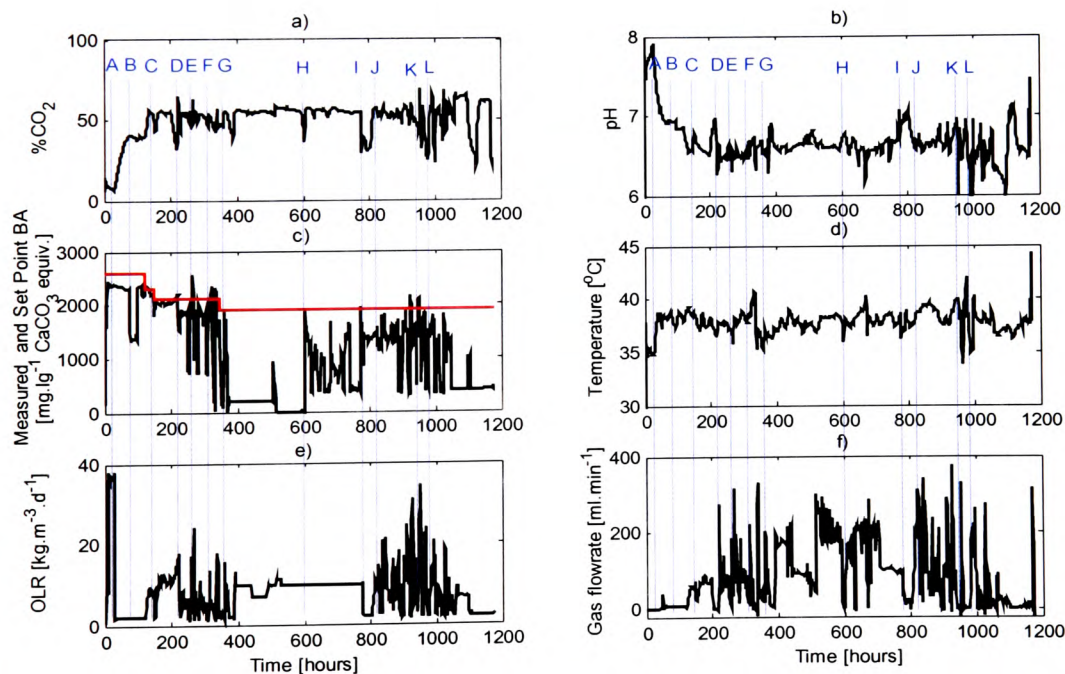

Figure 4.3.6 *Start-up 3* Performance of the optimised FAT controller

a) %CO_2, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

Table 4.3.6 *Start-up 3* **Perturbations: 3rd optimised start-up experiment**

A.	Start automatic operation.
B.	Acid supply to acidification chamber of BA monitor became blocked and was later cleared.
C.	BA monitor saturation chamber emptied as circulation pump (centrifugal) lost suction, thus preventing sample getting to saturation chamber.
D.	Feed to reactor stopped pumping and was later put right.
E.	Antifoam stopped pumping (ran out). Dosed reactor with BA. Manual operation till F.
F.	Back to normal automatic operation. Followed by erratic (for unknown reason), behaviour of BA monitor.
G.	System onto manual control as BA monitor U tube blocking and BA dosing to reactor not pumping. The period of constant OLR that follows showed that the reactor found the conditions more conducive to stable operation than the rapid variations in OLR caused by the disruptions in the BA monitor.
H.	Back to normal automatic control, shortly followed by a failure in the BA monitor, where the tubing between the saturation chamber and the acidification chamber had become blocked with bacterial growth. Increased concentration of bacteria in the reactor has increased the carryover of particulate to the BA monitor, despite the settler. which lead to serious reliability problems with the BA monitor. At this point, the control computer had crashed once more. Returned to manual operation
I.	Control computer restarted.
J.	Data logging computer crashed due to lack of memory, and continuing problems with blockages in the BA monitor.
K.	Pumping failure on BA dosing system.
L.	Pumping failure on BA dosing system. Periodic blockages in the BA monitor were experienced roughly on a daily basis, until the experiment was terminated 47 days after its start.

Start-up 4

The reactor was again seeded and the control strategy in *Start-up 4* was significantly altered from the previous start-up experiments. The primary difference was in that the actuation was achieved by dosing the reactor with a variable flow rate of BA at a concentration of 2222 mg.l^{-1} $CaCO_3$ equiv., while maintaining a constant HRT in an analogous fashion to the OLR actuation. The dosing of BA into the reactor had a far more direct influence on the measured BA than varying the OLR. The relationship between BA dosed and measured BA was naturally affected by the biological system in the reactor, but the CO_2, BA and VFA equilibrium and the hydraulic regime in the reactor were a physical/chemical systems with relatively rapid responses to change. The VFAs were produced and consumed by biological metabolism, but while in the liquid phase they were readily accessible to the physical/chemical process mentioned above. So dosing BA has a more direct effect on measured BA than changing the OLR and waiting for the acidogenic bacteria to adjust their production of VFAs to closer match the consumption of the same by the methanogens and as a consequence affecting the BA buffering in the reactor. This is clearly visible in the far tighter control achieved in *Start-up 4* which is shown in Figure 4.3.7 and shows closer following of the set point, by the measured BA, in spite of similar perturbations in the BA measurement signal to previous start-up experiments. The effect of perturbations is particularly evident from approximately 600 to 750 hours, and beyond approximately 1200 hours (Figure 4.3.7). Recovery elsewhere is relatively rapid.
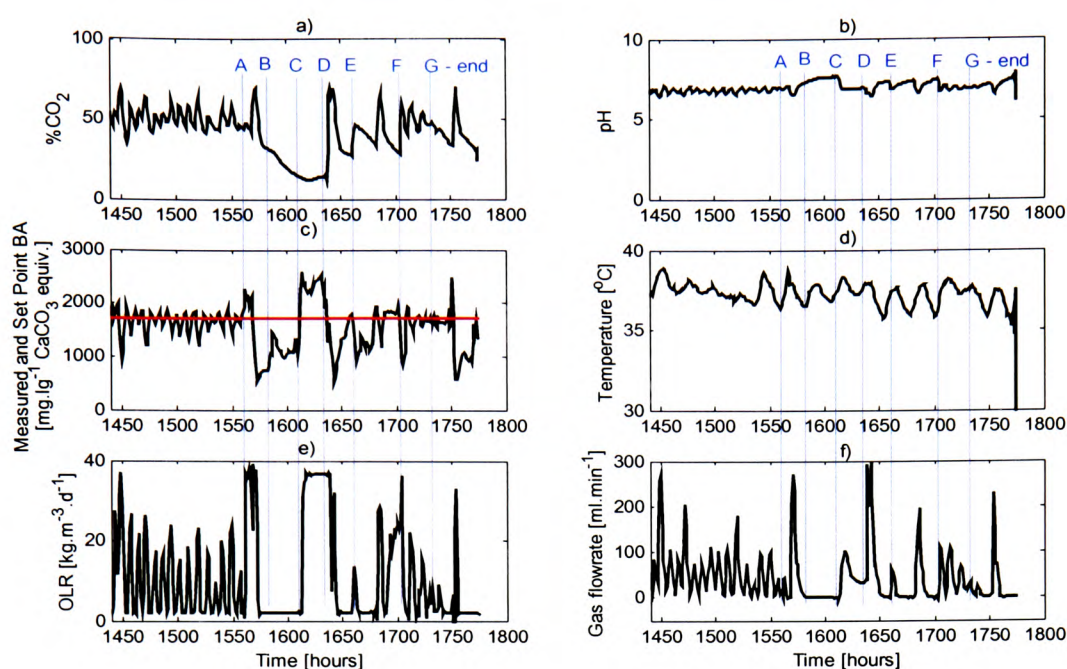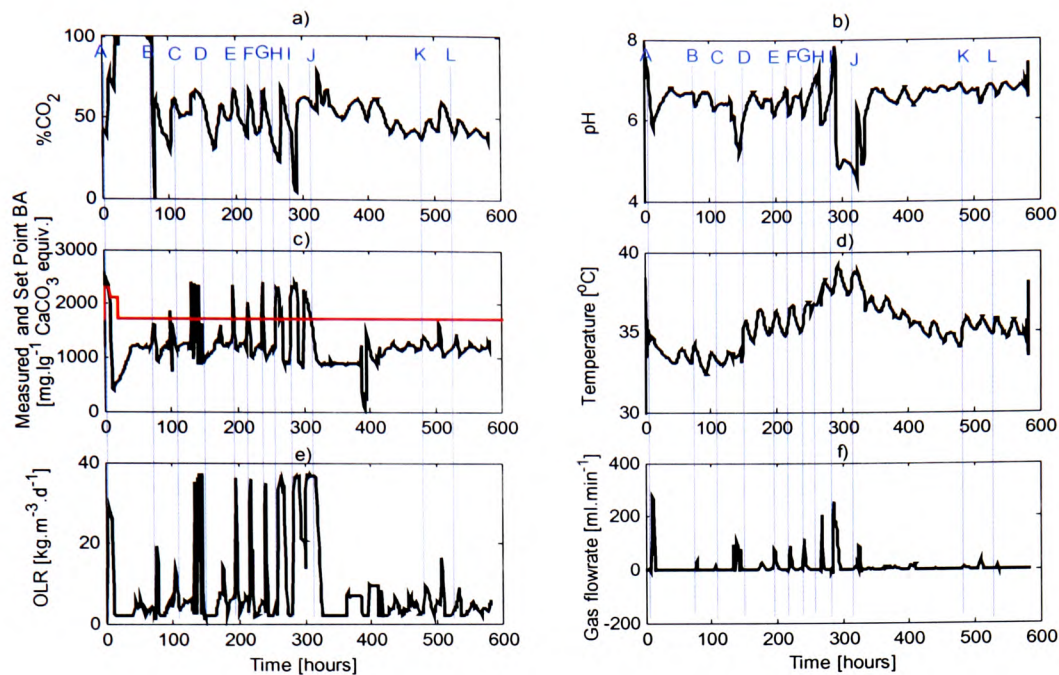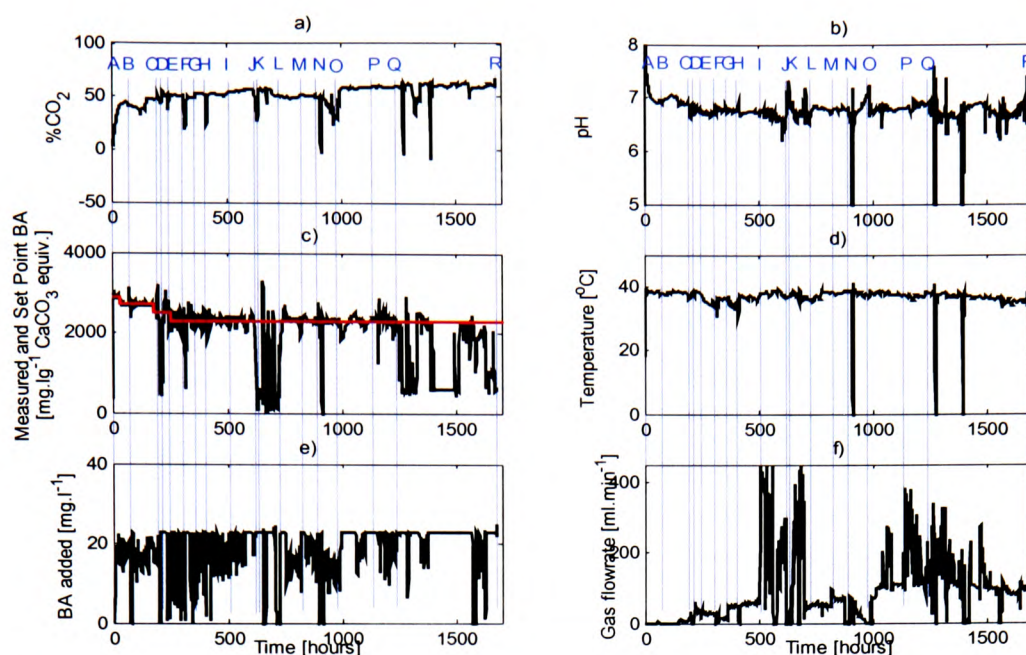
Figure 4.3.7 *Start-up 4* **Performance of the optimised FAT controller**

a) %CO$_2$, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

The OLR was set at (nominally) fixed levels, which are summarised in Table 4.3.7 and changed according to circumstances. In the main this was when the reactor was perceived as having improved in its ability to deal with the current loading rate, or when recovery from a perturbation warranted a reduction in loading rate.

The tendency to increase the gas production rate at the same time as the loading rate was increased and the %CO$_2$ remained reasonably steady at 50%, indicated that the biological performance of the reactor was increasing during this start-up. Arguably, the BA dosing shows signs of reduction as the start-up proceeds (Figure 4.3.7 c)), which would suggest a strengthening of the methanogenesis stage of the AD process. However, as is discussed by Rozzi *et al.* (1994), the dosing approach is philosophically a means of maintaining suitable environmental conditions for the bacteria, as opposed to removing the cause (of the tendency to sour) at source. The latter is the case when control actuation is achieved by varying the organic loading rate. The nature of the reactor and particularly the feed it received in this study was such that BA dosing at some level was required regardless of actuation strategy. A more complex feed than sucrose may generate buffering as a natural consequence of its breakdown, as would be the case for a feed containing protein for example. The cost of dosing may therefore become a significant consideration.

Table 4.3.7 *Start-up 4* **Perturbations: 4th optimised start-up experiment**

A.	OLR set to 2.5 kg COD m^{-3}d^{-1}
B.	Feed pump not pumping. Remedied by moving peristaltic tube.
C.	Changed peristaltic tube positions in BA monitor, feed and BA dosing pumps, causing a rise in measured BA.
D.	Liquid level in the reactor dropped because if either the water or BA pumps are not rotating (0 volt signal), the reactor could flow in reverse direction. The system was manually operated until refilled and then placed into normal automatic mode after approximately 1 hour. A non-return valve placed in the system to prevent this problem recurring.
E.	System stopped for short period (40 minutes) while 5 l (settled volume) of granules were removed. This was necessary as growth was causing potential problems of bacteria carryover to the BA monitor. The sludge blanket was still high, so the recycle was reduced by 30% as a temporary precaution.
F.	Over a 2 hour period, the system was stopped twice, and opened to remove more granules, (oxygen would have entered each time). Granules were visibly bigger than at seeding.
G.	OLR set to 6.7 kg COD m^{-3}d^{-1}
H.	Over 1 hour period, the system was stopped and a further 2.8 l (settled volume) of granules were removed, *Vup* was reset to 4.78 m.h^{-1}.
I.	OLR set to 10 kg COD m^{-3}d^{-1}
J.	pH probe cleaned. Liquid level low, so system filled while on manual control. Feed ran out soon after.
K.	The BA monitor was blocked on two consecutive days, leading to liquid in the solenoid valve, which was cleaned and reinstated. The peristaltic tubing in the BA monitor was replaced throughout and the monitor was recalibrated. Over 1 hour period, the system was stopped and a further 1 l (settled volume) of granules were removed. The recirculation rate was reduced by 57%. The system was run manually and the OLR was reduced to 5 kg COD m^{-3}d^{-1}. The *Vup* was increased to 100% a day later which appeared to reduce the headspace suspended solids, but also expanded the sludge blanket considerably. BA monitor problems persisted until L. and seemed to be foaming related. Antifoam increased
L.	Back to normal automatic operation.
M.	OLR increased to 8 kg COD m^{-3}d^{-1}
N.	Data logging computer crashed.
O.	Reactor leaking and liquid level below outlet port, hence gas phase open to atmosphere. OLR increased to approx. 8 kg COD m^{-3}d^{-1}.
P.	Pump failed in BA monitor, and peristaltic tubing in BA monitor changed.
Q.	Electricity fused, system put to manual control. This was followed by persistent problems with the BA monitor until R., probably caused by foaming in the chambers. The result was a fragmentation of the granules and significant washout of biomass. Channelling was also observed in the reactor during this period.
R.	Stopped on day 70

4.3.2 Detailed observations from *Start-up 1*

Figure 4.3.8 *Start-up 1* **from 0-120 hours**

a) %CO$_2$, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

Figure 4.3.8 shows the first 5-days of *Start-up 1*. It can be seen from the summary data presented in Figure 4.3.1 and Table 4.3.1 that aberrations occurred at about 55 hours and 73 hours, which would affect the evolution of the data series. Initially, very little gas production was evident and practically none recorded as gas flow rate during the entire 5-day period. However, it can be seen that the %CO$_2$, gradually increased over the first 60 hours, as the bacteria (previously dormant in a refrigerator for a year), recovered activity. It is noteworthy that feeding was essentially pulsed in character and occurred five times during the 5-day period and lasted approximately 5-hours. The amplitude of the pulses varied between about 5 and 15 kg m^{-3} d^{-1}. The pH can be seen to respond to the feed pulses by dropping slightly (circa pH 0.5). Already, at this early stage, it can be seen that the control is overly aggressive, in that errors between the measured and desired values of BA provoke large control actions on the OLR. The realisation that this was the case could not be made immediately. Ideally, the control system would have slowly increased the control action and hence the OLR as the bacteria became able to consume the substrate. However, sub-optimal

performance to an unknown extent, was expected, as the reactor under control was an unknown entity (with respect to performance) and had no part (other that physical dimensions etc), in the design of the control system. The degree to which the control was sub-optimal was expected to decrease as a function of the adaption characteristics of the control system. This in fact was the case, as can be seen from the data selected (for its minimal perturbations), in Figures 4.3.9 to 4.3.12. It can be seen that the OLR and by implication the control effort, became progressively more frequent, though still pulse-like in character. The deviation of the measured BA from the set point (though oscillatory), tended to improve and the gas production was seen to increase.

A comparison was made by Premier *et al.* (2001), between the first and fourth weeks of *Start-up 1*, showing that the mean OLR increased from 3.3 $kgCOD.m^{-3}.d^{-1}$, to 6.53 $kgCOD.m^{-3}.d^{-1}$, which was a continuing trend, somewhat retarded by the perturbations experienced.

Figure 4.3.9 *Start-up 1* **from 520-640 hours**

a) $\%CO_2$, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

Figure 4.3.10 *Start-up 1* from 1320-1440 hours

a)   %CO₂, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow
rate.

Figure 4.3.11 *Start-up 1* from 1430-1550 hours

a) %CO₂, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow
rate.
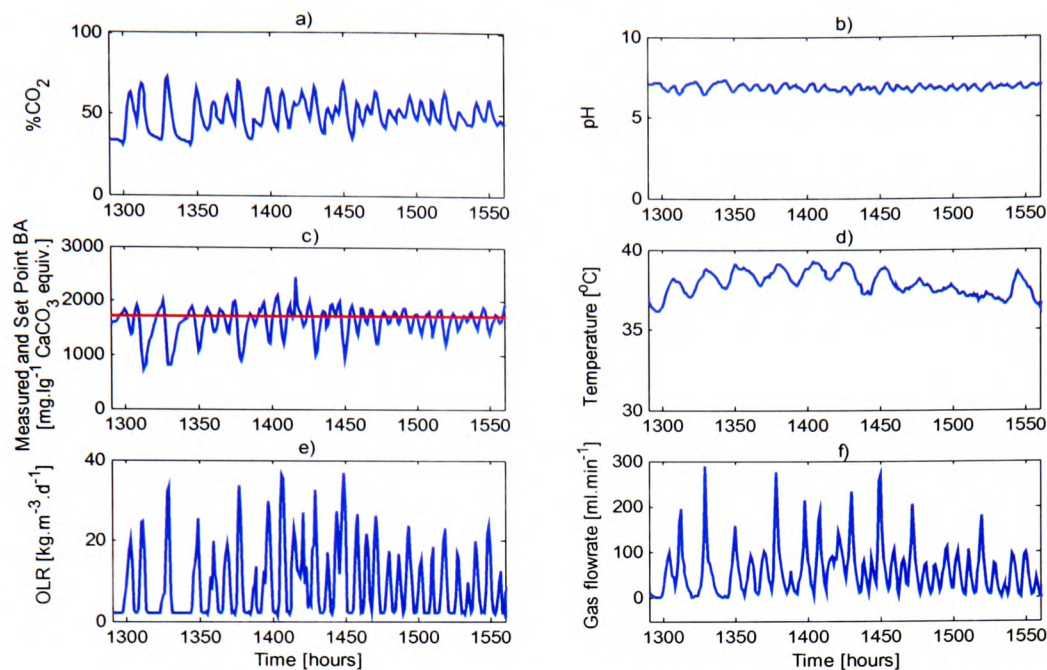
Figure 4.3.12 Sustained 11.25 day period of control during Start-up 1 from 1290-1560 hours
a) %CO₂, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

Figure 4.3.12 shows a period of 11.25 days toward the end of *Start-up 1* which was relatively undisturbed by instrumentation or ancillary equipment failures. The system gives the impression that it is operating slightly to the stable side of marginal stability, with under and overshoot of the measured BA compared to set point, reducing. It is possible that a prolonged period of failure free operation could have lead to convergence at a stable and acceptable operation, but the time taken to achieve this and the reliability of the system elements were beyond practical realisation.

Throughout *Start-up 1*, the affect of reactor temperature is difficult to discern, however by considering the cross-correlation of other data series with the reactor temperature, significant correlation is evident, (Figure 4.3.13). The diurnal variations are quite clearly visible in for example Figure 4.3.12 d), as are the variations due to weather patterns on a longer time scale. More accurate control could have reduced these fluctuations, but the 2°C daily variations and generally fluctuations between approximately 35°C and 40°C, while significant to microbial activity, are not excessive compared to practical temperature control of reactors. It is more difficult to ascertain if the correlation is caused directly by temperature variation, or if the modal frequencies of the system are similar to the frequency of temperature variations. The data in

Figure 4.3.13 is presented as normalised data such that the auto-correlation of reactor temperature at zero lag is exactly one, (which is also shown in this figure). It can be said that there is a relatively high degree of cross-correlation to temperature, particularly in the cases of $\%CO_2$, pH and BA. These are all parameters implicated in the $BA/CO_2/pH$ equilibrium (by definition) and are all susceptible to temperature through microbial metabolic rate and physico/chemical effects through dissolved CO_2 equilibrium in particular. This is particularly evident from the correlation of temperature to pH which is almost identical to the auto-correlation of the temperature. There is also a high likelihood that the pH probe was affected by temperature, which would result in a strong correlation as indicated.

There is a possibility that many of the failures experienced by the BA monitor due to blockages, particularly those caused by bacterial carry-over, could have been temperature related. The mechanism by which this may have occurred could be described as a sequence of events all traced back to reactor temperature thus: A rise in temperature would increase microbial metabolism, increasing acidogenesis and hence reducing pH. This would cause BA to breakdown and CO_2 to be evolved in greater proportion. The gas would further expand and disturb the sludge blanket causing carry-over of suspended solids to the BA monitor, leading to blockages.
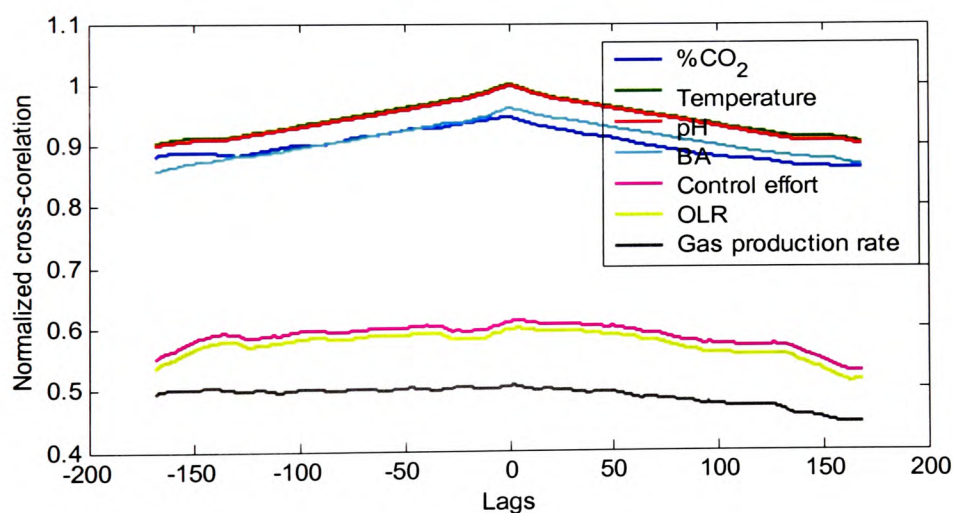
Figure 4.3.13 Cross-correlation between reactor temperature and various reactor parameters from 1290-1560 hours, looking 7-days into the past and future.
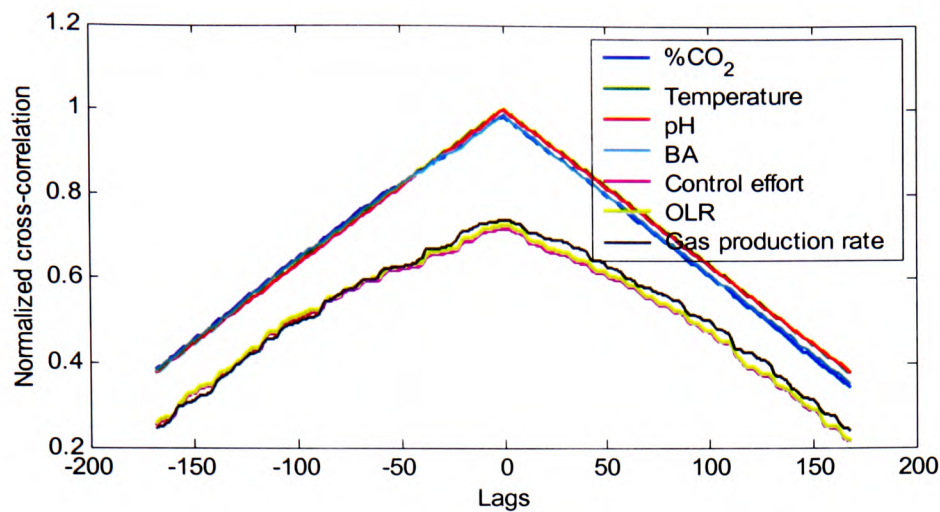
Figure 4.3.14 Cross-correlation between reactor temperature and various reactor parameters from 1290-1560 hours, in *Start-up 1*, looking 7-days into the past and future.

