Design of an integrated monitoring and optimal control system for supervisory operation of anaerobic digesters

A thesis submitted by

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Preface

This thesis describes research that was undertaken as part of an Engineering Doctorate in Biopharmaceutical Process Development which was carried out in collaboration with Perceptive Engineering Limited and sponsored by the Engineering and Physical Sciences Research Council (EPSRC).

The thesis initially aimed to take the format of a 'thesis by portfolio' which details a number of projects that are linked by the theme of advanced process control used/or with the potential to be used on industrial bioprocesses. The first project aimed to improve anaerobic digestion processes with an advanced control such as model predictive control. Due to the complex nature of the project, delays with industrial partners and early termination of the project by the industrial sponsor Perceptive Engineering Limited led to this project spanning the four year duration of the Engineering Doctorate programme.

Being an industrially focussed Engineering Doctorate, the projects reflect the requirements of industry, and various case studies were conducted as the aims of the project changed over the period of study to meet new research challenges within the company.

Publication list

The following articles by the thesis author, arising from the work herein, have been published.

Journal papers

1. G. Oppong, G. A. Montague, M. O'Brien, M. McEwan and E. B. Martin. Towards advanced control for anaerobic digesters: volatile solids inferential sensor, Water Practice & Technology Vol 8 No 1, 7-17 © IWA Publishing 2013.

Conference papers

1. Oppong, G., O'Brien, M., McEwan, M., Martin, E.B. and Montague, G.A. (2012). "Advanced Control for Anaerobic Digestion Processes: Volatile Solids Soft Sensor Development." 22nd European Symposium on Computer Aided Process Engineering, PART B, edited by Ian David Lockhart Bogle and Michael Fairweather. © 2012 Elsevier B.V. All rights reserved. Pages 967-971.

2. Oppong, Grace; McEwan, Matthew; Montague, Gary; Martin, Elaine

   Towards Model Predictive Control on Anaerobic Digestion Process. Dynamics and Control of Process Systems, Volume # 10 | Part# 1, 10th IFAC International Symposium on Dynamics and Control of Process Systems (2013), Conference Editor: Henson, Michael A., Pannocchia, Gabriele, Gudi, Ravindra, Patwardhan, Sachin C.

3. G. Oppong, M. McEwan, E. B. Martin, G. A. Montague

   'Towards Advanced Control for Anaerobic Digesters: Sludge Inventory Optimisation Simulation Study', AD13: 13th World Congress on Anaerobic Digestion – Recovering (bio) Resources for the World. Santiago de Compostela, Spain, 2013.

Abstract

Anaerobic digestion with biogas production has both economic and environmental benefits. 25 % of all bioenergy in the future could potentially be sourced from biogas (Holm-Nielsen *et al.*, 2009). Although anaerobic digesters have seen wide applicability, they typically perform below their optimum as a consequence of the complexity of the underlying process. This work involves the development of a generic advanced process control system for the optimisation of the performance of anaerobic digesters. There is a requirement for a configurable monitoring and optimisation system with associated sensors to optimise the production of biogas, combined with a degree of flexibility for quality and content of the digestate.

Several analyses are conducted to establish the baseline performance of the four benchmarked sites. Significant findings are revealed which include lack of superior technology between the four varying processes, differing performance due to optimisation activities through increased monitoring and whole plant optimisation such as energy usage and production. Potential improvements are presented including increased monitoring and a reduction in the variability of key parameters such as thicker percentage dry solids (% DS), steady feed rate, and temperature.

The lack of instrumentation in anaerobic digestion processes is a key bottleneck as sensors and analysers are necessary to reduce the uncertainty related to the initial conditions, kinetics and the input concentrations of the process. Without knowledge of the process conditions, the process is inevitably difficult to control. Financial gains that can be achieved through increased instrumentation were calculated to justify the business case for the need for process improvement. An instrumentation review is presented with the minimum and ideal instrumentation requirements for the AD process.

Improved monitoring is achieved through soft sensor development for volatile solids (VS), an important variable that is currently only monitored offline. The inferential sensor is developed using data from an industrial process and compared with the results from a simulation study where feed flow and biogas production rate are used for modelling VS.

This theme of improving monitoring with inferential sensors is continued with development of soft sensors with microbial data and data from different reactor designs.

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Nomenclature

AD	Anaerobic Digestion
AAD	Advanced Anaerobic Digestion
ADM1	Anaerobic Digestion Model number 1
APC	Advanced Process Control
ASM1	Activated Sludge Model number 1
BAFF	Biological Aerated Flooded Filter
BOD	Biochemical Oxygen Demand
BSM1 or 2	Benchmark Simulation Model number.1 or 2
CHP	Combined Heat and Power
COD	Chemical Oxygen Demand
C_P , C_PK	Process Capability Indices
CV	Control Variable
DoE	Design of Experiments
DS	Dry Solids
EEH	Enhanced Enzymic Hydrolysis
FT-IR	Fourier Transform Infrared Spectroscopy
GBT	Gravity Belt Thickener
GC	Gas Chromatography
GCMS	Gas Chromatography Mass Spectrometry
HACCP	Hazard Analysis and Critical Control Points

HPLC	High Performance Liquid Chromatography
HRT	Hydraulic Retention Time
IR	Infrared
KPI	Key Performance Indicator
LI-COR	
LR	Long range
LRQP	Long Range Quadratic Programming
LSL	Lower Specification Limit
MAD	Mesophilic Anaerobic Digestion
MBT	Methanobacteriales
MCC	Methanococcales
MIMO	Multiple Input Multiple Output
MMB	Methanomicrobiales
MPC	Model Predictive Control
MSC	Methanosarcinaceae
MST	Methanosaetaceae
MV	Manipulated Variable
NIRS	Near-InfraRed Spectroscopy
NWL	Northumbrian Water Ltd
OLR	Organic Loading Rate
Pc	Process Capability
PC	Principal Component

PCA	Principal Component Analysis
PEL	Perceptive Engineering Limited
PI, PID	Proportional Integral Derivative
PLC	Programmable Logic Controller
PLS	Partial Least Squares
$\boldsymbol{P_P}$, $\boldsymbol{P_P K}$	Process Performance Indices
QP	Quadratic Programming
ROC	Renewable Obligation Certificate
SCADA	Supervisory Control And Data Acquisition
SRT	Sludge Retention Time
SSM	Safe Sludge Matrix
SWOT	Strengths, Weaknesses, Opportunities, and Threats
TA	Total Alkalinity
THP	Thermal Hydrolysis Process
TSS	Total Soluble Solids
URS	User Requirement Specification
USL	Upper Specification Limit
UU	United Utilities
VFA	Volatile Fatty Acid
VS	Volatile Solids
VSS	Volatile Soluble solids
WwTP	Wastewater Treatment Plant

WwTW Wastewater Treatment Works

YW Yorkshire Water

Parameters and Symbols

AcH Acetic acid

BuH Butyric acid

CH_4 Methane

CO Carbon Monoxide

CO_2 Carbon dioxide

EtOH Ethanol

H, H_2 Hydrogen

H_2O Water

H_2S Sulphuric acid

K_2O Potassium oxide

k Rate constant

K Saturation constant

K_1 Saturation coefficient

K_s Half saturation constant

kLa Volumetric mass-transfer coefficient

N Nitrogen

NH_3 Ammonia

P_2O_5 phosphorus anhydride

ProH	Propionic acid
S	Substrate concentration
$\boldsymbol{SB}$	Growth limiting constant
$\boldsymbol{SO_4}$	Sulphate
tDS	Tonnes per Dry Solids
$\boldsymbol{\mu_{max}}$	Maximum specific growth rate

1 Introduction

1.1 Thesis motivation

There is a growing awareness that waste is an underutilised resource, with the emphasis shifting to process based solutions for recycling and recovery from disposal based solutions such as landfill. Combined with this, there is a new sense of direction and focus on utilising organic waste for the production of energy. One of the leading technologies to support this drive is Anaerobic Digestion (AD). The first anaerobic digester was built in 1859 in India (Marsh, 2008) and the technology has evolved and developed since this time, and resulted in making AD with biogas production gain both economic and environmental benefits. 25 % of all future bioenergy production can potentially be sourced from biogas and thus AD has a significant role to play in terms of contributing to the EU target of increasing the level of energy derived from renewable energy sources to a minimum of 20 % by 2020 (Holm-Nielsen *et al.*, 2009). However, limitation on the AD process such as partial decomposition of the organic fraction and slow reaction rates hinder the economic and environmental benefits. Due to the dynamic nature, the non-linearity and lack of knowledge of the AD process, there remains significant opportunities for improvements in operational efficiency (Appels *et al.*, 2008).

A number of reviews have concluded that to achieve optimal performance for AD, advanced control systems are required (Pind *et al.*, 2003; Jean-Philippe Steyer *et al.*, 2006; Ward *et al.*, 2008; Mendez-Acosta *et al.*, 2010). Advanced control strategies can offer an opportunity for the optimisation of processes such as anaerobic digestion that operate under strict regulatory constraints. The complex nature of the process dynamics provides sufficient motivation for the use of a model based control strategy. Through the use of mathematical simulation models, the application of model based control for the AD process can be investigated.

In 2009 a consortium was formed between Perceptive Engineering Ltd (PEL), Yorkshire Water (YW), Northumbrian Water (NWL) and United Utilities (UU). The objective was to optimise the AD processes of YW, NWL and UU through the implementation of multivariate advanced control. The final deliverable was a generic advanced control system that could be applied to a single phase or traditional Mesophilic Anaerobic Digestion (MAD) system and or a multiphase Advanced Anaerobic Digestion system (AAD). More specifically this would consist of a configurable, monitoring and optimisation unit coupled to instrumentation to optimise digestate quality and increase biogas yield quality. The end product named the ‘Perceptive AD-master’ is designed to openly communicate with existing automation instrumentation to enable good communication between instruments and control systems throughout the site and therefore provide an opportunity for plant wide optimisation. The AD-master would be integrated into existing PEL products and would aim to address the requirements of the AD processes as articulated by the consortium.

The three water companies in the consortium cover Yorkshire, the North-West and the North-East of England and are currently operating 50 digester plants. They provide the industrial AD processes and the technical expertise in terms of the operation of the ADs. PEL bring experience in the successful application of control solutions to various industrial processes, especially on bioprocesses and wastewater treatment processes (O'Brien *et al.*, 2011).

Being an industrially focussed Engineering Doctorate based within a consortium, the projects reflect the research requirements of industry, and changed over the period of study to meet new research challenges within the consortium. The User Requirement Specifications (URS) of the three water companies are very different, as the characteristic of the AD process differs within technologies, size, methods, site limitations and instrumentation. The overall outcomes of the project need to align with the individual aims of the water companies, and issues to be considered include sustainability, energy usage reduction and increased renewable energy production.

1.2 Aims and objectives

The ultimate goal of this project was to develop a multivariable control system for optimising the performance of anaerobic digester systems. The primary deliverable was a configurable monitoring and optimisation system that comprises appropriate sensors to enable the optimisation of biogas production. The system takes into account the requirement to accommodate a level of flexibility relating to the quality and content of the biogas and digestate. The approach adopted was a data based approach using multivariate statistical analysis for the development of a monitoring system and empirical time series modelling to capture the dynamic behaviour of the process, in preparation for the development of a Model Predictive Controller (MPC). Core challenges included the identification of appropriate sensors that are industrially robust, the modelling of an inherently non-linear biological process and the development of a robust anaerobic digestion controller with an optimiser that has widespread applicability for various AD technologies.

The first step was to assess whether there was a need for the application of advanced control on industrial AD processes and thus the first question that was addressed was "*Can an advanced control system improve the efficiency, stability and robustness of an AD process?*". This was undertaken through a literature survey, an analysis of current plant operations through process benchmarking of three industrial AD operations, an instrumentation review and a vendor review and questionnaire. The second question was "*What is the minimum instrumentation requirement to achieve the aims identified in the feasibility assessment?*" The instrumentation review and inventory simulation formed the basis of the approach in addressing this question. The final question was "*What is the level of improvement to be gained from advanced control?*" The control and monitoring approaches developed were tested on an inventory simulation system to calculate the level of improvement achievable from traditional control designs through to advanced control. The results generated from the inventory simulation were compared with simulation results using the Anaerobic Digestion Model No. 1 (ADM1) (Batstone *et al.*, 2002a) and this consequently led to the identification of further instrumentation requirements. A volatile solids (VS) inferential sensor model was developed to improve the level of digestate quality attribute instrumentation and advanced control capability.

A series of case studies were conducted using laboratory, pilot and industrial data to assess the effects of different process parameters on controlling and optimising the AD process. These aforementioned questions are introduced throughout the thesis and provide the knowledge and understanding to addresses the overarching aims of the project.

1.3 Thesis contribution

The work conducted in this thesis focuses on monitoring, modelling, control and optimisation of the AD process. Major research contributions include the benchmark analysis undertaken on four industrial AD processes in wastewater treatment plants in the United Kingdom and the development of an AD inventory simulation tool; that included a platform for testing and comparing various conditions on the system, thereby enabling the testing of control strategies and the understanding of optimisation studies. Furthermore a VS inferential sensor model was developed utilising data from an industrial process and simulated data that yielded a robust model for accurately predicting VS from easy to measure process parameters on the AD process. Finally two multivariate techniques of Principal Component Analysis (PCA) and Partial Least Squares (PLS) were applied to obtain additional process knowledge and also for the development of process models from laboratory data containing biological data including the population of methanogenic bacteria.

1.4 Thesis structure

The project was divided into four key phases (Figure 1.1): feasibility; design; implementation; and evaluation. Phase I; the feasibility study spanned years one and two of the Engineering Doctorate program, and included a literature review and the benchmark study of the four industrial sites that details the current state of instrumentation and control methodologies. This phase also contained an instrumentation review and vendor review and questionnaire. These tasks in phase I were necessary to establish the business case for phase II of the project.

Phase II; prototype development took place in year three and the URS was identified for the different members of the consortium which initiated the functional design specification. A complete prototype satisfying the URS could not be developed without improving the level of instrumentation on the process. This led to the development of the inventory simulation model which continued to year four where phase III activity of soft sensor development and case studies were conducted to increase the knowledge of the AD system as well as improve the level of instrumentation through soft sensors. The remainder of phase III activities; installation and testing prototypes and Phase IV activities; evaluation and market assessment, are not included in this thesis. Due to delays and difficulties within the project; the implementation and evaluation activities in phase III and IV were not conducted as part of this thesis.

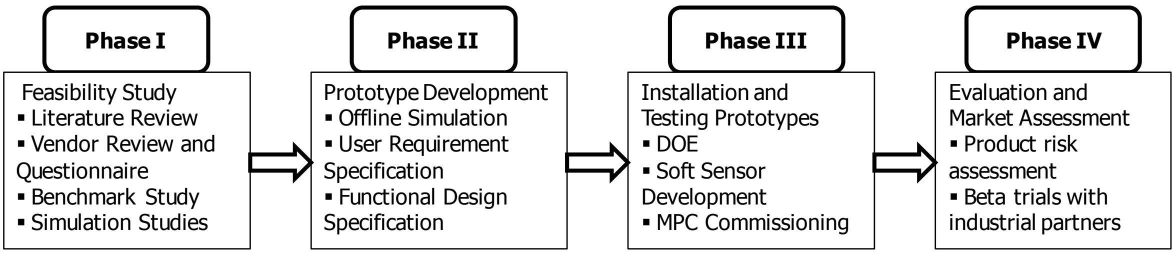


Figure 1.1 Project phases

Chapter 2 summarises the first part of phase I activities, the literature survey and instrumentation review in Chapter 3. The second part of phase I activities; the benchmark study are discussed in Chapter 5.

The various methodologies and approaches utilised in the thesis to fulfil the aims of the project are summarised in Chapter 4. Multivariate statistical analysis and inferential sensor development techniques are discussed in detail as well as advanced control methods with emphasis on model predictive control (MPC).

Chapter 6 discusses the inventory simulation which provided the platform for activities relating to the use of the control schemes and various scenario testing activities to be conducted on the AD process. The hybrid simulation model was developed using both established relationships for the AD system as well as process data from the benchmark study.

The inferential sensor development for the VS, which forms part of the phase III activities is discussed in Chapter 7, with a comparison of the inferential sensor developed with process data and with simulation data from the ADM1.

Finally Chapter 8 provides conclusions, summary and future work for the thesis.

2 Literature survey

2.1 Introduction

Traditionally the purpose of AD in Wastewater Treatment Plants (WwTPs) was for sludge stabilisation and odour reduction. Biogas production, solids destruction and pathogen reduction are now the key focus areas of research. This is particularly the case as the AD process is becoming more important as the world changes from disposal based solutions for biodegradable organic wastes such as wastewater sludge and food waste to production of renewable energy and high quality biosolids from these wastes. This drive has led to increased focus on AD and the technology is attracting industrial and academic interests worldwide.

There is currently active research being undertaken in this area by academics on every topic area of the process, such as co-digestion, microbial population dynamics, biorefinery, energy recovery, modelling and control and biodegradation. Leading themes of research can be categorised as modelling (with respect to the microbial community (Supaphol *et al.*, 2011; Guo *et al.*, 2015; Li *et al.*, 2015); co-digestion (Astals *et al.*, 2014; Jensen *et al.*, 2014; Astals *et al.*, 2015); pre-treatment methods (Ruffino *et al.*, 2014; Karray *et al.*, 2015); instrumentation (Ward *et al.*, 2011; Cadena-Pereda *et al.*, 2012); and temperature effects on AD systems (Bowen *et al.*, 2014; Vanwonterghem *et al.*, 2015).

These areas of research are linked to various AD characterisation or classification groups, however for the purpose of this literature survey, these will be limited to the classification groups of temperature, technology and the digestion process. Section 2.5 discusses AD classification by temperature and Section 2.4 discusses the technologies available. Modelling forms a central theme to this thesis and as such Section 2.3 discuses AD modelling approaches. The digestion process is at the core of all these classification groups and details of the process are summarised in Section 2.2.

2.2 The digestion process

Biochemical and physicochemical are the two general conversion processes for the AD process. The biochemical conversion process involves biomass growth and decay where bacterial cells excrete enzymes to disintegrate available organic materials. The physiochemical pathway involves association or dissociation and gas-liquid transfers. The main products of anaerobic digestion processes are biogas (comprised mainly of methane (CH_4) and carbon dioxide (CO_2)) for producing energy, digestate that is used as liquid fertiliser and fibre for compost.

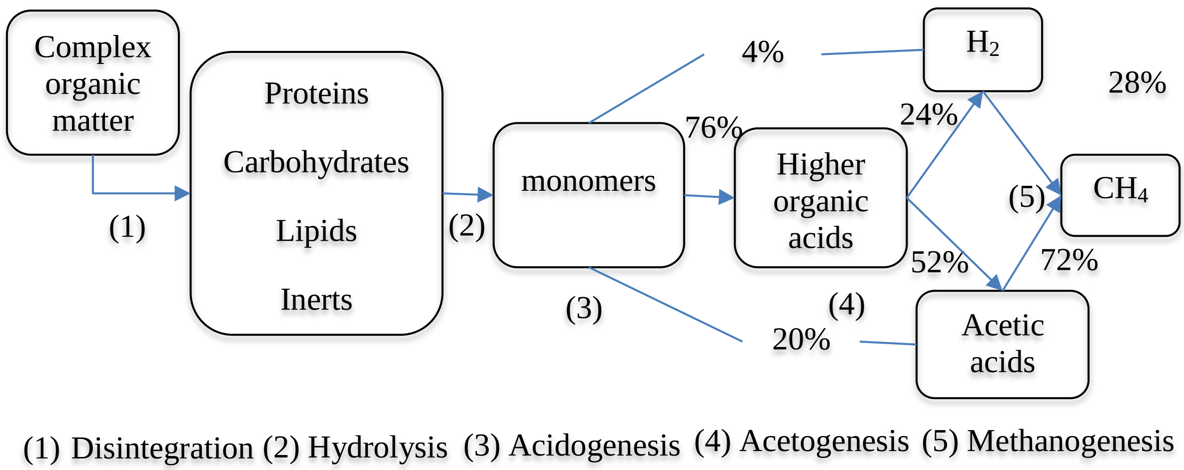


Figure 2.1The degradation pathways (Batstone *et al.*, 2002b)

Hydrolysis, acidogenesis, acetogenesis and methanogenesis are the four main steps in the process as depicted in Figure 2.1. The process of breaking down the organic polymers such as proteins, fats and carbohydrates into smaller monomers such as monosaccharides, long chain fatty acids and amino acids is characterised as hydrolysis. The hydrolysis process is achieved by the availability of extracellular enzymes produced by micro-organisms. In most models, this is the second step with disintegration being the first step. Disintegration may be an additional step in modelling to represent composite organic materials, which is important for waste activated and primary sludge digestion. In cases such as this, disintegration can represent the lysis of whole cells and separation of composites (Batstone *et al.*, 2002a). Acidogenesis ferments the sugars, amino acids and fatty acids produced during hydrolysis into VFA's, with the acetogenesis step consuming VFA's to produce CO_2, H_2 and CH_3COOH (acetic acid) molecules, which are then used by methanogenic organisms to produce CO_2 and CH_4 (Cioabla *et al.*, 2012).