The cross-correlation shown in Figure 4.3.13 considers the complete data set which constitutes *Start-up 1*, which when contrasted with Figure 4.3.14 which considers a subset of this data, shows that the cross-correlation which includes the perturbed periods of operation gives a higher correlation between $\%CO_2$, pH and BA against temperature, and somewhat similar correlations for the remaining parameters. It is believed that Figure 4.3.14 gives a better indication of the correlations than Figure 4.3.13 as the saturated signals will appear to increase the correlation significantly if they persist for significant proportions of the overall duration of the experiment. Never the less, the cross- correlations are apparently significant and the modelling used in the preparation of the control strategy and described in Section 3.3.3, is unable to take account of temperature variation, as this has not been included as a variable. As presented by Batstone *et al.* (2002), the five main influences of temperature on biochemical reactions are:

1. Increased reaction rate with increasing temperature (as predicted by the Arrhenius equation)
2. Decrease in reaction rate with increasing temperature above optimum ($>40°C$ for mesophilic and $>65°C$ for thermophilic)
3. Decrease in yields, and increase in half saturation constant due to increased turnover and maintenance energy with increased temperature
4. Shift in yield and reaction pathway due to changes in thermodynamic yields and microbial population
5. Increase in death rate due to increase in lysis and maintenance

They suggest that with temperature changes of ±3°C, AD can be modelled without temperature dependency, requiring only that suitably selected (for temperature) parameters be used in the model. For the most part, the data is close to this criterion but does drift over weeks and months. Even within the ±3°C, one would expect variations in the five main influences above to occur, and as a consequence, the normalisation of the data will lead to cross-correlation becoming evident.

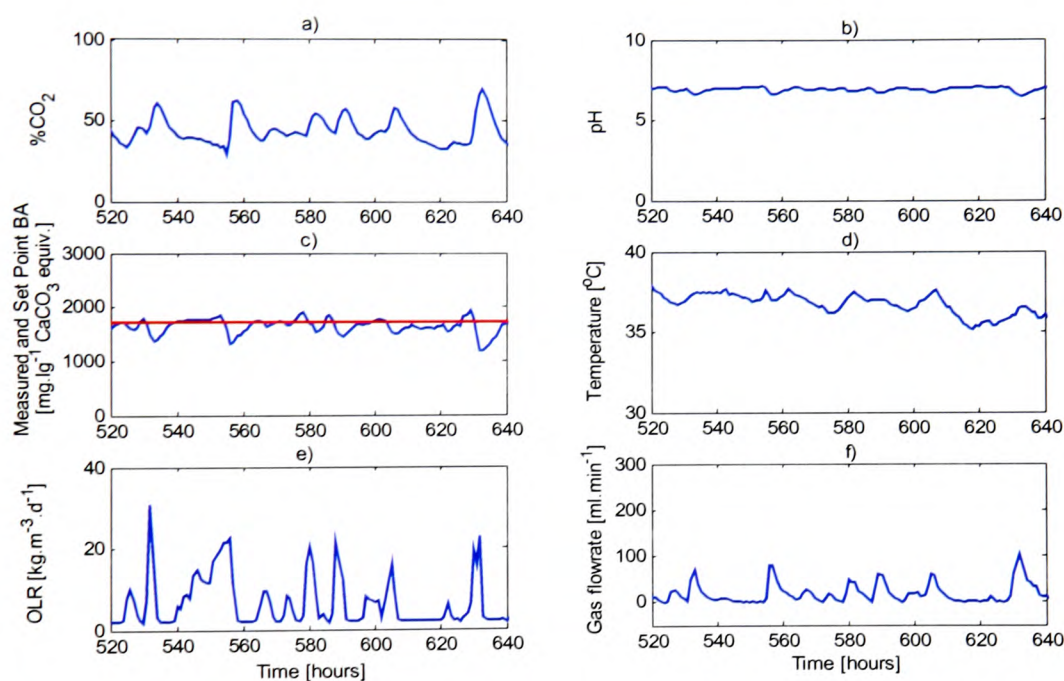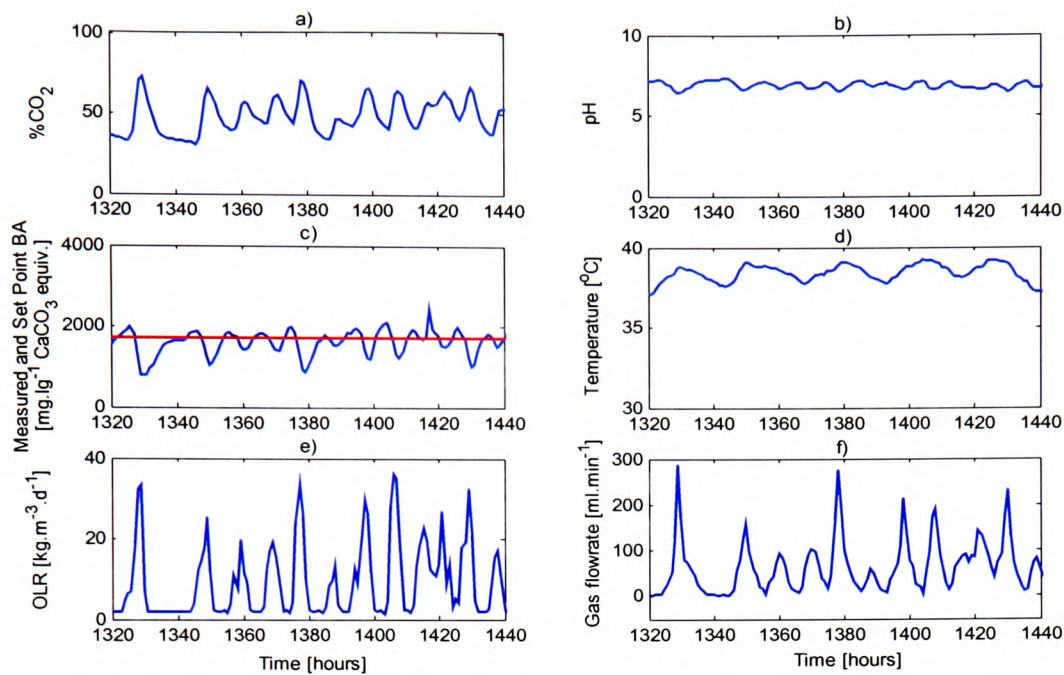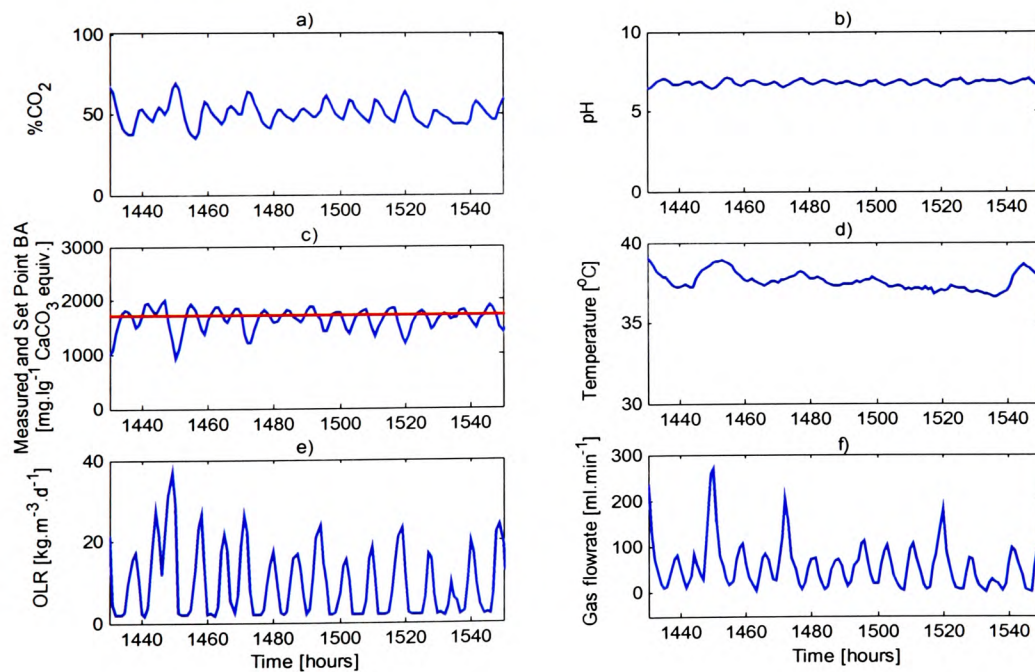### 4.3.3 Detailed observations from *Start-up 2*
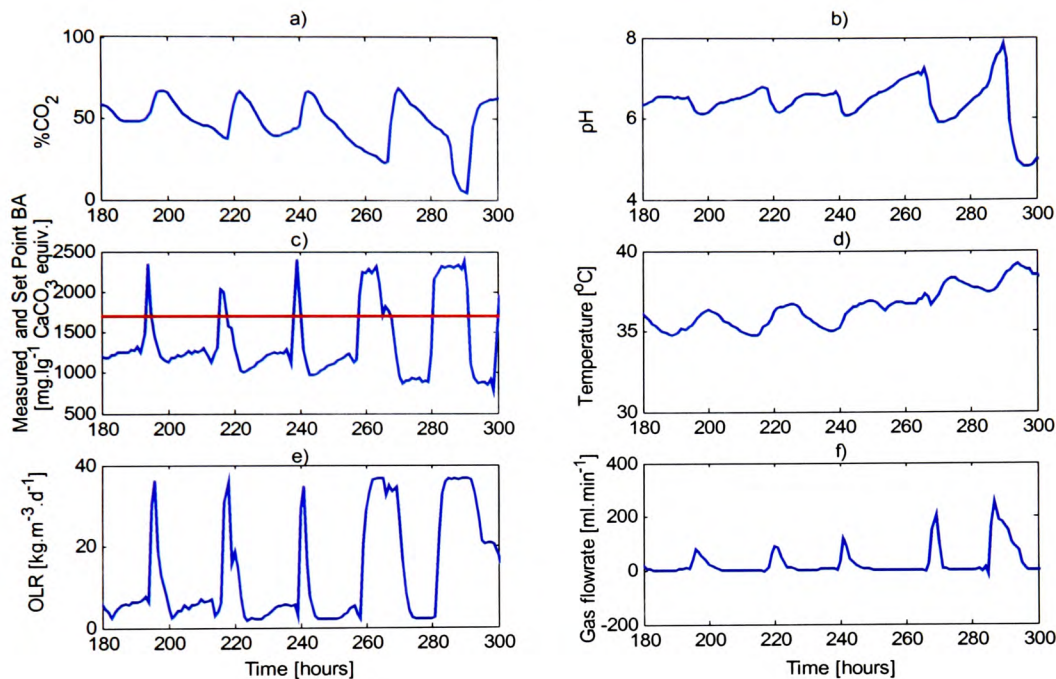
Figure 4.3.15 *Start-up 2* from 180-300 hours

a) %CO₂, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

Start-up 2 was run for considerably less time than *Start-up 1*. 12.5-days are presented in Figure 4.3.15 which should be considered in the context of Figure 4.3.5 which indicates that the BA monitor or its associated solids separation system caused perturbations at 170, 210, 235, 245 and 280 hours in the time series. These aberrations correspond to the sudden rise in measured BA and the consequential feeding that soon follows. The close following between BA and OLR indicate that the response is predominantly induced by proportional and derivative adaption elements, and the integral element has little chance to adapt over the time scale indicated and the repeated over and under shoot of the measured BA compared to the set point. The seed for *Start-up 2*, was the remaining bacteria, which had been considerably stressed from *Start-up 1*. The methanogens were

suspected to have been depleted significantly because of the feeding regime induced by the adaption parameters used in *Start-up 1*. The repeated and severe perturbations experienced by the system during *Start-up 2*, do not allow clear analysis of the controller performance, other than to say that the tendency was toward increasing feeding with time, with gradual increases in OLR, punctuated with large feeding 'spikes' at the points where the BA reading was unreliably high. This retarded the progress of the controller adaption and the pattern in essence, was repeated. It is believed that a long period of uninterrupted operation would have lead to a more sedate control performance compared to *Start-up 1*. It was noted that the reactor temperature would have the same relationships to the remaining data as discussed above. There is a clear correlation between the perturbations and the diurnal fluctuations in temperature and the rising trend in the OLR could be associated with the rising trend in temperature (at least to some unknown extent). The observed breakdown of the granules that released substantial fine suspended solid and caused the BA monitor problems, lead eventually to the termination of the experiment.

4.3.4 Detailed observations from *Start-up 3*

In the case of *Start-up 3*, the control and reactor arrangements were the same as *Start-up 2*, with variation of OLR as the control actuation and using the same adaption parameters as *Start-up 2*. The reactor however, was re-seeded with granules from a UASB reactor used to treat molasses waste as mentioned previously. Again, the experiment was perturbed frequently by instrumentation problems, so the 5-day period of operation, which was selected as being indicative of the controller performance is shown in Figure 4.3.16. Two perturbations occurred during this period at approximately 45 hours and 220 hours, and are summarised in Table 4.3.6 as events C and D. Beyond 230 hours, the cumulative effect of successive perturbations complicate the analysis of the data because of the cumulative damage done to the microbial consortium, from which it never had sufficient stable operating time to recover.

The key and interesting features of the controller performance shown in Figure 4.3.16 are the considerably improved set point following compared to *Start-up 2*, and the absence of the characteristic pulsed feeding regime experienced in *Start-up 1*. The OLR changes in a far less aggressive manner and shows an increasing trend until such time that the second perturbation occurs. The new seed seems to provide initial conditions from which the start-up can proceed fairly rapidly and it can be seen that the system reaches a sustainable (in the absence of measurement perturbations) OLR in the region of 10 kg m^{-3} d^{-1}. There is every reason to believe that this loading rate could be improved upon as the methanogenic bacterial populations increase

and the granules acclimatise and develop. This is of little consolation as once the system was badly over loaded at 220 hour and repeatedly so thereafter, the control was never re-established in the same way, but came to resemble the control achieved in *Start-up 2*.
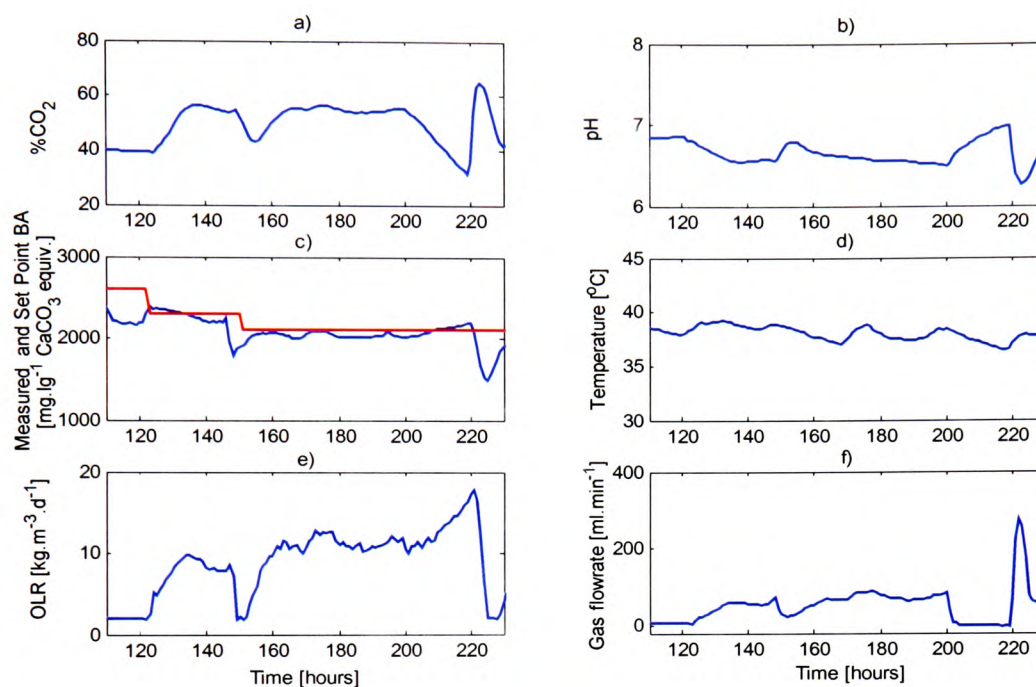
Figure 4.3.16 *Start-up 3* **from 110-230 hours**

a) %CO₂, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) OLR, f) Gas flow rate.

4.3.5   Detailed observations from *Start-up 4*

Start-up 4 was, in comparison to the previous start-up experiments, significantly more successful in maintaining reactor stability. Similar measurement perturbations were experienced to other experiments, yet the control strategy was better able to cope with such events. Once more the data presented here is selective, to minimise the confusion caused by the untoward events summarised in Figure 4.3.7 and Table 4.3.7 which include the complete time series. The reader is therefore able to refer to the complete data to establish the context of the selected data, as before.

The intention had been to raise the OLR in *Start-up 4* periodically as the operation of the reactor was seen to have stabilised. It was however, impossible to do this firstly because the perturbations described in Table 4.3.7 required the OLR to be reduced on occasions and secondly because the

peristaltic pump supplying the feed behaved in a temperamental manner, and did not deliver at a constant rate. The influent COD was measured off-line roughly 24 hourly, so it has been possible to calculate the OLR at these instances. There is still uncertainty between samples, so as a means to visualise and estimate the OLR, the calculated (raw OLR) data was filtered using a bi-directional filtering method (to avoid phase affects), and a 5th order Butterworth filter. Both the raw and filtered OLR are represented in Figure 4.3.17. The variation in OLR is to some extent more representative of real processes than a constant OLR would have been, as it is seldom possible to control the OLR of an effluent waste stream on a continuous basis.
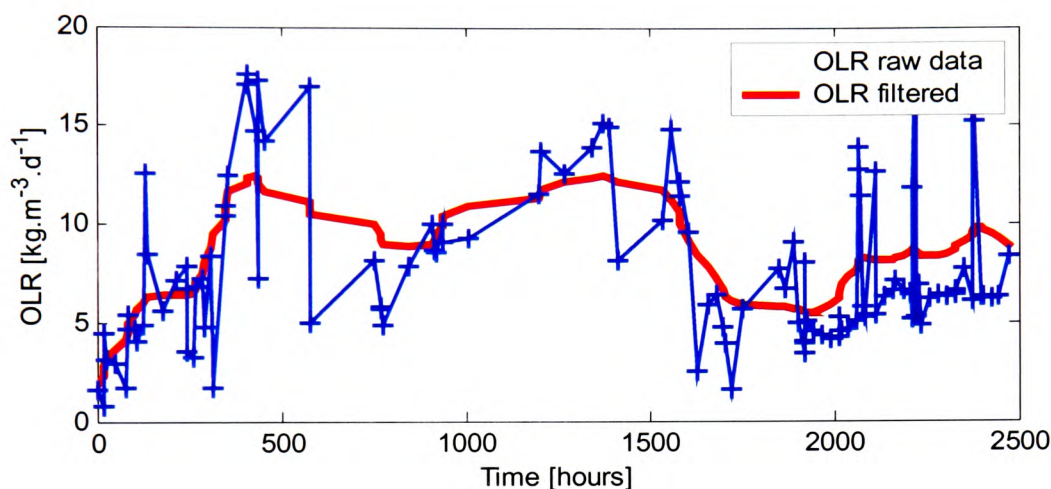
Figure 4.3.17 OLR calculated from influent COD, over duration of *Start-up 4*

The first 5-day window of data presented in Figure 4.3.18 is from early on in the experiment, with subsequent selections presented in Figures 4.3.19 to 4.3.21 following chronologically. All present 5-day periods, except Figure 4.3.21, which presents a 10-day period of uninterrupted operation.

The reader is reminded that the actuation in *Start-up 4* was different from all previous start-up experiments in that it used BA dosing as opposed to variations in the OLR to effect control over the buffering available in the reactor. Figure 4.3.18 shows 5-days data from the first week of the start-up. The reactor had been re-seeded in the same way and using the same seed sludge as in *Start-up 3* and the OLR was initially fixed at 2.5 kg COD m^{-3}d^{-1}. It can be seen (Figure 4.3.18), that the variations in BA added to the reactor are well able to maintain comparatively close following of the set point by the measured BA. A significant perturbation occurs at approximately 75 hour, but recovery is rapid, though some mild oscillation is apparently induced. It is notable

that the pH remains undisturbed and that gas is production for about 8 hours before this event then ceases.
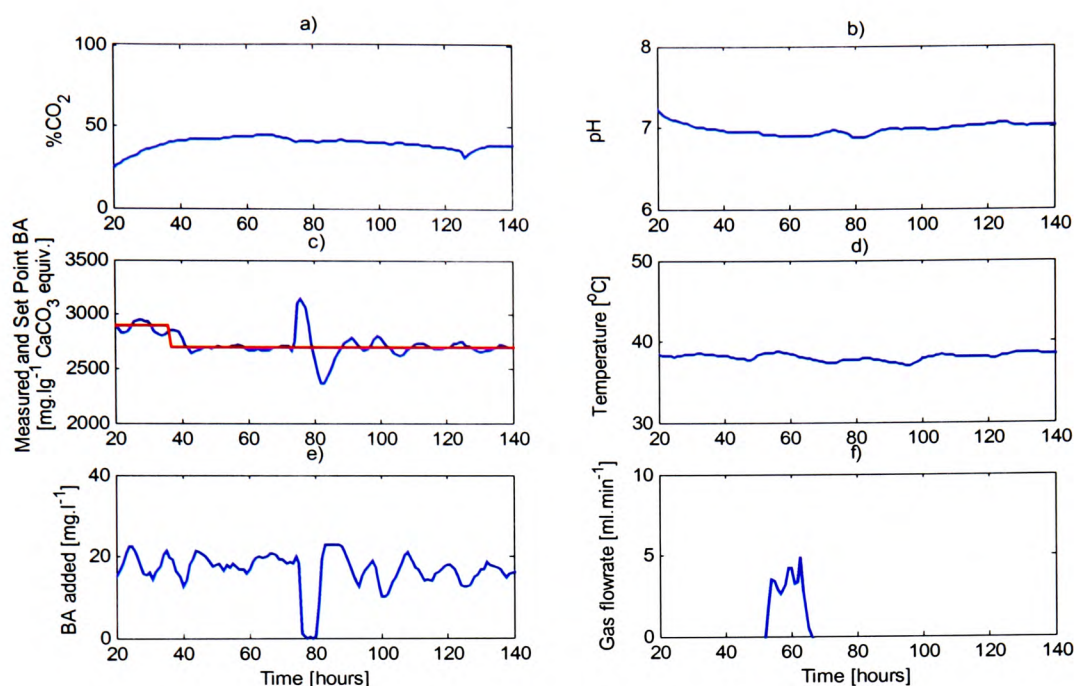
Figure 4.3.18 *Start-up 4* **from 20-140 hours**

a) %CO$_2$, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) BA added, f) Gas flow rate.

Figure 4.3.19 shows 5-days in the 3rd and 4th week of operation where gas production is sustained and reasonably constant until a small drop in BA due to increased loading rate to nominally 10 kg COD m^{-3}d^{-1} which causes maximum BA dosing. This continues for about 10 hours leading to an increased gas flow rate, in small part due to CO$_2$ evolution, but prior to this increase, the gas flow rate was probably under recorded as several episodes of sludge removal and level reduction were required, as detailed in Table 4.3.7. This is likely to be the reason that little change is evident in the %CO$_2$, plot a), indicating that CH$_4$ production was commensurately increased.

Although the measured BA is still oscillatory, it never exceeds about ±250 mg l^{-1} CaCO$_3$ equiv. error from the set point.
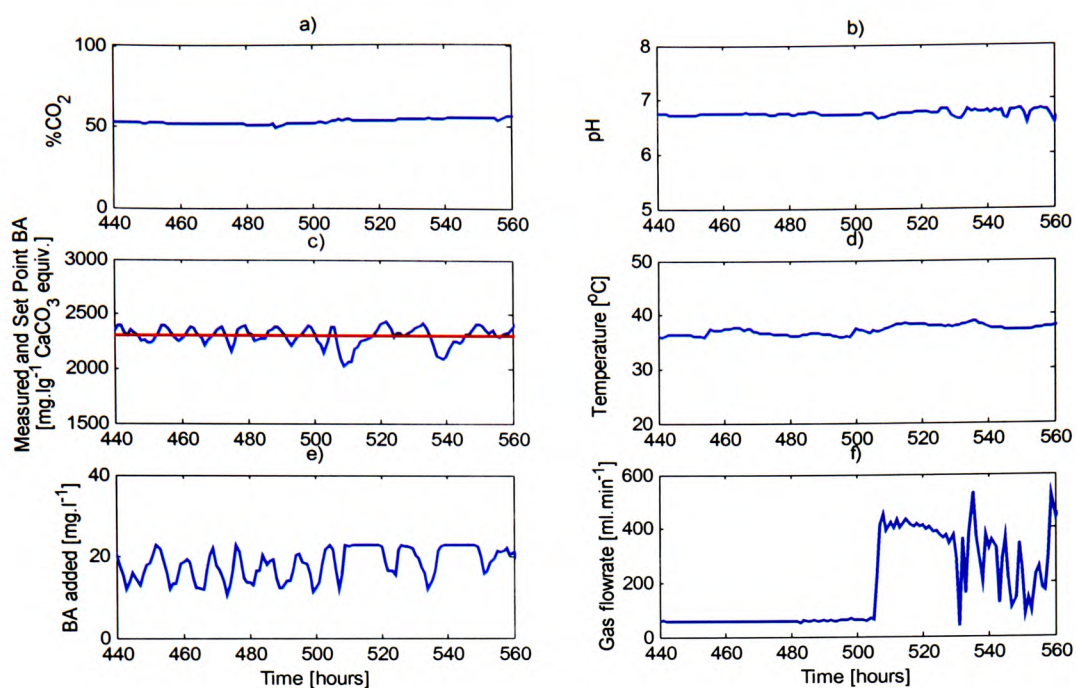
Figure 4.3.19 *Start-up 4* **from 440-560 hours**

a) %CO_2, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) BA added, f) Gas flow rate.
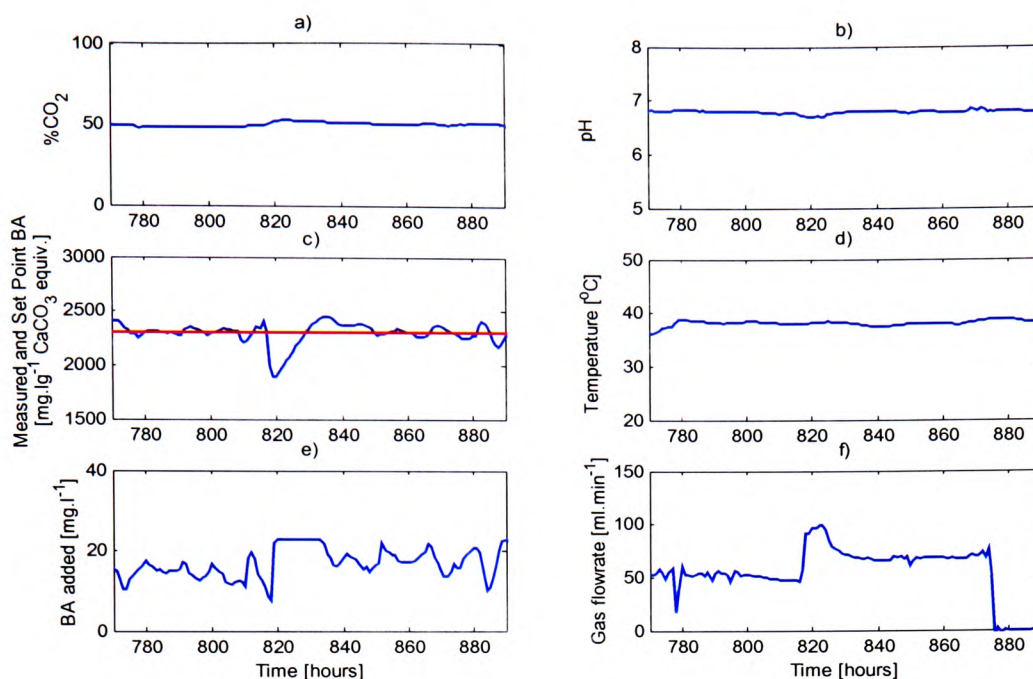
Figure 4.3.20 *Start-up 4* **from 770-890 hours**

a) %CO₂, b) pH, c) Measured (blue) and Set Point (red) BA, d) Temperature, e) BA added, f) Gas flow rate.