The degradation pathway and study of the micro-organisms involved in the AD processes are major areas of research. The AD process consists of complex microbiology comprising over 140 microorganisms (Batstone *et al.*, 2002a), and these microorganisms (bacteria) convert organic materials into biogas. The growth and balance of the different types of these micro-organisms are essential to the biogas production and can be inhibited by process parameters such as pH, alkalinity, concentration of free ammonia and volatile fatty acids (VFA) and light and heavy metals.

The AD system requires the acidogenesis and the methanogenesis stages to be balanced to avoid inhibition of methanogenic bacteria. A key task in the control of the anaerobic digestion (AD) process (automatic or otherwise), is the avoidance of inhibitory conditions. Inhibition is any situation which prevents a specific microbial growth and reproduction of the biomass that stabilises the sludge and forms biomethane. This is usually caused by the presence of inhibitory chemicals (high acids) or biologicals (hydrogen scavengers).

Inhibitors can be present in the AD process in the form of end products of feedstocks of inorganic, organic substances or microbial reactions introduced into the anaerobic digester. Anaerobic instability is the cause of the availability of various inhibitory substances. Examples of inhibitory substances include CO_2, ammonia and nitrogenous matter such as proteins and urea. The degradation of nitrogenous organic matter leads to ammonia production within the digester (Chen *et al.*, 2008):

$$\mathrm{C_aH_bO_cN_d} + \frac{4a - b - 2c + 3d}{4}\mathrm{H_2O} \rightarrow \frac{4a + b - 2c - 3d}{8}\mathrm{CH_4} + \frac{4a - b + 2c + 3d}{8}\mathrm{CO_2} + d\mathrm{NH_3}$$

Equation 2.1

Inhibition has been shown to be difficult to quantify, due to the complex nature of the digestion process mechanisms. These mechanism can be significantly affected by antagonism (the suppression of some species of micro-organisms by others), acclimation (adaptation to a new environment or a change to the old environment) and or synergisms (micro-organisms acting together for mutual benefit e.g. syntrophy) (Chen *et al.*, 2008). An example of an antagonistic and or synergistic effects in ADs is the impact of dual cations, where research has shown the effect of antagonism on combining potassium and calcium increased significantly when compared to effect of potassium alone (Kugelman and McCarty, 1965) .

The presence of inhibitory substances may cause shifts in the microbial population or bacterial growth, with shifts in the microbial population indicated by a decrease in the CH_4 gas production rate, or by an accumulation of organic acids. Therefore by measuring the gas production rate, the concentration of organic acids (VFAs), and or the presence of chemicals known to cause inhibition, the AD process can be stabilised and controlled.

The AD process is further exacerbated by complexities on a macroscopic level; the three-phase (solid-liquid-gas) AD process involves both sequential and parallel reaction pathways. The complexity and uncertainty in the dynamics of the micro-organisms involved in the process make the process difficult to model. When considering a single organism system, it is the case that no single kinetic model can describe the complexities of that single organism. It is therefore a major task for scientists and engineers to attempt to model multi-organism systems (Heinzle *et al.*, 1993).

2.3 Modelling

The need for continuous improvement on existing AD process operations and development of new processes with time, cost constraints and increase pressure on high product quality and availability of sustainable products, have driven the technology towards the use of model based process applications. Model building approaches still require simple methods with ease of application, 'the simpler the better' (Foss *et al.*, 1998).

Mathematical models can serve as useful tools to deepen the understanding of complex systems, and to facilitate operation and design of the process. If the behaviour of a system can be predicted, the production of outputs can be optimised and process failure can be prevented. However there is limited application of modelling approaches to AD processes. This is due to the complexity of the process which requires extensive input data, increased knowledge about the process dynamics and uncertainties within the model. Therefore the AD process has traditionally been considered as a black box system (Lidholm and Ossiansson, 2008).

There are various modelling approaches with differing ranges of accuracy and complexity dependent on the purpose of the model. For control purposes a possible complex, non-linear model with focus on the biochemical reactions with adequate monitoring can aid in developing an understanding of the process. The control and optimisation of AD systems requires an accurate dynamic model of the process. However modelling of AD systems often results in high order nonlinear models with several unknown parameters. This makes it difficult to control the process and therefore various system identification techniques need to be applied to the AD process.

Modelling AD processes is an active research area with various review articles, journals, thesis and book publications (Andrews and Graef, 1971; Lyberatos and Skiadas, 1999; Dochain and Vanrolleghem, 2001; Batstone *et al.*, 2002b; Zaher, 2005; Saravanan and Sreekrishnan, 2006; Donoso-Bravo *et al.*, 2011) which have been conducted studies into modelling the anaerobic digestion process and thus only a summary is given here.

Although extensive research into the microbiology of the process has been conducted, there is still a lot of uncertainty surrounding this area. For example, there are knowledge gaps such as the spatial distribution of individual organisms in flocs, granules and biofilms (Jean-Philippe Steyer *et al.*, 2006). This has a large effect on microbiological reaction rates, and for this reason 'first principles' modelling is not currently suitable for robust control. Given the importance of achieving a stable operating process, robustness is the key objective of any control system, with performance being important, but secondary for the improvement of ADs.

Andrews and his co-workers in 1974 worked on developing dynamic models for the purpose of process control for AD (Andrews, 1974; Graef and Andrews, 1974a). To date their models form the basis of most AD system models, and there has been little development of newer models. Most attempts to identify the biological treatment systems such as AD for the purpose of control, focus on the macroscopic fringes of the process dynamics without much impact on the microscopic level (Beck, 1986).

In depth research into conversion mechanisms including cell decay, lysis and hydrolysis indicated that hydrolysis of the dead particulate biomass is the rate limiting step and this kinetically controls the overall process (Pavlostathis and Gossett, 1986), whilst more recently methanogenesis has been shown to be the rate limiting step (Bowen *et al.*, 2014). However, it is evident that the rate limiting step varies for different conditions (Appels *et al.*, 2008). There are numerous models presented in the literature, from simple Monod kinetics (Siegrist *et al.*, 2002); first order models (Smith *et al.*, 1988); Andrews models (Graef and Andrews, 1974b); mass balance models (Bernard and Bastin, 2005b); through to more advanced models (Polit *et al.*, 2002; Ramirez *et al.*, 2009). However most of these models fail to accurately describe the digester dynamics, as they do not assess both random and deterministic factors affecting the microbial communities.

Various modelling complexities exist for AD system modelling; consideration of only the acidogenesis and methanogenesis steps is the lowest level of modelling complexity. Examples of these are given in Section 2.3.1. The highest level of complexity is considering the disintegration and hydrolysis steps, the anaerobic digestion model no.1 (ADM1) model in Section 2.3.2 details this and middle model complexities include the Siegrist model in Section 2.3.3.

2.3.1 Rate limiting step models

The rate limiting step is the slowest step which limits the overall process. Due to the multistep characteristic of the process, initial mathematical modelling approaches focused on the rate limiting step as this controlled the overall rate of the process. Volatile fatty acids (VFA's) were considered as the key parameter (Donoso-Bravo *et al.*, 2011) for modelling the rate limiting step. However as the rate limiting step changes under different operating conditions, this resulted in different models as the rate limiting step varies for different wastewater characteristics, loading rates, temperature and at different stages of the process. Examples of the various modelling approaches focusing on different rate limiting steps are summarised in Table 2.1. The table gives examples of models that assume substrate inhibited Monod kinetics of the methanogens (Graef and Andrews, 1974a); the Monod equation is commonly expressed as:

$$-\frac{dS}{dt} = \frac{k.X.S}{(K+S)} \qquad \text{Equation 2.2}$$

where the rate of uptake of substrate is given by dS/dt (mg $L.t^{-1}$), k is the rate constant (t^{-1}), S is the concentration of the substrate ($mg\ L^{-1}$), X is the concentration of the microorganism ($mg\ L^{-1}$) and the saturation constant is given by K.

Table 2.1 also show models that consider total VFA concentration as a key parameter (Hill, 1982) and Models using H_2 as the control parameter (Pullammanapallil *et al.*, 1991).

Table 2.1 Examples of Rate limiting step modelling

Model	**Bacteria group**	**Rate limiting step (Process)**	**Kinetic Function**
Graef and Andrews (Graef and Andrews, 1974b)	Acetoclastic methanogens	Methanogenesis	Andrews
Hill (Hill, 1982)	Acidogenic bacteria	Acidogenesis	Monod based
Smith (Smith *et al.*, 1988)	Rapidly degradable biomass	Hydrolysis	First order
Pullammanappallil (Pullammanapallil *et al.*, 1991)	H_2 utilising CH_4 bacteria	Methanogenesis	Monod (pH)

2.3.2 The anaerobic digestion model no.1 (ADM1)

There are several AD models developed in recent years, however these mainly consider a specific AD process or for a specific substrate; resulting in models that cannot be compared or transferred to solve other problems. The ADM1 is the commonly used AD model and consists of a complex multistep anaerobic process transformation model. This first generalised AD model was created by the International Water Association (IWA) task group for mathematical modelling of AD processes in 2002 (Batstone *et al.*). The model provides a common basis for AD model development and validation studies for ensuring more comparable results, and has been widely applied for predictions of real AD system behaviour with a sufficient level of accuracy to be useful in process development, optimisation, and control (Derbal *et al.*, 2009; Mairet *et al.*, 2011). It is a standard benchmark for developing operational strategies and evaluating process controllers for AD.

Although models have evolved to consider more process detail including more detailed kinetics such as the ADM1 (Batstone *et al.*, 2002b) model, they still fail to fully represent the complex nature of the AD system. Thus the best-fit of a model from a set of experimental data requires the optimum solution of the model parameter vector.

The first step to modelling is characterisation and fractionation of the influent as per the model input variables. This is followed by model calibration by estimating the most sensitive parameters of the model. Characterising the influent; this can be carried out in ADM1 by various means including physical-chemical analyses, physical-chemical plus online calibration, elemental analyses and input from another model. The ADM1 model includes:

- kinetics for disintegration of homogenous particles to carbohydrates, proteins and lipids, followed by hydrolysis of these particles to sugars, amino acids and fatty acids;
- Inhibition functions of metabolic activity by ammonia, pH, acetate and H_2, and nitrogen limitation;
- Description of gas-liquid transfer and ion association and dissociation;
- 32 dynamic concentration state variables, 26 state variables and 8 implicit algebraic equations;
- Exclusion of lactate formation, sulphate reduction, nitrate reduction, long chain fatty acid inhibition, competitive uptake of H_2 and CO_2 and chemical and biological precipitation.

As the model however does not include reduction of nitrate, precipitation, sulphur, intermediate components of lactic acid and ethanol; there are also several modifications and extensions of the ADM1 model which makes the model easier to implement for use in process control. Such modifications models include the ADM1xp which incorporates nitrogen (Wett *et al.*, 2006), this model can be modified further depending on the characteristics of the wastewater. Other common extensions of ADM1 include sulphate reduction (Batstone *et al.*, 2006) required for systems with high (greater than 0.002 mol SO_4 L^{-1} or 192 mg SO_4 L^{-1}) sulphate levels in the effluent (Hinken *et al.*, 2013). Implementation of winery wastewater in ADM1 has been implemented by various authors (Batstone *et al.*, 2004; García-Diéguez *et al.*, 2013), with ethanol as the main Chemical Oxygen Demand (COD) of the winery wastewater and microbial diversity modelling (Ramirez *et al.*, 2009).

2.3.3 The Siegrist model

In 2002 Siegrist (Siegrist *et al.*, 2002) published a slightly more simplified modelling approach in comparison to ADM1. The exclusion of valerate and butyrate as state variables was a key difference in this new model, with the hydrolysis rate modelled as a single step process with first order kinetics with respect to the concentration of particulate matter. The Siegrist model parameters are based on experiments, whereas the ADM1 uses review consensus. The Siegrist model was calibrated with lab scale experiments and validated with full-scale experiments. However the simplification in Siegrist model came with ignoring several processes and including several assumptions. The complex nature of the AD process means it cannot be modelled without several simplifications, assumptions and disregarding various processes. Examples of these include (1) the reactor is assumed to be completely mixed; (2) the liquid phase is considered to be dilute and the volume is assumed to be constant; (3) the sludge retention time (SRT) is equal to the hydraulic retention time (HRT); (4) fixed stoichiometry in the microbial processes and (5) kla (volumetric mass-transfer coefficient) value is only dependent on temperature (Lidholm and Ossiansson, 2008). These various assumptions result in limitations in the model.

2.3.4 TELEMAC Anaerobic Model no. 2 (AM2)

The TELEMAC (TELEMonitoring and Advanced teleControl of high yield wastewater treatment plants) Anaerobic Model no. 2 (AM2) focuses on Acidogenic and Methanogenic reactions and models the methanogenesis of volatile fatty acids (Bernard *et al.*, 2001). AM2 accounts for the likely inhibitory effects of accumulated VFAs which would result in reduced pH and accounts for this inhibition using Haldane kinetics:

$$\frac{dS}{dt} = \frac{\mu_{max}}{Y} \frac{SB}{K_S + S + S\left({S}/{K_1}\right)^n}$$

Equation 2.3 (Lokshina *et al.*, 2001)

Where μ_{max} is the maximum specific growth rate (h^{-1}); SB is growth limiting substance concentrations ($mg\ L^{-1}$); n is the Haldane index; Y is the growth yield ($mg\ L^{-1}$); K_S is the half saturation coefficient and K_1 is the inhibition constant. The AM2 is a mass balance cascade structure model based on 70 day dynamical experiments covering a wide operating range. The purpose of the model is to aid with the monitoring and control of AD systems. This is achieved by ensuring the experiments cover a range of experimental conditions and the validation step is performed with a wide set of transient conditions.

2.3.5 Further model extensions

Table 2.2 Model Reduction Approaches

Model reduction approach	**Method**	**Reduction**
Bernard and Basin (Bernard and Bastin, 2005b; Bernard and Bastin, 2005a)	AMH1	Uses principal component analysis (PCA) for reduction in the biochemical complexity
Hassam (Hassam *et al.*, 2012)	Homotopy	eigenvalue-state association to neglect the slow dynamic aspect of the model
Gracia-Dieguez (García-Diéguez *et al.*, 2013)	PCA	Extended PCA which can be used to capture minimum of 2 reactions
Rodriguez (Rodriguez *et al.*, 2008)	PCA	Uses PCA to determine the minimum number of reactions of 3 reactions

Due to the underlying complexity and model assumptions in ADM1, there have been several model modification and reduction approaches to aid with calibration and increased use in control approaches. Model reduction methodologies include projection methods and non-projection based methods. Projection based methods include Singular Value Decomposition or orthogonal decomposition methods. These model reduction methods aim to decrease simulation time, parameter estimation requirements, and implementation workload. The Siegrist model can be deemed as a simplification of ADM1 model as the model excludes butyrate and valerate components. Table 2.2 depicts examples of model reduction approaches for AD. The most detailed approach of these is represented by Rodriguez and co-workers (Rodriguez *et al.*, 2008), in this a PCA technique is applied to experimental data from pilot scale AD, treating diluted wine and compared with simulation data from the ADM1 model. The PCA technique is used to determine the minimum number of reactions to be included in the model structure to describe different percentage of data variability.

Since there are a large number of measured quality variables that are highly correlated approaches use PCA to examine the relationships between different reaction pathways as variables within the AD process data.

The general mass balance equation for describing the dynamic behaviour of a completely mixed stirred tank reactor in the liquid phase is given by Equation 2.4.

$$\frac{dx}{dt} = D \cdot (x_{in} - x) - Q(x) + K \cdot r(x) \qquad \text{Equation 2.4}$$

The $n \times 1$ vector of x describes the measurable concentrations of the species in the liquid such as ethanol, butyrate, propionate and acetate ($mg\ L^{-1}$). Q describes the loss of mass each species to transfer to the gas phase, r is the $p \times 1$ vector of conversion rates and K is the $n \times p$ matrix containing the pseudo stoichiometry associated with the macroscopic network. Equation 2.4 is then integrated between the time constants of t_0 and t and expressed by Equation 2.5. Equation 2.6a is obtained by applying moving average window of size T to the equation (1) between 0 and t for $t < T$ and Equation 2.6b obtained by integrating between $t - T$ and t for $t \geq T$.

The data was then normalised to remove the magnitude of the effects and rewriting the equation in the form of $u(t) = K \cdot w(t)$; for a set of N data of $u(t)$ the $n \times N$ matrix $U = [u(t_1)\ \ u(t_2) \ldots u(t_N)]$ is considered (Rodriguez *et al.*, 2008).

$$x_{(t)} - x_{(t_0)} - \int_{t_0}^{t} [D \cdot (x_{in} - x) - Q(x)]\, dt = K \cdot \int_{t_0}^{t} r(\cdot) dt \qquad \text{Equation 2.5}$$

$$u(t) = x_{(t)} - x_{(0)} - \int_{0}^{t} [D \cdot (x_{in} - x) - Q(x)] dt \qquad \text{Equation 2.6a}$$

$$w(t) = \int_{0}^{t} r(\cdot)\, dt$$

$$u(t) = x_{(t)} - x_{(t-T)} - \int_{t-T}^{t} [D \cdot (x_{in} - x) - Q(x)] dt \qquad \text{Equation 2.6b}$$

$$w(t) = \int_{t-T}^{t} r(\cdot)\, dt$$

Table 2.3 illustrates the various stoichiometric equations for ethanol digestion. The results obtained from the PCA show that over 70 % of the variability can be described by reactions 1, 2 and 7 alone (highlighted in the table) and these 3 reactions model can be adequate an adequate model of the system.

Table 2.3 Stoichiometries of 9 considered reactions for digestion of ethanol (Rodriguez *et al.*, 2008)

Reaction	**EtOH**	**BuH**	**ProH**	**AcH**	**H_2**	**CH_4**	**CO_2**	**H_2O**
R1. EtOH + H_2O → BuH + ProH + AcH + H_2	-1	0.100	0.042	0.737	1.758			-0.758
R2. BuH + ProH + H_2O → AcH + H_2 + CO_2		-1	-0.419	2.419	3.257		0.419	-2.838
R3. AcH → CH_4 + CO_2				-1		1	1	
R4. H_2 + CO_2 → CH_4 + H_2O					-1	0.25	-0.25	0.5
R5. BuH + H_2O → AcH + H_2		-1		2	2			-2
R6. ProH + H_2O → AcH + H_2 + CO_2			-1	1	3		1	-2
R7. H_2 + AcH → CH_4 + CO_2 + H_2O				-1	-2	1.5	0.5	1
R8. EtOH + H_2O → AcH + H_2	-1			1	2			-1
R9. EtOH + CO_2 → BuH + ProH + H_2 + H_2O	-1	0.413	0.173		0.653		-0.173	0.173

To summarise the current state of modelling approaches of AD process, the SWOT analysis in Table 2.4 highlights the strengths, weaknesses, opportunities and threats. In general the threats and weaknesses outweight the opportunities and strengths. These have been the main reasons for limited modelling success with the AD process. However with increasing focus, interest and funding of AD systems, from households to businesses and governments it should enable the strengths and opportunities to outweigh the weaknesses and threats due to knowledge and improved models.

Table 2.4 SWOT analysis of AD process modelling

Strengths	**Opportunities**
• BBSRC ADNet scientific network (Anaerobicdigestionnet.com, 2015) • Active research area with various publications; with a range of simple models to advanced models with benchmark models to compare new modelling approaches • Established AD modelling community from reputable institutions with models such as ADM1	• Requirement for robust models to understand the underlying complexity of the process • Opportunity for soft sensor development for VFA and H_2
Threats	**Weaknesses**
• Lack of adequate instrumentation and monitoring to generate process data that fully describes the process • Lack of collaborations requiring expertise from different subject areas including biologist, process engineers, civil engineers	• Lack of robust models explaining the complex behaviour of the AD process • Current models too large and complex and difficult to calibrate

2.4 AD technologies

AD systems can be configured in a number of ways:

1. Batch or continuous;
2. Plug flow or fully mixed;
3. Wet or dry;
4. Psychrophilic or Mesophilic or thermophilic;

5. Single stage or multi stage.

As an industrially focussed Engineering Doctorate, this literature survey reflects the research requirements of the industry and as such there is greater emphasis on AD technology in the wastewater treatment sector; which are generally configured as continuous, fully mixed, wet systems. Key differences in these technologies are variations of mesophilic or thermophilic (covered in detail in Section 2.5) and single stage or multi stage.

Traditional AD systems are single stage operation where the sludge is fed into a single digester for a period of time and through appropriate mixing and heating, biogas is produced. These systems are generally mesophilic AD (MAD) systems and a series of drivers have increased the complexities of AD technologies and resulted in increasing need for a more robust system through the separation of the key stage of the process.