The data presented in Figure 4.3.20 starts about 4 weeks and 4 days into the experiment and lasts for 5 days. Similar performance is maintained to that shown in Figure 4.3.19, though a measurement perturbation is evident at circa 817 hours. The gas production appears to stop totally, but this was caused by problems with the gas measurement system, caused by foaming in the headspace of the reactor. In fact the gas production was maintained.

Figure 4.3.21 shows the last 10-day period, which can be analysed before the system was compromised by repeated and severe perturbations of the measured BA. Never the less this period suffered disturbances at 980 and 1150 hours. It is fair to suggest that reasonable control was maintained over this period, despite the perturbations. The BA in the reactor can clearly be seen to oscillate about the set point, as has been the case in previous data during this start-up. This would often indicate a tendency to instability, or marginal stability. It can be argued however, that the oscillation is a function of the temperature variation and the corresponding effects (discussed above). These have been dealt with as disturbances, in the development of the control system, because no mechanism for temperature variation was included in the deterministic model. This is supported by the cross-correlation presented in Figures 4.3.22 and 4.3.23. Again, as in *Start-up 1*,

the cross-correlation of the indicated parameters with temperature are rather high. This is particularly true of the complete data set for *Start-up 4*, for the same reasons as mentioned previously, relating to Figures 4.3.13 and 4.3.14. The cross-correlation shown in Figure 4.3.23 considers only the period and data presented in Figure 4.3.21. It can be seen that some saturation occurs on the BA dosing, and that there have been periods where the process is recovering from perturbations.
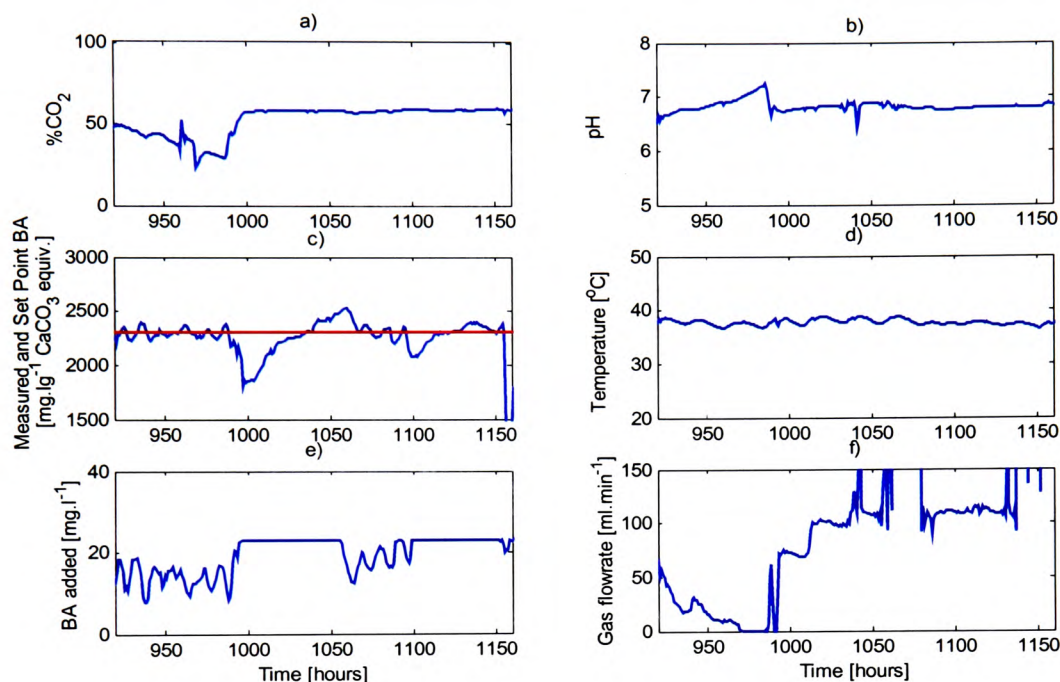
Figure 4.3.21 *Start-up 4* **from 920-1160 hours (10 days)**

a) %CO$_2$, b) pH, c) Measured (blue) and Set point (red) BA, d) Temperature, e) BA added, f) Gas flow rate.

The correlation analysis presented in Figures 4.3.22 and 4.3.23 shows that the dependence on temperature, though significant, is reduced compared to *Start-up 1*.

Overall, a comparison of the control performance between the two actuation methods, shows that the control strategy most likely to be successful is that which used BA dosing. It is possible to argue that the actuation by variation of OLR has not been fully tested despite the very long duration of *Start-up 1, 2 and 3*, as the lack of reliable operation of the process and instrumentation made the performance difficult to assess with confidence. The very fact that such unreliability was present indicates the need for control strategies capable of maintaining reasonable control at these critical episodes. The avoidance of 'run away' on the control action is important, but was not implemented in the work done in this project.
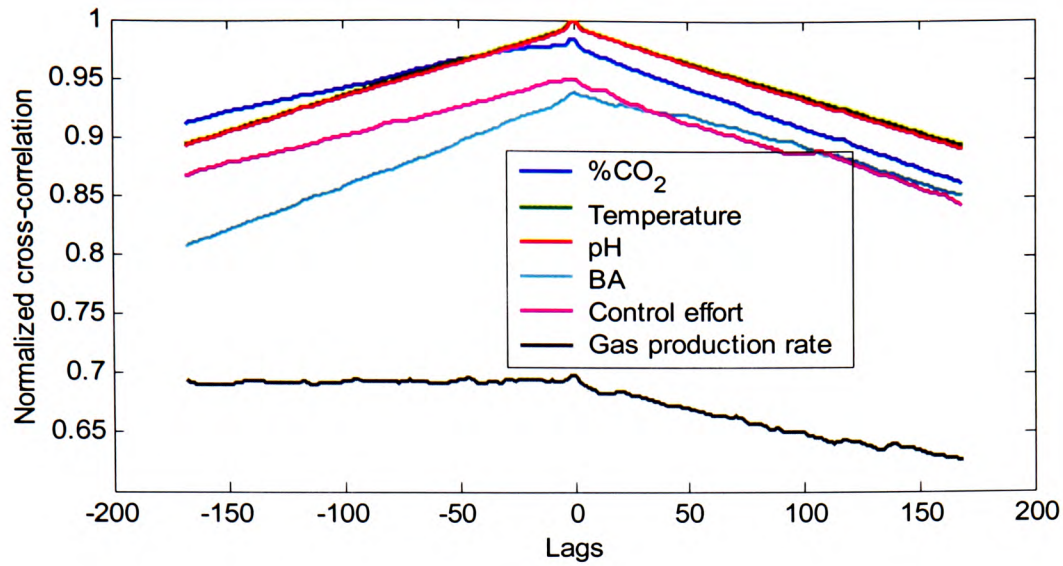
Figure 4.3.22 Cross-correlation between reactor temperature and various reactor parameters during whole of *Start-up 4*, looking 7-days into the past and future.
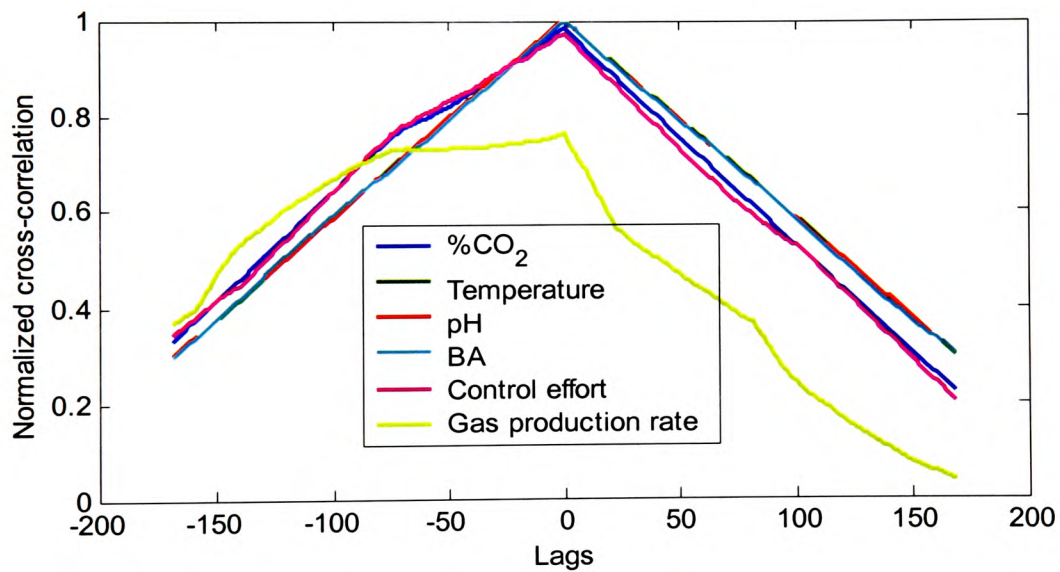
Figure 4.3.23 Cross-correlation between reactor temperature and various reactor parameters during 920-1160 hours (10 days) of *Start-up 4*, looking 7-days into the past and future.

4.3.6 Consideration of the effect of gain discrepancies between the control and monitoring computers

The simulation illustrations presented in Figures 4.2.17 to 4.2.19 can be compared with the data from *Start-up 1,2 and 3* and if the aberrations caused by failures in the BA measurement are considered, it can be argued heuristically that the data is similar to that generated by the simulations. The discovery of the discrepancy has made the data appear more predictable with respect to the modelling that was employed and as a result, the confidence that the control strategy could be made to deliver significant improvements once the control effort gain discrepancy were corrected, has been increased.

Comparing Figure 4.2.17 b) with the data from *Start-up 1* in Figures 4.3.1 to 4.3.4, shows significant similarities in the 'saw-tooth' responses evident in both simulated and real data. The periodicity of the responses is also similar though they become more frequent as the microbial populations strengthen in the experimental work. Again there is intuitively and arguably an equivalence between the simulations and the experimental data. The same correlation is evident when the detailed and selected data is viewed in Figures 4.3.8 to 4.3.11.

The data from *Start-up 2 and 3* are more difficult to correlate to the performance of the simulations, though the responses appear to be more closely related to the 'corrected' system that they were to the 'uncorrected' system simulations. Figure 4.2.19 still exhibits the characteristic 'saw-tooth' response and when compared to Figure 4.3.5, some evidence of this trend can arguably be said to exist. It is however the case that, the set-point is not reached for most of the duration of the experiment, which is not predicted by the simulation. The data from *Start-up 3* in Figure 4.3.6 tells a similar tale, though the detailed enlargement presented in Figure 4.3.16 does show some tendency to behave like the simulation.

It should be noted that the same error did not exist in the case of *Start-up 4*, which dealt with BA dosing as a control action, and as a result, the performance was significantly better, though still oscillatory, as discussed previously.

5.0 CONCLUSIONS AND RECOMMENDATIONS

This Chapter seeks to draw conclusions based on the four broad objectives set out in Section 1.3 (and in boxes below). The first of these set out parsimoniously to establish if very simple models would be able to represent the AD process with sufficient fidelity to be usefully employed in both control system analysis and synthesis. Based on the outcome of this study, the second objective would select a suitable modelling method from literature or otherwise, for use in the design of a suitable control strategy which would start to fulfil the third objective. The third objective contained the main thrust of the project, and its ultimate ambition, which was a cost effective control system with industrial applicability and transferability between different high rate anaerobic digesters. The fourth objective was to experimentally investigate a philosophical approach, leading toward the ultimate ambition. This in essence, was to apply a specific control strategy parameterised using an specific model, which in turn is calibrated on an arbitrary but representative reactor and applied to a different (in design and operation), reactor.

The recommendations that follow are made with the same objectives in view and are intended to give direction to future work, without trying to be comprehensive and exhaustive. This thesis is considered to be the first stage of a development process, which will lead to the transferable generic anaerobic digester controller, which is the ultimate ambition of the work. An exhaustive list of possible directions of study would not serve this ambition well.

5.1 CONCLUSIONS DRAWN FROM THE INVESTIGATION INTO BLACK BOX MODELLING

> *Objective i.*
>
> AD is well known to be a non-linear process, but the degree to which this process could be modelled parsimoniously using linear and non-linear, black box models was not clear from the literature. Therefore the first objective was to discover if simple models of the type mentioned were sufficiently accurate to represent an anaerobic digester subject to relatively high loading and stressed conditions over many weeks (which would also consider time variations in the reactor behaviour). An existing fluidised bed reactor was used in this study, in the belief that the results would be reasonably transferable to any high rate reactor, which was well mixed.

The identification of low order linear, uncoupled black box models of various common structures such as ARX, ARMAX and Box Jenkins, from on-line sensors and data logging for BA, $\%CO_2$, gas production rate and TOC, proved to be both possible and practicable. However the simplest model structure of choice was the ARX structure. ARX models in particular were parameterised using data resulting from substantively different variations in organic loading rates compared to

temporally separate (by multiple retention times), verification data, generated on the same fluidised bed anaerobic digester. Predictions 30 minutes ahead, displaying significant accuracy, were demonstrated, despite the expected non-linearity, time variation and coupling between the measured data streams.

A comparison of ARX models which all used the same lag space, training and validation data was performed for linear SISO ARX, linear MIMO ARX and non-linear feed forward neural network ARX models. This showed that the performance of the linear SISO ARX, measured using correlation analysis was comparatively good in the case of BA, but less able to represent the %CO_2 and gas production rate than the other models. The comparative study did not include TOC.

The correlation analysis showed that the linear SISO model produced auto-correlation and cross-correlation functions, which remained within the 95% confidence limits for the most part. The linear SISO model for %CO_2 on the other hand, produced correlation functions predominantly outside the 95% confidence limits. In the case of gas production rate, the linear SISO ARX model showed performance comparable with the non-linear neural network ARX model, though inferior to the linear MIMO ARX model, in terms of the correlation functions.

In comparing the more complex structure of the non-linear neural network ARX model and the linear MIMO ARX model, it is evident from the correlations that the Neural network model was superior with respect to BA, but inferior with respect to gas production rate.

The results of the comparison of models with the underlying ARX structure showed that the selection between them is not straight forward, though it might be deduced that on the basis of correlation performance alone, the neural network and MIMO models would be preferred to the SISO model, because of the poor performance of this model with respect to %CO_2. Of the three models considered, the MIMO model would be preferred in situations where black box approaches are relevant, for its combination of its relative simplicity, accuracy and transparency.

The limitation of the black box approach lies in the fact that long prediction horizons degrade the performance of the model progressively, such that at the point where pure simulation is performed (infinite prediction horizon), the accuracy is greatly diminished. Some similarity in the dynamic behaviour or the underlying data generating mechanisms of the anaerobic process used remains. Reducing the horizon of the simulation to one step (30 minutes) ahead improves the accuracy of

the model to the point that it can be considered a relatively accurate representation of the system. The limited pure simulation accuracy makes these ARX models less suitable than alternatives for use in the synthesis of control systems, though they could form part of the control strategy where online data is available, such as in self-tuning systems.

5.2 CONCLUSIONS DRAWN FROM MODEL SELECTION FOR CONTROL STRATEGY DEVELOPMENT

Objective ii.

Having determined the success or otherwise, of the simple black box approach, the second objective was the establishment of a suitable modelling strategy which could be used in the design of a control strategy.

Deterministic dynamic models of varying complexity have been published along with calibrations, verifications and validations, to afford a large pool of candidate models with a high degree of transparency. These are considered preferable, for reasons of transparency, to models, which are in general terms fuzzy, such as fuzzy logic, neural network, expert systems and their hybrids and derivatives. In the context of this study, they are also considered to be preferable to the black box models, which were the subject of Section 5.1.

The selected model of Marsili-Libelli and Beni (1996) embodied the parsimonious attributes of minimum substrates, products and associated bacterial populations, while at the same time including the physical-chemical equilibria necessary to represent all the parameters of interest in the experimental work which was conducted. The model was calibrated using the same anaerobic digester used in the identification of black box models, and as such was known by the author and afforded continuity in model development.

It was possible to investigate the control strategy which was developed, by using simulations which included the Marsili-Libelli and Beni (1996) model. A relatively 'relaxed' control strategy demonstrated a notional lower limit of likely behaviour, which was then compared to the more aggressive control, derived from the numerical optimisation procedures based on the simulation model. The performance of the optimised control strategy was a significant improvement over the heuristically parameterised 'relaxed' controller.

Simulations were able to explain the reason for oscillatory behaviour in the experimental work and to verify that unmodelled dynamics and transmission delays in the software communications caused this behaviour.

The simulations of a discrepancy in the control effort gain were able to demonstrate that the control that should have been expected was inadequate, but this analysis paradoxically improves the confidence that can be placed in the ability of the modelling to represent the system.

5.3 CONCLUSIONS DRAWN FROM CONTROL STRATEGY DEVELOPMENT

Objective iii.

The third objective was to select and investigate a suitable control strategy by simulation techniques using Computer Aided Control System Design (CACSD) tools. The control strategy would be developed with an ultimate goal (partly beyond the current study), to deliver a generic control system, which could be shown to be applicable to anaerobic digesters which are different in design and operation. The control system should require a minimum of instrumentation, expertise and prior knowledge of the reactor and should be able to control the anaerobic digester from commissioning and start-up to steady state under realistic loading conditions.

The Fast Adaption Trajectory (FAT) adopted increased the propensity to instability, but allowed closer following of the desired value.

Tight optimisation constraints imposed through the selection of a cost function would lead to high adaption mechanism gains, which in the event of unmodelled dynamics, could cause stiff behaviour at the point of implementation on an anaerobic digester.

Sub-optimal performance should be expected, as the real world anaerobic digester was unlikely to be accurately represented by the Marsili-Libelli and Beni (1996), even if the same digester were used. This is because of variations in the operating conditions of the reactor and the consequent development of the microbial consortium it contained.

Within broad but ill-defined bounds, the control strategy is expected to adapt the control action to give sub-optimal, yet acceptable control on a variety of different high rate anaerobic digesters with a well-mixed content.

The strategy adopted required only a single sensor (BA monitor), neglecting the independent temperature control function and was aimed at a notional ill-defined reactor, which would be operated automatically from commissioning by non-expert personnel. The nature of the control strategy would tend to maximise the loading rate as a natural consequence of an improving biological performance, until steady state was achieved.

5.4 CONCLUSIONS DRAWN FROM THE TESTING OF THE CONTROL STRATEGY DEVELOPED

Objective iv.

The control strategy would at this point, be tested on a laboratory scale reactor and its performance investigated.

The performance of the control strategy was overwhelmingly dependent on the reliable and reasonably accurate operation of the BA monitoring system. No mechanism was included in the control strategy to mitigate the effects of failure of the measured variable, and as a consequence, signal saturation due to failures, induced a control action response, which effectively over loaded (in some way), the reactor. Failures in other ancillary and auxiliary equipment had similar affects. For the system to be made industrially applicable, system (particularly BA monitor) failures will need to be detected and 'holding actions' taken till the problem can be remedied. A BA monitor designed for greater rates of flow from a larger reactor, is likely to be more reliable, as blockages will occur less frequently.

The unmodelled dynamics (particularly those evident in the measured variable and those caused by an implementation discrepancy in the gain of the control effort) have caused poor controller performance. The generic controller should be parameterised using a model which includes any significant delays and adopts a 'two standard deviations – worst case' philosophy in defining the dynamics of the system. This will lead to sub-optimal and less aggressive control in general, but will avoid the behaviour observed in *Start-up 1*.

The following arguments are made assuming that the measured variable remained reliable. Though this was not the case, there were numerous periods during the experimentation when stable operation allowed the characteristic behaviour of the controller to be deduced. The controller implemented in *Start-up 1*, which used OLR control actuation, showed that even in a situation where there had been significant omissions in modelling the system dynamics, sub-optimal control could still be shown. The control action was impulse-like and aggressive, but improvement occurred over time (albeit measured in weeks and months). The control was however poor and stemmed from the optimisation with unmodelled dynamics, which gave high adaption mechanism gains in the FAT controller. Re-optimisation, including measurement delays, showed (particularly in *Start-up 3*), that the control action was considerably improved and prolonged operation would have been expected to lead to increasing loading rate till steady state. In *Start-up 4*, the actuation was changed to BA dosing, and showed good control could be

maintained over the reactor, and that the OLR could be increased progressively in the space of weeks.

Comparisons between the OLR actuation and BA dosing actuation show that tighter control can be maintained over the reactor system used in the experimentation in the latter case.

Reactor temperature was considered to have a significant affect on the control systems in all the start-up experiments and oscillation in *Start-up 4* in particular, were in part at least, derived from temperature effects even though these variations were of the order of $\pm 1^{\circ}C$ over a days operation and approximately $\pm 2.5^{\circ}C$ over longer periods.

The experimentation has demonstrated that it is possible to control a reactor from the commissioning stage or re-start and see improvement in the biological performance. However complete start-up and steady state operation was not achieved because of the lack of reliability of the system elements, in particular the BA monitor, at this scale and flow rate of sample.

5.5 RECOMMENDATIONS FOR FUTURE WORK

While the control system has shown that it could control the EGSB reactor used in the experimentation, it has not yet been shown that this can be sustained up to high loading rates in the region of 20 kg $COD.m^{-3}.d^{-1}$ and above. All the experimentation used sucrose as the basic feedstock and required BA addition to maintain buffering. The simplicity of the feed obscures its problematic characteristics, which are less conducive to stable operation than many more complex feed mixtures and compounds. The control experimentation has been dogged by unreliability, which have highlighted an already known fact, which is that failures will occur during operation, and the control system should have the ability to detect and mitigate against their worst effects. While the experimentation has investigated the transferability of the control strategy between reactors of different specification, it has done so only to a limited extent. That is, the control strategy from commissioning for the sucrose fed EGSB reactor of 30 l liquid volume was developed using a model calibrated from a fluidised bed reactor fed on a simulated yeast waste, having a liquid volume of 6 l. The scope for considering other reactor specifications is therefore very large. The control strategies were not tested (in a predefined and planned manner), with regard to over loading during the experimentation reported here. Disturbances such as toxic, hydraulic and over loading and sudden changes in feed characteristics (say from sucrose to lactose predominance), are common episodes in the treatment of industrial and municipal effluents. As

such, knowledge of the ability of the control strategies to reject such disturbances is important in the understanding of the control performance. Some of this work has since been done as part of a separate PhD study.

Given the considerations above, the following recommendations for further work are presented:

1. The monitoring of the bicarbonate alkalinity as a single measured control variable would appear to be beneficial. It is clearly important that the instrument used should be reliable, and it is recommended that a thorough re-engineering of the BA monitor used is essential if it is to continue to be employed. One of the main reasons for the BA monitor failures was the blockage of small orifices with particulate carried over from the EGSB reactor. It is therefore important that a reliable filtration of separation system should be purchased or developed, which is able to cope with continuous operation. The prospect of increased flow rates from pilot of full-scale reactors would also improve the reliability of the monitor used in this work. Alternative methods to monitor BA, based on titration methods, are available and just such a device has been loaned to the University of Glamorgan by INRA (Narbonne, France), and should be investigated for their suitability in the generic control strategy.

2. Condition monitoring of AD has been considered by a number of researchers. These techniques should be considered for integration into the generic control strategy in order to prevent the excessive over or under feeding/dosing of the reactor in the event of a system failure.

3. It is recommended that the generic control strategy using OLR variations for actuation, should be reappraised in light of the recommendations 1., 2. and the discrepancy in the control action gain, the latter being discovered after the experimentation and which should be eliminated in future work.

4. The BA dosing strategy should be tested for its ability to deal with organic, hydraulic and toxic over loads, as well as its ability to cope with a sudden change in feed characteristics from say a sucrose to a lactose feed over a short period of time (say 2 hours). An experiment could be designed which took a reactor from start-up on sucrose feed, through various over loads and feed changes.

5. The generic control strategy should be tested for its transferability between high rate anaerobic digesters of different specification (including full scale), which would require re-optimisation of the adaption parameters to be performed using the existing fluidised bed reactor model and consideration of transport and instrumentation delays. This should be a

relatively trivial matter, which could be embedded into a tool which could be supplied as a generic controller for AD and may have commercial potential.

6. During the experimentation it was found that the pH was highly correlated to the BA, at least for the sucrose feed used. Furthermore, the reliability and accuracy of the pH meter was very good, as was the response time of this instrument. It is worth considering other measured variables such as pH and VFAs, despite their possible disadvantages, while adopting a similar philosophical approach to that used for BA in this work.

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APPENDIX A

A1 LIST OF SOFTWARE INCLUDED

Table A1 Software included in CD Appendix

Filename	Description
mitdig.mdl	Simulation of MIT rule
modmit.mdl	Simulation of normalised MIT rule
modmit2.mdl	Simulation of normalised MIT rule with grossly simplified AD model
ddemrac_4.vi	Virtual instrument for testing the effect of DDE communications
modmit6.mdl	Controller model for testing the effect of DDE communications
mrac_ugsb_startup_1.mdl	Controller –experiment 1
mrac_ugsb_startup_2.mdl	Controller –experiment 2
mrac_ugsb_startup_3.mdl	Controller –experiment 3 – *Start-up 1*
mrac_ugsb_startup_4.mdl	Controller –experiment 4– *Start-up 2*
mrac_ugsb_startup_5.mdl	Controller –experiment 5– *Start-up 3*
mrac_ugsb_startup_6.mdl	Controller –experiment 6– *Start-up 4*
mrac_1.vi	Virtual instrument interface – experiment 1
mrac_2.vi	Virtual instrument interface – experiment 2
mrac_3.vi	Virtual instrument interface – experiment 3– *Start-up 1*
mrac_4.vi	Virtual instrument interface – experiment 4– *Start-up 2*
mrac_5.vi	Virtual instrument interface – experiment 5– *Start-up 3*
mrac_6.vi	Virtual instrument interface – experiment 6– *Start-up 4*
Datalogger7.vi	Virtual instrument data logging – experiments 1-5
Datalogger8.vi	Virtual instrument data logging – experiments 1-5
trackflorPID.m	Optimisation routine for optimisations a) and b)
trackflorPIDb.m	Optimisation routine for optimisations c), d) and b)
trackflorPID2nd.m	Optimisation routine for optimisations f) and g)
track2florPID2nd.m	Optimisation routine for optimisations h), i), j) and k)
ddeadc.m	Dynamic data exchange M-File – from LabVIEW™ VI
ddedac.m	Dynamic data exchange M-File – to LabVIEW™ VI
ddetest1.mdl	Demonstration program for Fnc BLOCK used in DDE
bishnorm.m	Data normalisation function
myfilt_2.mat	Filter coefficients used with filtfilt.m
florence_Simuls_Sin_Ponly_1st.mdl	Simulation model – experiment 1
florence_Simuls_Sin_PID_2nd.mdl	Simulation model – *Start-up 1, 2 and 3*
ControlSimulationModel_2_Discr.mdl	Simulation model – Discrepancy in OLR gain
florence_optim4_BA_PID_2nd.mdl	BA Control action optimisation model
narbonne.m	Cauchy model to validate the methodology
Narbonne_model.mdl	Simulink™ equivalent to narbonne.m
pH_BA.m	M-File for determining pH and BA based on Marsili-Libelli and Beni (1993a)
florence_model_verification.mdl	2 population lumped parameter model of the AD Process, including a model of BA
ControlSimulationModel_1.mdl	Control simulation study over 1500 hours – P+I adaption mechanism
ControlSimulationModel_2.mdl	Control simulation study over 1500 hours – P+I+D adaption mechanism (aggressive controller)

A2 TEST SYSTEM FOR CONTROL IMPLEMENTATION

The following shows the software items used in the testing of the direct data exchange between the MatLAB/Simulink™ implementation of the control strategies and the LabVIEW™ vitrual instruments which would be used with a data acquisition card during experimentation.