Process development for MAD systems began in the 1960's where further understanding of the need for heating, mixing and feeding systems became apparent (Noone, 2006). At this stage the main driver was reduction of odour. The 70's and 80's focused on separate processing inputs and their interactions and the drive during this period was the EU directive on improving pathogen quality and bacteriological of digestate sludge for land application (Noone, 2006). Current regulations and policies, such as the climate change act (*Climate Change Act*, 2011), EU and UK targets for energy from renewable sources and the Renewable Obligation Certificates (ROCs) (ofgem, 2011b) system is driving the technology towards higher efficiencies, improved yields and tighter regulations to make the technology more attractive from both a technical and financial perspective.

Advanced anaerobic digestion (AAD) may be loosely defined as a treatment process which improves the conversion of the organic material into biogas. AAD techniques are typically multi-stage and require additional techniques to separate the different stages of the process with pre-digestion techniques of thermal hydrolysis or enzymic hydrolysis and improve substrate composition contact between the microorganisms and the organic material. The two key steps in the digestion process are the acid forming stage (acidogenesis), and the methane forming stage (methanogenesis). Different conditions such as temperature and pH are required for the optimisation of these stages (Appels *et al.*, 2008). For example, there is a requirement for different optimum pH values for the various phases of the digestion process. The hydrolysis and acidification phases require lower pH values between 4.6 and 6.3, whereas the optimal pH range for the methane formation stage is between 7.0 and 7.7. Separation of these stages enable optimisation of each stage without hindrance on the other and therefore multi-stage AAD technologies generally yield more biogas, higher digestate and biogas quality with greater stability and robustness of the overall process than traditional single stage processes.

The two leading AAD approaches are enzyme hydrolysis technology and thermal hydrolysis. Other approaches include Ultrasound, Microsludge, OpenCEL, and Cell Rupture. Thermal Hydrolysis Processes (THP) are typically large scale AD plants, with 15 plants in the UK, 14 in the rest of Europe and four in the rest of the world (CAMBI, 2011). There are over 200 AD systems in the UK using the enzymic hydrolysis (Monsal, 2011). These are thus established and proven technologies with new plants currently under construction for both technologies.

2.5 Temperature

AD generally operates in three temperature ranges of psychrophilic 4-20 °C, mesophilic 20-40°C and thermophilic 40-70°C (Batstone *et al.*, 2002b). Mesophilic and thermophilic systems are the normal operating temperature ranges with mesophilic system being the most common and stable. The stability of mesophilic anaerobic digestion (MAD) systems is a result of the wider diversity and robustness of bacteria to grow at mesophilic temperatures and also that they are more adaptable to changes in environmental conditions (Angelonidi and Smith, 2014).

Different optimum temperature values exist for different phases of the digestion process, as methanogenic bacteria especially are very sensitive to temperature fluctuations therefore temperature should be kept to within ±1˚C (Appels *et al.*, 2008). Local temperature variations may well indicate the presence of poor mixing, or dead spots in the digester. Optimisation of the heat balance is important in improving the digester operation and efficiency as a whole.

Temperature has a significant effect on biogas production. Budiyono and co-workers (Budiyono *et al.*, 2010) conducted experiments in a 400 ml digester using cattle manure. The experiment was run at 38.5˚C and room temperature. Comparison of the average gas production gave 5.8 ml gVS^{-1} per 1˚C increase in temperature. This value is however based on the specific experimental set up and cannot be used generally as the size of the digester and the feed affects conversion rates. Research has shown that in general biogas production follows a sigmoid function as in a batch growth curve. Biogas production is very slow at the beginning and end period of observation. A second report by Alverez and Liden (Alvarez and Lidén, 2008) stated that by reducing the temperature from 35˚ to 25˚C caused a 30 % reduction in volumetric biogas production rate was observed for a Llama-cow-sheep manure bench top digestion process (Alvarez and Lidén, 2008). However a 7˚C reduction from 25˚C to 18˚C caused a 51 % reduction in the biogas volumetric production rate. This is expected as an increase in temperature improves the kinetics in the system and hence increases the degradation rate. However the results also showed high CH_4 content which increased at low temperatures. The CH_4 content in the biogas increased from 49.9 % to 61.1 % between 35˚C and 18˚C. This counteracts with the fundamentals of a decrease in volumetric gas production rate. The volumetric CH_4 production rate was reduced from 2094 ml at 35˚C to 1676 ml CH_4 per day at 25 ˚C representing a reduction of 20 % (Alvarez and Lidén, 2008). A further reduction of 47 % from 1676 to 894 ml CH_4 d^{-1} was seen when the temperature was reduced from 25 to 18˚C. Thus biogas production rate increases with decreasing CH_4 composition for temperatures within the mesophilic digestion region of 30˚C to 35˚C. An optimum temperature must be established at which high CH_4 composition and biogas yield are simultaneously optimised. The profitability of the anaerobic digestion process is strongly affected by the percentage of CH_4 present in the resulting biogas. Any advanced control scheme must therefore optimise both CH_4 and biogas yields.

2.6 Conclusions

AD technologies continue to be an attractive topic for scientists, engineers, industries and governments, as they struggle to learn and understand the complexities of the process and drive scientific and engineering development. They also align with government drivers to reduce fossil fuels, find alternative energy sources and reduce waste to landfills. The technology is experiencing major transitions through increased focus on AD for combating climate change and biorefinery developments. The dynamics of the process continue to increase with high uncertainties and increasing complexities; the technology continues to develop with increase new industrial processes.

Through conducting the literature survey it was found that instrumentation with respect to sensors is a key limitation of industrial scale ADs. Various online sensors for key variables exist at laboratory or experimental scale but are mainly offline analysis methods and are not currently available on industrial scale application. The possible reason for this may be due to cost, reliability, or market demand for example the need for monitoring of the hydrolysis and fermentation stages which may require the integration of spectroscopic sensors or soft sensors to efficiently predict important parameters such as alkalinity and VFA. Efficient monitoring of these parameters is deemed important for future research development (Ward *et al.*, 2008). This issue has led to the need for a detailed instrumentation review (summarised in Chapter 3) to establish the gaps and opportunities in this area.

Following on from the instrumentation review, a vendor review was conducted to identify the key technology players in the field with two questionnaires aiming to: (1) gain input from the AD technology providing vendors and (2) understand the reasons for the variation in the application of the various technologies to support the project. The vendors included AD original equipment manufacturers (OEMs), pre-treatment technology providers and various other suppliers for the process specifically for the WWT market. This task was carried out to obtain input from the technology providers on how their technologies could be integrated into the Perceptive AD master and the AD process overall to meet the aims of the project. The key targeted technology providers were Monsal and CAMBI. These two companies provide leading advanced anaerobic digestion (AAD) technologies. Examples of their technologies are covered in the benchmark study in Chapter 4. Involving the process designers was paramount to the project as it allowed the opportunity to improve the process from the design level.

Response from the questionnaires through emailing and cold calling the vendors was low and as a result, vendors were then targeted at several AD events and conferences. The limited response received was inadequate to obtain insights from the vendors to support the research and these are not presented in this thesis.

3 Instrumentation review

3.1 Introduction

This instrumentation review discusses the minimum and ideal instrumentation requirements for an AD process. The economic and environmental benefits of biogas production from an AD process are well understood and in recent years significant technological developments for increasing the efficiency, yield, stability and robustness of the system has increased the need for better monitoring of the process (Olsson *et al.*, 2005).

Current regulations and policies such as the climate change act (*Climate Change Act*, 2011), EU and UK targets for energy from renewable sources and the Renewable Obligation Certificates (ROCs) (ofgem, 2011b) system are driving the need for higher efficiencies, and improved biogas yields. These requirements make the investment in control and monitoring technologies more attractive. This is supported by various studies both in industry and academia. Due to the low energy efficiency for converting biomass to electricity of only 13 % (Warthmann and Baier, 2013), there is an opportunity to improve the efficiency and yield; monitoring and control will play a crucial role.

The lack of process control handles, instrumentation, and developed control algorithms have been addressed to some extent in the past 10 years (Boe *et al.*, 2010; Palacio-Barco *et al.*, 2010; García-Diéguez *et al.*, 2011; Cadena-Pereda *et al.*, 2012; Vanwonterghem *et al.*, 2015). The current gap in instrumentation technology was the lack of availability of rapid intermediate sensors to detect overloading conditions. To date there are a limited number of sensors that can measure total or individual organic acids; with some available on commercial production sites and others under development (Pind *et al.*, 2003).

There are on-going research projects in this area in both academia and industry, with new types of instruments being commercialised frequently due to regulatory and process improvement demands. There are wide varieties of instruments available at the laboratory scale which is not yet applicable at an industrial scale. The gap between laboratory and industrial scale instrumentation, control and automation is more significant for AD than for most fields, as digestion at laboratory scale is much more stable and easy to control than at an industrial scale (Horan, 2009).

An additional challenge has been dealing with the lack of reliability of existing sensors, and the potential effect that they may have on a closed-loop control system and fault detection algorithms have proven not to be satisfactorily reliable to detect faulty on-line sensors. Robust control strategies based on on-line sensors include algorithms for automated detection of faulty sensors. Sensor faults typically include drift, offset shift, scaling shift, fixed value, complete failure, and calibration errors

Stability of the AD process may be indicated by biogas production rate, and effluent VFA or effluent COD or TOC concentrations. When attempting to control parameters, typically limited manipulated variables are available, with feed flow being the most commonly used. Other manipulated variables include temperature, stripped gas, agitation and mixing.

Plant wide optimisation needs to be taken into account for the implementation of any control scheme. It is evident that energy balance is an important plant performance indicator, particularly where CHP operation is utilised for the downstream process (Horan, 2009). For this reason, the monitoring of the energy used and produced by the various heat and power units is necessary. Flow and temperature probes are reliable and well established within the industry and in such situations where instrumentation is unavailable; it should be implemented to enhance energy utilisation.

3.2 Instrumentation technology providers

A common aphorism in the field of control instrumentation is "To measure is to know". In the past, the availability of sensors was a key obstacle for control and automation of WwTPs. Measurements for treatment systems were mainly limited to pH, flows and dissolved oxygen (DO). This situation has improved over the last 10 years, and currently sensors for biochemical oxygen demand (BOD), COD, ammonia, nitrate, nitrite and phosphate are now available for on-line monitoring of wastewater treatment.

The book entitled "Instrumentation, Control and Automation in Wastewater Systems" gives a good account of developments in this area up to 2005 (Olsson *et al.*, 2005). Key conclusions with respect to the state of instrumentation, control and optimisation up to 2005 were:

- Limited usage of sensors for closed loop control approaches
- Improved ease of data collection and visualisation through the adoption of supervisory control and data acquisition (SCADA) systems

- Process or plant wide control and optimisation approaches are new areas for development
- 50 % of control loops surveyed were found to be in manual mode
- Lack of on-line sensors no longer deemed as the main limitation for on-line control, process flexibility recognised as a greater limitation.

Table 3.1 Examples of technology providers for AD systems

Company	**Instrument**	**Details**
Bioprocess Control Ltd	Biogas OptimizerTM (*Products | Bioprocess Control*, 2016)	A SCADA solution which allows process diagnosis, decision support and optimisation; and Automated Methane Potential Test System (AMPTS) system
SCAN	Spectrolyser, pHlyser, ammolyser, chlorilyser, and turbilyser (SCAN, 2011)	Spectral probes, ion selective probes, electrochemical sensors, optical sensors
Geotech	GA3000 and GA4000 (*Products Archive - Geotechnical Instruments (UK) Ltd*, 2016)	Simple fixed position biogas analyser and laser diode analyser for highly accurate CH_4 analysis
Endress Hauser	Flow, level, pressure (*Level, flow, pressure, temperature measurement | Endress+Hauser*, 2016)	Data logging and digital communications
Hitech Instruments	GIR5000 ('GIR5000 series - Biogas & Landfill analysers - Multiparameter analysers for biogas applications,' 2016)	Designed specifically for biogas applications and measures CH_4, CO_2, and O_2 or H_2S
AppliTek	Anasense (AppliTek, 2009)	Monitors VFA, bicarbonate and alkalinity

Various companies have portfolios of instrumentation specifically to address the needs of the water industry. Although the state of instrumentation for process units such as activated sludge plants (ASPs) has improved considerably, there is still a lack of suitable instrumentation for ADs. Table 3.1 depicts different technology providers for AD systems; such as the spectrolyserTM which is specifically designed for WwTP (SCAN, 2011). This SCAN spectrometer probe has proven to be reliable for the online monitoring of BOD, COD, Total Soluble Solids (TSS), pH, nitrate and temperature (O'Brien *et al.*, 2011) for the treated effluent stream of an ASPs. The multi parameter probe uses UV-Vis spectrometry over the range 220-720 nm or 220-390 nm and can be mounted in the media or in a flow cell with automatic cleaning using compressed air (SCAN, 2011). Instrumentation such as this has made some ASP control solution implementations possible yielding, improved process efficiency.

Another example of on-line instrumentation developed specifically for monitoring AD systems is the Anasense® from AppliTek. An example of the Anasense Control Unit is shown in Table 3.2. This system is used in the TELEMAC supervision system to monitor VFA, bicarbonate and alkalinity. The TELEMAC project is aimed at bringing new methodologies from the IT and science sectors to water treatment, and compares a group composed of leading scientist and engineers offering an advanced remote management system for anaerobic WwTPs which do not benefit from a local expert in wastewater treatment. The TELEMAC system involved new sensors for improved monitoring of the process dynamics and with automatic controllers that stabilise the treatment plant (Bernard *et al.*, 2004).

Table 3.2 Example of instrumentation control units

		
CH_4 analyser from Nova Analytical Systems Inc. (Nova analytical systems, 2010).	Anasense from AppliTek NV (AppliTek, 2009)	pH or Redox (ORP) & Conductivity analyser from ABB (*pH / ORP transmitters - Analytical Measurement | ABB*, 2016)

The HK microwave dry solids measurement system shown in Figure 3.2 is manufactured in Germany by Harrer and Kassen and distributed by Process Instrumentation UK Ltd. This analyser is typically commissioned for a cost < £10,000 and the instrument is capable of measuring % DS within the range 0 % to 40 % DS. A low power oscillator in the microwave measuring instrument is used to generate an electromagnetic wave which is then transmitted into the sludge via an antenna. The wave is transmitted through the dielectric properties of the sludge. This is received by a second antenna and the phase delay and power level of the wave received are proportional to the concentration of the product (density) or the dry solids (UK, 2011).

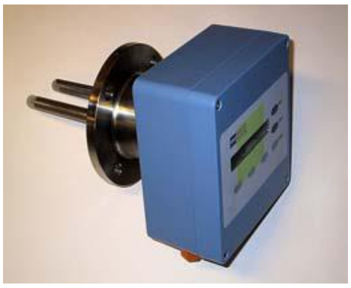


Figure 3.1 The HK microwave dry solids measurement system (UK, 2011)

The ISO 15839:2003 standard is the most complete protocol for sensor characterisation in water quality for on-line sensors and analyser equipment for water specifications as well as performance tests (Iso.org, 2015). Most of the instruments detailed in the survey conformed to this standard. Sensor characteristics covered by the standard include performance metrics of range, linearity, accuracy, drift and speed of response.

The provision of more standard measurements such as temperature, pressure, liquid level, and flowrates are not considered in this survey, as such instruments are readily available, with state of the art technology found on many plants. Physico-chemical measurements such as pH, conductivity, redox, CH_4, H_2S, H_2, CO_2 and bio-chemical measurements of BOD and TOC are readily available with state of art technologies. Measurements of suspended solids, bicarbonate alkalinity, digester gas and UV absorption have application only in certain areas. Measurements systems which require further development work include sludge morphology, calorimetry, COD and VFA.

An important precursor step in the development of robust control solutions to ensure enhanced AD operation is the development of robust sensors and analysers. Challenges limiting the success of control strategies in AD typically include uncertainty in the process kinetics and uncertainty in the input and output flows and concentrations. The availability of reliable sensors can help overcome these limitations. Sensors can be categorised into two groups (1) reliable simple sensors for operator support and regulatory control of the process and (2) advanced sensors tools for auditing, optimisation, modelling activities (Vanrolleghem and Lee, 2003).

3.3 Sensors and instruments

This section provides a discussion on instrumentation in the solid, liquid and gas phases of the AD process. Variables can be measured in the gas or liquid phase. Liquid phase measurements include VFAs, pH, COD, dissolved H_2 and alkalinity, whilst gas phase measurements consist of flowrates, and composition of species such as CH_4, H_2S, H_2, CO_2 and siloxanes (Ward *et al.*, 2008). Sensors for physical parameters such as flowrate are of importance in the process. Gas flowrate measurements are provided using differential pressure techniques, turbine sensors or magnetic flow sensors.

Figure 3.1 illustrates the various parameters measured in the solids phase as well as liquid and gas phases.

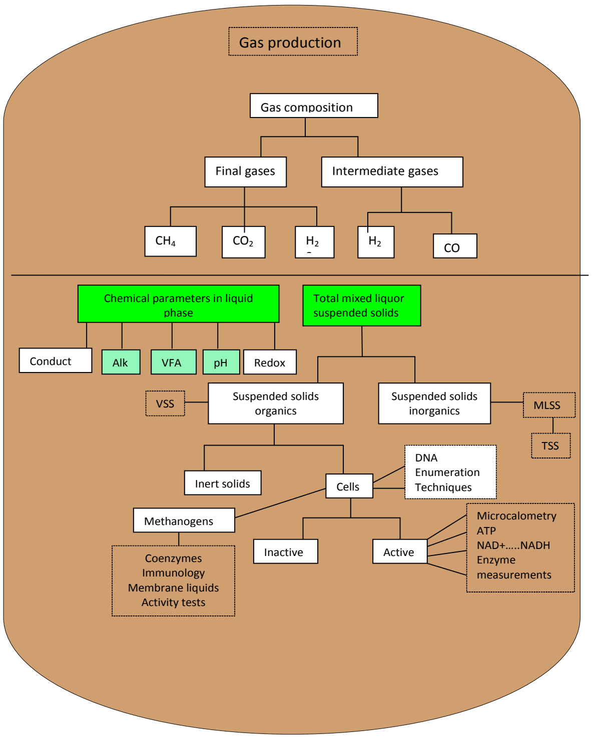


Figure 3.2 Digester gas, liquid and solid phase measurements (Switzenbaum *et al.*, 1990)

3.3.1 Gas phase sensors

Gas measurements are usually much easier in comparison to analytical measurements in water and other liquids. Gas production is one of the fastest acting and most commonly applied parameters for monitoring and controlling AD processes. Gas flow on-line parameters are used is in various studies. As fluctuations and measurement noise in gas flow measurements are common, low pass filtering is often necessary in order to provide a smooth gas flow measurement necessary for controlling the process.

Due to the explosive nature of biogas; many gas analyser instruments are ATEX (Explosive Atmospheres Directive) certified. This is a European Union Directive which requires employers to protect workers from the risk of explosive atmospheres (Hse.gov.uk, 2015). Table 3.3 depicts gas phase measurement, with their level of accuracy, example instruments and whether these instruments are readily available online or not. The easiest of these measurements is gas flow; the digester off-gas stream is a slightly more benign environment for online sensors. Many different industrial gas measuring instruments are readily available and most of these instruments require a gas flow of about 5 L min^{-1} or more for analysis. The most common laboratory instruments are volumetric displacement and can measure gas flow at very low concentrations. The measured gas flow signal can be affected by noise, usually due to the effects of foaming. This noise typically requires online filtering to provide a useable signal (Pind *et al.*, 2003).

Biogas flow monitoring systems are readily available and widely applied in industry and the accuracy of these instruments is affected by temperature values due to dilution of water vapour in the gas with increased temperature which can increase from 8 % at 35^{o}C to 17 % at 55^{o}C. Prices range considerably between portable devices and fixed point or wall mounted modular devices and continuous process monitoring; with the Gas Data GFM416 biogas analyser costing around £3200.

Table 3.3 Gas phase measurements

	Technology Types or Method	**Ranges or Level of Accuracy**	**Reliability and Cost**	**On-line or Process Dynamics**	**Examples**
Gas flow	Volumetric displacement instruments, thermal dispersion devices, orifices plates, pilot tubes and turbine meters	Range: 0-500 Nl min^{-1}. and ± 0.5 % repeatability, 5 L·min–1-0.1mL·min–1(Guwy *et al.*, 1995)	£3000-5000	Speed of response typically 30 seconds	Geotech-GA3000, HiTech-GIR5000, Gas Data-GFM416 (*Products Archive - Geotechnical Instruments (UK) Ltd*, 2016)
CH_4 and CO_2	Volumetric displacement measurement, GC, IR adsorption analysis methods	CH_4 0-60 % and CO_2 10-50 % of total gas.	£800-1500	Readily available both lab and industrial scale	LI-COR, CEA CH_4, Servomex Ir1520
H_2	Mercury-mercuric oxide detector cell (0.01ppm), thermistor metal conductivity	0-4 % range typically by volume	£350-500		None found
H_2S	Measure H levels using electronic sensors or gas measurements, electrochemical sensors	In concentrations between 0-50 ppm in gas produced	£200-500	GC and FT-IR analysis, applied to 6 sites (Arnold and Kajolinna, 2010)	None found

The removal of CO_2 can be controlled by manipulating the pH and alkalinity. Therefore control of gaseous CH_4 composition can be maintained to some degree. The use of CH_4 production is commonly employed as the output parameter for control. The CO_2 and CH_4 composition can be measured using gas chromatography (GC) - mass spectrometry (MS) or GC- flame ionisation detector (FID) methods and infrared measurements. Measurement of CH_4 composition in AD biogas may be achieved by passing the biogas through a column or bed of soda lime to scrub off the CO_2. A simple volumetric measurement of the CH_4 can then be conducted. The profitability of the AD process is strongly affected by the percentage of CH_4 present in the resulting biogas. An advanced control scheme should look to optimise the relative biogas CH_4 compositions. These instruments are also relatively reliable provided they do not suffer from foam infiltration (Horan, 2009).