Ddemrac 4.VI
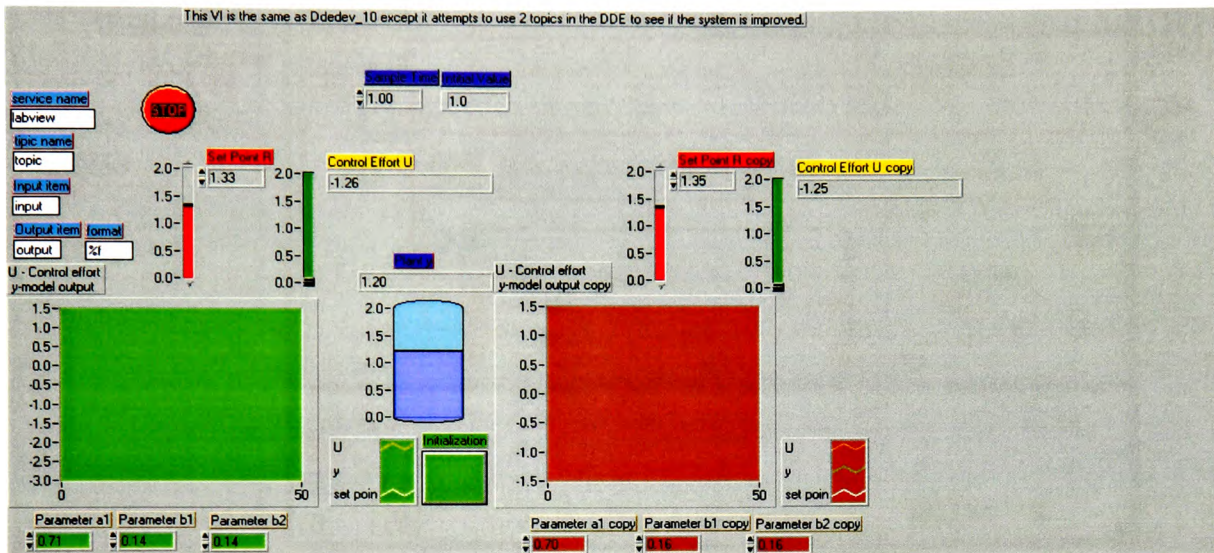
Figure A2.1 Ddemrac_4.vi panel
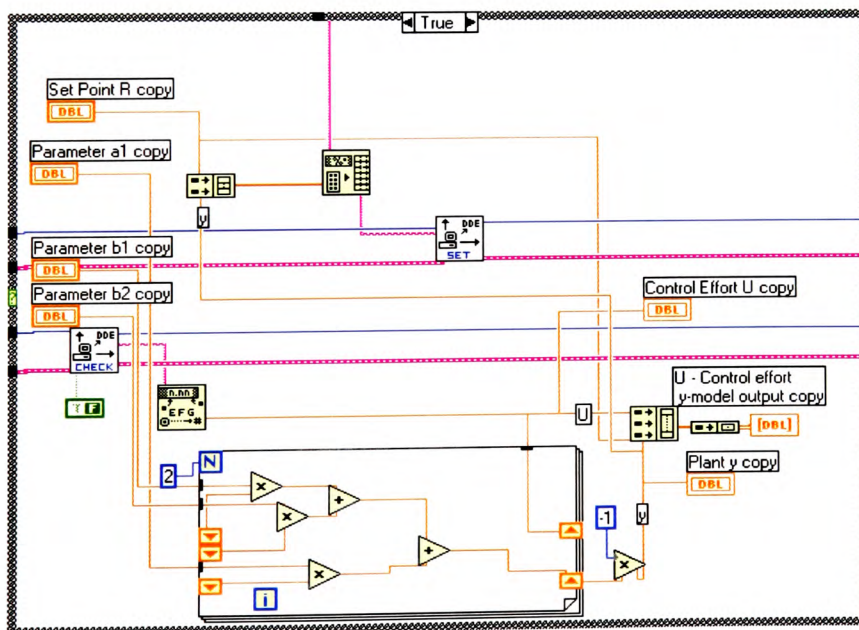
Figure A2.2 Ddemrac_4.vi diagram (true case)

Figure A2.3 Ddemrac_4.vi diagram (showing false case)

Modmit6.mdl

Figure A2.4 Modmit6.mdl Simulink™ model of control strategy development
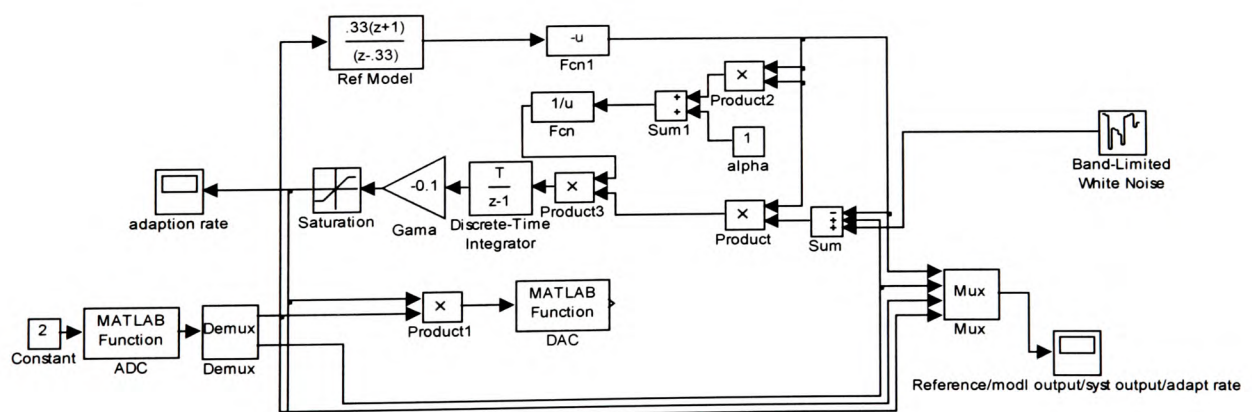
APPENDIX B

PUBLICATIONS ASSOCIATED WITH THE STUDY

This appendix contains copies of the papers published during the execution of the Ph.D. project, which are presented chronologically as follows:

Premier, G. C., R. Dinsdale, A. J. Guwy, F. R. Hawkes, D. L. Hawkes and S. J. Wilcox (1997). Simple black box models predicting potential control parameters during disturbances to a fluidised bed anaerobic reactor. Water Science and Technology 36: 229-237.

Premier, G. C., R. Dinsdale, A. J. Guwy, F. R. Hawkes, D. L. Hawkes and Wilcox. S. J. (1999). A comparison of the ability of black box and neural network models of ARX structure to represent a fluidised bed anaerobic digestion process. Water Research 33: 1027-1037.

Dinsdale, R. M., Premier, G. C., Hawkes, F. R., and Hawkes, D. L. (2000). Two-stage anaerobic co-digestion of waste activated sludge and fruit/vegitable waste using inclined tubular digesters. Biosource Technology 72: 159-168.

Premier, G. C., Monson, K., Hawkes, F. R., Hawkes, D. L. and Wilcox S. J. (2000). Controlling the start-up of an EGSB anaerobic digester using on-line bicarbonate alkalinity monitoring and an adaptive control scheme. 1st World Water Congress of the International Water Association (IWA), Paris, IWA

Premier, G. C., Monson, K., Hawkes, F. R., Hawkes, D. L. and Wilcox S. J. (2001). Controlling the start-up of an anaerobic digester using a single control variable controller optimised using a non-specific model. 9th Anaerobic Digestion Conference, Antwerp, IWA

SIMPLE BLACK BOX MODELS PREDICTING POTENTIAL CONTROL PARAMETERS DURING DISTURBANCES TO A FLUIDISED BED ANAEROBIC REACTOR

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ABSTRACT

Models of the anaerobic digestion process which predict digester behaviour sufficiently accurately could be used in process control. Although the process is generally considered to be non-linear, it could possibly be represented by an adaptive linear model, where the model adapts rapidly enough to represent the process at differing operating conditions and times in its operating life. Simple linear black box models of low order were investigated, predicting over a limited horizon and relying on current and recent data values to refine the prediction. Independent black box ARX models were identified for gas production rate, % CO_2, bicarbonate alkalinity and Total Organic Carbon using on-line data from a fluidised bed reactor at varying organic load. Model predictions looked ahead one sample step (30 minutes) and when validated using data obtained in a different time period (separated by 4-8 weeks) gave significant predictions in each case. All the models consisted of only second or third order polynomials. The non-linear nature of the process was found to have little effect over the operating conditions investigated. Also the variation of the process within a 4-8 week period was not sufficient to cause the models to predict badly. © 1997 IAWQ. Published by Elsevier Science Ltd

KEYWORDS

Anaerobic digestion; linear models; on-line measurement; prediction; identification.

INTRODUCTION

Anaerobic digestion is generally considered to be a non-linear, time varying three-stage process (e.g. Emmanouilides and Petrou 1997, Simeonov et al. 1996). The process depends on a synergistic relationship between bacterial populations and is influenced by physico-chemical conditions and the reactor process. A number of dynamic structured mathematical models have been described for anaerobic digestion (e.g. Costello et al. 1991, Jones et al. 1992, Vavalin et al. 1996) based on Michaelis-Menten kinetics. Such models may require information, such as bacterial kinetic parameters, substrate and product concentrations and bacterial mass balances, which is not easy to determine. One approach adopted by Simeonov et al.

(1996) was to use an identification process to estimate some of these parameters in a non-linear and time-varying scheme. Marsili-Libelli and Beni (1996) similarly identified parameters in mass balance type models. Hoh and Cord-Ruwisch (1996) proposed a reversible kinetic model which allows for the effects of substrate inhibition without the need to determine a large number of parameters experimentally. A common aim of these modelling studies (e.g. Jones *et al.* 1992) is to identify a dynamic model which would be suitable for on-line estimation and forecasting, providing accurate predictions of digester behaviour sufficient for use in process control and controller design.

Models are always an approximation of real world systems and as such can only be judged on their fitness for purpose. When used in control, the model is not necessarily used to achieve a deeper understanding of the underlying process. It is perhaps wise to use the simplest model which is able to represent the system to an arbitrary accuracy specified by the designer. Furthermore the need for a non-linear model may not be paramount if the process can be represented by a piece-wise linear model, which would be the case if the model were to adapt rapidly enough to represent the process at differing operating conditions and times in its operating life. Given that this is possible, a Model Reference Adaptive Control (MRAC) scheme could be employed. Fuzzy (Marsili-Libelli and Muller 1996) and Expert systems (Chynoweth *et al.* 1994) are two alternative approaches which like neural networks show considerable scope.

The work of Marsili-Libelli and Muller (1996) was based on the type of reactor and influent described in this paper. The operation of the laboratory scale fluidised bed reactor used here on the same influent made up batch-wise has been previously described (Guwy *et al.* 1997). Significant variations in biogas composition resulted from batch-wise preparation of the feed, and in the work presented here these changes due to feed acidification were eliminated so that the effects of step changes in loading rate could be observed. This paper investigates whether a fluidised bed anaerobic digester can be represented adequately by simple linear black box models of low order. The models are employed to predict over a limited horizon and rely on current and recent data values to refine the prediction.

MATERIALS AND METHODS

Reactor operation and instrumentation

The reactor and influent to the process have been previously described (Guwy *et al.* 1997). The anaerobic digester system, operating at 37°C, consisted of two perspex 7 litre fluidised bed reactors connected in parallel (11 litres total liquid volume, 3 litres gas headspace) using a Siran® sintered glass carrier (Schott Glaswerke, Germany) to give a total collapsed bed volume of 3 litres. A 1031 EHEIM recycle pump (supplier Monside Ltd, Letchworth, Herts., UK) was used to recycle the liquor contents through the reactor system at an up-flow velocity of approximately 0.55 m min^{-1}. The reactor had been operated on the same influent continually for two years before the experiments described here took place. At the end of the experimental period the biomass content of the bed was measured. Samples were washed in deionised water and analysed for volatile suspended solids (VSS) by standard methods (APHA 1985).

The influent was a simulated baker's yeast wastewater having a COD of approximately 6,700 mgO$_2$l^{-1} with a steady state loading rate to the reactor between 17.6 - 18.8 kgCODm^{-3} day^{-1} with a corresponding hydraulic retention time 9.1 - 8.2 hours. The influent was made up in a concentrated form with a COD of approximately 247,000 mgO$_2$l^{-1}, delivered using a Watson-Marlow (Falmouth, UK) pump (type 503u) and diluted with water delivered by a Watson-Marlow 503u pump at the point of delivery to the reactor. It was not found necessary to refrigerate the feed as at this concentration no COD reduction with time or acidification due to microbial growth was detected.

The percentage of carbon dioxide and the hydrogen concentration in the biogas were monitored on-line using an ADC monitor type SBG100-002-15290 (ADC Ltd. Hodderson, UK) and a GMI Exhaled Hydrogen Monitor (Gas Measurements Ltd. Renfrew, Scotland) respectively. For hydrogen measurements hydrogen sulphide was removed from the biogas by passing through a saturated solution of copper sulphate and

calibration of the monitor with standard gases was performed at least once per month. The biogas flowrate was measured with a low flow on-line gas meter (Guwy *et al.* 1995). The pH was measured by a Kent EIL9142 meter using an Ingold Xerolyte electrode (type HA405-DXK-S8/120). A bicarbonate alkalinity (BA) monitor described previously (Guwy *et al.* 1994) was used on-line in the effluent stream, measuring BA as $mgCaCO_3l^{-1}$.

TOC was measured using the high temperature IR method using a Rosemount-Dohrmann DC 190 (Sartec Ltd., Borough Green, UK) with an autosampler injection system (50µl volume). Effluent (20 ml min^{-1}) was filtered using a 15µm nylon fabric (Sericol Industrial Fabrics, Broadstairs, UK) held in a chamber designed by the Institute for Biotechnology, KFA, Julich, Germany, and fitted in our laboratory with a rotating brush for automatic cleaning. The effect of the filter unit was to reduce the measured COD strength of effluent by 15, equivalent to settling the effluent for one hour or filtering with a Whatman G/FC filter. Excess filtrate was returned to the reactor. For TOC analysis a continuous stream (6.3 ml min^{-1}) of filtered effluent flowed through a mixed 9ml continuous flow cell positioned in the autosampler tray. The sampling frequency corresponded to the time taken by the instrument for a complete IC, TC and TOC analysis, approximately 8-11 minutes. Data was collected using software supplied by Rosemount-Dohrmann allowing transfer to a spreadsheet for evaluation.

Non-steady state operation

The experiments reported here were performed over an 8 week period during which the reactor was run continually. Data used for parameter estimation for modelling CO_2, BA and gas responses were separated by one month from the model validation data and for the TOC model the data were separated by two months. Changes in organic loading rate (Bv) were brought about with minimal changes in hydraulic retention time by adjusting the feed pump flow delivering the concentrated feed to the reactor. The pump delivering dilution water remained at a fixed rate (19.5-21.7, average 20.8 ml min^{-1}) so that hydraulic retention time decreased by a maximimun of 10% from the average of 8.5 hours during the shock. The feed pump voltage was directly related to the flow and hence Bv. Table 1 shows the experiments used for parameter estimation and validation of the predictive models.

Table 1. Experiments used for parameter estimation and validation of models

Expt.No.	Min. Bv gCODl^{-1}d	Max. Bv gCODl^{-1}d	Description
1	26.5	70.2	series of step changes in Bv of varying amplitude and duration; black box parameter estimation for BA, %CO_2 and gas production rate models
2	17.8	38.6	series of step changes in Bv of varying duration; black box parameter estimation for TOC model; validation of the models of BA, CO_2, and gas production rate
3	16.1	69.9	two step changes in Bv of similar duration and amplitude; validation of TOC model
4	17.6	75.0	single step change in Bv (8.8h duration); validation of the models of BA, CO_2, and gas production rate

Data logging and processing

Data from the instrumentation were logged on a PC with an interface card (MIO 16) using LabVIEW™, both supplied by National Instruments (Newbury, UK). Sensor data, time and date were logged into files for

off-line processing. The virtual instrument (VI) was configured to sample all the on-line sensors (except TOC) at 2 minute intervals. This sample rate was very fast and although high sampling helps to increase confidence in the sampling of a continuous data stream it can lead to intrinsic problems in oversampling discrete systems as discussed by Wellstead and Zarrop (1991). The post processing of the data involved filtering to enhance the signal and re-sampling to produce a more appropriate sampling rate for the process dynamics. The time series were digitally filtered using a zero phase, forward and reverse low-pass filter which was parameterised by the Yule/Walker recursive least squares approach as described in the MatLAB signal processing toolbox (Krauss *et al.* 1995). The data were then re-sampled at 30 minute intervals which was considered to be a reasonable compromise with respect to the digester dynamics.

Linear model identification

This is the process of producing a linear mathematical model which is able to predict future values of the data to an arbitrary degree of accuracy.

Model Structure. A black box approach was used, where an input (x) and Gaussian white noise (e) are mapped through transfer functions G(z) and H(z) and added to give a resulting output (y), as discussed by Ljung (1987) and Soderstrom and Stoica (1989) The system is shown schematically in Figure 1.
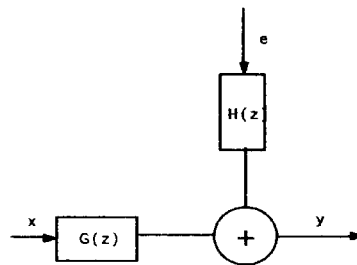
Figure 1. Black box model structure.
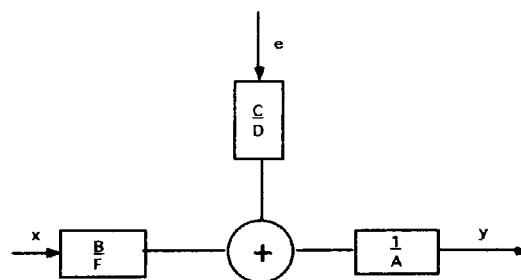
Figure 2. General family of model structures.

A General Family of Model Structures. The black box model can be represented more flexibly by representing the transfer functions as ratios of polynomials in z^{-1} (which can be considered as the delay operator), as shown in Figure 2.

The family of models can be written as:

$$A(z)y(t) = z^{-k} \frac{B(z)x(t)}{F(z)} + \frac{C(z)e(t)}{D(z)}$$

where: $A(z) = 1 + a_1z^{-1} + a_2z^{-2} ... + a_{na}z^{-na}$, $B(z) = b_1 + b_2z^{-1} ... + b_{nb}z^{-nb+1}$ and similarly for $C(z)$, $D(z)$ and $F(z)$, and where z^{-nk} represents a pure delay as a multiple of sample periods. The model structure can be selected to include as many or as few of these black box parameters as is necessary to produce a sufficiently accurate model. Model structures are discussed at length by Ljung (1987 and 1993) and by Soderstrom and Stoica (1989).

RESULTS AND DISCUSSION

Reactor operation

The operation of this reactor using similar influent made up every 4-5 days in a refrigerated feed tank gave changes in biogas H_2 and CO_2 content due to changes in VFA content of the feed (Guwy et al. 1997). responses. Feed delivery here eliminated these changes and stable baseline values for BA, gas flow and biogas H_2 and CO_2 content were obtained. The TOC:COD ratio for the effluent was 1:3.1. The attached biomass content of the reactor system was determined to be 16.6 gl^{-1}VSS, although the washing process was observed to remove biomass from the sample which was then not measured.

The ARX model structure and parameter estimation

The ARX model, which stands for Auto Regressive with eXtra (or eXogenous) input $B(z)x(t)$, was found by trials to be the most appropriate model structure. More complex model structures were able to reduce the sum of squared errors when tested against verification data, however the added complexity of the model was not justified by the improvement in forecasting. The model structure can be written as:

$$A(z)y(t) = B(z)x(t-nk) + e(t)$$

where $y(t)$ is the predicted value. Model predictions looked ahead one sample step i.e. 30 minutes.

Figure 3 shows the gas production rate and % CO_2 varying with organic load represented by the feed pump voltage and these data were used to estimate the black box model parameters for the respective models.
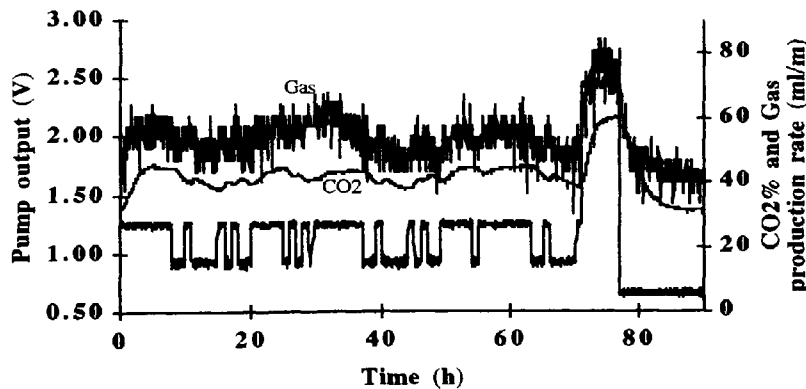
Figure 3. Experiment 1 data for parameter estimation: gas production rate and %CO_2.
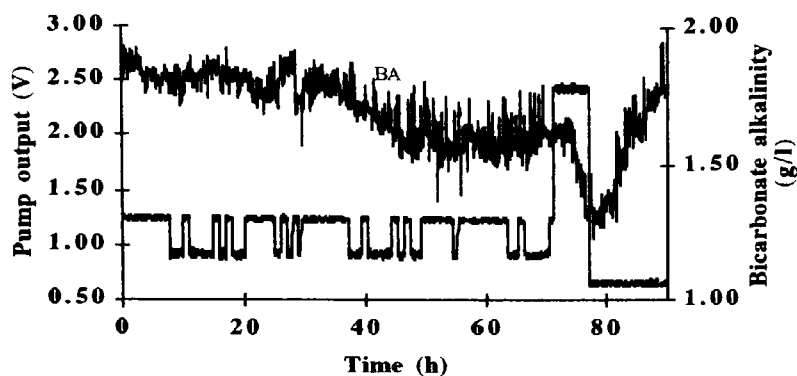
Figure 4. Experiment 1 data for parameter estimation: bicarbonate alkalinity.

Figures 4 and 5 show the data used in parameter estimation for the BA and TOC models respectively. There would be little chance of extracting a comprehensive model for the process with such excitation as there is a need to excite all the modes of the system. Such a disturbance is known as persistently exciting and is essentially the only way to experimentally search the entire state space. This would require exhaustive testing and would include running the digester to failure. Not withstanding the limitations of the models, by using data measured on-line, it was possible to make significant predictions of BA, CO_2, gas production rate and TOC using independent ARX black box models. All the models consisted of only second or third order polynomials, with a single sample period delay between the input (loading rate) and the output (the relevant parameter e.g. BA).
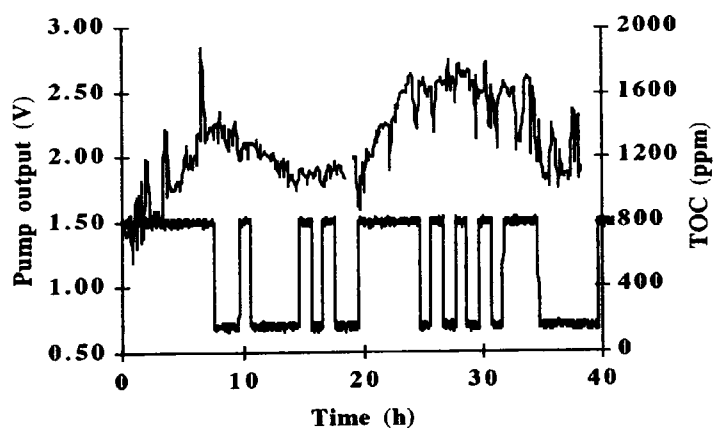
Figure 5. Experiment 2 data for parameter estimation: TOC.

Validation of models

The validation of the CO_2 and gas production rate models (Figure 6) and the BA model (Figure 7) showed that it was possible to predict with a relatively high degree of accuracy the future value (30 minutes ahead) when subjected to loads comparable to those used in the parameter estimation. This was despite the fact that

the models were essentially structurally simple (ARX) and assumed to be totally uncoupled. Figure 8 shows predictions of TOC using step changes greater than those used in the parameter estimation data. The predictions show again a relatively high degree of accuracy, as do the models for the other parameters, BA and gas production rate, when similarly tested with a large step change (Figure 9). In validation, no attempt was made to match initial conditions.

The horizon over which predictions are made (30 minutes) is considered to be ample in terms of time required to execute recursive parameter estimation for such linear models with a view to their use in a MRAC scheme similar to that proposed by Emmanouilides and Petrou (1997), but using a linear model as the reference model instead of a neural networks as these have inherent problems of initial training and subsequent recursive parameter (weights and biases) estimation. Looking more than one step ahead leads to a progressive deterioration in accuracy of prediction when using the above black box models.