Carbon Monoxide (CO) is another unwanted by-product in the gas phase, and low concentrations of CO may be detected. CO however has low solubility and is easily measured. Control of CO variable was not investigated as yields are typically deemed negligible (Horan, 2009).

Much of the research into new sensors has concentrated on the analysis of intermediate compounds. These compounds, for example VFA and H_2 can contribute to or cause inhibition, which significantly reduces sludge stabilisation and biogas yields. Measurement of the intermediate compounds in the liquid phase and the final gases (H_2, CH_4, CO_2, and H_2S) is important for characterising the state of the process. H_2 is produced as an intermediate component, which is immediately consumed by another phase of the digestion process. H_2 rapidly dissociates from the liquid phase to form H_2 gas. This liquid-to-gas transfer occurs in a highly non-linear manner, meaning that the H_2 responds to a disturbance in a highly dynamic manner, both in the liquid phase and in the gas phase. Because of this, H_2 in the gas phase is not indicative of a stable or unstable process. By monitoring (and possibly controlling) the H_2 content, it is possible to monitor or control the various phases in the process. Conversely dissolved H_2 is not as dynamic, and studies of dissolved H_2 have been shown to correlate to the organic loading rate (OLR). Dissolved H_2 concentration can be predicted by calculating the biogas composition under the assumption of the equilibrium between gas and liquid phase using Henry's law (Vanrolleghem and Lee, 2003), as a crude estimation.

3.3.2 Liquid phase sensors

Monitoring of the intermediate chemical species that are created within the digester vessel and then immediately consumed within the same vessel (or an immediate downstream vessel) can provide key information on microbial activity. The intermediates produced are degraded from soluble and insoluble proteins, carbohydrates and lipids. Monitoring of these intermediates is carried out in the liquid phase, within the digester vessel itself. Instrumentation for the monitoring of the biological intermediates such as VFA and bicarbonate alkalinity is an active research area. Soft sensors for VFA and alkalinity have been developed to enable better monitoring of the process. Finally the analysis of the fermentation stage of the digestion process is achieved through techniques such as photometric cuvette tests, ion chromatography, or titration methods.

VFAs are fatty acids with a carbon chain of less than six. These are deemed to be the most important intermediates in the process. The conversion of VFAs to CH_4 and CO_2 is conducted through the acetogenesis and methanogens stages. The monitoring of the VFA composition gives important information about the state of these stages. As the composition of the feedstock entering the digester can vary greatly, the general interpretation of the VFA concentration can become highly problematic. For example, an increasing VFA content may be due to a change in the feedstock, or alternatively it may be due to a change in the microbial balance between the different stages. These two different causes require diametrically opposite control actions, therefore VFA monitoring at multiple points in the process is important for optimal control of the AD process. The most important drawback to fulfil automatic control of VFAs is the lack of on-line measurement devices, and the potentially high cost of those instruments that are available.

Current methods for VFA measurement include distillation, calorimetry, GC and various titration techniques. Of these approaches the titrimetric methods are considered to be more rapid, simplest and most cost effective. Most of these assume that VFAs are mainly composed of acetic acid (Bouvier *et al.*, 2002). In the literature several publications have reported the on-line monitoring of VFA’s through titrimetric methods (Bouvier *et al.*, 2002; Feitkenhauer *et al.*, 2002).

Table 3.4 Liquid phase measurements

	Technology Types or Method	**Ranges or Level of Accuracy**	**Reliability or Cost**	**On-line or Process Dynamics**	**Examples**
VFA	Distillation, calorimetry, chromatography and	VFA accumulation reflects a kinetic	£12000-20000	HSGC (Kanokwan et al., 2007), FT-IR spectrometer as an on-line	Anasense® (AppliTek,
Ammonia	Ion selective, and electrochemical based	100–1100 mg-N · L–1; Colorimetric range:	£12000-20000		Anasense® (AppliTek,
H_2	Amperometric probe (50 nM), H_2 or air fuel cell		Typically an estimate from	Available on lab scale and estimation mechanism for	None found
BOD	Spectrometer: measure optical spectra from 200	Not an usual parameter for AD	None found	Lab scale in-house developed biosensor (Liu et al., 2004)	Carbolyser (SCAN, 2011)
COD or TOC	Spectrometer measure optical spectra from 200	COD: 0-1500 mg L^{-1} O2 and 2 % accuracy.	£25000-£30000	FT-IR spectrometer as an on-line sensor	Carbolyser (SCAN, 2011)
Alkalinity, PA, TA	Total buffer capacity	1000-3000 mg L^{-1} typically	None found	FT-IR spectrometer as an on-line sensor	Anasense® (AppliTek,

Off-line measurements of VFAs for verifying the state of the biomass within the AD has been applied in control studies. In these studies, the control algorithm has been based on other measured on-line parameters of inorganic chemical components, such as redox potential, ammonia, pH, and alkalinity. Another approach has been VFA estimation using a modified nitrate sensor for measuring nitrate reduction through a denitrifying organism immersed in partially digested feedstock's in an excess of nitrates. Measuring nitrate reduction through titration is proportional to the organic carbon (Ward *et al.*, 2008). Titrimetric methods can also be applied for the analysis of total and partial alkalinity.

VFAs are formed during the acidogenesis and acetogenesis stage. A stable efficient fermentation process yields VFA component (acetic, propionic, butyrate etc.) values between 500 to 3000 mg L^{-1} as the equivalent amount of acetic acid. There is equilibrium between the production of acid by hydrolysis and acid degradation by methanation. An acid concentration above 10000 mg L^{-1} results in pH drop usually below 7 and results in a reduction in CH_4 concentration. This parameter could potentially be monitored and controlled using the Anasense instrument.

The pH level in the digester is a particularly important parameter for monitoring and control. In general the ideal range of pH is between 6.6 and 7.6. If the pH is particularly low, then the methanogenic bacteria essential to the final stage of CH_4 production will be inhibited. Currently there are a wide range of sensors available for the measurement of pH, however many pH probe electrodes are prone to electrode poisoning due to the harsh environments in the digestion process. The hydrogen sulphide (H_2S) concentration present in the sludge causes electrode poisoning to most pH monitoring instrumentation. The Hach Lange pHD sc digital differential electrode for pH and redox measurement is designed to overcome this problem. The reference system of the pHD sc electrode does not come into contact with the fluid that is being measured and avoids the problem of electrode poisoning.

The measurement of carbohydrate levels in the digester vessel is also considered. Substrate carbohydrates may be in either soluble or insoluble form. The measurement of soluble carbohydrate is comparatively much easier, using methods such as high performance liquid chromatography (HPLC) which may be applied on-line. In comparison insoluble carbohydrates require complicated pre-treatment methods, after which they can be measured using HPLC, colorimetric methods or GCMS. Because of the pre-treatment requirements, on-line measurements are not possible. Even for offline lab measurements, the costs for these measurements are sufficiently high and hence these measurements are only conducted on a small scale. Currently there is no direct on-line measurement of the composition of either H_2S or CH_4 in the liquid phase (Vanrolleghem and Lee, 2003). Any future developments in the measurements of these parameters may yield new potential control strategies.

Temperature sensing probes are relatively cheap and reliable, and the digester vessel can be instrumented with a number of these at various positions both radially and axially around the circumference of the vessel. Local temperature variations may well indicate the presence of poor mixing, or dead spots in the digester. Temperature probes should also be mounted in the hot water circuit entering the digester, and possibly on the biogas streams leaving the digester. This would allow the online calculation of the digester heat balance. Optimising the heat balance is essential to optimising the digester operation as a whole.

The use of gas flow measurement as an on-line parameter is found in numerous studies. This is regarded as a key monitoring parameter (in conjunction with the sludge feed rate), as it is a relatively fast indicator of changes in the microbial population.

Soluble H_2 is an intermediate species which is both produced and immediately consumed in the AD process. Gaseous H_2 concentration may be measured using a mercury-mercuric oxide detector cell; an exhale H_2 monitor; or palladium metal oxide semiconductors (Pind *et al.*, 2003). H_2 has a very short relaxation time as shown in Table 3.5 and the content in the gas phase could be between 20-30 ppm to 400-600 ppm which makes measurements much easier in the gas phase.

Table 3.5 Theoretical relaxation times for some AD parameters (Switzenbaum *et al.*, 1990)

Substrate	H_2	Glucose	CO_2	Acetate	Propionate	CH_4
Relaxation time	15 seconds	3 minutes	1 hour	2 hours	4 hours	2 days

H_2S is produced as a result of the degradation of sulphide containing compounds such as proteins in small quantities. H_2S forms a small proportion of the overall biogas composition.

3.3.3 Solid phase sensors

For the AD process, the 'solid phase' refers to solids carried in liquid suspension, either in the feedstock, digestate, or in the main body of the digester vessels. Solid measurements are usually conducted on feedstock prior to entering the digester and then post digestion, so as to ensure that the instruments can be accessed for maintenance purposes. The main purpose of measuring the solids before and after digestion is to evaluate the percentage solids reduction, which indicates the level of microbial activity in the digester. Accurate measurement of the solid component properties is more difficult compared to gas or liquid measurements. Solid phase parameters for measurements include percentage dry solids (% DS), cell enumeration, deoxyribonucleic acid (DNA) sequencing, protein content, bacterial lipids, adenosine tri-phosphate (ATP), enzyme activities, methanogenic activity measurement, micro-calorimetry, co-enzymes, C1-carriers of methanogens and immunology of methanogens. In general these parameters are not often used for automatic control as these are usually measured off-line with long analysis periods and complex systems for measurement (Moletta, 1998). Laboratory analyses for the characterisation of bacteria or the organic compounds are mostly carried out for research purposes and typically not an actively monitored process parameter.

One of the newer sensor types is near-infrared spectroscopy (NIRS), which is used in a variety of industries for classifying or predicting the characteristics of complex media and bulk solid materials. NIRS is a non-destructive optical technique, which produces a spectrum as its output, as such NIRS requires a multivariate technique such as partial least squares (PLS) regression to map the spectral output to one or more measured physical parameters. NIRS has the advantage of being able to measure several parameters simultaneously providing a calibration model is prepared for the parameters of interest. The need for a calibration model is a drawback for the NIRS technique, as each type of waste may require its own calibration model and a biochemical methane potential (BMP) test may still be required to obtain the reference value. NIRS has been used to monitor ADs mostly for determining VFA content and BMP.

Table 3.6 Solid phase measurements

	Technology Types or Method	**Ranges or Level of Accuracy**	**Reliability and Cost**	**On-line or Process Dynamics**	**Examples**
Total organic carbon (TOC)	Spectrometer: measure optical spectra from 200 to 750 nm directly in liquid	Range: 0-10000 ppm; Accuracy: 2-3 %	Average price £25000	FT-IR spectrometer as an on-line sensor	SCAN: Carbolyser
VOC	Spectrometer: measure optical spectra from 200 to 750 nm directly in liquid	Not an usual parameter for AD	None found	GC and FT-IR analysis, applied to 6 sites (Arnold and Kajolinna, 2010)	None found
Indirect measurement of organic matter	Assessment of VS and total solids (TS)	Not a usual parameter for AD, calculation on the inlet feed to digester, varies dependent on feed.	None found	None found	None found

One key variable for the digestion process is the % DS fed into the digester. Typically this parameter is measured off-line, and these spot sample results are then used to adjust the sludge dewatering process accordingly. The optimum solid content obtained for biogas production is in the range of 7 to 9 percentage dry solids (% DS) (Balsam, 2002). This is the amount of solids in sludge, which contain organic matter of proteins, carbohydrates, fats, nutrients. Due to the function of water in the digester, the total solids (TS) content will directly correspond to water content. Water content is an important parameter as it enables the movement and growth of bacteria, facilitating the dissolution and transport of nutrients and contributes to the metabolic reactions as most of these are dependent on the hydrophobicity of the organic material. Water can also reduce the limitation on mass transfer of non-homogenous or particulate substrate (Budiyono *et al.*, 2010). % DS information may be used to estimate the organic loading to the digester. The organic loading rate (OLR) is a key parameter for the operation of the digester. An OLR greater than 3 kg VS ($m^3.d^{-1}$) may lead to overloading of the digester which will in turn require a reduction in the sludge feed rate to allow the digester to recover.

Online DS meters for the sludge feed stream are available, and are relatively reliable. These sensors are designed to work with sludge dry solids contents in the range 0 % to 10 %. This sensor information may be used to estimate the organic loading of the digester which is a key parameter for operating the digester; a loading rate above 3 kg VS ($m^3.d^{-1}$) may lead to overloading of the digester which will in-turn require a reduction in the sludge feed rate in order to allow the digester to recover.

In the UK, the use of treated digestate sludge as an agricultural fertiliser is governed by the 'Safe Sludge Matrix' (SSM). This is a set of rules governing what type of crops that different sludge can be applied to. A 'conventionally treated sludge' is one in which at least 99 % of pathogens have been removed. An 'enhanced treated sludge' is one in which at least 99.9999 % of pathogens have been removed. Table 3.7 shows the UK Safe Sludge Matrix (Chambers *et al.*, 2001). The matrix sets out the types of crop groups which may be treated with conventional, enhanced or untreated sludge.

The main driver for determining how a digester is operating is ensuring that the digested sludge is compliant with sludge stabilisation requirements. Beyond the requirements for pathogen reduction there is no other direct specification for digestate quality in general use. As it is deemed to be a waste product, digestate is excluded from the main farm quality assurance scheme and this is the main obstacle for applying digestate use on agricultural land (Booth, 2009). This will inevitably change due to increased regulations and the move towards selling digestate as a product.

Table 3.7 The safe sludge matrix (Chambers *et al.*, 2001)

Crop group	**Untreated sludges**	**Conventionally treated sludges**	**Enhanced treated sludges**
Fruit	×	×	√ 10 month harvest interval applies
Salads	×	× (30 month harvest interval applies)	√ 10 month harvest interval applies
Vegetables	×	× (12 month harvest interval applies)	√ 10 month harvest interval applies
Horticulture	×	×	√
Combinables and animal feed crops	×	√	√
Grass and forage (grazed)	×	× (deep injected or ploughed down only) 3 week no grazing and harvest interval applies	√ 3 week no grazing and harvest
Grass and forage (harvested)	×	√ (no grazing in season of application) 3 week no grazing and harvest interval applies	√ 3 week no grazing and harvest

Regulations such as these articulated in the Code of Good Practices (CoGP) and SSM are used for sludge stabilisation in the UK. Treatment processes for sludge are managed by the principles of hazard analysis and critical control point (HACCP) management. HACCP applies risk based management and control procedures to manage and reduce potential risks to human health and the environment. The HACCP approach is adopted and applied to sludge treatment, to ensure that the microbiological requirements set out in the SSM are achieved and that the appropriate quality assurance and risk management and reduction procedures are in place. This ensures that if the digestate is being spread on agricultural land, it complies with the relevant microbiological standards (Davis *et al.*, 2010).

The SSM however does not include specific sludge quality indices. In an attempt to remedy this, the waste resources action program (WRAP) created an industry specification, the Publicly Available Specification (PAS 110) (WRAP, 2010) which producers use to verify that digestate produced is of consistent quality and fit for purpose. Some of the parameters from the PAS 110 guidelines include limits for toxic elements such as copper, zinc and lead; limits for digestate stability characteristics such as VFA and residual biomass potential as well as declaration of nutrient characteristics of total nitrogen, phosphorus and potassium (NPK) values (WRAP, 2010). In March 2011, the Andigestion plant in Devon became the first AD plant to achieve digestate certification and the site is approved under the Biofertiliser Certification Scheme (BCS). BCS was built on from PAS 110 and offers a tool for classifying digestate (Organic-farmers-and-Growers, 2011).

To comply with these guidelines, adequate instrumentation for the measurement and monitoring specified parameters may be required in the near future, with a key challenge being the ability to reliably and accurately measure these parameters. Currently composition can be analysed within the laboratory as opposed to online in the digester and hence soft sensors may be developed to as surrogate measurements.

3.3.4 Software sensors

There are limitations in the availability of reliable on-line sensor instruments for those parameters discussed previously. It is possible that these limitations may be overcome through the development and deployment of software-based sensors (also known as 'inferential sensors' or 'soft sensors').

A software sensor associates a hardware sensor and an estimation algorithm (software) to provide on-line estimate of an un-measurable variable (Chéruy, 1997) and this will be discussed in detail in Chapter 7. The key to a successful software sensor is to make use of multiple instances of cheap, reliable, and easy to maintain sensors (such as flows, temperatures and pressures) together with an appropriate multivariate model or algorithm, in order to estimate some hard-to-measure parameter in real-time. Development of software sensors for AD is an active research area, with new models and techniques being published frequently. There are many common models used in developing soft or inferential sensors.

The phenomenological or model driven approach, which is commonly based on first principle models, describes the underlying physical and chemical background of the process. As these models are usually based on the ideal steady-state of the process (which for AD is largely unknown), this makes their use as the basis for soft sensors in AD problematic.

The data driven approach employs a range of data analysis techniques including univariate or multivariate statistical analysis, artificial neural network and fuzzy models, and rely on a historical record of past behaviour of a particular process to estimate future behaviour. These are more popular as they are perceived to describe the real process condition as the data used is measured within the processing plant.

There is an increasing need for model based estimators to reliably predict costly or unavailable measurements on the basis of related but less expensive on-line sensor values (Theilliol *et al.*, 2003). An example of such a system is a model which calculates the risk of foaming due to microbiological causes. As causes of foaming in AD are not in complete agreement; this model has encapsulated invaluable empirical knowledge of key factors, with organic loading rate (OLR) and filamentous microorganisms present in the activated sludge system, as the inputs to the model. This case study was used to evaluate the performance of the model used in the IWA Benchmark Simulation Model No. 2 as a framework (Alex *et al.*, 2008a). Simulation results for one open loop configuration and two close loop control strategies proved the usefulness of this approach for the estimation of the risk of foaming in AD’s (Dalmau *et al.*).

Currently the use of soft sensors on industrial scale processes is limited, mainly due to the difficulty in developing robust models and in validating cause sensor information. It is common practice to analyse samples off-line to compare results to the soft sensor value to ensure that the reliability of the soft sensor.

The development of a software sensor typically requires an intensive laboratory sampling campaign to develop the sensor, as well as periodic lab samples to validate the software sensor values, and to provide 'bias correction' for unmeasured drifts in values.

As such, the software sensor approach would be more suitable for parameters which are frequently measured, such as VFA or pathogen levels in digestate.

3.3.5 Sensor requirements for advanced control

As a result of this instrumentation review and the benchmark study in Chapter 5, ‘minimum’, ‘essential’ and ‘nice to have’ instrumentation requirements for considering the implementation of any advanced control scheme are summarised in Table 3.8.

Table 3.8 Summary of instrumentation

	Minimum	**Essential**	**‘nice to have’**
Input	Pressure or level measurements	% DS	Chemical composition
	Feed flowrate	TOC	COD
Process state	Temperature	VFA	Redox potential
	pH	Bicarbonate alkalinity, alkalinity, total alkalinity	Ammonia
			Intermediate gases of H_2 and CO
Output	Biogas composition (CO_2, CH_4 and H_2S)	Heating and cooling elements	
	Biogas flowrate	VS	

The minimum instrumentation requirements are readily available easy to measure instruments which provide basic monitoring of the input, process state and output parameters of the system. In addition to the minimum level of instrumentation, essential instrumentation requirement includes sensors that characterise the digester environment and give some indication of the microorganism activity, such as VFA, or bicarbonate alkalinity. Additionally, sensors mounted prior to the AD to give the characteristic of the quality of incoming sludge (such as % DS, bicarbonate alkalinity) would enable a reduction in the uncertainty in the process. Within the context of an advanced control scheme, manipulated variables could be adjusted in response to these measured disturbances, in order to meet control strategies. As these new sensor types become readily available, there is still a barrier of reliability, accuracy, and cost to overcome and gain widespread usage in monitoring, control and optimisation of AD systems. This is considered as the main hurdle for new instruments developed for bicarbonate alkalinity and VFA. Sensors that are non-essential or 'nice to have' for control include ammonium which exists in a pH dependent equilibrium with ammonia. An increase in the pH shifts the equilibrium to favour ammonia. Ammonia is toxic to bacteria and acts as an inhibitor when present in the process. However ammonia inhibition is only more evident in protein rich feedstocks (Wiese and Ralf, 2007). Online monitoring of ammonia content ensures a trouble free operation and ammonia probes are relatively commonplace in activated sludge plant operation, with the same probes being applied to digester sludge streams.