The validation data sets were chosen to force the models to predict at operating conditions which were not used in parameter estimation of the models, which would, if non-linearity were significant, cause the model to deviate in its predictions. The non-linear nature of the process was found to have little effect over the operating conditions investigated. Also the variation of the process with time (1-2 months) was not sufficient to cause the models to predict badly.
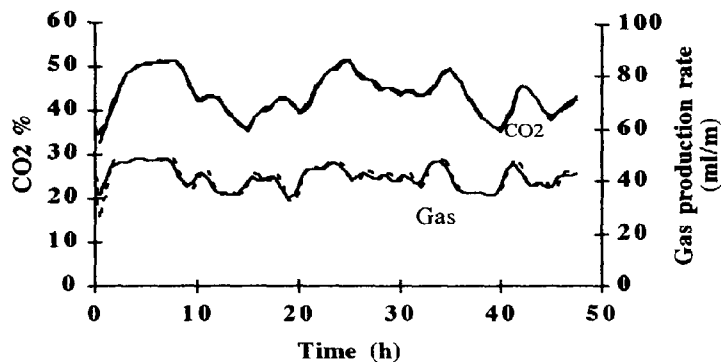
Figure 6. Experiment 2 validation of gas production rate and $\%CO_2$ models. Dashed lines show predictions 30 minutes ahead.
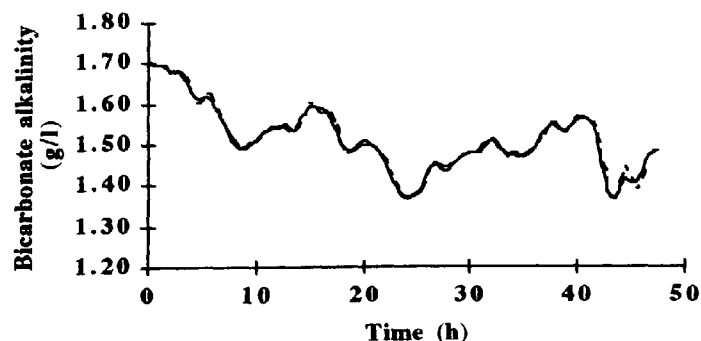
Figure 7. Experiment 2 validation of BA model. Dashed line shows predictions 30 minutes ahead.
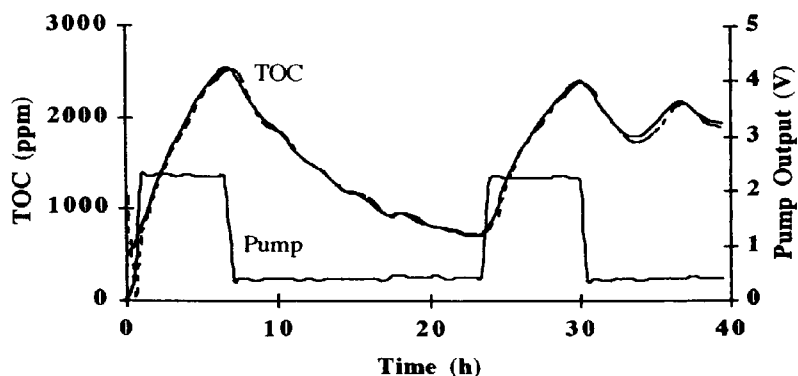
Figure 8. Experiment 3 validation of TOC model. Dashed line shows values 30 minutes ahead.
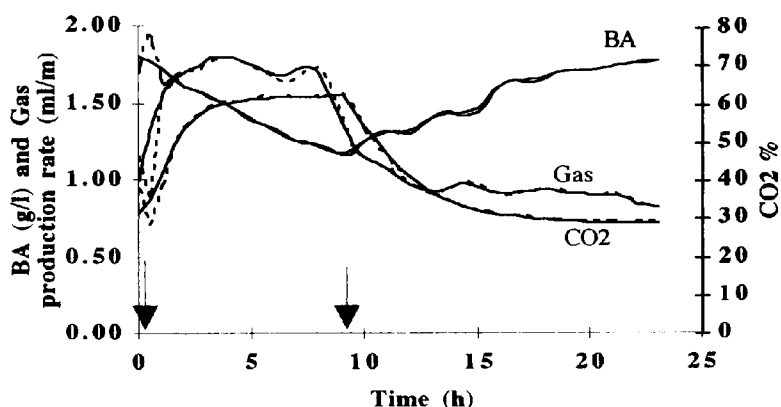
Figure 9. Experiment 4 validation of gas production rate, BA and $\%CO_2$ models (arrows denote step load). Dashed lines show values 30 minutes ahead.

It thus appears that simple, linear, independent black box models of gas production rate, $\%CO_2$, BA and TOC are able to represent the anaerobic digestion process under the conditions tested with an accuracy which may be sufficient as the basis for process controller design.

CONCLUSIONS

Using on line sensors and data logging for BA, % CO2, gas production rate and TOC, in a fluidised bed anaerobic digester, it was possible to identify black box ARX models which were linear, uncoupled and of low order, for each data stream. The black box parameters were determined from data which resulted from substantively different variations in Bv compared to the verification data and separated by multiple retention times from it. The models were shown to predict 30 minutes ahead with significant accuracy despite the assumed non-linear, coupled and time varying characteristics of the anaerobic process.

ACKNOWLEDGEMENTS

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A COMPARISON OF THE ABILITY OF BLACK BOX AND NEURAL NETWORK MODELS OF ARX STRUCTURE TO REPRESENT A FLUIDIZED BED ANAEROBIC DIGESTION PROCESS

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Abstract—The performance of three black box models which were parameterized and validated using data collected from a laboratory scale fluidized bed anaerobic digester, were compared. The models investigated were all ARX (auto regressive with exogenous input) models, the first being a linear single input single output (SISO) model, the second a linear multi-input multi-output (MIMO) model and the third a nonlinear neural network based model. The performance of the models were compared using correlation analysis of the residuals (one-step-ahead prediction errors) and it was found that the SISO model was the least able to predict the changes in the reactor parameters (bicarbonate alkalinity, gas production rate and % carbon dioxide). The MIMO and neural models both performed reasonably well. Though the neural model was shown to be superior overall to the MIMO model, the simplicity of the latter should be a consideration in choosing between them. A simulation with an horizon approaching 48 h was performed using this model and showed that although the absolute values differed significantly, there were encouraging similarities between the dynamic behavior of the model and that of the fluidized bed reactor. © 1999 Elsevier Science Ltd. All rights reserved

INTRODUCTION

The difficulty in establishing mathematical models based on the underlying biochemical processes in an anaerobic reactor is evidenced by the large volume of literature directed to this end. The nonlinear and time varying characteristics of anaerobic digestion processes are well documented (Costello *et al.*, 1991) so that deducing adequate models of such characteristics, by parameterizing large deterministic models (derived from an understanding of the biological, chemical and physical processes) is difficult because of the large number of parameters involved (Kotze *et al.*, 1969) although it is likely to remain a worthwhile objective. The volume of data required to determine kinetic and other constants is prohibitive, in all but the most extensive studies (Simeonov *et al.*, 1996) and when this is added to the fact that the system is (to an unknown and system specific extent) not stationary (i.e. is time dependent) it follows that the model parameters would need to be identified recursively. To do this recursive identification, the system should ideally be persistently excited (in the sense that all the dynamic modes of

response are present in the data). An alternative may be to assume that time variation is simply a disturbance on the system, which may or may not be dependent on measurable state variables (or process parameters).

Boskovic and Narendra (1995) have investigated the performance of various linear and nonlinear controllers for the control of batch fermentation processes by simulation and concluded that in certain circumstances neural networks have superior performance. Some authors (Jeppsson and Olsson, 1993) have taken the view that reducing the order of the model, such that measurable physical variables are sufficient to recursively identify the model parameters, is an appropriate approach to the reduction of model complexity. This is in effect simplifying the process model to the point that repeated and frequent estimation of the model (which includes significant *a priori* knowledge) can be achieved. The benefits of models with structures and parameters which are related to real system variables are significant in the understanding of process behavior (from simulations). However, it is conceivable that a black box approach (Ljung, 1987) (as opposed to the grey box, reduced order type models of Jeppsson and Olsson, 1993) could

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be useful in situations where the input/output relationships are of overriding importance and the significance of the model parameters is not under consideration. This situation arguably arises in the control of such processes, where a fast, workable and robust solution is of more importance than depth of understanding and model elegance.

Given that a black box approach is acceptable in a particular situation, the model could be one of many possible structures. Previous work has investigated the use of simple linear model structures (Premier *et al.*, 1997) and their ability to represent key variables in an anaerobic process. This paper seeks to compare discrete time SISO (single input, single output) with MIMO (multi-input, multi-output) linear models and SISO nonlinear models based on feed forward neural network architectures. It is noted that the learning techniques adopted in neural network connectionist work (Levenberg–Marquate, detailed in Ljung, 1987 and used in this study) have similarities with the parameter estimation techniques used by engineers and mathematicians (Miller *et al.*, 1990). In both cases, the objective is to estimate the values of a parameter vector in response to the performance of an objective function. Also in both cases (teaching in neural networks and parameter estimation in system identification) a set of example data is necessary and a best-fit model is sought from a set of possible models represented by the model structure.

Three model structures have been considered in this paper and the performance of the models were compared using correlation analysis. All are ARX models (auto-regressive with exogenous input) specifically SISO and MIMO and a comparable (same order) ARX neural network model. The functions operating on the regression vectors (past data samples) are linear polynomial functions (in the cases of SISO and MIMO linear ARX models) and a nonlinear neural network.

MATERIALS AND METHODS

Anaerobic reactor

The fluidized bed anaerobic digestion system which formed the basis of the study was described by Guwy *et al.* (1997). The total volume was 14 l, of which 21% was gas headspace volume. The solid support medium was Siran[w] sintered glass (Schott Glaswerke, Germany) fluidized by recycling reactor liquor at an up-flow velocity of approximately 0.55 m min^{-1}. The bacterial population was well adapted to the feed, which had remained unchanged for two years prior to the experimental period described here.

The influent was a simulated baker's yeast wastewater having a COD of approximately 6700 mg O_2 l^{-1} with a steady state loading rate to the reactor between 17.6–18.8 kg COD m[-3] day^{-1} with a corresponding hydraulic retention time of 9.1–8.2 h. The influent was made up in a concentrated form with a COD of approximately 247,000 mg O_2 l^{-1}, delivered using a Watson-Marlow (Falmouth) pump (type 503u) and diluted with water at the point of delivery to the reactor. The pump delivering

dilution water remained at a fixed rate (19.5–21.7, average 20.8 ml min^{-1}) so that hydraulic retention time decreased by a maximum of 10% from the average of 8.5 h during the shock. The feed pump voltage was directly related to the flow and hence the digester loading rate (Bv).

The percentage of carbon dioxide and the hydrogen concentration in the biogas were monitored on-line, as was gas flow. The bicarbonate alkalinity of the reactor effluent was monitored continuously using an on-line bicarbonate alkalinity (BA) monitor described previously Guwy *et al.* (1994) measuring BA as mg $CaCO_3$ l[-1]. Further details of the reactor, instrumentation, influent and test regime are given in Premier *et al.* (1997).

Data selection and processing

Raw data were collected, on-line, from the fluidized bed reactor by a virtual instrument, implemented using LabVIEW[TM]. The data were then processed off-line, using a separate software application, MatLAB[TM]. Significant levels of measurement noise were present on the data and were dealt with by filtering with a Butterworth filter of 5th order. The sampled data were filtered in both chronological directions in order to remove any phase effects. After filtering, the data were normalized with respect to its mean and standard deviation, with a particular view to improving the performance of the neural network training (Bishop, 1995).

A different set of data was required to effect the parameter estimation (and network training) from that used in validation. The "training" and "validation" sets were chosen for their significant temporal separation (approximately four weeks during which time the digester was fully operational) which might have allowed process time variance the opportunity to develop.

Model structures

The ARX structure (Ljung, 1987) uses delayed inputs and outputs in order to determine a prediction of the output at one (or more) sample interval(s) in the future. It is of the form

$$\hat{y}(t) = \hat{f}[x(t)], \tag{1}$$

where $\hat{y}(t)$ represents the model prediction, $x(t)$ represents the regression vector of current and past inputs, outputs and additive prefiltered noise and $\hat{f}(.)$ is some function of $x(t)$.

In the case of linear black box models, this function consists of linear polynomial quotients. In the multivariable case (MIMO) equation 1 represents a matrix equation with definable cross coupling between the data sets. For the case of nonlinear connectionist models in this paper, the function is a neural network of multi-layer perceptron architecture with a single hidden layer of nonlinear squashing activation function neurons and a linear output layer (Norgaard, 1995).

The linear ARX models

Parameter estimation of the linear ARX models followed a standard minimization of the sum squared errors approach (Wellstead and Zarrop, 1991). In the absence of noise, the model could be determined directly from linear algebra from very few data points, in a relatively trivial manner. In the ARX structures, it is assumed that the noise, which is always in evidence in experimental data (to a varying degree) is equivalent to prefiltered white noise where the poles of the filter are identical to those of the resulting ARX model. Practically, this means that iteration may be necessary to ensure that deviation from this assumption does not have a deleterious effect on the model predictions. Again, because of the noise we are forced to use an overly determined data set and to solve using the least squares approach.

The linear SISO ARX model. This is of the form

$$\hat{y}(t) + y(t) (a_1 q^{-1} + a_2 q^{-2} + \ldots a_{n_a} q^{-n_a})$$

$$= u(t - n_k) [b_1 + b_2 q^{-1} + \ldots b_{n_b} q^{(-n_b + 1)}] + e(t),$$

where $a_1, a_2, \ldots, a_{n_a}$ and $b_1, b_2, \ldots, b_{n_b}$ are constant coefficients which form the parameters to be estimated $\hat{y}(t)$ is the one-step-ahead prediction of $y(t)$ the actual output. q^{-1} represents the delay operator. $u(t)$ is the input, $e(t)$ is the additive noise, n_k number of delayed samples (minimum = 1); n_a length of the output regression vector and n_b length of the input regression vector + 1.

The linear MIMO ARX model. Similarly, the MIMO ARX model is of the form

$$\mathbf{A}(q)\, y(t) = \mathbf{B}(q)\, u(t) + \mathbf{e}(t),$$

where

$$\mathbf{A}(q) = \mathbf{I}_{n_y} + \mathbf{A}_1 q^{-1} + \ldots + \mathbf{A}_{n_a} q^{-n_a}$$

and

$$\mathbf{B}(q) = \mathbf{B}_0 + \mathbf{B}_1 q^{-1} + \ldots + \mathbf{B}_{n_b} q^{-n_b}$$

As detailed in Ljung (1993) the parameter vector is determined in a similar way to the SISO ARX, with the difference that the parameter vector $\theta = [\mathbf{A}_1, \ldots, \mathbf{A}_{n_a}, \mathbf{B}_1, \ldots, \mathbf{B}_{n_b}]$ consists of matrices (bold type). θ will include parameters which cross-couple the data streams, such that the effect of past values of $\%CO_2$ for example can be made to have an effect on the prediction of bicarbonate alkalinity and gas production rate.

The neural network ARX model

This model is after Norgaard, 1995

$$\hat{y}_i(w, W) = F_i\left(\sum_{j=1}^q W_{ij} f_j\left(\sum_{l=1}^m w_{jl} z_l + w_{j0}\right) + W_{i0}\right).$$

Where: $\hat{y}_i(w, W)$ is the prediction of the model as a function of network weights. F_i is the output layer activation function, which is linear in this paper. W_{ij} are the weights through which the hidden layer is connected to the output layer. W_{i0} acts as a bias. f_j is the hidden layer activation function, which is a tanh function in this paper. w_{jl} are the weights through which z_l is connected to f_j. therefore w_{j0} acts as a bias. z_l represents the feature vector of length m, presented to the input of a feed forward neural network.

Training and validation data

The data used in parameter estimation (and training) is described by Premier et al. (1997) and is shown in Fig. 1. The data are normalized using its mean and standard deviation, however the ranges of the absolute values of the data are shown in Table 1.

The same data gathered from these experiments were used to determine the linear model parameters and the neural network model weights. Model validation was performed using the same validation data set (Fig. 2) in all cases.

System identification procedure

Having determined appropriate data sets for the training and validation, all the selected models were trained and validated with the same data sets, to allow a basis for comparison.

The number of previous samples in the regression vectors for inputs and outputs (lag space) was determined using a function implemented by Norgaard attributed to He and Asada (1993). This confirms a heuristic approach taken in Premier et al. (1997) on the basis of observation of the data time series. A MatLAB® function

(*LIPSCHIT*) implemented by Norgaard, determines an index, which is high when the regression space is insufficient and becomes constant at a lower value. when increasing the lag space has no further significant effect on accuracy in representing the data.

The number of regressors effectively defines the model structure for the SISO linear ARX model, but the MIMO linear ARX model still requires a decision as to the cross coupling between a particular output prediction (say $\%CO_2$ for example) and previous samples of the other time series (BA and gas production rate in this example). In all cases, second order polynomials (in the delay operator) were used.

In the case of the neural network model, the training algorithm was based on the Levenberg–Marquadt nonlinear least squares technique, while the remaining models were parameterized using a linear least squares approach, as implemented by Ljung (1993).

RESULTS AND DISCUSSION

The ARX model structure was selected on the basis of a brief study of the behavior of a number of linear SISO black box models (such as the AR, ARMAX, OE and Box Jenkins). The iterative procedure indicated that the linear ARX model's performance was for the most part superior to the alternatives. As suggested by many authors (including Bishop, 1995) Occam's razor, which paraphrased affirms that the simplest adequate solution is the best, was employed and the ARX structure was extrapolated to include the MIMO and neural network models.

The choice of second order functions in the delay operator (q) means that the models have a regression vector looking back over two samples which, at a sampling time of 30 min, will include data collected over an hour. Increasing the order of the models would probably lead to lower NSSE's (normalized sum of squared errors) but would to an increasing extent cause over-fitting to the data and hence the model would be unrepresentative of the underlying dynamics of the process. The dimensionality of the neural network model is also dependent on the size of the parameter vector (i.e. the number of weights and biases) so is not directly comparable with the linear models, although significant similarity exists, as shown in equation 1. The technique employed by Norgaard (1995) to determine the length of the regression vector, was to calculated the index of He and Asada (1993) and to look for a knee point in the index, beyond which, increasing the regression vector would have little effect. More weight was given to the insight obtained by investigating the responses of the process to a step input, which on a heuristic level appeared similar to overdamped second order systems.

The sampling time of 30 min is considered to be relatively short, however a compromise was sought between that suggested by the process dynamics and that suggested by the dynamics of the slowest instrumentation (bicarbonate alkalinity monitor of Guwy et al., 1994).

(a)

(b)
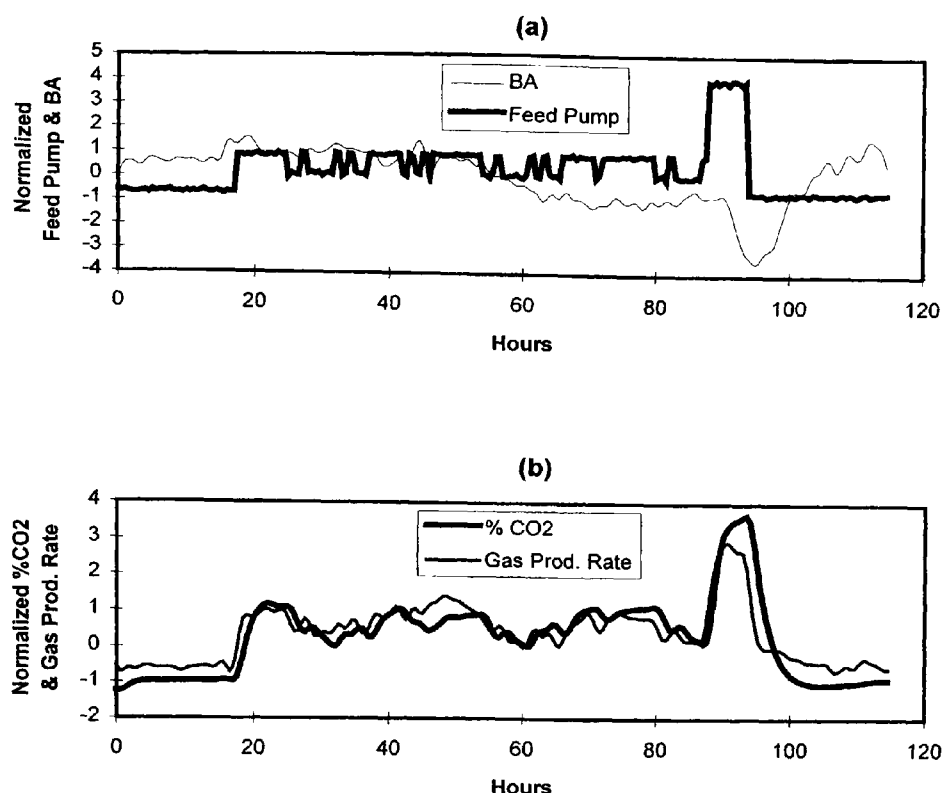
Fig. 1. Data used in parameter estimation on neural network training for system identification. (a) Normalized feed pump control voltage and bicarbonate alkalinity. (b) Normalized % carbon dioxide and gas production rate.

The time varying characteristics of the fluidized bed reactor are not known, so the time lapse between the data sets for training and validation were a matter of judgment. It is of course possible that the data selected, were not separated sufficiently in time to account for microbial population changes, or that the populations were by chance similar in their dynamics for both sets of data. The time variance was assumed to be unpredictable, though dependent on the reactor's operating history (loading, environmental and inhibitory episodes). Variations over-time in parameters such as biomass yield or endogenous decay coefficients etc., were assumed to be small and as such could be treated as system disturbances. Furthermore, it was assumed that the loading regime which extended over approximately 3 months, was sufficiently varied so as not to favor the development of special-

ized (and perhaps fragile) consortia of microbial populations.

ARX model predictions

Comparison of models. Figures 3, 4 and 5 show the bicarbonate alkalinity (BA) one-step-ahead prediction as an example (for the three alternative ARX models investigated) compared to the measured validation data set. It would be possible to compare the models predictions to the parameter estimation/training data, however one would expect a good fit in this case as the objective is to minimize the sum of the errors squared. The validation set is of key significance, as it indicates the ability of the model to generalize (or represent an "unseen" data set). The validation data and the corresponding predictions seem at first sight to be very close to each other, which is often the case with one-step-ahead

Table 1. Maximum and minimum true values of parameter estimation and validation data

Data series	Parameter estimation data		Validation data	
	maximum	minimum	maximum	minimum
Feed pump (volts)	2.5	1.6	1.5	0.7
Bicarbonate alkalinity $(g \, l^{-1})$	1.8	1.3	1.7	1.38
%CO$_2$	60	32	52	33
Gas production rate $(ml \, min^{-1})$	80	40	39	19
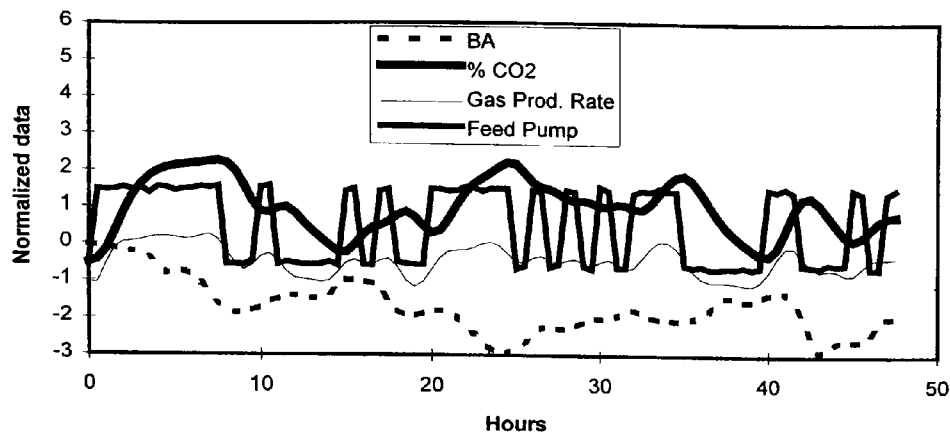
Fig. 2. Normalized bicarbonate alkalinity, CO_2, gas production rate and feed pump data used in the validation of the ARX models for system identification.

prediction, where the step size is of relatively short duration. It is difficult to assess the performance of the model by looking at such plots and statistical techniques are normally employed. Figures 3–5 do indicate however, the excellent predictions achievable with short temporal prediction horizons.

In the case of the % carbon dioxide and gas production rate, the results were similar in their deviation to those in Figs 3–5 and, in the interest of brevity, have not been shown.

Nonlinear (Neural Network) ARX Model for Bicarbonate Alkalinity

The neural network regressors were chosen to be the same as those used for the linear ARX model, these being two previous inputs, two previous outputs and a single delay. The architecture of the network was initially a fully connected feed-forward network, with one hidden layer of 10 hyperbolic tangent activation function neurons and an output layer of one linear activation function neuron.

The predictions obtained from this model (when considering the auto-correlation of residuals and cross-correlation of the input to the residuals, which are explained below) were poor. The auto-correlation, in particular, remained consistently outside the 95% confidence band, implying that the

model was over-fitting the data. The solution proposed by Norgaard is to reduce the dimensionality of the network by applying an OBS (optimal brain surgeon) algorithm, which is used to "prune" the weights to the point where near optimal results are obtained. This involves retraining (for a limited number of epochs) the network, as its structure is altered by removing a single weight at a time and keeping track of test errors, to see at which point they are minimized. In doing so, the predictive performance of the neural model was improved significantly and the results are shown in Fig. 5. The model structure was reduced to eight weights in total for the bicarbonate alkalinity neural model.

Nonlinear (Neural Network) ARX Model for % CO_2 and Gas Production Rate

A similar procedure was followed for these data streams, with similar results, although in both cases, the number of weights left after pruning was almost double that of the bicarbonate alkalinity.

Correlation analysis

For the purposes of comparison, it is necessary to consider measures of performance from one model structure to another. Investigations of nonlinear ARMAX (auto regressive with moving aver-
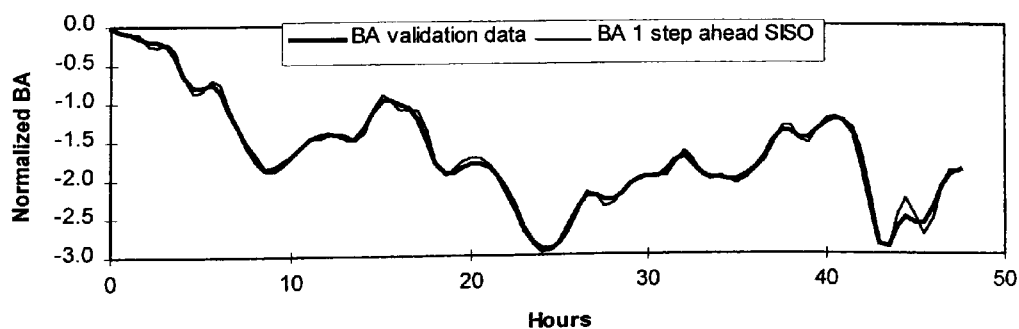
Fig. 3. Bicarbonate alkalinity predictions for a linear ARX SISO model.
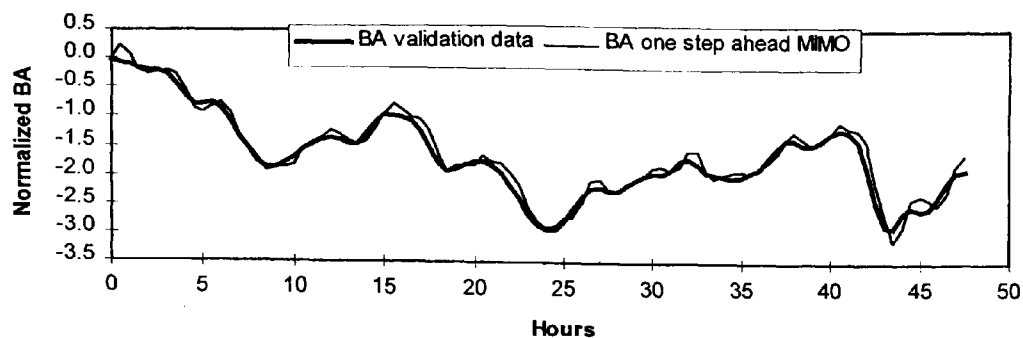
Fig. 4. Bicarbonate alkalinity predictions for a linear ARX MIMO model.

age and exogenous input) model performance, using synthesized and experimental data, were conducted by Chen *et al.* (1990) who applied a number of statistical tests which were based on correlation analysis and the χ^2-tests. It is common in system identification to consider the correlation analysis as the primary measure of model performance in particular the auto-correlation of the residuals (errors between predictions and real validation data) and the cross-correlation of the input (feed pump) and the residuals.