As biogas production requires anaerobic environment better yields, redox potential is recommended to be below 330 mV. Feedstocks containing oxygen, nitrate groups and sulphate extensively affect the redox potential and thus the pH, as such redox potential is also recommended as 'nice to have' measurement.

Choosing an ideal sensor for application on existing or new plants need to be conducted with great care. The recommendation for minimum, 'essential' instruments listed in table 3.8 are provided at any site considered for a pilot study.

Conclusions

AD is not a new technology, however due to the biological nature of the process, the relatively harsh environment and the lack of robust validation methods for new instruments, there is a general lack of available instrumentation for measuring the biological and chemical state in the digester vessel. In addition, gaps in the core knowledge of the underlying mechanisms involved make it difficult to quantify the need for a specific instrument. Continuous developments are ongoing with respect to more robust, sophisticated sensors in order to provide insight into the major uncertainties and disturbances in the AD process. However there is a requirement for further development by both academics and industrialists to improve the reliability of new instruments and also the applicability of the information provided by these instruments for automated monitoring and control systems. Clearly the benefit of applying new instrumentation is improved monitoring and better operator understanding with more flexibility with respect to the operation of the process. Additionally, new sensor data provides information to further understand and improve the process. In most cases, biological and chemical laboratory data such as alkalinity and VFA concentrations is used as 'backup information' to better inform daily operation, rather than for closed loop optimisation. Use of such data for developing soft sensor models may provide frequent prediction of VFA to improve the daily operation and control of the process. Hence, information from such a sensor should be collected, interpreted, and acted upon in real-time, within the framework of an advanced control system to optimise the process.

Recent developments from Bioprocess Control (with the Automatic Methane Potential Test System), AppliTek (with the Anasense instrument) and others are paving the way for online monitoring and control of AD systems. As these instruments have not achieved widespread industrial usage, it is difficult to assess the reliability and accuracy of them. For example, the Anasense® instrument has been validated on both pilot scale and industrial scale by its developers. Their conclusion was that the system requires further developments in order to improve its robustness, especially in the presence of highly charged cations (Molina *et al.*, 2004). This demonstrates that robustness is a significant hurdle for some newly developed sensors.

The recommended essential sensors for AD control shown in Table 3.8; beyond this, the minimum level of instrumentation for attempting advanced control in AD should include (1) some means of measuring the disturbances being applied to the process; the most significant disturbances being the rate, concentration, and nature of the feedstock. Whilst the flow is commonly measured, the concentration and the composition often are not measured. Installation of online dry solids meters for this purpose is recommended. Additionally it may be possible to characterise the composition of the feed by accurately tracking the relative proportions of primary, secondary and co-digestion feedstocks being applied to the digester. In addition to this, measuring the ammonia content of the feedstock with an ammonia probe may yield considerable benefits. (2) Some means of measuring and or characterising the biological or chemical conditions within the digester itself. By monitoring and controlling such measurements, the stability of the digester can be maintained. Of the available sensors, pH and ammonia probes appear to offer the best chance of producing repeatable and reliable information. The Anasense®

probe for measuring VFA's is an exciting development, but it may not be sufficiently robust to allow for industrial process control. Furthermore if such an instrument is trialed, then there should be a parallel development of a software based sensor, which may prove to be considerably more reliable. Chapter 7 volatile solids soft sensor development aims to increase the level of monitoring on the process and further development of soft sensors can help improve the level of monitoring significantly.

Additional improvements can be gained by closely working with instrumentation providers such as Geotech to develop more robust reliable instruments. As part of this research, Perceptive Engineering Ltd engaged with Geotech to trial the Capilex VFA instrument. Trials with the instrument were not conducted during the period of this thesis; however increase collaborations between AD processers, Universities, instrumentation and technology providers can improve the development of increase robust instruments and the level of monitoring on the AD system.

4 Methodology

4.1 Introduction

Traditionally AD systems have been constructed as large civil engineering projects and the need for monitoring, control and optimisation has been a low priority and as such retrofitting new instrumentation can be difficult. New AD systems currently being built are however more automated and involve input from cross disciplinary fields. Although some of the systems involved in this study are fairly new, there is still a limited degree of instrumentation and monitoring. Therefore, there is a need to use techniques to extract as much information from the process as possible to improve the monitoring and control of these complex systems. There are a considerable number of approaches available and the information extraction techniques applied here include principal component analysis (PCA), partial least squares (PLS), recursive least squares (RLS) neural networks (NN), model predictive control (MPC), quadratic programming (QP) and various data pre-processing strategies.

Bioprocesses in general are inherently difficult to control, but there has been a range of successful approaches reported in the pharmaceutical and food industries. In common with other bioprocesses, the characteristic of the AD bioprocess, which exhibits varying dynamics and complexity, makes it difficult to monitor and control.

Data driven methods for developing soft sensors and process models for process monitoring and control through multivariate statistical analysis are widely applied and well established techniques. Within the AD community however, soft sensor application on industrial processes are limited. The industries perception of the AD process is changing and moving away from the AD process being a waste reduction process to a manufacturing process with high value output products, for which there is increasing need to improve the process through enhanced instrumentation and control.

The overall aim of the research presented in this thesis is to design an integrated monitoring and optimal control system for the supervisory operation of anaerobic digesters (AD). There are several sub-objectives required to achieve this aim:

1. Quantification of the baseline performance of existing plants;
2. Review of existing instrumentation;
3. Modelling of the AD plant behaviour, with the emphasis on biogas production, digester stability and quality attributes of digestate and biogas;

4. Soft sensor development to improve monitoring and measurement systems as required;
5. Assessment of the challenges of a generic AD controller and or optimiser;
6. Optimal integration of AD systems within wastewater treatment works (WwTW s);
7. Assessing the opportunities for an advanced controller on AD systems;
8. Prototype development of controller or optimiser system fulfilling the aims of the user requirement specification (URS);
9. Controller performance evaluation and system improvement.

This will form a complete engineering cycle of specification, design, modelling, implementation and testing as depicted in Figure 4.1. The specification stage involves quantification of the baseline performance, review of existing instrumentation and assessment of the challenges of a generic controller. The design phase will involve using the results of the specification stage to formulate the URS developed through the benchmark analysis (Chapter 5). Modelling for the controller and soft sensors constitute the modelling step. Prototype development of the advanced controller will form the development stage which will then be tested and evaluated through integration of the system on WwTW and controller performance evaluation.

Quantification of baseline performance of existing plants has enabled key strengths, weaknesses, opportunities and threats affecting the project aim to be identified. Example of strengths include: (1) identification of several commonalities within the results from the four main WwTWs such as variability in certain measurements makes it easier to transfer models from one plant to the next, (2) significant bottlenecks identified for each site and (3) quick fix money saving solutions identified, giving greater value to the overall project. Several opportunities were also identified along with various weaknesses and threats and these are summarised in Table 5.6. One of the key weaknesses found was lack of instrumentation which resulted in the benchmarked systems not being fully evaluated on a physiochemical and biological scale. This also posed a greater threat as without adequate instrumentation on the process to monitor key parameters; the aims of control cannot be achieved. This led to the need to fully review instrumentation on the AD process. Soft sensor application on the AD process was identified as a key means of overcoming the instrumentation limitation on the process, while at the same time recognising that soft sensors are also reliant on instrumentation.

As a consequence a number of studies were carried out to develop soft sensors for volatile solids and volatile fatty acids (VFA).

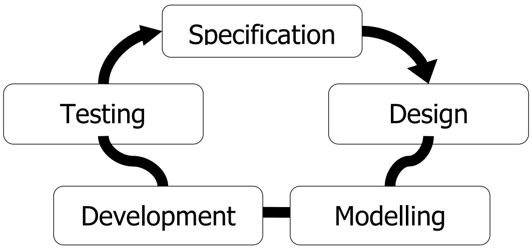


Figure 4.1 The engineering life cycle

Several methods were required to achieve the aims of the nine objectives, which included quantitative and experimental mixed techniques with various methods to evaluate, compare and contrast behaviour. The approaches can be classified into three main groups comprising of (1) system identification (2) modelling and (3) controller design methods. These will be covered in detail in Section 4.2.

4.1.1 Research questions

Advanced control such as model predictive controller (MPC) has had much industrial success. The feasibility study carried out as part of this research revealed that due to the nonlinearity, complex dynamic and highly constrained characteristic of the AD process, an advanced controller may be able to optimise and improve the process significantly. MPC can be the route to implement advanced control and Perceptive Engineering Ltd, the industrial sponsor for this project has the capabilities in MPC applications to support the project. Therefore the question here was; is MPC the best controller regime for AD, and if so, to what degree can MPC improve the process by?

In addition, the feasibility study revealed that due to a lack of instrumentation, the AD process is difficult to control. Therefore can a conventional controller optimise the process through improved instrumentation and better monitoring? From the instrumentation review, the minimum level of instrumentation required for the efficient monitoring of the AD systems was discussed. Once these sensors are applied, how useful is the data generated and how can the information from the data be used to improve the control of the process?

There are questions associated with the overall aim of the project, concerning the different technologies and complexities of AD systems. How transferrable are the findings from the benchmark, inventory control and soft sensor studies applied to different AD systems so far? Is the same level of instrumentation required for the different AD technologies? What are the similarities between AD systems and what are the significant differences? If there was a different population of microorganisms would the same parameters need to be monitored and controlled?

The process of developing the research started with the conceptual phase of formulating the ideas into a realistic research design. Following successful application of advanced control solutions on wastewater treatment processes (WwTP) (activated sludge processes in particular) by Perceptive Engineering Ltd (O'Brien *et al.*, 2011); market research analysis was conducted considering the opportunities for advanced control on ADs. The consortium was formed and the aims of the feasibility studies were then set. Through the initial literature review, the scope and significance of the problem was understood and the gaps in the current state of art were identified.

4.1.2 Research design

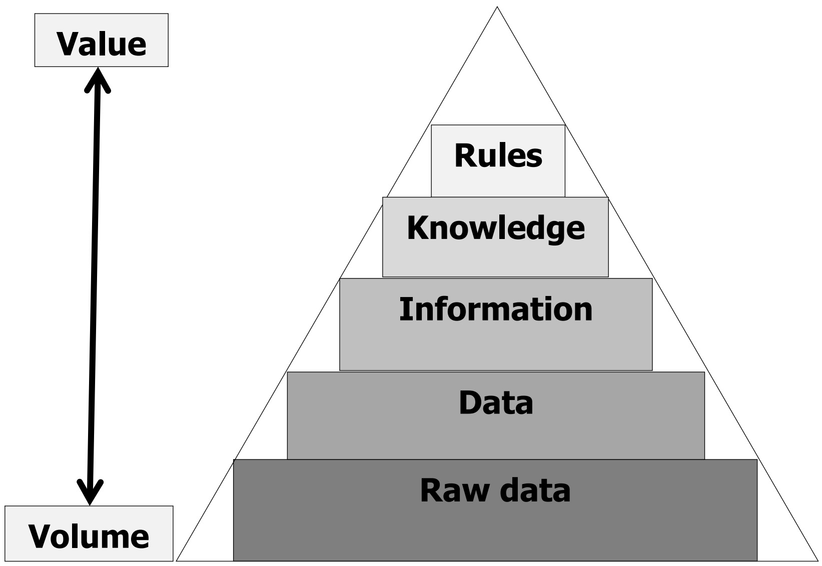


Figure 4.2 Knowledge extraction from data pyramid (Xue Zhang Wang, 1999)

The overall research aim of this project is to evaluate whether an advanced controller such as MPC can improve the AD process. Determining whether the aims have been achieved will require three fold technical justifications of assessing the improvements observed through MPC; the financial case to ensure that the payback period for installing the controller is within the time frame set by the consortium and the application is ethical, sustainable and transferrable to other AD systems. Critical to the success of this is instrumentation, access to industrial AD processes and knowledgeable engineers.

Figure 4.2 demonstrates the stages of data mining from which information and knowledge are extracted from raw data. This is the underlying theme throughout the various studies undertaken within this project. Data can exist in any form with no significance, knowledge or information beyond its existence. Thus raw data may exist in large volumes whilst yielding little known value or useful transparent information that can easily be understood. Selection of raw data and pre-processing provides data that can be transformed into information. Rules and decision making tasks can then be performed from interpretation of the information into knowledge, enabling data to be transformed from a data rich source into information rich output moving up the pyramid.

From the lower levels of the pyramid upwards; the value in knowledge increases whilst the volume of data decreases. On industrial AD processes hundreds of parameters may be measured, of these only a limited number may be of interest for operating the process. Managers and high level decision makers may monitor or require knowledge from only a couple of key performance indicators (KPI's) to make decisions about the process. Thus the knowledge of the process increases whilst the volume of data decreases. Within this project, large volumes of data were collected during the feasibility stage to gather information about the various processes. This was used as knowledge for building models from which rules such as controller settings, ranges for operating parameters and measures of performance indicators could be set to evaluate the system behaviour. In terms of the modelling aspects of this project, at one site data from approximately 800 signals were obtained and of these only 50 signals were deemed useful for assessing the status of the process. For the soft sensor study only 8 process data signals were selected from which the final model only used two signals which related to the output parameter. Thus the use of low volume data to obtain knowledge from an initial high volume of data is a common theme within this research.

4.1.3 Overview of applied methods in thesis

A range of techniques are applied to fulfil the needs of the studies within the project. These will be covered in detail within the different sections of the thesis and a summary is given here. The various methods include: system identification; methodology for soft sensor development; benchmarking of industrial processes; controller design; and optimiser design. The five steps to be followed for building models, making use of the methods and achieving the aims of this project are:

1. Selection of raw data (raw process data for benchmark, DoE and perturbed or excited plant data);
2. Data pre-processing;
3. Knowledge interpretation (model building);
4. Information transformation (soft sensor development);
5. Decision making from established rules (advanced controller application).

Selection of raw data is a critical point in the overall research to avoid the concept of 'rubbish in, rubbish out' outcome of process data modelling. The nature of the results generated from the various modelling techniques will depend heavily on the quality of data used for the modelling. Following selection of useful data, inadequate data pre-processing can result in unreliable models. Knowledge interpretation from these models is also essential and requires deep understanding of the AD system.

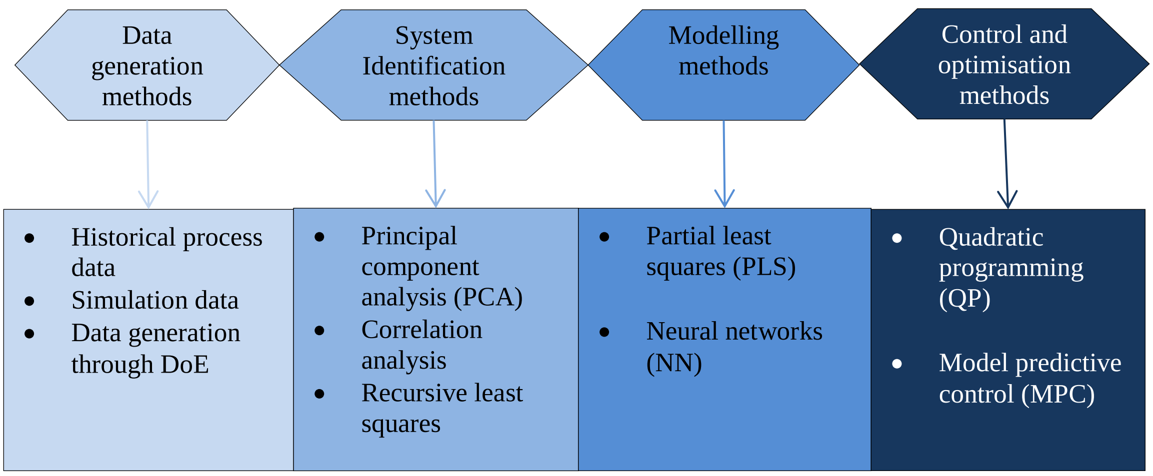


Figure 4.3 Levels of methods

In moving towards improved operational objectives it is necessary to consider data generation, system identification, modelling and control and optimisation methods.

These are shown in Figure 4.3. Data generation methods applied here include the use of historical process data, simulated and excited or DoE generated process data. Due to the large operational difference in laboratory scale AD and industrial ADs, laboratory assessments are not considered for this research. Historical process data is first used, as years of data are freely available. Simulations are also used to generate data, as these are cost effective ways of obtaining data; however they are not as accurate representation of industrial ADs due to modelling difficulties arising with bioprocesses.

System identification is the approach of building mathematical models of dynamic systems based on observed data from the system (Lennart, 1999). System identification forms a major part of this research. Once data has been generated, a series of system identification methods can be applied to gain knowledge about the process. This broad area covers many methods including linear, nonlinear, parametric, nonparametric, hybrid structures. The simplest approach to system identification is impulse response identification, where the impulse needs to be large enough to enable the response to be greater than the noise within the system (Dimitry, 2005).

4.2 Modelling

Science is generally based on inference of models from observations and studies on their properties. The models become the paradigms, hypothesis, laws of nature and interpretation of the true system. The model thus is the concept of how variables relate to each other when they interact with the system. As true representation of the system cannot be achieved through models; models are evaluated on their usefulness rather than truth (Appels *et al.*, 2008). The system characteristics that model approximates can be defined by:

- Linearity - obeying the principles of superposition with additive and scaling properties;
- Causality - if output depends only on the present and or past values), stability (if the system does not diverge;
- Memory - whether the system depends on the present value alone or can it depend on the past and future values too;
- Time invariant - lack of time dependency on the system, such that the system’s response to a given input does not depend on the time the input is applied.

These system properties must be considered when building the model. The model building has three basic entities; these include (1) the data set, (2) the model structure and (3) model identification methods. This can consist of many steps and thus within this research the model building approaches cover the stages of problem statement, defining the modelling environment, conceptual modelling, model representation, implementation, verification, initialisation, validation, documentation and model application.

4.2.1 Model identification techniques

The control and optimisation of AD systems require an accurate dynamic model of the process. However modelling of AD systems often result in high order nonlinear models with several unknown parameters.

Least squares (LS) is the most popular cost function for parameter identification in AD models. LS generally describe the approach of solving an overdetermined system of equations through an approximation. The aim of the method is to minimise the sum of the squares of the residuals rather than solve the inexactly specified system (Cleve, 2004). The LS estimation can be constructed in the simple form of

$$\boldsymbol{y} = \mathbf{Ax} + \boldsymbol{v} \qquad \text{Equation 4.1}$$

Where y constitutes sensor measurement, x is the estimator, v is the unknown noise or measurement error and the ith row of A characterises ith sensor. The estimation is conducted by choosing $\hat{x}$ that can minimise $\| A\hat{x} - y \|$. This is the deviation between what is actually observed by (y) and what can be observed if $= \hat{x}$, with no noise where $v = 0$. The LS estimation is thus $\hat{x} = (A^T A)^{-1} A^T y$. This gives the maximum likelihood estimation of the parameters (Stephen, 2008).

With regards to a control solution for the AD process, it is useful to have a model of the AD system available online that updates as the process changes. Methods for solving such problems are usually called adaptive methods. Identification techniques for such systems are termed recursive identification methods (Lennart, 1999). Recursive least squares (RLS) is a recursive variant which improves the efficiency of LS algorithm. The RLS algorithm works by moving through a time history dataset and continually updating model coefficients as it passes through the dataset. The algorithm uses the covariance matrix weight factor, which determines how quickly the model coefficients are changed. Recursive identification tools are common for handling systems with varying dynamics as in the case of the AD process. A new parameter set can be estimated for each observation. While the update of parameters may be attractive, there are a number of shortcomings including:

- Numerical instability and sensitivity to outliers;
- Sensitivity of RLS to the initial conditions of the algorithm;
- Slow tracking capability for time varying parameters (Jiang and Zhang, 2004).

However RLS is still a popular approach for online parameter estimation applications and as such the method is used widely in this research.

4.2.2 Soft sensor based methods

The behaviour of a process is indicated by the state of the process and the process inputs that impact on it. The states of many secondary 'explanatory' variables reflect the states of the primary variables. Secondary variables are variables whose values can be explained by changes in other variables such as primary variables. With the abundance of computer aided tools available, the concept of inferential or software measurement is well defined and inferential model building techniques are commonly applied. However while the concepts are common, there are still key design factors to consider. These include the characteristic of the data, the need for robust pre-processing techniques to carefully remove noise and outliers within the data. The selection of the correct secondary outputs and inputs for model building, in combination with process knowledge is essential in generating a model that is both mathematically applicable and sound from an engineering perspective. The model must then be tested for reliability based on how the estimator deals with measurement problems, delays, infrequent sampling and the irregular return of information.