The auto-correlation function of the residuals should ideally resemble an impulse. This would indicate that the residuals are "white", i.e. no correlation exists between the residuals and any time shifted replica of the series. There should also be no correlation between the residuals and any linear or nonlinear combinations of past inputs and outputs (Chen *et al.*, 1990).

If the identification of an ARX model were successful, then one would expect the residuals to be unpredictable. The predictability and hence deviation from optimum can be assessed by using correlation analysis. Specifically the auto-correlation of the residuals should exhibit correlation only when the time series are not time shifted (one to the other). Similarly, in cross correlating, no correlation should exist between the residuals and the system input signal (feed pump). If the correlation functions are within a confidence interval of 95% of the conditions mentioned, then it is reasonable to

accept the model as a fair representation of the system.

A comparison of the predictions of the models was performed by analyzing the residuals. The results for bicarbonate alkalinity, %CO_2 and gas production rate are presented in Figs 6, 7 and 8, respectively. It can be seen from Figs 6–8, that the SISO ARX model fails to achieve the 95% confidence criteria for %CO_2, although it gives adequate results for the BA and gas production rate. Comparing the MIMO ARX to the neural network ARX model, it would seem that the former is able to represent the system with inferior accuracy in the case of BA and better accuracy for % CO_2 and gas production rate. While it may be possible that the neural network could be improved by optimizing the training process and network structure iteratively, the same can be said for all the models. It is not clear to what extent the models are optimized, which is usually the case in identification.

The underlying biochemical processes point to there being significant coupling in the data streams measured. It is perhaps not surprising therefore that the MIMO and neural network models which both include cross coupling, out perform the linear SISO model overall, with the %CO_2 for the latter being significantly outside the confidence limits.

It is worth restating (in order to highlight the increased computational effort) that in order to obtain the performance presented in this paper, when using the neural network ARX model, a
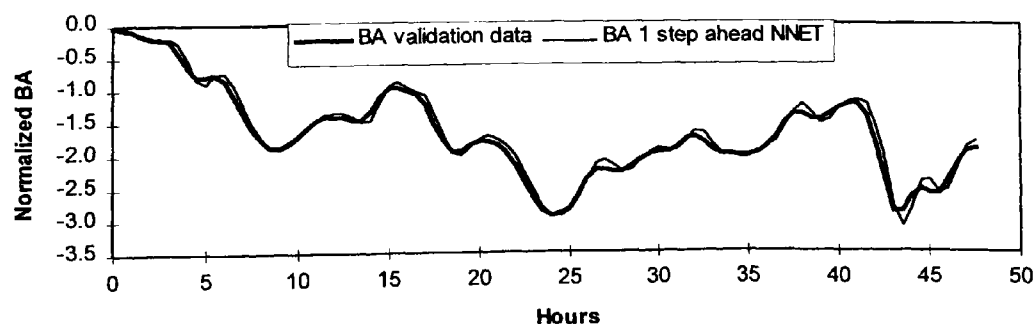
Fig. 5. Bicarbonate alkalinity predictions for a nonlinear ARX neural network model.

(a)

(b)

Fig. 6. Correlation analysis for bicarbonate alkalinity using nonlinear, MIMO and SISO ARX models. (a) Auto-correlation of residuals from prediction of validation data. (b) Cross-correlation of pump to the residuals from prediction of validation data.

pruning algorithm was employed. This reduced the number of weights and biases so that the model was not over-fitting the data. Prior to its use the results from the correlation analysis were consistently outside the 95% confidence limits.

Given that the MIMO model is generally less complicated than the nonlinear neural model, while producing comparable predictions, its use should be considered with some favor. To investigate the behavior of the MIMO model, it is useful to consider its performance in predicting over a long period of time. Figure 9 presents a pure simulation using the MIMO ARX model, which uses only initial (input and output) data as starting conditions and from then on uses the predicted data and the input (feed pump) in order to predict subsequent steps ahead. If the MIMO model was a perfect representation of the data generating mechanism of the anaerobic process, then the predicted response

would be coincident with the validation data. It is unlikely that this would be achieved as the model is linear and is attempting to represent a nonlinear process. It is only feasible with the one-step-ahead prediction, because this technique is essentially a piece-wise linearization of the process dynamics by continually using the most recent measurements in making a prediction a short step in time ahead. Having accepted the limitations of a pure simulation, the general behavior (rather than the absolute values) indicate that the model is at least similar dynamically to the anaerobic process under consideration. The least accurate predictions are those for bicarbonate alkalinity [Fig. 9(a)] which indicates significant deviation after about 15 h. It is possible that the prevailing bacterial stress levels of the validation data set were higher than those of the parameter estimation data set, which is supported in part by the fact that the bicarbonate alkalinity of

(a)

(b)

Fig. 7. Correlation analysis for % carbon dioxide using nonlinear, MIMO and SISO ARX models. (a) Auto-correlation of residuals from prediction of validation data. (b) Cross-correlation of pump to the residuals from prediction of validation data.

the parameter estimation data set reacts after a delay of *ca.* 5 h data [most visible after the final shock at 90 h on Fig. 1(a)]. The response of the bicarbonate alkalinity to the end of the shock load is much quicker, with a delay of less than 1 h. The implication is that the biological system is able to cope with the increased loading rate for about 5 h before the bicarbonate alkalinity starts to reduce. In the case of the validation data set however, the bicarbonate alkalinity begins to reduce more rapidly, indicating that the system is less able to generate bicarbonate alkalinity. The delay (which may vary within each data set) is therefore built into the ARX models through the parameter estimation data and is an example of the time variance of the system.

The ARX model structure presupposes that the noise is filtered when passing through the system, by a transfer function which has the same poles as

the ARX model. If this assumption is not valid, the resulting model accuracy is deleteriously affected. There are no simple means known to the authors for determining the consequence of the noise filtering, other than observing the performance of the resulting model and determining if the model is "good enough".

A comparison of three ARX models has been presented. All the models were parameterized and validated using the same data and in an attempt to make the resulting models comparable, the regression vectors (past data samples) were the same for all the models and all the data streams. While it is not claimed that the models were in any sense optimal, the approach of maintaining constant those parts of the identification procedure which were common to all models, has produced results which may form the basis of a selection procedure with respect to the three model structures used.

(a)
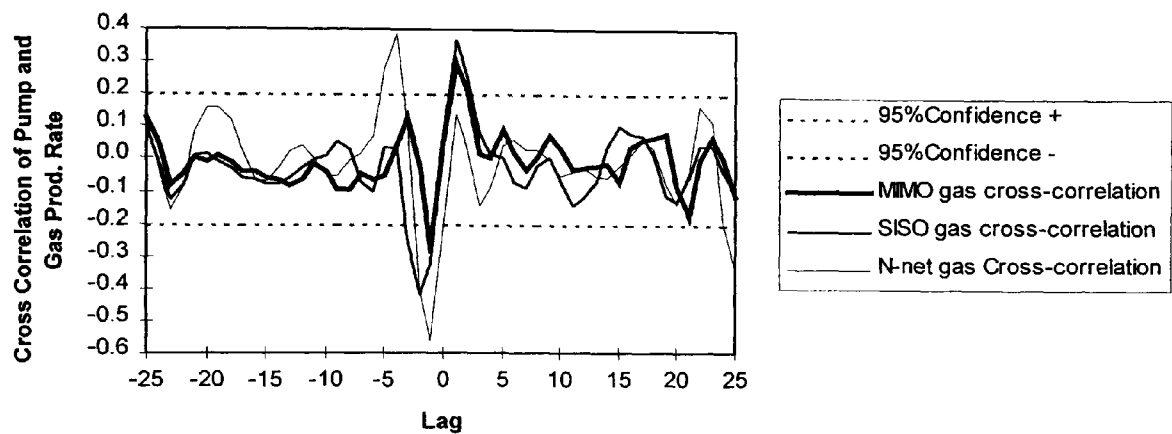
(b)
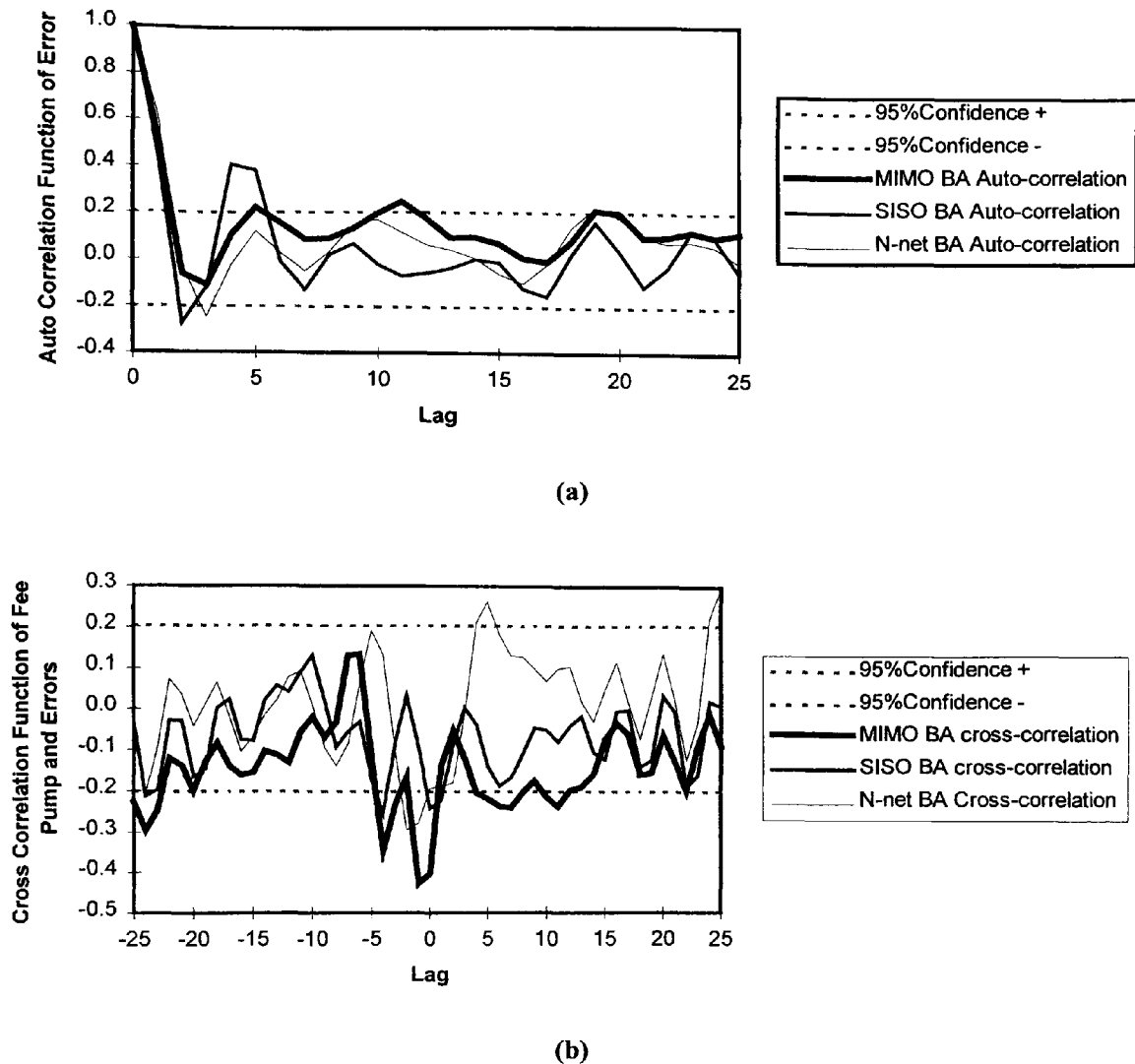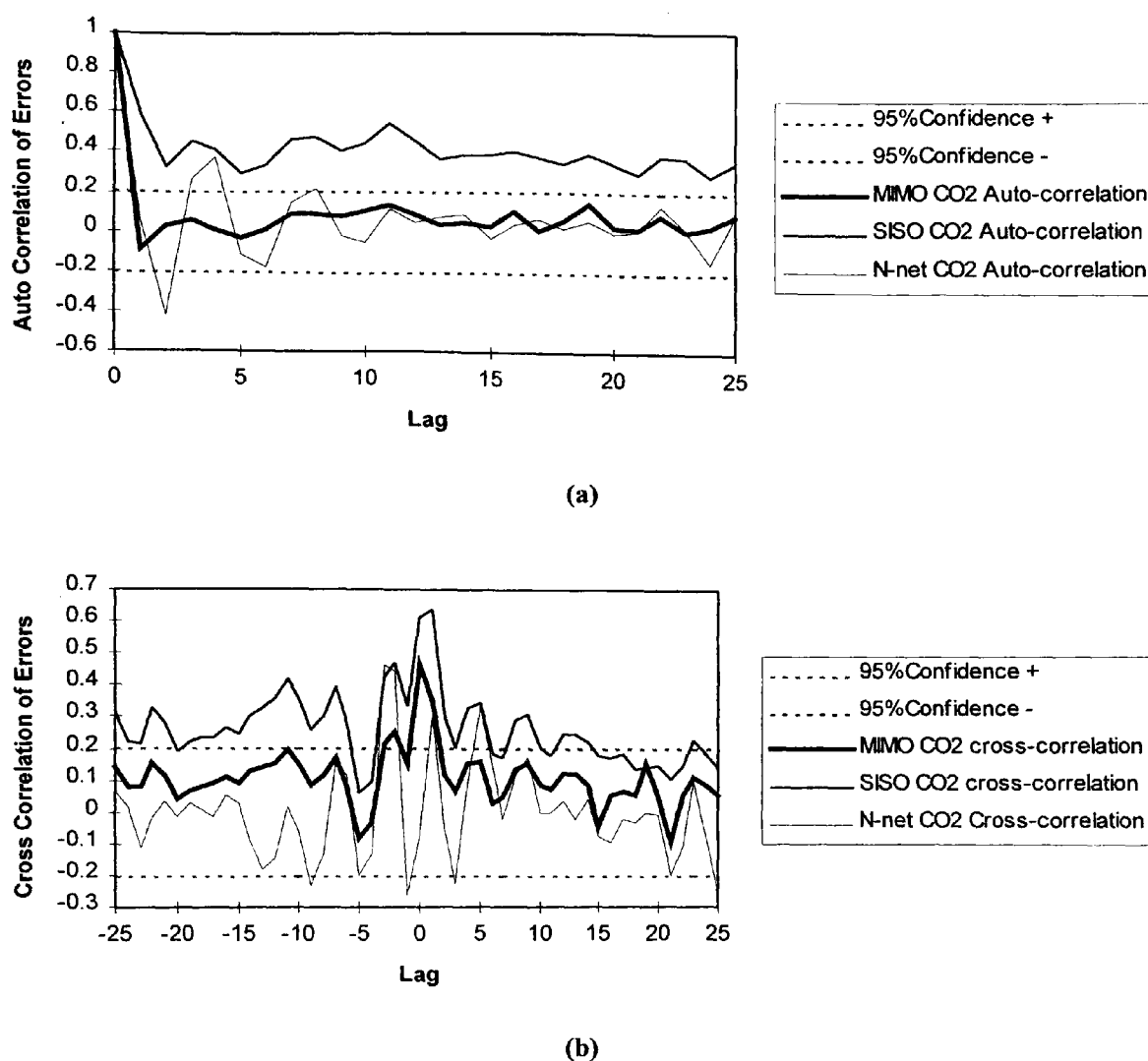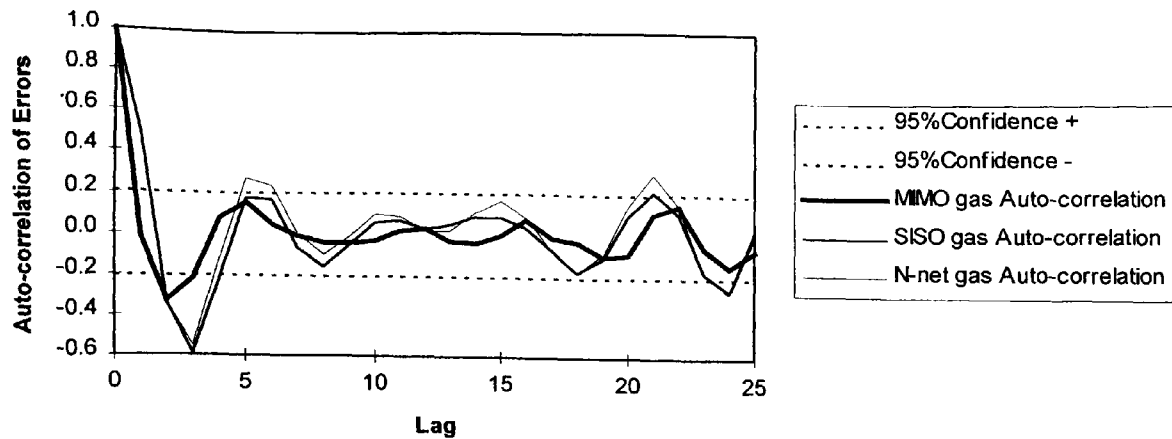
Fig. 8. Correlation analysis for gas production rate using nonlinear, MIMO and SISO ARX models. (a) Auto-correlation of residuals from prediction of validation data. (b) Cross-correlation of pump to the residuals from prediction of validation data.

It can be seen that the performance of the MIMO model was superior to that of the SISO and comparable with the neural network approach when considering the 95% confidence intervals on the correlation analysis of the residuals. Overall, the neural network had higher performance than the linear models, however the added complexity of the neural network model and associated identification process is not considered to warrant its adoption, unless the accuracy of the model is a paramount factor. If recursive identification is to be performed, where the neural model would require repeated retraining, it is likely that the improvement in performance indicated by the results, may lead to the computing overheads becoming a significant mitigating consideration. Not only would the training of the network require a considerable number of presentations of the data (epochs) but a large amount of training data would be needed to ensure

adequate training. These are in contrast to well established recursive identification algorithms used in linear black box techniques which require very little historical data to be stored and are fast in their execution (Soderstrom and Stoica, 1989). There are however training techniques which significantly increase the speed of training neural networks, such as that proposed by Venugopal and Pandya (1992) and provided the sampling time is similar to that chosen in this paper, processing time should not be a significant problem with modern computers.

CONCLUSIONS

The comparison of a linear SISO ARX, linear MIMO ARX and nonlinear feed forward neural network ARX model (all using the same lag space, training and validation data) showed that the linear

(a)

(b)

(c)
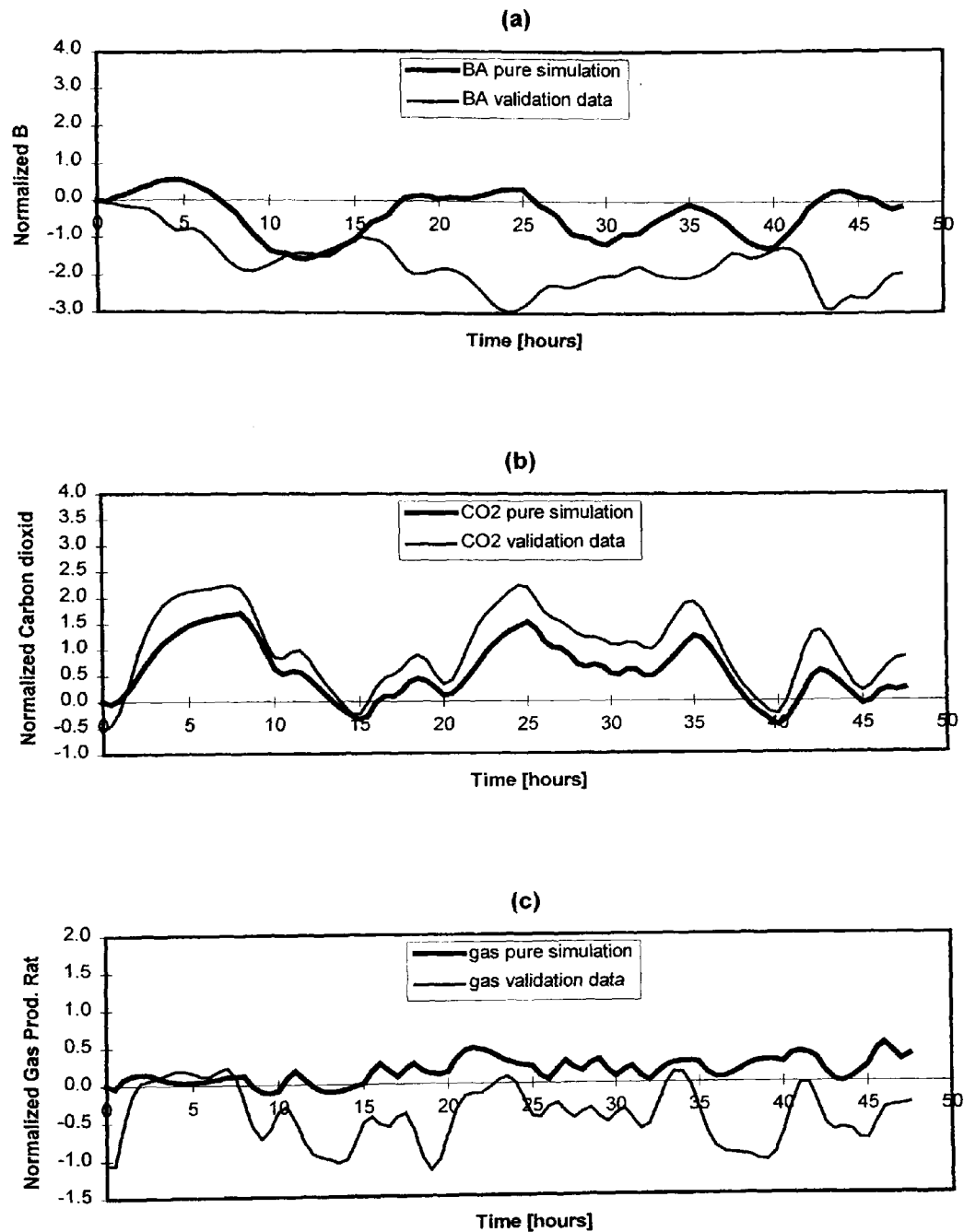
Fig. 9. Comparison of validation data with predictions from a pure simulation, using the MIMO ARX model. (a) Bicarbonate alkalinity, (b) carbon dioxide, (c) gas production rate.

SISO ARX model's performance, measured by correlation analysis, was comparatively good in the case of bicarbonate alkalinity, but less able to represent the %CO_2 and gas production rate than the other models. For the linear SISO model bicarbonate alkalinity, the auto-correlation function remained within the 95% confidence limits for the most part, as did the cross correlation function. In the case of the %CO_2 prediction by the SISO model, the correlation functions were predomi-

nantly, outside the 95% confidence limits. The correlation analysis for the gas production rate showed that the performance of the SISO model was comparable with that of the neural network model, though inferior to the MIMO model.

The neural network and MIMO models had comparable performance with respect to correlation analysis, though the MIMO model had better performance in the case of the gas production rate and worse in the case of BA. Based on the results there

would be no generally superior choice of model, however the neural network and MIMO models would both be preferred to the SISO model, because of the %CO_2 correlation analysis of the latter.

Of the three models investigated, the MIMO model would be preferred in situations where black box approaches are relevant, for its combination of its relative simplicity, accuracy and transparency.

In considering the pure simulation using the MIMO model, it is concluded that the model dynamics are (although not accurate) similar to those of the fundamental data generating mechanisms of the anaerobic process used in the experimental work. Reducing the horizon of the simulation to one step (30 min) ahead improves the accuracy of the model to the point that it can be considered a relatively accurate representation of the system.

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BIORESOURCE
TECHNOLOGY

Two-stage anaerobic co-digestion of waste activated sludge and fruit/vegetable waste using inclined tubular digesters

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Abstract

The anaerobic co-digestion of a 10% total solids (7.4% VS) waste activated sludge/fruit and vegetable mixture with approximately 25% of the VS arising from the fruit and vegetable waste was studied in duplicate two-stage systems. Acidogenic CSTRs and methanogenic inclined tubular digesters operated at 30°C achieved stable anaerobic digestion at an overall system loading rate of 5.7 kg VS m^{-3} d^{-1}, overall HRT of 13 days (3 day acidogenic HRT, 10 day methanogenic HRT), with 40% VS destruction and a system biogas yield of 0.37 m^3 kg VS^{-1} added. The biogas methane content was 68% and bicarbonate alkalinity in the methanogenic stage was over 4000 mg CaCO$_3$ l^{-1}, although TVFA levels were relatively high at 1300 mg l^{-1}. By increasing the overall system HRT to 17 days (system OLR 4.3 kg VS m^{-3} d^{-1}) with the methanogenic HRT increased to 13 days, the average TVFA in the methanogenic stage was reduced to 300 mg l^{-1} and the overall VS destruction was 44%. Using these results an embodiment design was developed for a full-scale plant. The duty cycle was such that HRTs could vary from 4 to 26 days in the case of the acidogenic stage and 10 to 65 days in the case of the methanogenic stage. © 1999 Elsevier Science Ltd. All rights reserved.

Keywords: Anaerobic digestion; Two-stage; Waste activated sludge; Inclined tubular digester; Fruit/vegetable waste

1. Introduction

Owing to tighter environmental legislation in Europe, increasing numbers of aerobic plants are predicted to be built to treat wastewaters before their discharge to the environment. However the operation of these plants results in the production of large quantities of waste activated sludge (WAS) which due to the same legislation also presents difficulties for disposal because of the closure of some traditional disposal routes (Davis, 1996). In the UK the volume of sludge is expected to grow by 60% to 1.6 million tonnes dry solids per annum (Davis, 1996). Legislation has also increased the cost of disposal of other organic wastes such as municipal solid waste (MSW) to landfill. In Europe the organic fraction of municipal solid waste can form up to 37% of the collected MSW. Because of the closure of these traditional disposal routes alternative routes for the disposal of these organic wastes such as co-digestion are being sought (Mata-Alvarez et al., 1992; Kiely et al., 1997;

Griffin et al., 1998; Zhao and Kugel, 1996; Callaghan et al., 1999). Anaerobic digestion has been applied to MSW (see e.g., Fruteau et al., 1997; Nopharatana et al., 1998), to market wastes, the latter being highly digestible (Mata-Alvarez et al., 1992) and other fruit and vegetable wastes (e.g., from food production, Raynal et al., 1998).