Process stability is a measure of the consistency of the process with respect to process characteristics; a stable process behaves consistently over time. In the digestion process the different environmental condition requirement for the acid and methane forming bacteria is the major cause of instability in the process, this is followed by inhibition and foaming. Due to the large instability in AD processes, it is common in practice to construct digesters larger than the optimal size to reduce the impact of instability. This is expensive with respect to construction, operation and maintenance. By monitoring key variables in the process, instability can be reduced, but to do so requires knowledge of the causes of instability.

Digester instability can be a result of hydraulic, organic and toxic overloading (Graef and Andrews, 1974a). Hydraulic overloading is a result of an organisms inability to reproduce before being washed out due to the reduction in the residence time. The residence time is defined as the reactor volume divided by the influent sludge flowrate. Organic overloading is a result of build-up of volatile acids which can cause inhibition to methanogenic organisms. Toxic overloading is generally caused by feeding the digester with materials which can kill methanogenic organisms. These may include heavy metals, ammonia, detergents, organic chemicals and cations. Thus monitoring of key parameters that can provide indication of instability in the digester can improve the monitoring to avoid digester failures.

Table 4.1 Examples of modelling techniques on AD systems

Measurements	**Estimation methods**	**Uncertainty**	**Reference**
CH_4	Non-linear regression with the Marquardt-Levenberg algorithm	Covariance matrix-FIM	Lokshina et al. (2001)
TSS, VSS, Biogas, COD, VFA and gas composition	Least squares criterion	Confidence region and linear confidence interval	Kalfas et al. (2006)
Biogas	Gradient search technique	Confidence region	Batstone et al. (2009)

Various methods have been used for software or inferential sensor developments. Table 4.1 lists examples of AD system modelling techniques for estimating some useful AD parameters, and some of these techniques will be explored in detail in Chapter 7.

4.2.3 Control approaches on AD processes

The term advanced control can be misleading in its meaning. In its early days it was taken to mean any alternative control to the traditional three term (proportional, integral, derivative) controller. However it can describe the practice of using elements from various disciplines that include control engineering, decision theory, artificial intelligence, statistics, signal processing, hardware and software engineering.

The three phase AD process involves sequential and parallel reaction pathways. The complexity and uncertainty in the dynamics of the microorganisms involved in the process make it difficult to model. In comparing multi-organism systems to single organism systems, it is widely accepted that no single kinetic model can describe all the complexities of the single organism system; it is therefore a major task for scientists and engineers to model multi organism systems. Initial attempts to model the AD process concentrated on the rate limiting step, but this varies for different conditions. In general hydrolysis is the rate limiting step. Most of these models in literature (Appels *et al.*, 2008) are very specific and steady state in nature. These are simple models, and most tend to fail to accurately describe the digester dynamics. The aims of these models are generally to achieve the following:

- Estimation of process states such as reactor volume, biogas production, its compositions and retention time etc. for determining the performance of a specific system;
- Allow sensitivity analysis to be conducted for various process parameters;
- Allow assessment of model differences and knowledge of where the process can be improved;
- Whole plant optimisation capability providing understanding of how the digestion process can affect the downstream processes (Appels *et al.*, 2008).

Within the AD process, the acid and methane forming microorganisms differ in physiology, nutritional needs, growth kinetics and sensitivity to environmental conditions. Maintaining the balance between these microorganisms is crucial to gain stability of the whole process and this is generally the primary cause of digester instability (Jean-Philippe Steyer *et al.*, 2006). The complexities of the AD process increases the number of control objectives, thus from the feasibility results undertaken so far, an ideal control scheme for the process should aim to have the following objectives:

1. Pathogen reduction to meet compliance;

2. Optimise biogas production;

3. Optimise CH_4 composition;

4. Optimise the multiple attributes of digestate quality;

5. Improve the energy balance of the AD process and with other processes on the site to optimise efficient use energy;

6. Align gas production with ‘triad’ periods to gain maximum revenue;

7. Align combine heat and power (CHP) unit with AD for optimum energy production;

8. Limit inventory disturbance to the upstream and downstream process (several hierarchal control objectives);

9. Control of temperature to a minimum variation;

10. Control of % DS to enable optimum organic loading rate (OLR) feed without overloading digester;

11. Control of retention time to meet compliance and optimise throughput;

12. Control of feed flow with minimum variability to improve stability;

13. Odour reduction control;

14. Foam reduction control.

Some of these objectives conflict with each another and require sophisticated control systems to achieve the best balance of the objectives. There is thus a requirement for a complex multi objective controller. An ideal controller will therefore need to meet or balance all these objectives or as many as possible. Most industrial AD control applications mainly include simple PI and PID controllers to control temperature and levels, however there are examples of pilot and laboratory scale artificial neural networks (ANN), fuzzy logic, linear and nonlinear model based control (Pind *et al.*, 2003) on industrial AD systems and these tend to be single objective in nature. This limitation of a single input, single output control strategy, often linear in form is insufficient to handle a complex process such as AD.

The AD process has large unknown number of microorganisms in a population from various sources and different processing units. The lack of complete knowledge of the system environment and direct cause and effect relationships of the various parameters make the task of achieving the goals of the project complicated. Varying AD configurations, system characteristics, structures (due to physical, geographical and legislative factors) and input characteristics limit the use of generic models to achieve the aims of control for AD systems (Wahab *et al.*, 2007). These have resulted in varying range of control strategies and structures applied.

4.3 Advanced control

Process control in bioprocesses aims to influence the individual behaviour of the different living cells in the digester by controlling their extracellular environment (Boudreau and McMillan, 2007). The extracellular environmental state condition can be determined by process variables. These process variables must be measured or inferred from other measurements to enable them to be controlled. Process control aims to transfer variability from process output to the process inputs subject to measurement resolution, noise, loop dead time, repeatability and controller tuning (Boudreau and McMillan, 2007).

4.3.1 Model predictive control

MPC also known as receding horizon control (RHC), dynamic matrix control (DMC) and generalised predictive control (GPC) consists of control algorithms which numerically solve an optimisation problem at each step (Dimitry, 2005). The algorithm used in this research is based on the minimisation of the cost function:

$$J = \sum_{i=1}^{N} [e_{i+1} P e_{i+1}^{T} + \Delta u_i Q \Delta u_i^{T}] \qquad \text{Equation 4.2}$$

Where the weighting matrices are given by P and Q over the horizon, N. Δu is the vector of the current and future control moves subject to constraints, e is the vector of the setpoint tracking errors, i is the sample point.

MPC models provide the exponential and ramping time response for deviations about operating points. MPC involves the operation of multivariable controllers under process constraints (Sandoz *et al.*, 2000). These constraints may be ‘hard’ constraints of manipulated variable (MV) minimum and maximum limits, incremental move limits, as well as 'soft' constraints such as the controlled variable (CV) minimum and maximum limits. This makes the MPC controller ideal for constraint optimisation problems found in the AD process. There are several methods available to manage such constraints, such as long range (LR), quadratic programming (QP) and a combination of these two; long range QP (LRQP).

The PerceptiveAPC (*Perceptive Engineering Ltd*, 2012) MPC solution uses the QP constraint management method. The QP solver aims to optimise by minimising or maximising a quadratic function of multivariable form, subject to linear equality and inequality constraints.

QP can be incorporated into MPC for constraint linear control, which is the general, conventional approach. General objectives of an MPC includes (i) input, output constraints violation prevention (ii) driving CVs and MVs to steady state optimal values, (iii) prevention of excessive moves of MVs and controlling the plant when signals and actuators fail. There are therefore trade-offs and approximations to translate these objectives into a mathematical problem statement for defining the character of the controller. Different possible solutions exist for defining this and therefore naturally there are several MPC control formulations. Perceptive Engineering Ltd has several model forms incorporated into PerceptiveAPC which include finite impulse response (FIR), autoregressive with exogenous inputs (ARX), linear and nonlinear modelling with NN. The steady state and dynamic optimisation objective is achieved with QP and output horizon through finite horizon. Most MPC products are based on linear empirical models, however nonlinear processes such as the AD can be represented by a discrete time nonlinear model such that:

$$\boldsymbol{x_{k+1}} = \boldsymbol{f}(\boldsymbol{x_k}, \boldsymbol{u_k}), \boldsymbol{x_k} \in \mathbb{X}, \boldsymbol{u_k} \in \mathbb{U}, \qquad \text{Equation 4.3}$$

Where $x_k \in \mathbb{R}^{n_x}$ and $u_k \in \mathbb{R}^{n_u}$ are the plant states and control action at time k.

$$\mathbf{min} \quad \sum_{\boldsymbol{i=0}}^{\boldsymbol{N-1}} \boldsymbol{l}(\boldsymbol{z_i}, \boldsymbol{v_i}) \qquad \text{Equation 4.4}$$

$$\boldsymbol{s.t} \quad \boldsymbol{z_{i+1}} = \boldsymbol{\bar{f}(z_i, v_i)}, \quad \boldsymbol{i} = \boldsymbol{0, \dots, N-1}$$ Equation 4.5

$$\boldsymbol{z_0} = \boldsymbol{x_k},$$ Equation 4.6

$$z_i \in \mathbb{X}, \; v_i \in \mathbb{U}$$

Where N is the horizon length, x_k is the initial condition which is the plant state at time step k. z and v are used as the predicted state and control in the formulation of the MPC, to differentiate between the actual plant state x and control u. The plant model equation and the objective function is represented by $\bar{f}(.,.)$. This function is commonly linear $(Az_I + Bv_i)$ for most industrial applications (Rui, 2010).

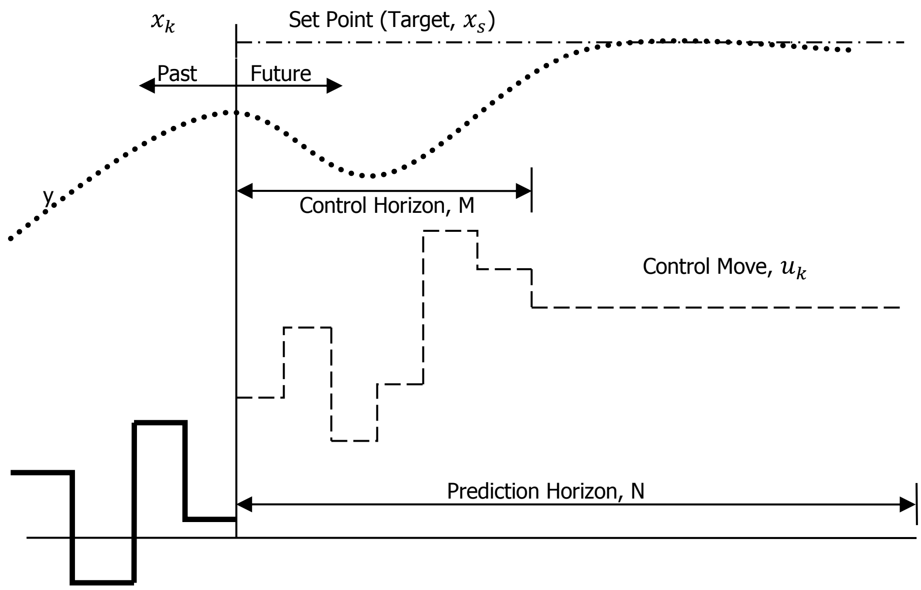


Figure 4.4 Moving horizon strategy of MPC

Figure 4.4 demonstrates the moving horizon approach for MPC. The prediction horizon predicts future variation of the controlled variables to a finite time. A series of control moves are calculated for the manipulated variable, and predict incremental changes in process outputs from incremental changes in process inputs. It is incremental in the sense that manipulated variables at each sampling time are updated by the optimisation algorithm, where the cost function of minimisation is the difference between predicted outputs and the set points. Each consecutive optimisation therefore differs as the prediction horizon recedes in time. In general MPC control may use incremental models of FIR and ARX. These models use current and previous values of process cause signals to predict process effect signals.

There are a series of calculations involved in MPC control execution; this is depicted in Figure 4.5. Step one requires knowledge of the current state of the process such as the state of the inputs of disturbance, manipulated and output control variables. The steps that follow generally aim to ensure the status and direction of the process is moving towards steady state and dynamic optimisation (Qin and Badgwell, 2003).

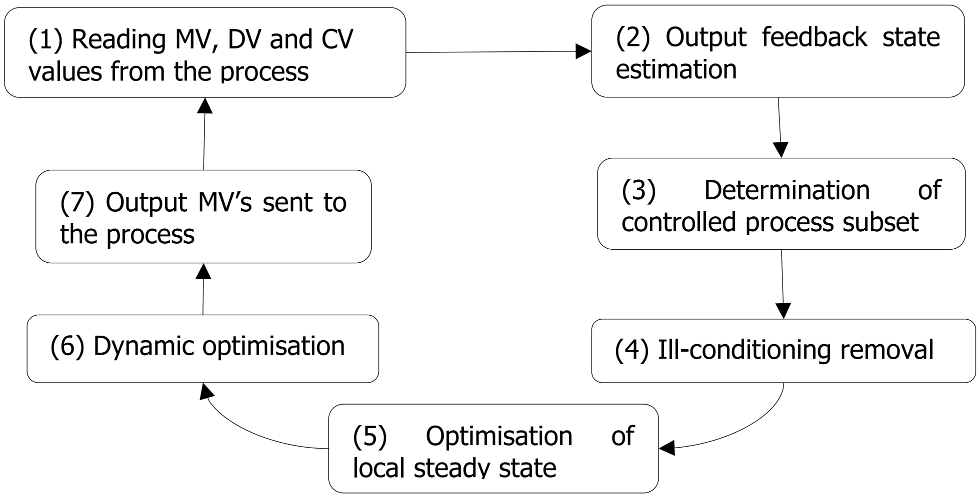


Figure 4.5 Series of flow of calculations conducted for MPC control (Qin and Badgwell, 2003)

State estimation aims to estimate the dynamic state of the system. Failure to include this concept into the MPC may result in the need for further instrumentation to estimate additional process measurements. Other effects may include (1) for integrating or unstable processes, the use of ad hoc fixes to remove offsets and (2) limitations on unmeasured disturbance models. Thus most industrial MPC control calculation design incorporates some feedback mechanism.

The determination of the controlled process subset requires the controller to determine which MV's to be moved and which CVs to be controlled. This will include the selection of high and low level control outputs.

Ill-conditioning occurs where a small error in the calculation can result in larger errors. In the case of MPC, small changes in the controller error can lead to large MV moves with a high condition number in the process gain. Such situations require examination of the condition number at each control execution in order to exclude the ill-conditioning impact.

The majority of industrial MPC controllers execute local steady state optimisation at each control cycle. This enables the steady state inputs and outputs to be close to their targets. The controller may use a linear program (LP), QP or both to conduct the optimisation and this dependent on the provider and or the nature of the problem.

In terms of dynamic optimisation, changes are made to the MVs to drive the process to the set steady state by the MPC controller without violating constraints. The constraints can be hard (should never be violated), soft (some violations are allowed) or set point approximations where there is penalisation on deviations above or below the setpoint (Qin and Badgwell, 2003).

Common reasons for failures in industrial applications of MPC include; constraints, unique performance criteria, process nonlinearities, model uncertainties and cultural reasons with regards to education, people or financial reasons (Qin and Badgwell, 2003). The cultural reasons such as education, the people or financial reasons are very critical to the success of the controller in the long term. This is because with a good understanding of the process from the control engineers, a reasonable MPC with little model uncertainties can be designed and implemented. The controller is then left with operators, who will manage and make use of the controller dependent on their training and the level of time available to maintain the controller which may be financially constrained. As per the simulation activities conducted so far, some of these are eliminated; however the nonlinearities and model uncertainties present in AD systems may make it difficult to achieve a successful application of MPC.

4.3.2 Dynamic model structures

FIR and ARX are popular linear model structures. Process models are central to MPC and FIR is a popular model structure of choice for MPCs, due to the ease of fitting complex dynamic systems without the selection of a model structure. FIR uses lagged inputs for capturing the system dynamics of the process and therefore is commonly non-parsimonious and a large amount of model parameters are needed. These follow a more complex modelling approach and includes large data sets whereas parsimonious models like ARX aim for simplicity (Nounou and Nounou, 2007). ARX uses both lagged inputs and outputs to represent the output and offers greater simplicity. Parsimonious models also offer models with few degrees of freedom, which can avoid over-fitting a situation where the model works well in a given range but breaks down in predictability outside that range. The FIR model can be described as:

$$\boldsymbol{y}(\boldsymbol{k}) = \sum_{\boldsymbol{j}=\boldsymbol{1}}^{\boldsymbol{N}} \boldsymbol{B}_{\boldsymbol{j}}\boldsymbol{u}(\boldsymbol{k}-\boldsymbol{j}) + \boldsymbol{v}(\boldsymbol{k}) \qquad \text{Equation 4.7}$$

Where N corresponds to the settling time and $u(k)$, $y(k)$ and $v(k)$ are the process input, output and noise vectors respectively. B_j is the matrix of the coefficients to be identified models of the FIR can only be applied to stable processes (Qin, 1998; Nounou and Nounou, 2007).

The ARX model structure predicts the process and the future trajectory of the effect signals using current and past process cause signals. For a multivariable system such as the AD, ARX can be represented by:

$$\boldsymbol{y}(\boldsymbol{k}) = \sum_{\boldsymbol{i}=\boldsymbol{1}}^{\boldsymbol{n_y}} \boldsymbol{A_i} * \boldsymbol{y}(\boldsymbol{k}-\boldsymbol{i}) + \sum_{\boldsymbol{j}=\boldsymbol{1}}^{\boldsymbol{n_u}} \boldsymbol{B_j} * \boldsymbol{u}(\boldsymbol{k}-\boldsymbol{j}) + \boldsymbol{v}(\boldsymbol{k}) \qquad \text{Equation 4.8}$$

Where $u(k)$ and $y(k)$ are the inputs and outputs of the process data vectors. $v(k)$ is vector representing the noise and A_i and $B_j$represent matrices for the model coefficients and n_y and n_u are the time lags for the inputs and output variables. This method allows use of steady-state regression techniques for modelling dynamic processes (Qin, 1998; Su *et al.*, 2009). Modelling in this form has been applied to AD processes (Premier *et al.*, 1999).

4.3.3 The quadratic programming algorithm

The aim of the quadratic program optimiser is to move the process to a steady state optimum operating point. The constraint controller key objective is to hold process variables at specified setpoint values or within their constraint limits subject to the actuation variable constraint limits (*Perceptive Engineering Ltd*, 2012).

$$\boldsymbol{J} = \sum_{\boldsymbol{i}} \boldsymbol{a_i} * \boldsymbol{M_i} + \sum_{\boldsymbol{j}} \boldsymbol{b_j} * \boldsymbol{A_j} \qquad \text{Equation 4.9}$$

Where M_i represents the process variables, A_i as the actuation variables and the cost assigned to the process and actuation variables as a_i and b_i. The optimum is maximised subject to process and actuation constraints. The algorithm is available in most industrial MPC frameworks where the dynamic model associated with the constraint controller is used to generate the steady state model for use in the optimiser directly. The QP algorithm is used in the inventory simulation study Chapter 6; to optimise the system and compare an MPC with and without an optimiser.

4.4 Multivariate statistical analysis

Decision making activities in terms of the monitoring and control of AD processes require chemical measurements that are reliable and that can be used to enhance the process control understanding. Rapid technological advancements have resulted in large volumes of data being stored and retrieved easily, enabling an increase in the application of data based modelling.

The growing use of data based modelling over the past forty years has resulted in the advancement of mathematical and logic based methods. The success of data based technologies is however a result of how accurately and successfully a system is defined and measured. There has been considerable success in multivariate calibration, multivariate process modelling & monitoring & pattern recognition, calibration & discriminant analysis as well as structured modelling (Wold and Sjostrom, 1998). Pioneers such as Svante Wold and Bruce Kowalski combined mathematical modelling, multivariate statistics and chemical measurements to develop the field of chemometrics. These achievements were only possible due to the use of established methods such as principal component analysis (PCA) and partial least squares (PLS).

The basis of identifying a good quality model relies on the quantity and quality of the data used for the modelling. It has been suggested that the input data must have a minimum of 5 measured changes that are of the order of 5 times larger than the noise associated with the input (Boudreau and McMillan, 2007). The historical data generated for the feasibility studies lacked this quality attribute and therefore a DoE was required to improve the quality of the data. This can be carried out by conducting step or pseudo random binary sequence (PRBS) tests. The generation of such data can take months to years for a system such as the AD.

A further challenge is that some critical parameters such as those affecting the safe sludge matrix requirement cannot be changed as it will yield non complying product. These impose constraints and set the boundaries on the process. Thus processes models such as those for AD are bounded and limited by the degree to which the process can be excited.