Anaerobic digestion is commonly used to treat a mixture of primary and secondary sludges, as it results in a smaller amount of waste with reduced polluting power, odour potential and number of pathogens, and greater dewaterability. A renewable energy by-product, biogas, also results. Activated sludge alone, unmixed with municipal primary settled sludge, is widely reported to show only 30–45% reduction in VS during conventional anaerobic digestion, despite having a higher ultimate biodegradability (Ghosh, 1991). Pre-treatment procedures to improve the anaerobic biodegradability of WAS have been reported, with thermal pre-treatment being the most common (Huag et al., 1983; Tanaka et al., 1997; Li and Noike, 1992). Shimizu et al. (1993), Tiehm et al. (1997) and Wang et al. (1999) showed beneficial effects of ultrasonic lysis on subsequent anaerobic digestion. Other pre-treatments have been

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considered, e.g., by Novelli et al. (1995) who studied the solubilisation of municipal sludges using alkaline pre-treatments, and Hwang et al. (1997) using pressure to disrupt cells. These procedures are somewhat energy-intensive or costly (Takashima et al., 1996). The latter workers attempted membrane retention of particles and alkaline hydrolysis of the digested sludge, but overall degradation was not much improved over the long-term. Use of a specially adapted thickening centrifuge to partially lyse cells mechanically is reported as a promising technology, increasing the methane yield, and the digestibility from 59.5% to 76.6% (Dohanyos et al., 1997).

Two-stage anaerobic digestion where the digestion process has been divided up into a acidification stage and a methanogenic stage, has been shown to improve biogas production from a mix of primary and WAS (Chang et al., 1989) and for WAS alone (Ghosh, 1991). The latter worker showed, using 7.5% TS WAS, that a two-stage system eliminated problems commonly experienced with foaming and could give a VS reduction of 56% as commonly calculated or of 73% calculated from the mass balance. However, for WAS alone, only small improvements in VS destruction from a two-stage system were reported by Bhattacharya et al. (1996), and by Shimizu et al. (1993) using sonicated WAS. A two-stage system applied to fruit and vegetable wastes (Mata-Alvarez et al., 1993) in the absence of pH control to maintain a low pH in the acidogenic stage did not work effectively to give acidification, and thus showed no significant advantage over a one-stage system.

As part of the WAS treatment system the sludge is often thickened by the use of a centrifuge or belt press. The use of a thickened sludge would offer a number of advantages such as smaller reactor size, therefore reduced capital and running costs. If the sludge is to be transported to a central digester, thickened sludge would also result in lower transportation costs. The aim of this paper was to study (at laboratory-scale), the anaerobic digestion of high TS content waste (10% TS), composed of WAS and vegetable waste, in methanogenic inclined tubular digesters with an acidification stage CSTR. Inclined tubular digesters (ITD) have a number of advantages: they can be used to treat high total solid wastes, have a tendency to retain particulate matter, have a small gas/liquid interface to minimise scumming and, as they do not require agitation, offer the advantage of lower energy input over CSTR type reactors (Chapman, 1986). The laboratory-scale results were then used to design, to embodiment stage, a full scale plant large enough to treat the biological sludge from an ANANOX™ process (Garuti et al., 1992) and putrescible wastes, (e.g., market waste) in a sensitive Mediterranean area with a seasonal peak population of 8000 p.e.

2. Methods

Waste activated sludge (WAS) was collected from an activated sludge plant owned by Hyder plc. treating domestic and industrial waste, without primary settlement, in oxidation ditches operating at a 1 day HRT, approximately. The sludge had been dewatered by the addition of polyelectrolyte (OCI Posifloc CEF B90, OCI Ltd., Castleford, UK) at a dosage rate of 3 kg t^{-1} TS and passage through a belt press giving 16% TS. The assumption was made that WAS was comparable with the biological sludge from an ANANOX™ process, as they are both composed of settled suspended bacterial biomass. Sludge was frozen until required and after defrosting was diluted with tap water to approximately 11% total solids. The fruit and vegetable waste consisted of homogenised plums (185 g), lemons (76 g), lettuce (369 g), tomatoes (190 g), courgettes (85 g) and bananas (95 g) to give 86 g l^{-1} TS (76 g l^{-1} VS). The feedstock was made up by adding approximately 75% by volume of 110 g l^{-1} TS, 73 g l^{-1} VS, waste activated sludge to 25% by volume of fruit and vegetable waste. This gave a feedstock for the acidification reactors with an average 100 g l^{-1} TS content and 74 g l^{-1} VS content, of which approximately 25% VS was from the fruit and vegetable waste.

The two acidogenic reactors consisted of 5 l Quickfit vessels maintained at $30 \pm 2°C$ and stirred continuously at 125 rpm by a RZ50 Heidolph Stirrer (LabPlant, Huddersfield). From day 0 to day 88 the reactors had a 2.4 l working volume and from day 100 to day 159 the reactors had a 3.2 l working volume. The reactors were seeded by filling to the working volume with feedstock, then left to acidity for three days before the commencement of feeding seven days per week. From day 0 to day 74 the acidogenic reactors were operated at a 3 day HRT and OLR of 26 kg VS m^{-3} d^{-1}. Samples were analysed for VFA composition and pH. Samples were also taken from day 55 for TS and VS analysis.

To investigate the effect of changes in HRT, from day 75 acidogenic reactor 1 was converted to a 2 day HRT (OLR 39 kg VS m^{-3} d^{-1}) by feeding twice a day and acidogenic reactor 2 was converted to 1 day HRT (OLR 78 kg VS) by feeding 3 times a day. Over this two week period the reactors were not fed at weekends. Samples were taken each time the acidogenic stage was fed, to be analysed for VFA composition and pH. The acidogenic reactors were restarted on day 100 by seeding with 3.2 l of feedstock as described by the procedure given above and operated until day 159. A 3 day HRT over a 5 day week was used from day 103 to day 159 by feeding 1100 ml Monday to Thursday and 1340 ml on Friday, averaging a 4 day HRT over a 7 day week.

Two 8 l inclined tubular digesters (ITD 1 and ITD 2) with an aspect ratio of 10 (body length of 1000 mm with an internal diameter of 100 mm), and 20° angle of in-

clination, as designed by Chapman (1986), were used as methanogenic stages (Fig. 1). The two ITDs were fitted with 5 sample acquisition ports (P1–P5) as shown and were maintained at 30 ± 2°C. The reactors were seeded by adding 6.5 l of anaerobically digested WAS/vegetable waste mix from a previous experiment which was made up to 8 l with 5% TS WAS sludge. The anaerobically digested seed sludge originated from a laboratory digester, seeded with municipal anaerobically digested sludge, which had been fed WAS/vegetable waste for 6 weeks and left unfed at room temperature for 5 months prior to use. From day 1 to day 74 ITD 1 and ITD 2 were fed every day including weekends with output from the acidogenic reactors. The reactors were started up at an 18 day HRT, and over a 32 day period the HRT was gradually decreased to a 10 day HRT while maintaining biogas % methane, reactor pH and stable or increasing gas production rates. The reactors were operated at a 10 day HRT from day 33 to day 74, feeding with output from the acidogenic reactors operated at a 3 day HRT. Gas was collected from the body of the reactor and the weir sections as shown in Fig. 1. Gas samples were analysed daily for methane and CO_2. Gas production was monitored on a daily basis by the use of oil-filled analogue gas meters (Alexander Wright, London, UK). Samples of effluent were taken on a regular basis for the determination of pH, TVFA and bicarbonate alkalinity. From day 55 to day 74 samples for total solids and volatile solids destruction were taken. The methanogenic reactors were unfed from day 75 until day 103. From day 103 to day 159 the ITD reactors were fed only on week days, by feeding 850 ml of acidogenic reactor contents on Monday to Thursday and 1340 ml of acidogenic reactor contents on Friday, giving an average HRT calculated over a 7 day week of 13 days. The ITD reactors were then left at 30°C from day 160 to day 213 with all ports, except the gas port, stoppered to prevent evaporation. On day 213 the reactor contents were analysed for TS and VS to determine the ultimate biodegradability of the substrate.

Total and volatile solids analyses were performed in triplicate on a single grab sample according to standard methods (APHA, 1989). Temperature and pH measurements were performed according to standard methods (APHA, 1989) and bicarbonate alkalinity (partial alkalinity) by titration to pH 5.75 (Jenkins et al., 1983). Gas composition and VFA analysis were determined by gas chromatography (Peck et al., 1986).

3. Results and discussion

3.1. Acidogenic reactors

The initial WAS/fruit and vegetable feedstock averaged pH 5.3 (ranging from pH 5.1 to 5.8, 18 samples SD = 0.3) with average TVFA levels of 1170 mg l^{-1} (Table 1). The performance of the acidogenic reactors is presented in Table 1. A pH controller was not used to control either the acidogenic or methanogenic stage or neutralise the feed, so the pH level in the reactors was allowed to float. In the acidogenic stage the pH floated between pH 4.4 and pH 6.2 despite an increase in TVFA from 1170 mg l^{-1} in the feed, to over 6000 mg l^{-1} in the reactor in most cases. The average pH varied little between the acidogenic reactors at 4, 3, 2 or 1 day HRT averaging 5.1 to 5.6 in all the reactors. A pH of 5.6 was achieved in a 3 day HRT CSTR acidifying WAS without pH control (Ghosh, 1991), so that the addition here of fruit/vegetable matter to 25% of total VS had little effect. A number of studies have found acidogenic reactors to operate successfully at pH of between 5.0 and 6.0 while utilising primary sludge (Eastman and Ferguson, 1981; Elefsiniotis and Oldham, 1994) or WAS (Ghosh, 1991). Results from this study would support this, as significant levels of acidification were achieved for around 160 days without the use of a pH controller, suggesting that pH control was not necessary for the acidogenic stage.

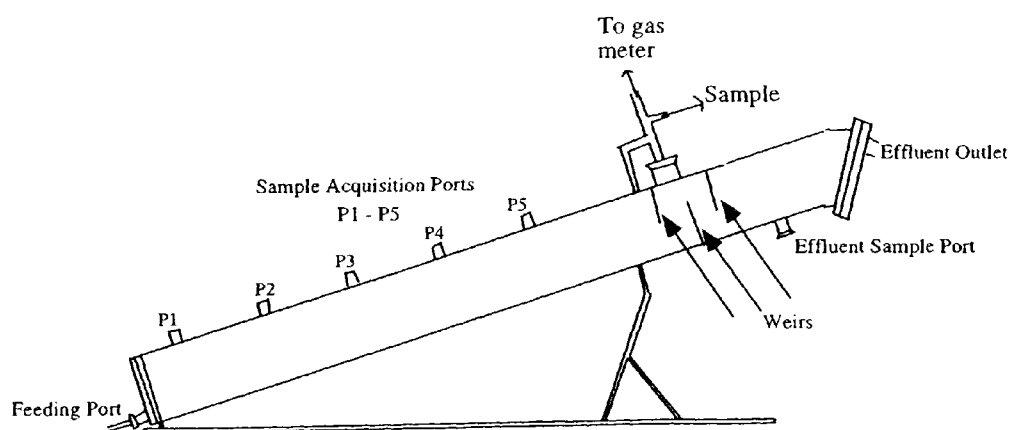At a 3–4 day HRT an average of 6400 mg l^{-1} TVFA was produced. This corresponds to a VFA yield of 0.09

Fig. 1. Inclined tubular digester (ITD).

Table 1
Performance of acidogenic reactors[a]

	Feed	3 day HRT (days 1–74)	4 day HRT (days 103–159)	2 day HRT	1 day HRT
Mean pH	5.3 (20)[b] SD 0.3	5.3 (78) SD 0.2	5.63 (70) SD 0.4	5.1 (16) SD 0.2	5.3 (24) SD 0.4
pH range	5.2–5.8	4.7–5.8	4.8–6.2	5.0–5.4	4.4–5.4
TVFA (mg l⁻¹)	1170 (12) SD 750	6150 (36) SD 1880	6620 (51) SD 1500	6100 (8) SD 1970	4400 (11) SD 1880
Acetate (mg l⁻¹)	598 SD 415	3570 SD 1370	4077 SD 1180	3042 SD 1693	2608 SD 1457
Propionate (mg l⁻¹)	292 SD 193	480 SD 320	475 SD 200	584 SD 283	198 SD 19
i-Butyrate (mg l⁻¹)	28 SD 19	110 SD 50	151 SD 72	89 SD 48	84 SD 54
n-Butyrate (mg l⁻¹)	143 SD 101	1380 SD 500	1100 SD 270	1173 SD 517	826 SD 628
i-Valerate (mg l⁻¹)	70 SD 46	200 SD 120	280 SD 130	167 SD 100	151 SD 107
n-Valerate (mg l⁻¹)	37 SD 31	460 SD 280	520 SD 240	528 SD 201	250 SD 130

[a] SD = Standard deviation.
[b] () = Number of samples.

g VFA g⁻¹ VS added. The VFA yield of WAS in acidification reactors has been reported to vary from 0.11 to 0.59 g VFA g⁻¹ VS added (Chiu et al., 1997). All C_2–C_5 VFAs were detected, however the VFAs were primarily acetic acid (60%) and n-butyric (20%) (See Table 1). Ghosh (1991) achieved levels of up to 9500 mg l⁻¹ TVFA, consisting mainly of acetic, propionic and n-butyric. Table 1 shows TVFA levels in reactors operating at a 3 day and 2 day HRT were similar, however TVFA levels decreased significantly from 6100 mg l⁻¹ to 4400 mg l⁻¹ with operation at a 1 day HRT.

3.2. Methanogenic reactors

The output of the acidogenic reactors was fed directly to the methanogenic stage without any pH adjustment. From day 1 to day 33, ITD 1 achieved daily gas production of 1.6 l l⁻¹ d⁻¹ and ITD 2 1.3 l l⁻¹ d⁻¹. The methane content of gas from ITD 1 was 69% CH_4 (9 samples SD = 4) and for ITD 2 70% CH_4 (10 samples SD = 3). From day 33 the loading rate was increased to 6.0 kg VS m⁻³ d⁻¹ and the HRT decreased to 10 days. By day 36 the average gas production had risen to 2.0 l l⁻¹ d⁻¹ and remained at around this value until day 74. Thus after 32 days start-up with decreasing HRT from 18 to 10 days, using seed from a working digester which had remained unfed for 3 months, the reactors could be successfully operated at a 10 day HRT.

The data for the period day 53 to day 70 at a 10 day HRT are presented in Table 2. During this period daily gas production for ITD 1 was 2.1 l l⁻¹ d⁻¹ (15 samples, SD = 0.3). The average gas composition of 68% CH_4

was the same as achieved by Ghosh (1991) using WAS. Using the gas production figure from ITD 1 and the loading to acidogenic stage, the biogas yield for the whole system was 0.37 m³ kg VS⁻¹ added.

During the period days 37–70 high levels of TVFA of up to 2350 mg l⁻¹ were experienced in both ITDs indicating that the reactors were not operating at their optimum. An average of 1300 mg l⁻¹ TVFA was found in ITD 1 and an average of 1800 mg l⁻¹ TVFA was found in ITD 2 (Table 2) between days 53 and 70. In contrast, levels of 172 mg l⁻¹ TVFA were found in the methanogenic stage at a 10 day HRT and 6.2 kg VS m⁻³ d⁻¹ organic loading rate by Ghosh (1991) indicating that lower levels of TVFA are possible for WAS alone. However the pH and the bicarbonate alkalinity of the methanogenic ITD reactors were high indicating good process stability. The pH in ITD 1 and ITD 2 averaged pH 7.8 (39 samples, SD = 0.2) with bicarbonate alkalinity averaging 4800 mg $CaCO_3$ l⁻¹ in ITD 1 and 4100 mg $CaCO_3$ l⁻¹ in ITD 2. A pH of 7.7 in the methanogenic reactor of a two-stage process was reported by Ghosh (1991) without the addition of alkali. This work indicates that reactors could be operated with 25% of VS as fruit and vegetable waste also without any addition of alkali. However, despite the high TVFA, a VS destruction of 43% for ITD 1 and 39% for ITD 2 were achieved. The VS destruction of WAS ranges from 16% to 50% (Parkin and Owen, 1986), although in a two-stage system up to 56% was achieved by Ghosh (1991). The ultimate biodegradability, on day 213 after being left unfed for 54 days at 30°C, measured as the % VS reduction in ITD 1 was 47% and 41% in ITD 2. Thus

Table 2

Performance of methanogenic reactors[a]

Parameter	10 day HRT		13 day HRT	
	ITD 1 (days 53–70)	ITD 2 (days 53–70)	ITD 1 (days 141–159)	ITD 2 (days 128–159)
% Methane	68	67	68	70
	(14)[b]	(14)	(5)	(7)
	SD 4	SD 5	SD 4	SD 4
TFVA levels (mg l⁻¹)	1300	1800	530	250
	(8)	(5)	(10)	(16)
	SD 500	SD 690	SD 364	SD 250
VS destruction (%)	43	39	43	44
	(6)	(6)	(5)	(6)
	SD 7	SD 6	SD 5	SD 4
Bicarbonate alkalinity	4800	4100	7290	9090
(mg CaCO₃ l⁻¹)	(4)	(4)	(4)	(4)
	SD 1100	SD 1200	SD 2250	SD 1320

[a] SD = Standard deviation.
[b] () = Number of samples.

it appears that increasing the HRT above 10 days in the inclined tubular digester would give little improvement of overall VS destruction.

In an attempt to reduce the effluent TVFA levels from the methanogenic stage the methanogenic HRT was increased from 10 to 13 days with the acidogenic stage at a 4 day HRT. The effect on the VFA level of ITD 1 can be seen in Fig. 2 and ITD 2 in Fig. 3. At the 13 day HRT the TVFA levels in ITD 2 rose to 2900 mg l⁻¹ on day 110 but fell to 1500 mg l⁻¹ on day 124. The average TVFA for ITD 2 from day 128 to day 159 was 250 mg l⁻¹ (Table 2). This was taken to be the steady-state period, during which ITD 2 achieved a VS destruction of 44%. Operation at a methanogenic-stage HRT of 13 days rather than 10 days (system HRT 17 days rather than 13 days) did not significantly improve %VS destruction, but significantly lowered TVFA content, so that the resulting effluent was less odorous.

In ITD 1 the TVFA rose from 400 mg l⁻¹ on day 115 to 7800 mg l⁻¹ on day 117 to a peak of 10 000 mg l⁻¹ on day 127 (see Fig. 3). The reactor was found to have undergone a severe shock, with the effluent pH fallen to pH 5.8 on day 117 with a reduction in methane content from 41% on day 115 to 15 % on day 117. ITD 1 had low pH at port P1 (pH 5.42) and pH 5.78 at port P5 on day 117. This was in contrast to ITD 2 which had a pH of 7.46 and 7.75 at these two ports on day 117. Despite the low pH of the acidified influent, lack of stirring in the reactors and high TS content, ITD 2 always maintained the pH within the optimum range for methanogenesis, although a slight pH gradient was seen with a lower average pH at port P1 (pH 6.9) and pH 7.8 at P5. The average effluent pH of ITD 2 was pH 7.7 (21 samples, SD = 0.2) from day 128 to day 159.

To recover ITD 1, on day 117 the reactor was fed with 850 ml of acidogenic-reactor effluent with 40 g
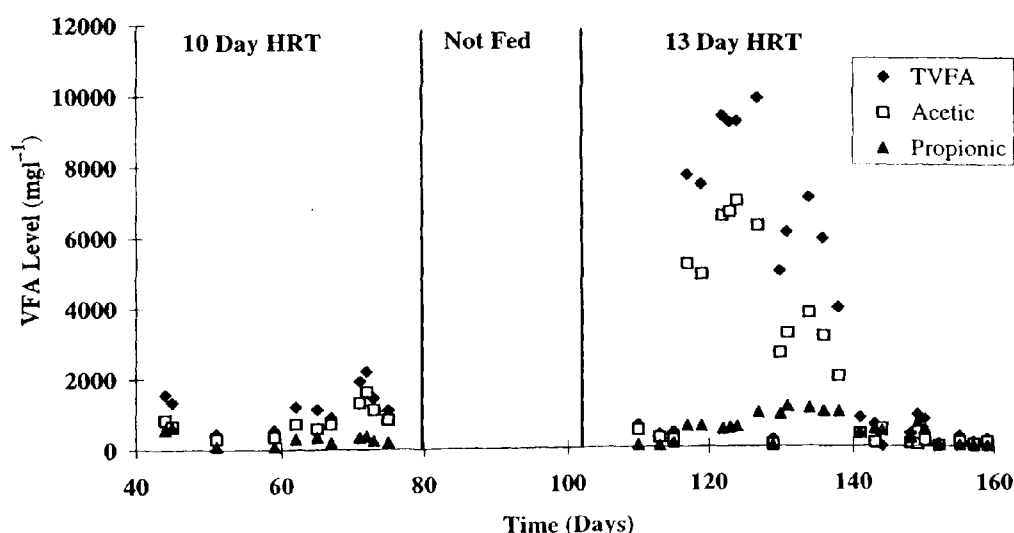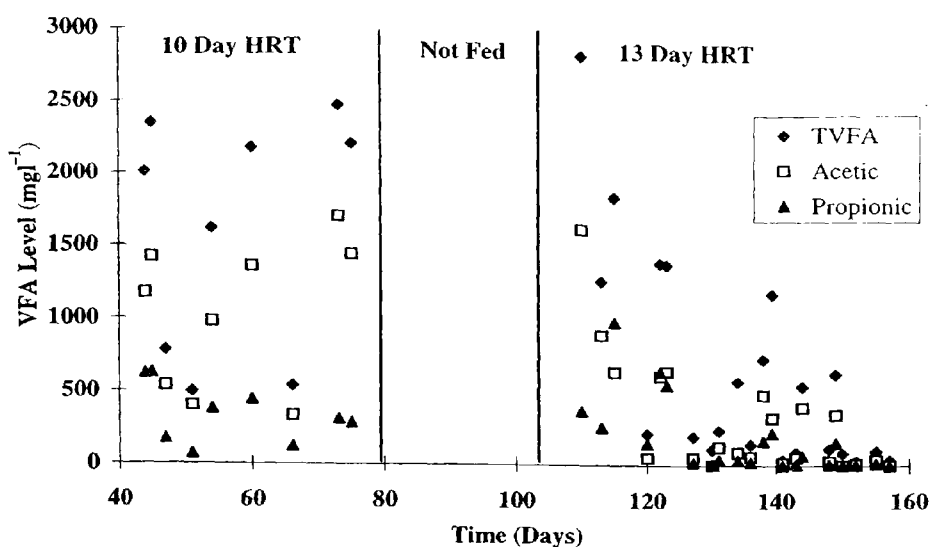

Fig. 2. VFA Levels in ITD 1.

Fig. 3. VFA Levels in ITD 2.

sodium bicarbonate and subsequently 1.1 l of ITD 2 effluent. On day 120 and 122 ITD 1 was fed with 425 ml of acidogenic reactor effluent and 450 ml of ITD 2 effluent. The normal feeding regime was restarted on day 127. Using this regime the lower section of the reactor pH was above pH 7 on day 118 and by day 128 the entire length of the reactor was at pH 7 or above, although the effluent pH was below pH 7 until day 128. From day 141 to day 159 the average effluent pH of ITD 1 was pH 7.7 (14 samples, SD = 0.2).

The TVFA levels in ITD 1 had fallen sharply to 800 mg l^{-1} by day 141 (Fig. 2). The average TVFA from day 141 to day 159 (Table 2) was 530 mg l^{-1} and average VS destruction was 43%. The average gas composition was 68% and 70% methane respectively in ITD 1 and ITD 2 in the periods of stable operation. Thus despite having had TVFA levels of 10 000 mg l^{-1}, within 10 days the reactor could be returned to a 13 day HRT by addition of sodium bicarbonate and methanogenic effluent from normal operation. It appears useful to retain approximately 20% of the digester volume of digested effluent on site for the purposes of recovery of the reactor from acid-generating shocks.

3.3. Embodiment design

The difficulties of designing plant for the treatment of domestic sewage in sensitive coastal areas with a seasonal dramatic increase in population are well recognised (see e.g., Castillo et al., 1997). The results from these laboratory scale investigations were to form the basis of design of the full scale plant which would be capable of treating sludge from an ANANOX™ process (Garuti et al., 1992) and market waste produced by a Mediterranean tourist resort with a seasonal population peak of 8000 p.e. but a rural winter population circa

1200 p.e. The resort studied was remote and a conservation area, so problems were experienced with solid-waste disposal. Fruit/vegetable market waste was identified suitable for disposal by co-digestion, alleviating problems experienced acutely in the summer months. This conceptual exercise is representative of many small coastal and island resorts in the Mediterranean.

Ghosh et al. (1975) and Ghosh (1991) discussed the advantages and disadvantages of two-stage digestion as a means to improve digestibility and system design. A degree of uncertainty existed prior to the laboratory-scale tests, with regard to suitable retention times in the acidogenic reactor. Using a model of the acidogenic stage based on the work of Eastman and Ferguson (1981) the acidogenic stage performance was simulated in order to ascertain that the hydrolysis could be achieved during a retention time similar to the 3.1 days reported for WAS by Ghosh (1991). The model used has been summarised in Table 3. The values, units and assumptions made in the modelling are shown in Table 4.

The simulation showed that:

- The concentration of degradable particulate would reduce rapidly and asymptotically to zero, such that an SRT of 3 days would affect most of the reduction by solubilisation.
- The concentration of viable anaerobic biomass would be at a maximum at an SRT of approximately 1 to 2 days, and reduce gradually with increasing SRT.
- As would be expected, the products of acidogenesis would increase in response to the solubilisation of degradable particulates.

The model supported use of a HRT of around 3 days for the acidogenic stage when operated at 30°C. The sludge production from the ANANOX process was based on knowledge of the resort's population and was agreed as part of the design specification by the com-

Table 3

Summary of acid stage model (after Eastman and Ferguson (1981))

Particulate COD:

$$F = \frac{F_0}{1 + k_h \theta}$$

(1)

Soluble substrate COD:

$$S = \frac{K_s\left(1 + \frac{X_0}{X} + k_d\theta\right)}{\theta(\mu' - k_d) + \frac{X_0}{X} - 1}$$

(2)

Biomass COD:

$$X = \frac{Y(F_0 - F + S_0 - S) + X_0}{1 + k_d\theta}$$

(3)

Products COD:

$$P = P_0 + (F_0 - F) + (X_0 - X) + (S_0 - S)$$

(4)

F = effluent concentration of degradable particulate COD
F_0 = influent concentration of degradable particulate COD

S = effluent substrate concentration COD
S_0 = influent substrate concentration COD

X = effluent viable biomass concentration COD
X_0 = influent viable biomass concentration COD

P = effluent product concentration COD
P_0 = influent product concentration COD

k_h = first order hydrolysis rate constant
μ = maximum specific growth rate
K_s = substrate concentration at 1/2 max. specific growth rate
k_d = decay coefficient
Y = yield coefficient
θ = hydraulic retention time (= solids retention time in CSTR type system)

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missioning agents (ENEA, Bologna, Italy). The projected flow rates over the year are shown in Table 5 where the two stages of the sludge treatment system were sized at 5 m³ for the acidogenic stage and 12.7 m³ for the methanogenic stage, in order to give peak HRT of 4 and 10 days, respectively. The methanogenic inclined tubular digester design had an internal diameter of 1.3 m, an internal length of 10 m and a 20° inclination.