4.4.1 Principal component analysis

PCA was developed in 1901 by Pearson (Pearson, 1901) with the geometric optimisation explanation and later Hotelling's in 1933 (Hotelling, 1933) reported the algebraic derivation of PCA. Given a set of data consisting of a large number of interrelated variables, PCA aims to reduce the dimensionality of the problem whilst retaining the major sources of variation in the data set (Jolliffe, 2005). For a vector of x with p random variables, if the variance of p random variables, the structure of the covariances or the correlations between the p variables are of interest, then for a large complex p variables, it is best to look for some of the p derived variables that preserve most of the information given by variances and correlations or covariances (Jolliffe, 2002). PCA concentrates on variances and places less emphasis on covariance and correlations (Jolliffe, 2002). However although PCA focuses on variance, it does not ignore correlations and covariance (Jolliffe, 2005).

The inferential sensor study uses PCA to examine the relationships between variables within the AD process data, since there are a large number of measured quality variables which are highly correlated. Through the approach of PCA, dimensionality of the multivariate data is reduced whilst still retaining the original variables as each principal component is a linear combination of the original variables. This enables the representation of the original data set containing correlated variables, in a new ordinate system that is characterised by uncorrelated variables called principal components (PCs).

$$\boldsymbol{X} = \boldsymbol{T}\boldsymbol{P}^{\boldsymbol{T}} + \boldsymbol{E} \qquad \text{Equation 4.10}$$

Where X is the process variables, T is the score matrix, P is the loadings matrix and E is the errors. X may be decomposed through singular value decomposition (SVD) or nonlinear iterative partial least squares (NIPALS). The procedure was carried out using Matlab software with the PLS toolbox (Wise *et al.*, 2010). The data was first autoscaled before applying PCA since the variables have different units. As PCA aims to capture variation, autoscaling enables all variables to be treated on an equal basis in the analysis and therefore variables that have greater variation due to the magnitude of the variable do not dominate variables with a smaller order of magnitude of variation.

PCA has various assumptions, which include linearity, large variances having important structure and PCs are orthogonal. There are methods available for modelling nonlinear systems with nonlinear PCA approaches (Martin, 2010). Process knowledge is required to determine whether PCs with low variance are noise.

PCA is a common and flexible approach used for data compression, information extraction and preliminary visualisation of samples (Wold *et al.*, 1987; Jolliffe, 2005). The application of PCA may reduce the dimensionality of the multivariate data into a smaller number of PCs than original variables. It enables the representation of the original data set containing correlated variables, in a new reference system that is characterised by uncorrelated variables of PCs. The PCs are linear combinations of the original variables calculated hierarchically and are mutually orthogonal. The greatest amount of variation contained in the original data set is captured by the first PC. Subsequent PCs captures the next greatest possible amount of variance. Once obtained, the loadings and scores can be graphically represented to observe any trends or groupings in the data set, in form of variables and sample respectively.

4.4.2 Partial least squares

Although PCA may be a popular approach in chemometrics for treating sets of data subject to high dimensionality; it does not offer prediction of a response variable. Partial least squares or projection to latent structure (PLS) models predict a process output from linear combinations of a reduced set of independent variables, namely latent variables. These are typically steady state methods, which eliminate correlations between inputs (Boudreau and McMillan, 2007). Predictive models can be constructed for highly collinear systems and involve many factors. PLS is therefore less use for understanding underlying relationships within a set of data but rather has a general purpose for response prediction (Tobias, 1995). PLS was pioneered in the econometrics field by Herman Wold in the late 1960s and later found application in the chemical field by his son S. Wold and others such as H. Martins and B. Kowalski (Wold, 1966; Wold *et al.*, 1973; Kowalski *et al.*, 1982; Wold, 2004).

The method of PLS aims to relate two data matrices of X and Y by means of a linear multivariate model. This method is applied in this research for building predictive models because of its usefulness in dealing with noisy and collinear data (Ericksson *et al.*, 2006). As discussed previously MLS has the tendency for over-fitting, where there may be too many observations. In such cases, there may be a low number of factors (latent variables) that account for most of the variation in the response. PLS extracts the latent factors which account for most of factor variation and thus avoids the overfitting issues if the model structure is selected appropriately.

For processes with large a number of factors where collinearity may exist and process relationships are not well understood such as the AD process, PLS is a useful tool for constructing predictive models of such systems (Tobias, 1995). Principal component regression (PCR) aims to find factors that capture the greatest amount of variance in the predictor (X) variables, whilst multi linear regression (MLR) attempts to find a single factor which best correlates the predictor and the predicted variables. PLS relates to both PCR and MLR and attempts to maximise covariance (Wise *et al.*, 2006). Selection of latent variables (LV) in PLS models is very important as selection of too few or too many can result in under or over fitting of the model, resulting in a model that fits the sampled data perfectly but fails to predict new data well. Over fitting violates parsimony and may lead to poor future performance.

If all the variables in the block are measured in the same units, then no scaling is required. When the variables in a block are measured in different units, then variance scaling may be used. This is conducted by dividing all the values in the variable by the standard deviation of that variable to enable the variance of each variable to be a unity. Furthermore variables can be given different weights depending on their influence on the model.

4.4.3 Inferential measurements

Information is used for operating the plants through monitoring and control as well evaluating the performance of the plant. Predictive models, namely soft sensor, virtual online analysers or inferential sensor can also be built from this information. Modelling of these sensors can follow the data driven approach or model driven. Model driven soft sensors generally are of the form of first principle modelling, which describe the physical and chemical characteristics of the process. The highly dynamic and complex characteristic of industrial processes makes use of such model types difficult for practical use. Data driven soft sensors are therefore more common on industrial processes and generally use PCA and regression techniques.

The general approach for soft sensor development is depicted in Figure 4.6 A robust soft sensor must aim to predict with accuracy, precision and reliability but also cope with measurement noise, data outliers, drifts, missing values and data colinearity

(Kadlec, 2009). Inferential measurements improve reliability and reduce process composition noise but drift and unknowns are inevitable. Data pre-processing techniques used included visual inspection, removal of bad data, outlier detection and treatment, data cleaning including filtering and data alignment to reflect process operation. This process was applied to the simulated and industrial process data selected for the inferential sensor modelling. Once the simulation and process data was available, the model development commenced with initial data inspection.

As the offline process data used for the inferential sensor development was measured infrequently with large variability in when the measurements were conducted, this made modelling with PLS difficult and therefore less likely to be used in basic process control.

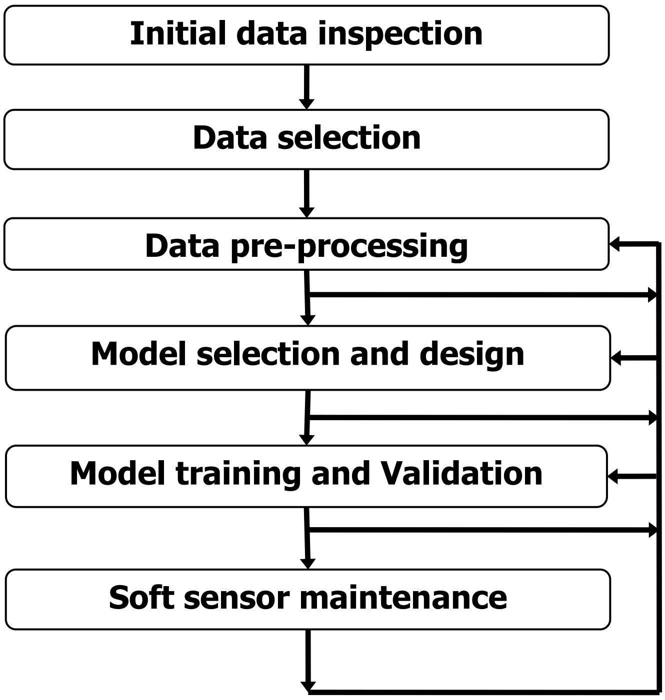


Figure 4.6 Schematic of inferential sensor development process

4.5 Conclusions

This chapter presented a brief summary of key methods used in this thesis. Multivariate statistical analysis techniques are used in Chapters 5 and 7 with soft sensor development in Chapter 7. Multivariate statistical analysis methods are used in this thesis due to the limitations of increased uncertainty in parameter values and variability imposed by models designed with widespread applicability such as ADM1. The virtual plant model ADM1 has many advantages as described in section 2.3.2.

5 Benchmark study

5.1 Introduction

The benchmark study, discussed in this chapter formed the backbone of the feasibility study. Between the three water companies, four sites were selected (1) Blackburn wastewater treatment works (WwTW) (2) Mitchell Laithes WwTW (3) Bran Sands WwTW and (4) Lancaster WwTW. An initial benchmark analysis was undertaken on the Lancaster mesophilic anaerobic digestion system, but it was later upgraded to the Monsal Enhanced Enzymic Hydrolysis (EEH) and a further benchmark analysis was conducted. However due to this change the site excluded from the analysis undertaken in this chapter but the data from this site is included in Chapter 6, with respect to the soft sensor development activities. The general findings from the site contribute to the overall business case and together these four sites provide a good representation of the various AD technologies available to the water industry.

The aim of the benchmark study is to establish baseline performance using process data for the existing plants generalised delay steady state behaviour and in the presence of controlled disturbances. Benchmarking allows the assessment of best practice and the identification of any bottlenecks inherent to the process as well as providing insight into the culture with respect to the daily operation of the process. The benchmark study addresses the following goals:

- Comparison of the operational objectives, review current process operational performance and defining, quantifying, and qualifying the performance metrics;
- Investigate the performance of the existing regulatory control system and identify areas for improvements in terms of advanced control monitoring;
- Determine the level of accuracy and precision for current instrumentation and sampling methods for determining systematic and random errors;
- Calculate process capability and performance indices for key process variables.

A crucial part of the benchmarking exercise is focus on monitoring and measurement systems with respect to control as identified in Chapter 3; this is addressed through the assessment of (i) process performance (outputs of the process); (ii) the inputs required to achieve the outputs and (iii) other parameters to ensure that performance is delivered (Ahmad and Benson, 1999). The robustness of these measurements depends on a number of factors including the availability of data that provide relevant information, and the ability to trust the data. Online measurements form the basis of control systems and thus obtaining data from reliable and correctly appropriately operated measurement systems is crucial. There is a requirement to avoid systematic measurement errors. Calculating the uncertainties in the instruments allows the controller to be parameterised and hence operate close to the constraints.

The use of historical process data to benchmark a site enables the determination of the behaviour of the plant and allows the modelling of its performance through the data generated from the various processes. There are several challenges with this approach:

- The availability of the necessary sensors for monitoring key performance indicators (KPIs);
- Accuracy and validity of the measurement systems for the evaluation of systematic errors;
- Precision and reliability of the measurement systems to account for random errors.

Without testing the various measurement systems against these challenges, an assessment of the accuracy and reliability of the data generated cannot be undertaken. The data used for the analysis is thus assumed be a good representation of the process, prior to the analysis.

For the identification of relevant KPIs to satisfy the project aims, a hierarchy of KPIs were identified Figure 5.1. Every organisation will have a set of KPIs to measure their performance and progression. These may include lost time, employee motivation, customer written complaints and net energy usage etc. Within the water industry these may be sewage treatment works breach of consents, water quality, sewer flooding incidents and pollution incidents. With respect to the AD project, corporate KPIs for the water companies include a reduction in net energy usage and reduction in CO_2 emissions. Electricity consumption generally accounts for over 70 % of the water companies CO_2 emissions and hence reducing the reliance on imported electricity is important for the companies involved, and this can be achieved through the utilisation of the biogas produced from the AD process. The energy generated is mainly used on site with excess exported to the national grid. The objective for the 3 water companies is then to optimise the AD and combined heat and power (CHP) processes to reduce their reliance on imported energy. This also satisfies government incentives with respect to increasing renewable energy resources (ofgem, 2011b). Exported electricity from AD processes is of greater value compared to electricity generated from conventional fossil derived sources, as per the renewable obligation certificate (ROCs), feed in tariffs (FITs) and renewable heat incentives (ofgem, 2011a). Maximum energy production and minimum energy usage thus form the basis of the corporate KPIs. Business unit KPIs differ between the 3 companies. United Utilities (UU's) aim is to improve digestate quality, whilst the exploration of co-digestion opportunities of other waste streams with sewage sludge is a priority for Northumbrian Water Ltd (NWL). Yorkshire Water's (YW) objectives are the overall optimisation of the AD process with CHP operation. From these business KPIs, various control KPIs are formed and setpoints to be investigated are generated.

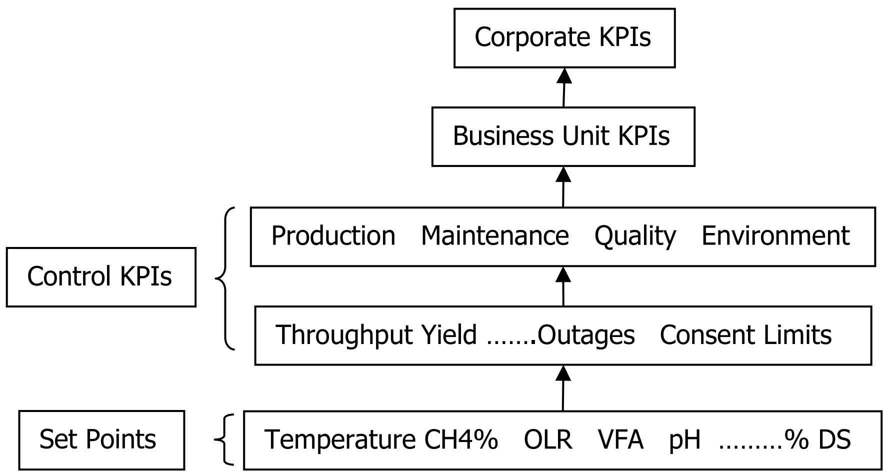


Figure 5.1 The hierarchy of KPI

The benchmark analysis is conducted using Perceptive's Advanced Process Control (APC) software systems (*Perceptive Engineering Ltd*, 2012). Various statistical process control (SPC) techniques were implemented to analyse the process audit data, process capability (PC) form the core of the analyses. Pc describes the minimum variability that occurs when the process is in a state of statistical process control. This is true for processes where process variability is only due to random and common causes intrinsic to the process. Combining the capability standard deviation with customer specification, setpoint or the objective function gives an index which illustrates the best quality control possible for the process. This enables the identification of any risk in using the current quality control to achieve the specification.

Process performance indices (Pp and Ppk) and process capability indices (Cp and CpK) are two metrics that relate specification and variability (Shunta, 1997). These two metrics together provide information that can be used to guide quality control improvements through (i) reviewing the current performance of the process, (ii) estimating any potential improvement in quality and (iii) providing a guide on how improvements can be achieved. Cp describes the minimum variability occurring while the process is in a state of statistical process control. This is defined by equation 5.1 as the difference between the upper and lower specification limits (USL-LSL) divided by six sigma (6σ). Cp considers only the spread of the data in relation to the specification limits. This is the state where variability is caused by random or common causes inherent within the process, thereby giving an index for the best possible control. A high value of Cp corresponds to a process capable of meeting the specification. Generally, the rule of thumb is if Cp<1 then the process is unsatisfactory and Cp>1.6 indicates a process with high capability with Cp between 1 and 1.6 in the medium range of capability.

$$C_{\square} = \frac{(allowable\ range)}{6\sigma} = \frac{(USL - LSL)}{6\sigma} \qquad \text{Equation 5.1}$$

Nevertheless, Pp measures all sources of variability in describing the average operation by the current control system. Ppk gives an indication of how well the controls maintain the variability within the desired range. These metrics combined can be used to assess whether the performance of the process meets its capability. Table 5.1 can be used as a guide to assess the capability and performance of the process (Shunta, 1997) by evaluating several KPIs from the process data.

Table 5.1 Process capability analysis

		Does performance meet capability?	
		No (Ppk<<Cp)	**Yes (Ppk~Cp)**
Does capability meet specification?	**No (Cp<1)**	Change process Improve control	Change process
	Yes (CP>>1)	Improve control	Little incentive for improvement

5.2 *The benchmark sites*

5.2.1 Blackburn WwTW

The Blackburn anaerobic digestion (AD) process was commissioned in 2006 following an upgrade from a traditional single phase MAD system to the Monsal EEH MAD technology. The site in Lancashire handles around 13,500 tDS of sludge per year, for approximately half a million people in the Blackburn and South Lancashire area. Figure 5.2 illustrates a simplified process flow for the advanced digestion process where the red lines indicate flows of the pre-digested sludge, purple lines indicate the flows of digestate, green lines indicate flows of biogas, and blue lines indicate heating water flows. The site utilises its own primary and secondary sludge, plus imported sludge and cake from other sites, as well food waste. All the feed streams pass into the balancing tank and are then thickened by the gravity belt thickeners. The impact of the different waste streams on the digestion process cannot be evaluated as the quantity and quality of the different streams being mixed are not recorded.

The dataset was extracted from United Utilities's OSIsoft[1] PI (Process Information) historian which records data from various AD process control systems of the Blackburn WwTW SCADA system, programmable logic controller (PLC) and the laboratory information management system (LIMS) as well as from calculated KPIs. Approximately 396 signals were collected from 14 January 2010 13:00 to 14 July 2010 12:00, totalling 188 days of data used for the benchmark study.

5.2.2 Mitchell Laithes WwTW

The digestion process at Mitchell Laithes WwTW is a traditional MAD. A simplified diagram of the process is shown in Figure 5.3. The site located in Dewsbury treats imported sludge from nearby WwTW and the sites own generated sludge. The data set used for the analysis was extracted from Mitchell Laithes SCADA system with 110 signals collected over a period of 150 days from 29th October 2010 at 00:00 to 1st June 2011. The level of instrumentation at this site is limited and consequently, the KPIs of volatile solids destruction, digestate chemistry, gas composition and the level of foaming within the digester could not be investigated. This made it challenging to evaluate the performance of the digestion process and hence most of the analysis mainly identified bottlenecks in instrumentation and inventory.

[1] OSIsoft is a software company manufacturing the PI system of real-time data infrastructure solutions