Two serpentine heat exchangers were designed using dynamic models of the two stages, in order to simulate the bulk fluid temperatures from start-up through to steady operation. The aim (based on a knowledge of temperature effects on the anaerobic process (Malina, 1964)), was to maintain the temperature of the digester contents to within ± 3°C of the set point temperature (35°C). Closed-loop PID control systems were employed in the simulation, paying due regard to heater saturation and limiting the maximum temperature of the heating water to avoid damage to viable biomass and avoid fouling (50°C) in the reactors. The peak power (i.e., saturation) requirements suggested by the simulations

were 3 kW and 5 kW for the acidogenic and methanogenic stages, respectively. The most significant uncertainties in the heat-exchanger design were the rheological properties of the digester contents (since considered by Moeller and Torres (1997)).

The gas produced by the digesters at peak loading was estimated from the laboratory-scale results to yield approximately 6.7 kW. This would mean a significant deficit for heating the reactors, particularly when considering system efficiencies. Furthermore the temporal lag between the need for heating and the supply of digester gas would further increase the need for a gas boiler suitable for an alternative gas supply. In winter the ITD methanogenic stage would operate with a 65 day HRT and the acidogenic stage at 26 day HRT, and it is possible that operation below design temperatures would be satisfactory.

The functionality of the process would depend on the timed delivery of feed to the individual stages. The feed was to be conditioned by an angle disintegrator which would deal with the large particles of vegetable waste from markets and similar sources, while a centrifugal

Table 4
Model parameters and assumed data

Parameter	Value	Units	Assumptions	Reference
F	Eq. (1)	g COD/l	Hydrolysis rate limited process	Eastman and Ferguson (1981)
F_0	75.5	g COD/l	Based on 8% TS and determined using ratio of TS:VSS from batch tests	Batch tests at Uni of Glamorgan
S	Eq. (2)	g COD/l	Hydrolysis rate limited process	Eastman and Ferguson (1981)
S_0	$f(\Delta S, S)$	g COD/l	$\Delta S = S_0 - S$ remains constant due to microbial metabolism and estimated from reduction in ΣCPL	Eastman and Ferguson (1981), Ghosh (1991)
ΔS	4.9	g COD/l	$\Delta S = S_0 - S$ remains constant due to microbial metabolism and estimated from reduction in ΣCPL	Eastman and Ferguson (1981), Ghosh (1991)
X	Eq. (3)	g COD/l	Hydrolysis rate limited process	Eastman and Ferguson (1981)
X_0	0	g COD/l	No viable biomass in feed	
P	Eq. (4)	g COD/l	Hydrolysis rate limited process	Eastman and Ferguson (1981)
P_0	2.58	g COD/l	P_0 = influent VA COD+ unutilised soluble COD	Eastman and Ferguson (1981)
k_h	0.125	h^{-1}	Hydrolysis rate similar to primary sludge digestion	Eastman and Ferguson (1981)
μ'	6.2	d^{-1}	As compared to 2.7–3.4 d^{-1} for methane formers	Metcalf and Eddy (1994), Eastman and Ferguson (1981)
K_s	0.142	g COD/l	Assumed same as Aerobic K_s	Gosset and Belser (1982), Metcalf and Eddy (1994)
k_d	0.013	h^{-1}		Eastman and Ferguson (1981)
Y	0.4	g cell COD/ g COD utilized		Eastman and Ferguson (1981)
θ	0.3–10	d		

decanter was to be used to further dewater the feed to 10% TS and hence minimise the digester volumes. These physical processes would aid cell lysis and consequently acidogenesis. Fluid transfer would be effected by progressive cavity pumps, which would be controlled by logic controllers in conjunction with automatic valves.

The reactors were sized for the worst case and this imposed HRT varying from 4 to 26 day and 10 to 65 day for the acidogenic and methanogenic stages, respectively. The acidogenic reactor could be operated partly filled at off-peak periods, and its spare capacity used to

buffer peak loads and protect the methanogenic reactor. Table 5 indicates that the peak loading would occur from mid July to late August. The acidogenic reactor is expected to operate successfully at all likely conditions. Table 5 shows that the methanogenic reactor is required to adjust from loading at a 19.5 day HRT to a 10 day HRT within 2 weeks (15–31 July). Start-up from no load to a 10 day HRT in 1 month was achieved in the work reported here at laboratory-scale. With careful monitoring it is possible that this time could be reduced, particularly as the reactor as proposed would be con-

Table 5
Seasonal variation in sludge production by the ANANOX™ process and of fruit and vegetable waste used to size the anaerobic digestion stages[a]

Month	ANANOX sludge (m^3 d^{-1})	Vegetable waste (kg d^{-1})	Total feed[b] (m^3 d^{-1})	Acidogenic stage 5 m^3 HRT (day)	Methanogenic stage 12.7 m^3 HRT (day)
January	0.09	86	0.176	26.0	65.0
February	0.09	86	0.176	26.0	65.0
March	0.09	86	0.176	26.0	65.0
April	0.09	86	0.176	26.0	65.0
May	0.09	86	0.176	26.0	65.0
June	0.18	129	0.309	14.9	37.2
1–15 July	0.40	171	0.571	8.1	19.5
15–30 July	0.81	347	1.150	4.0	10.0
August	0.81	347	1.150	4.0	10.0
September	0.20	129	0.329	14.0	35.0
October	0.09	86	0.176	26.0	65.0
November	0.09	86	0.176	26.0	65.0
December	0.09	86	0.176	26.0	65.0

[a] HRT based on nominal peak HRT of 4 days (acidogenic phase) and 10 days (methanogenic phase).
[b] Assuming vegetable waste has a density of 1000 kg m^{-3}.

tinuously fed at a low load, and it is recommended that experienced staff should be on hand in mid-July for several weeks until sufficient process management information is gained. It is also recommended that approximately 20% of the digester volume of successfully-digested stabilised effluent be retained onsite during this period, together with sodium bicarbonate, since as reported here addition of these successfully recovered the ITD within 10 days from shock giving a dramatic rise in TVFA. In the unlikely event of a stress to the methanogenic digester, facility will be provided to recycle the effluent from either stage back to the ANANOX™ process.

4. Conclusions

An embodiment design for a full-scale methanogenic inclined tubular digester with a prior acidogenic stage, treating the sludge from an ANANOX™ process with 25% VS from added fruit and vegetable wastes has been developed for use in a sensitive coastal area with a seasonal population.

In laboratory-scale studies of this system, stable anaerobic digestion was achieved in a two-stage system at an overall system loading rate of 5.7 kg VS m^{-3} d^{-1}, overall HRT of 13 days (3 day acidogenic HRT, 10 day methanogenic HRT), with 40% VS destruction and a system biogas yield of 0.37 m^3 kg VS^{-1} added, although with relatively high effluent TVFA.

Increasing the overall system HRT to 17 days (system OLR 4.3 kg VS m^{-3} d^{-1}) with the methanogenic HRT increased to 13 days much reduced the average effluent TVFA, giving VS destruction of 44%.

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CONTROLLING THE START-UP OF AN EGSB ANAEROBIC DIGESTER USING ON-LINE BICARBONATE ALKALINITY MONITORING AND AN ADAPTIVE CONTROL SCHEME

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ABSTRACT

The start-up phase of Anaerobic Digestion (AD) reactors is a critical period during which special efforts are made to ensure stability. Maintaining control is essential and is usually done manually at the expense of human effort and start-up time. Automatic control of the AD process with on-line monitoring of Bicarbonate Alkalinity (BA), should speed up the start-up procedure and make it a less labour intensive and uncertain phase of operation. This poster proposes to show the start-up of an Expanded Granular Sludge Bed (EGSB) Laboratory scale AD process which is controlled by a Model Reference Adaptive Controller (MRAC), using a simple adaption mechanism.

KEYWORDS

Anaerobic digestion; control; MRAC; bicarbonate alkalinity

INTRODUCTION

The control of anaerobic digestion (AD) start-up is an important research objective for many groups who are seeking to identify robust and workable implementations for the treatment of waste waters from a number of sources, (e.g. Moller and Jorgensen (1997); Perrier and Dochain (1993)). The non-linear and sometimes brittle nature of the AD process has been known for some time and is a limiting consideration in the design of reactors, (e.g. Denac et al. (1990); Monroy et al. (1996); Ryhiner et al. (1992)). Usually the research has been aimed at maintaining the stability of the system when faced with various perturbations such as fluctuations in loading rate, toxicity of the influent, temperature variations and so on. These often lead to increased levels of Volatile Fatty Acids (VFA's) which are a sign of an unstable reactor. The VFA's unfortunately are not easily measured 'on-line' and it is arguable that the levels of VFA's of the different species will be sufficient to determine the state of the AD process. BA however, is measurable on-line, with a good degree of accuracy and with a sensor which is reasonably robust in its operation, (Guwy et al. (1994)). The maintenance of a BA buffering margin is a means of controlling the pH drop caused by a build up of VFA's, (McCarty (1964); Rozzi et al. (1985)). It is possible to control the buffering by adding bicarbonate to the reactor contents. Such a control action could maintain conditions suitable for the microorganisms, but would not alter the metabolic imbalance. Alternatively, the rate of production of the VFA's can be adjusted by altering the loading on the reactor by changing (for example) the dilution rate, (Rozzi and Passino (1985)). In this work, the latter concept has been used during the start-up phase when in practice the load to the reactor could be varied.

When starting an AD process for the first time, the bacteria introduced as an inoculant are often sourced from a process operating on a significantly different waste. The bacterial populations may undergo significant acclimatisation, and the loading rate may need to be incremented from a low level and at a slow rate. Ensuring that the rate of increase is as high as possible to give rapid start-up is not a trivial matter (even under automatically controlled conditions). However, the use of automatic control will allow the process to increase loading continuously and at short sampling intervals (in the case of this work, hourly, unlike manual operation which is not usually so frequent). The rate of loading is incremented automatically only if the margin of stability (BA buffering) is increased beyond a desired level, (set point). In the case of poorly buffered effluents (e.g. many food processing and chemical industry wastewaters, including those with no nitrogenous compounds to generate ammonium bicarbonate), the buffering must come from BA dosing. It is possible to maintain the level of dosing constant while using the loading rate to control the state of the process, as was done in this work.

REACTOR OPERATION

A 30 litre Expanded Granular Sludge Bed (EGSB) reactor was used (Fig. 1), seeded with granules from a UASB reactor at Davidson's Paper Mill (Aberdeen, Scotland). (Details of both EGSB and UASB reactors can be found in Grasius et al. (1997)).The reactor was fed a constant 20 ml/min of a 3.36 g/L $NaHCO_3$ solution, (BA of 2000 mg/L $CaCO_3$) with a variable flow of a concentrate (x20) of a simple salts medium containing 1% glucose (W/V) (Cohen et al. (1980)) combined with an inversely proportional volume of tap water to give a constant inflow volume of 21.5 ml/min into the effluent recirculation tube. Upflow velocity (Vup 4.78 m/h) and retention time (24 hours) were constant. Peristaltic pumps and tubing (Watson and Marlow Ltd., Falmouth, UK) were used throughout.
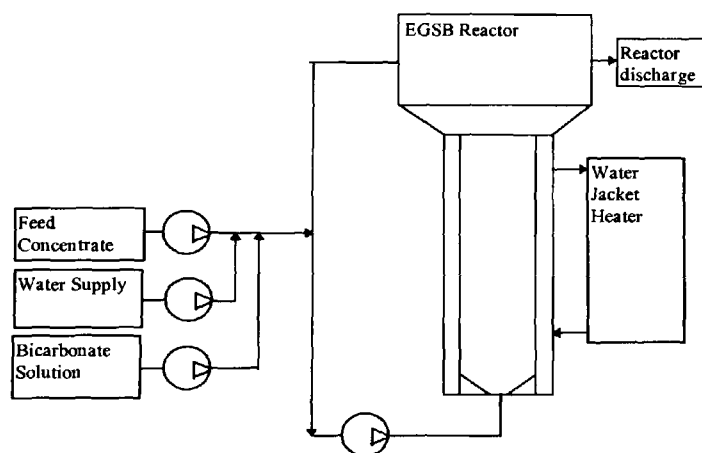

Figure 1. Schematic diagram of EGSB reactor

THE MONITORING AND CONTROL SYSTEM

The monitoring system was designed to log data from a number of on line sensors, using a personal computer equipped with a virtual instrument software program (LabVIEW™) and the control system was implemented on a separate personal computer for convenience. BA, the most important parameter with regard to the control system was measured on-line, as described by Guwy (1994). Other parameters (sampled at 1 minute intervals) monitored on line were pH, gas

phase hydrogen concentration, gas production rate, % carbon dioxide in the biogas and reactor temperature. The sampling rate of the control computer was independent of the monitoring computer and was every 1 hour. The monitoring computer had both A/D and D/A I/O facilities, (National Instruments, UK). The BA signal was provided to the control computer, which in turn provided the monitoring computer with the control effort calculated by the controller at each sample. The control effort was converted to appropriate voltage signals to run the water and concentrate feed pumps such that the volumetric flowrate remained constant, but the feed strength varied. The control computer used a similar I/O card and virtual instrument package to effect the I/O function. The control algorithm was programmed using a graphical, block oriented Computer Aided Control System Design (CACSD) package, (MatLAB/Simulink™). Communications between the software packages was achieved using the Direct Data Exchange (DDE) facilities provided by both. The BA set point could be adjusted within LabVIEW™ on the control computer. The setpoint and measured value (BA) were then provided to the control algorithm at each sampling interval as shown in Figure 2. The current control effort was passed back to LabVIEW™ for delivery to the monitoring computer.
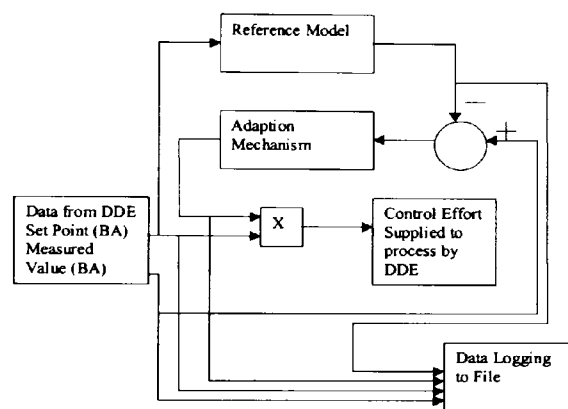

Figure 2. Block diagram of the Adaptive Control strategy

The adaption mechanism is the *normalized MIT* (Massachusetts Institute of Technology) *rule* as discussed by Åström and Wittenmark (1989). It should be noted that the stability of the system is not guaranteed.

EXPERIMENTAL PROCEDURE

The adaptive controller was initialised using a model. This allowed the duration of the initial 'learning' and settling of the control system to be reduced. The controller was then switched to on-line data and the controlled start-up of the process was begun. The set point was adjusted to the desired buffering, which was below the known level of BA, which was being supplied to the reactor at a constant rate. This ensured that feeding would commence. The experiment progressed unaided apart from regular checks and maintenance on instrumentation and the taking of samples for off-line assays (COD, VFA, pH and BA).

RESULTS

Figure 3 shows the data logged by the system. From zero to about 80 hours, the controller was initialised using a linear model of the BA response.
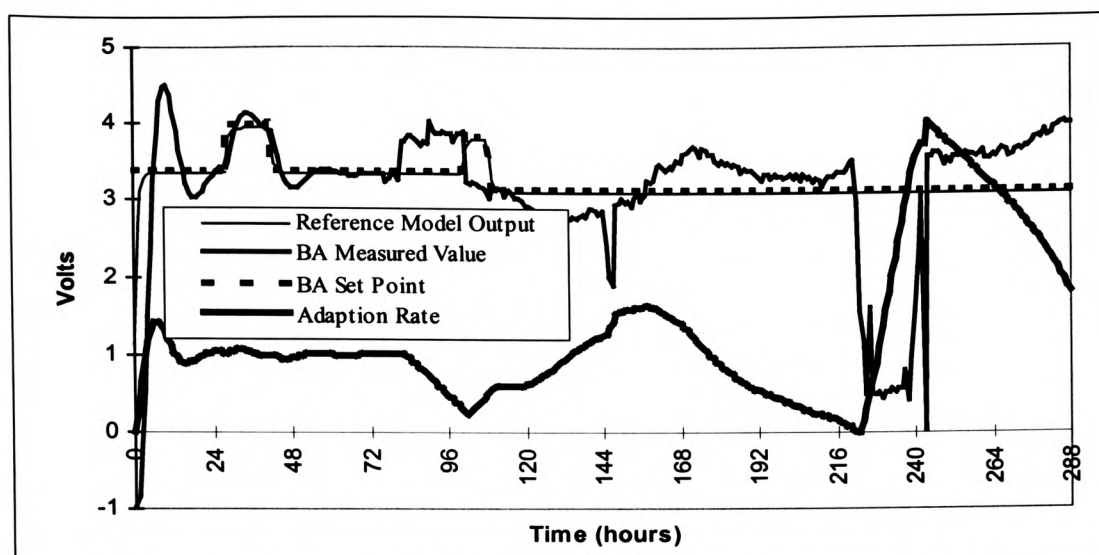
Figure 3. Plot showing the BA Set Point, Measured Value of BA, Reference Model Output and the Adaption Rate

The initialisation was not done in real time, but at a highly accelerated rate such that each hour passed in 2 seconds. Once initialised, the controller was switched onto real time and simultaneously started to control the real process. At about 100 hours, the BA set point was increased to begin feeding the process. After a further 10 hours (approximately), the set point was reduced once more and from this point the set point remained unchanged. The adaption rate acts as a simple gain, multiplying the set point, to give the control effort. As the adaption rate decreases, so the loading rate on the reactor is increased. All the signals in Figure 3 are displayed as voltages. At 150 hours, the measured value experienced a sudden drop due to a blockage in a pipe in the BA monitor. At approximately 225 hours, the BA measured value dropped dramatically and remained so for about 15 hours. This was due to the BA monitor running out of CO_2 which is required to saturate the samples.

DISCUSSIONS AND CONCLUSION

It is evident from Figure 3 that the adaptive controller "learns" the appropriate action during initialization, up to about 80 hours. The reference model is somewhat ambitious, particularly during startup when there is impaired metabolism from an under developed bacterial population. Never the less, when the controller begins to control the process (after 80 hours on the time axis), the control action is sensible and tends to minimize the error between set point and measured value, regardless of absolute values. Uncharacteristic failures in the monitoring of the BA signal had the consequence of shutting down the feeding, but at the same time changing the adaption rate in a fail safe direction. It is possible to conclude at this stage that control can be maintained during start-up. The experimentation and controller development are on-going and it is expected that further data and conclusions will be available by the time of publication.

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The controlled start-up of an anaerobic digester using a single control variable controller optimized using a non-specific model

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ABSTRACT

Start-up of an anaerobic digester can be considered to be a prolonged and particularly critical shock-loading regime. The first start-up (e.g. from commissioning with an inoculant) is accompanied by considerable uncertainty. A control strategy that could bring the digester to its nominal loading rate, under controlled and reasonably optimal conditions, from the point of initial commissioning, would be a useful device for minimizing risk and human effort. Such a strategy is presented here, based on an MRAC controller designed using a model parameterized on a different anaerobic digester. A 30 1 EGSB reactor was used to test the strategy and it was found that the loading rate increased with time as the inoculant developed toward a working anaerobic culture.

KEYWORDS

Anaerobic digestion; control; start-up; MRAC; bicarbonate alkalinity

INTRODUCTION

The use of automatic control of anaerobic digestion (AD) has enjoyed significant success, employing a number of control strategies (e.g. Steyer et al. (1999), Perrier and Dochain (1993)). Start-up of an AD reactor can be considered to be a prolonged and particularly critical shock-loading regime and the first start-up of such a process would be accompanied by considerable uncertainty. In general, the design of the control strategy requires a representative model of the reactor and its associated processes. If a model were available, it is likely not to have been parameterized for the specific digester. Considering the likely scenario at the point of commissioning, knowledge of the specific reactor will be limited to design specifications. In the case of restart, historical operating data would also be available. The accuracy of a model depends on the source of the data from which it is parameterized. These models may be traditional in their structure as in Andrews (1968), or fuzzy in a general sense (e.g. Marsili-Libelli and Muller (1996) or Premier et al. (1999)). We should expect that the AD process will be time varying and therefore batch tests would be unrepresentative, as the microbiological culture would not have developed to represent the full load working digester. On-line identification would take care of time variations, but usually depends on a number of on-line measurements, and consequently considerable instrumentation. It would be beneficial to the AD operator and commissioner to be able to control the start-up over its entire duration, using a minimum number of on-line sensors and relying as far as possible on the generation of model information from a system other than the one being commissioned. Start-up control of biological reactors has been considered by a number of authors such as Moller and Jorgensen (1997); Renard et al. (1991). As is the focus of this work, Rozzi et al. (1994) in particular used Bicarbonate Alkalinity (BA) as a control variable, but used a markedly different control strategy. Maintaining a BA buffering margin is a means of controlling the pH drop caused by a build up of Volatile Fatty Acids (VFAs), (McCarty (1964); Rozzi et al. (1985)).

The use of VFAs as a control variable has been shown to be practically achievable (as demonstrated by Renard *et al.* (1991), using propionate concentration), particularly since titration based, on-line measurement of VFAs has been shown to be feasible (Dehaas and Adam (1995)). BA gives similar information to the VFAs but is affected by the carbon dioxide equilibrium in the reactor, through carbonic acid. The activity or stress levels, (particularly of the methanogens) is therefore intrinsically part of the BA measurement, which has been shown to be readily measured on-line, (Guwy *et al.* (1994); Rozzi and Labellarte (1984); Tomei *et al.* (1994)).

METHODS

Reactor operation

The reactor considered in this work was of an Expanded Granular Sludge Blanket (EGSB) design, running at mesophilic temperature. The EGSB had a liquid volume of 30 l and was inoculated with granules from a UASB reactor at Davidson's Paper Mill (Aberdeen, Scotland). Both EGSB and UASB reactors are explained in Grasius *et al.* (1997)). The reactor was fed a constant 18 ml/min of a 3.73 g/L $NaHCO_3$ solution, (BA of 2222 mg/L $CaCO_3$) with a variable flow of a concentrate (x20) of a simple salts medium containing 1% glucose (w/v) (Cohen *et al.* (1980)) combined with an inversely proportional volume of tap water to give a constant inflow volume of 21.5 ml/min into the effluent recirculation tube. Before this start-up, the bacteria were kept at room temperature and not fed for 1 year. Up-flow velocity (Vup 4.78 m/h) and retention time (24 hours) were constant. Peristaltic pumps and tubing (Watson and Marlow Ltd., Falmouth, UK) were used throughout.

Modelling the process

The digester model used was that published by Marsili-Libelli and Beni (1996), which was essentially a two population model of the anaerobic digestion process which employed both Monod and Haldane kinetics. The model was parameterized using data from a fluidized bed reactor as described by Guwy *et al.* (1997). It includes the CO_2/pH/Bicarbonate alkalinity ionic equilibrium with other cation species also considered. The important fact is that the model was parameterized on data generated by a lab scale fluidized bed anaerobic digester and not the EGSB digester, which is the focus of this work.

Controller design and optimization

The controller was based on the Model Reference Adaptive Control (MRAC) scheme presented by Åström and Wittenmark (1989). The adaption mechanism was numerically optimized using the cost function: $J = 0.1(2 - \dot{X}_m) + |e_m| + 0.001|\dot{U}|$, with terms relating to the methanogenic bacteria (X_m), growth rate (maximizing) and minimizing the so called model error (e_m) and rate of change of control effort (U).

RESULTS AND DISCUSSION

Figure 1. presents the first 4.5 days of operation (approx.), while Figure 2. presents a similar time span in the fourth week. In the first week a 'technical hitch' caused the BA to increase suddenly by approximately 300 mgCaCO₃/l, when 'fixed' the BA dropped by a similar amount to the original value, as indicated in Figure 1. The two data series illustrate clearly that the controller increased the ORL in such a way as to continually develop the methanogenic population. It can be seen from Figure 2. that the recovery rate has increased compared to that of Figure 1., which implies that the methanogenic population has become more efficient at

2

converting the VFAs, thus raising the BA. The mean ORL increased from 3.3 kgCOD/m³/day in the first week to 6.53 kgCOD/m³/day in the fourth week.
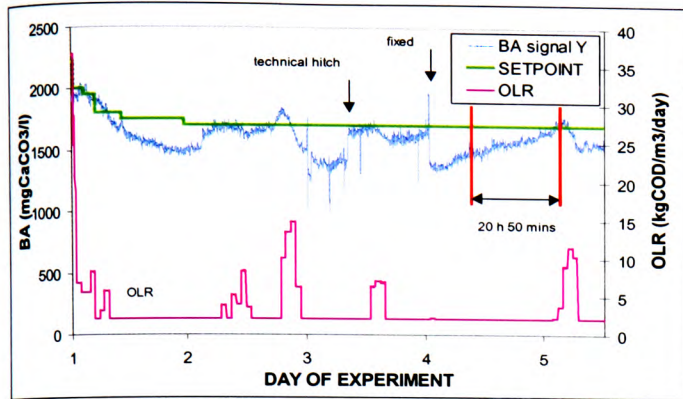

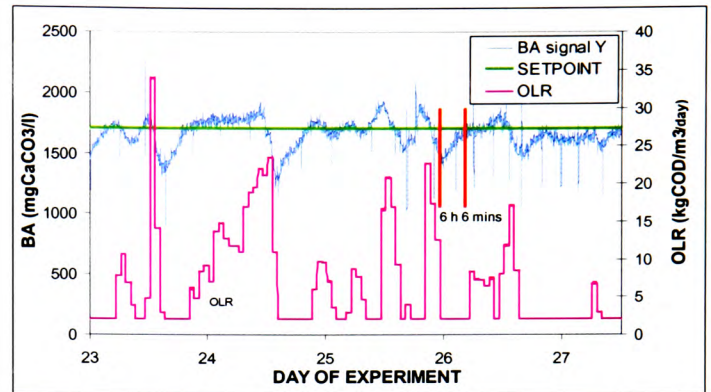**Figure 1. BA/SETPOINT/OLR Relationship during first week**

Figure 2. BA/SETPOINT/OLR Relationship during fourth week

CONCLUSIONS

It can be concluded that the control strategy maintained a BA buffering level over the first four weeks of operation considered here, during which time the OLR increased and the methanogenic population showed signs of strengthening.

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