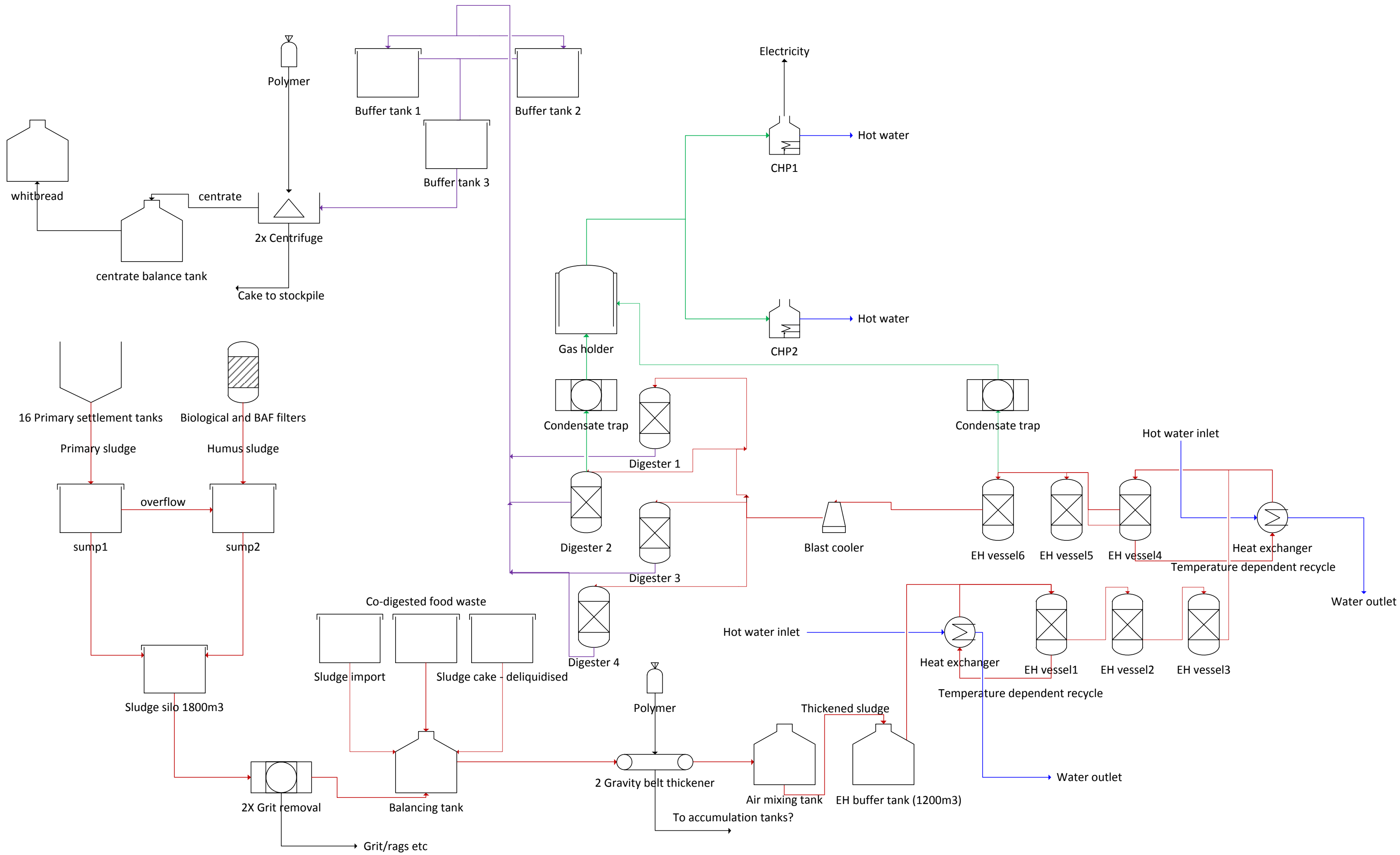


Figure 5.2 Schematic of blackburn anaerobic digestion process

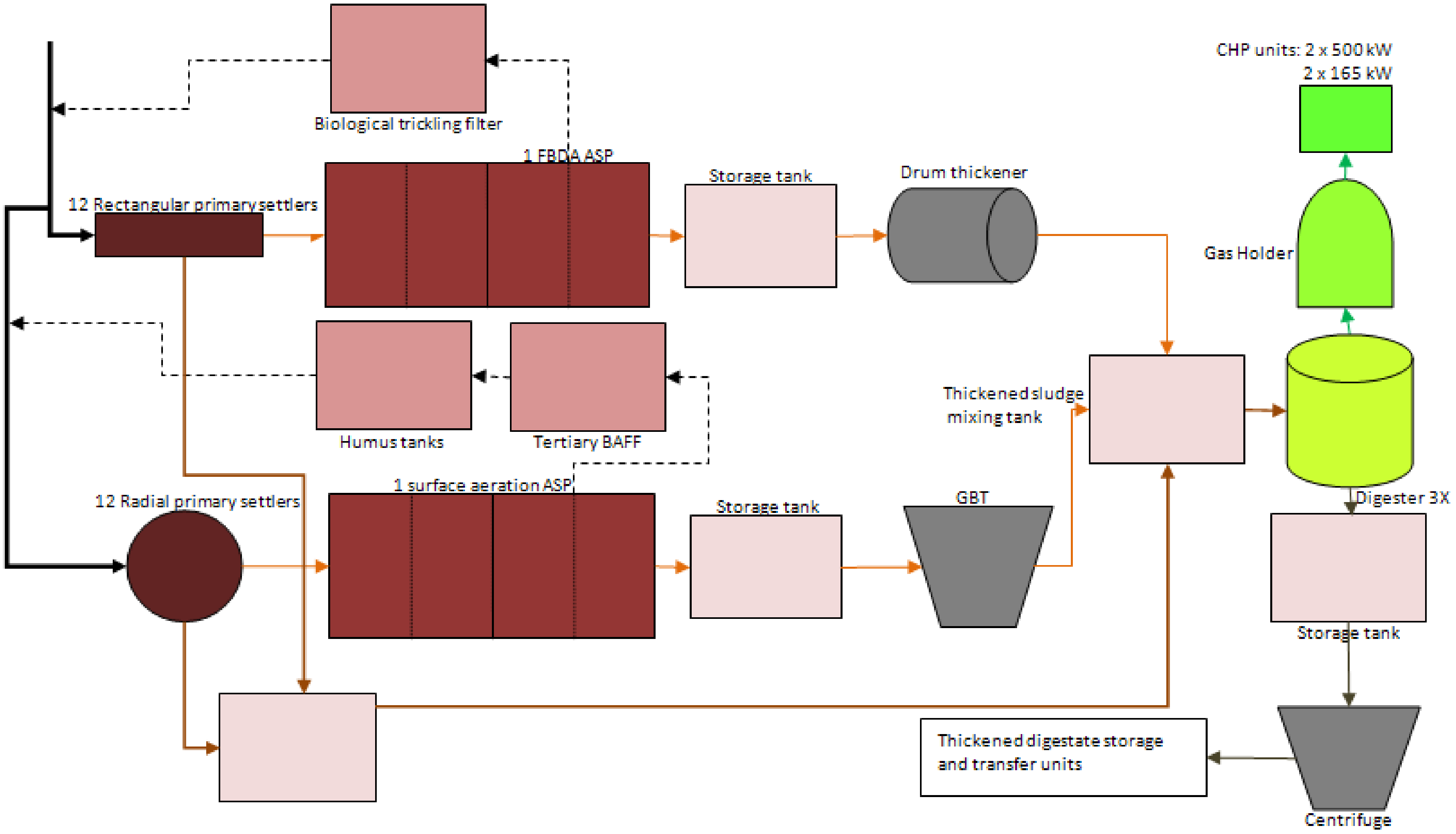


Figure 5.3 Schematic of Mitchell Laithes AD process

5.2.3 Bran Sands WwTW

The Bran Sands WwTW is one of Northumbrian Water's regional sludge treatment centres (RSTC). The 50 acre site was previously partly used for sludge drying. The company made a strategic decision to invest in a thermal hydrolysis process (THP). Part of the remit was to utilise as much of the equipment from the old drying plant as possible which included instrumentation used for the thickening processes. The dryers are still available on standby should the thermal hydrolysis AD breakdown. The site is manned 24 hour and treats both domestic and industrial waste. A simplified outline of the process is given in Figure 5.4.

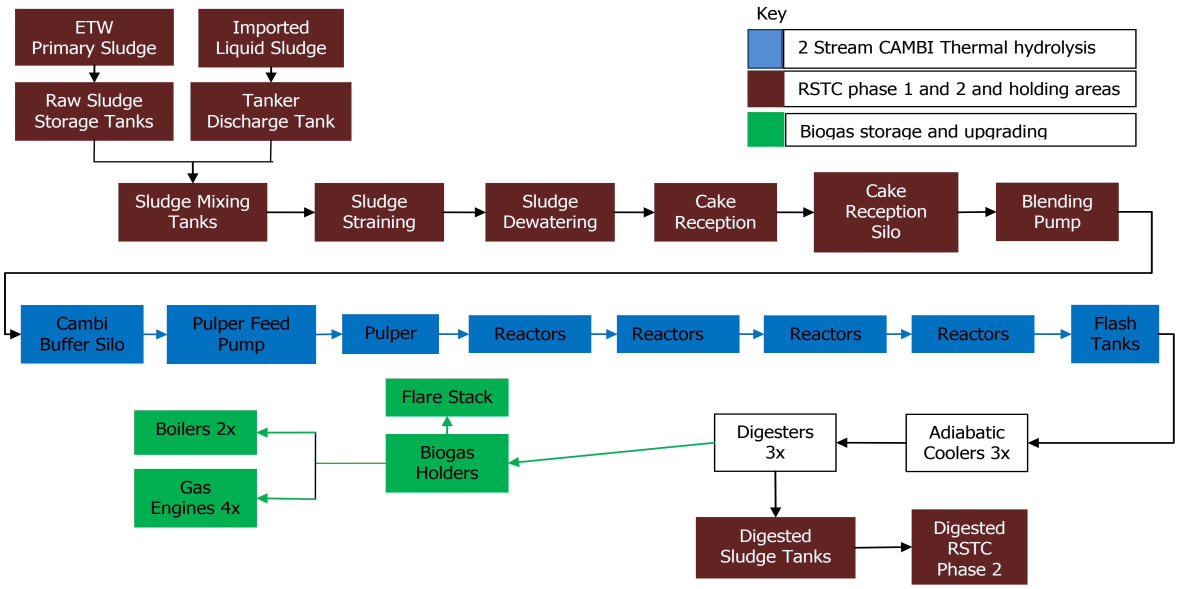


Figure 5.4 Schematic of Bran Sands AD process

Northumbrian Water identified a number of issues they were working to address prior to the benchmark study taking place. These included the following:

- High operator variation leading to increased variation in the process;
- Uncertainty in how to reduce faults and daily breakdown in the operation of the pumps and belt thickeners;
- Uncontrollable high levels of foaming and uncertainty to the causes of foaming;
- Variability in terms of quantity and quality of the imported cake potentially resulting in blockages through an increase in 'rags' (accumulation of sticks, plastics and other materials typically larger than 6mm) in the system and increased process downtime caused by 'rags' in the strain tank;

- Design limitation of the AD plant. Insulation for boilers and pipes required;
- Combined Heat and Power (CHP) units: Performance affected by boiler demand for biogas supply and heat balance, moisture in the biogas affects performance significantly and operators need to drain moisture traps continuously to reduce this affects.

Four operators from the site were tasked with resolving some of these issues and their findings although excluded from the results of the benchmark study help to build the business case for the site for sludge inventory control which aided the inventory simulation study in Chapter 6.

The data set used for the analyses was extracted from the site's data historian. The site uses three different systems for monitoring, control and data storage. These are the XCS5 which is located in the wastewater treatment area, Intouch which was previously utilised in the old drying plant and which is now used for the belts and dewatering units for the AD process and finally XCS6 (Oracle) which has been implemented on the advanced digestion process. 392 signals were extracted during a period of 89 days between 5th January 2011 to 5th April 2011 and these were imported into the PerceptiveAPC software for analysis. Laboratory data from the operators was also included with 113 signals between 7th September 2009 to 24th April 2011. The data obtained both from the laboratory and the data historian was subject to significant amount of missing data, variation in sampling time and hence required pre-processing prior to analysis.

5.3 Benchmark data analysis methodology

The benchmark analysis was conducted in PerceptiveAPC (*Perceptive Engineering Ltd*, 2012), Minitab 16 Statistical Software (Microsoft-cooporation, 2006) and Matlab (Mathsworks, 2012). PerceptiveAPC suite of products consists of real time and off-line development tools for different industrial sectors and process types (Perceptiveapc.com, 2015) including:

1. PharmaMV for the pharmaceutical sector;
2. WaterMV for the water industry;
3. BatchMV for batch production;
4. ADvisorMV for optimisation of AD systems.

PercepticeAPC offers modelling, visualisation and analysis tools which combine multivariate statistical analysis and model predictive control (Perceptiveapc.com, 2015). Featuring:

- Process analysis: use of univariate and multivariate statistical methods for detecting outliers, conducting correlation analysis and statistical normality etc.;
- Process monitoring: single and multivariable alarm thresholds, fault detection and diagnoses;
- Process modelling: empirical linear and non-linear regression techniques which include sensitivity analysis and cross validation metrics;
- Process control: a range of industrial control algorithms ranging from PID to model predictive control;
- Process optimisation: calculation of optimum solutions for improved control (Perceptiveapc.com, 2015).

The data from each site was loaded into PerceptiveAPC separately at 5 minutes sampling interval for the online data which in intervals of seconds. It was decided that due to the slow dynamics of the Ad system, 5 minute sampling interval was adequate. Several key steps were followed to pre-process the data to enable analysis on the data as the process data generated is generally very noisy and contains errors, missing data and outliers; it therefore required various pre-processing techniques to refine the data. The systematic pre-processing procedures followed were:

1. Visual inspection;
2. Handling missing data;
3. Outlier detection;
4. Data alignment;
5. Offline data pre-processing to reflect the online data.

The first step for data pre-processing was visual inspection to inspect the full dataset and identify the signals which required further data pre-processing. The inspection required use of knowledge of the process so far, the specification ranges for different parameters and discussion with operators to discuss the data. The visual inspection revealed long periods of missing data; high ‘spikes’ in the data such retention values and measurements at zero which related to instruments which were out of service. There are large sections of data missing in the signals due to a possible power or operational failure or site shut down as shown in pink on Figure 5.5. Due to the large level of missing data, the data selector was used to remove the data completely from the analysis. On visual inspection of time series plot of the missing data, it was evident that some of the samples were outliers or errors.

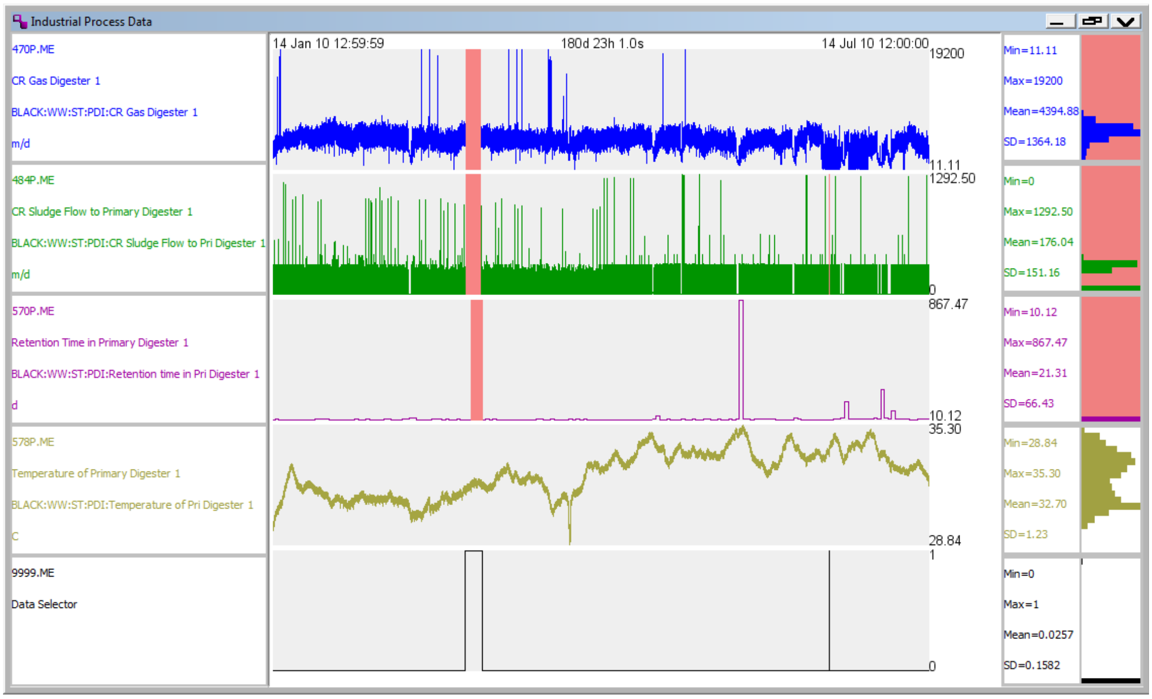


Figure 5.5 Use of data selector to pre-process process data

In Figure 5.5; plot of retention time for primary digester 1 is shown as 570D.ME. On the plot there is a signal peaking at 867.47 days for retention time. This is a clear error as normal operating range for retention time is between 20 to 25 days or less for EEH digesters. Removal of the missing data and extreme outliers resulted in selection of 88.2 % of the data for analysis (these are signals that equal 1 on the data selector signal) with 11.8 % of the data removed.

Data alignment of the process data was required to align cause and effect signals. This is shown in Figure 5.6 for temperature where the original data 570A.ME has been shifted to yield 570P.ME to reflect temperature effects on biogas production.

Outlier detection is one of the initial steps in data analysis for obtaining a coherent data set. It is common that what may be seen through visual inspection as noise or error may not be necessarily bad data and that these outliers can carry important information about the process. As such removal of what may be deemed to be as outliers can lead to a model giving incorrect results, misspecification and biased parameter estimation (Ben-Gal, 2005). The univariate hampel filter (Hampel, 1971; Hampel, 1974) addresses the issue outliers have on the robustness of an estimator. The hampel filter approach was then used to remove further outliers such as the spikes in feed and gas data. Figure 5.6 depicts various signals along with their pre-processed signal.

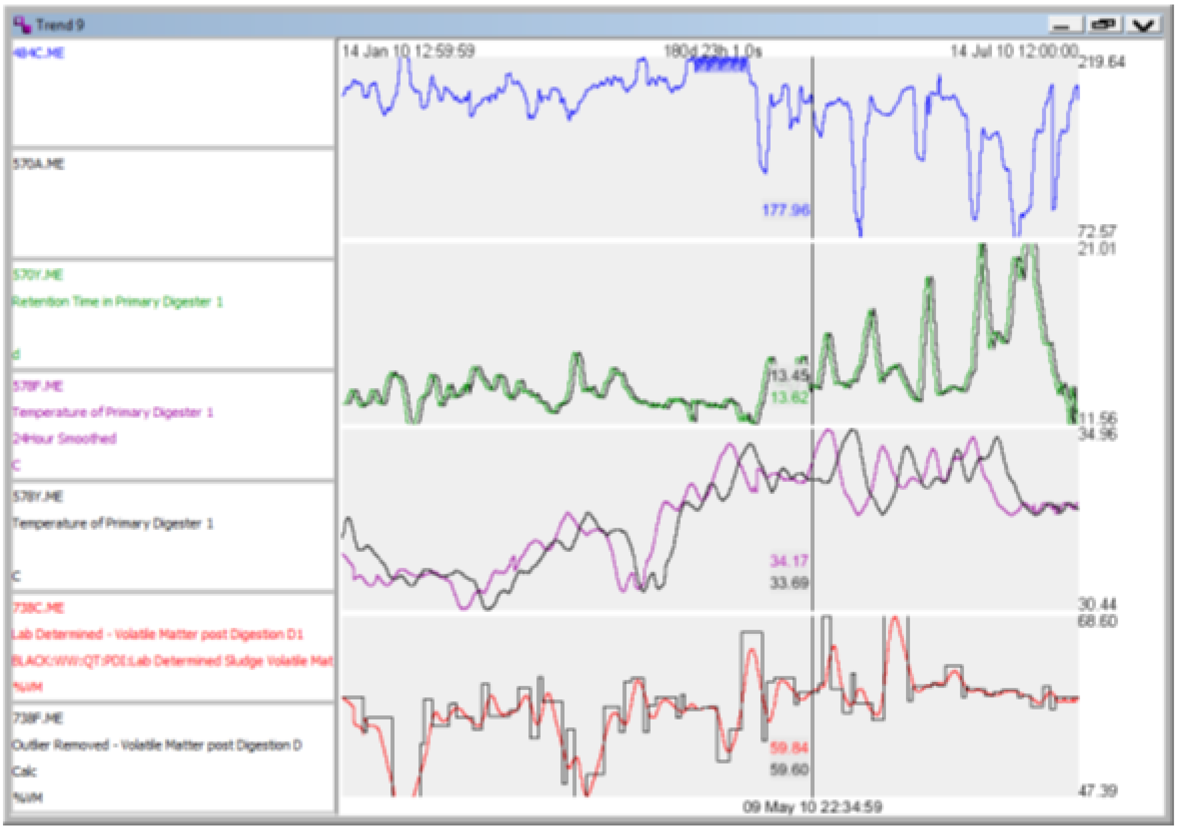


Figure 5.6 Data pre-processing analysis

The offline samples are collected 2-3 times a week and the last sampled value is held until the next sample point. This results in process parameters remaining constant until the next sample is taken hence to enable better modelling with the online process data, a ramp function was used in PerceptiveAPC. The pre-processed data in Figure 5.6 (red plot) for volatile solids is ramped to the next sample point and therefore only holds the peak positions. Figure 5.6 shows examples of the signals from the industrial process: biogas production (blue), digester feed flowrate (green), retention time (purple) and digester temperature (dark green). There are missing values (pink) for some of the online data due to plant shutdowns. Additionally there are spikes in the data and outliers including a large spike in the retention time at 857 days, which is not a feasible value. The periods covering the missing data and the spikes were excluded from the analysis.

Table 5.2 List of Key Performance Indicators (Horan, 2009)

Parameter	**Range**	**Units**
Biogas yield	0.1-1	m^3 kg VS^{-1}
Energy produced per kg vs^{-1}	Various	KW KG VS^{-1}
Energy generated	0-4x10^4	KW hr^{-1}
H_2S	<1000 ppm	For some CHP units
H_2 and CO_2	1-5 % and 0-50 %	% in biogas
Methane yield	50-80	% in biogas
	0.2-0.8	m^3 kg^{-1} VS_{app}
	100-286	m^3.CH_4.VS.COD_{fed}
% gas flared	0-100	Varies
Gas Holder level	Process dependent	Varies
HRT	14-25	days
Alkalinity	1000-3000	Mg L^{-1}
Temperature	30-40 for MAD systems	^oC
Polyelectrolyte usage	0-300	Kg day^{-1}
Optimum feed rate	0-500	m^3 day^{-1}
Feed TS (%)	4-8 %	% of total volume
VS removal	50-65 %	%
VS destruction	30-90 %	%
Digestate quality	Various means to satisfy PAS 110	Varies

Using the process design specification settings and list of typical key performance indicators in Table 5.2, time series analysis was conducted on the datasets to determine the internal structure of the data. The results for these are discussed in Section 5.4.

5.4 Benchmark results

5.4.1 Blackburn enhanced enzymic hydrolysis MAD

Time series plots were conducted for each of the samples to investigate the data. Several key findings were identified and a summary of these key findings are discussed in this section.

Currently the % DS is controlled manually by the process operators through adjusting the amount of polymer in the gravity belt thickeners (GBTs), which reduce the sludge volume through removal of water and thickening of the sludge. For this process the % DS has a specification range of 5 to 7 %. The process capability chart Figure 5.7, illustrates the offline % DS for the Blackburn site Figure 5.7a and the online % DS for Mitchell Laithes Figure 5.7b. The red lines indicate the lower and upper specification limits and the black distribution curve indicates the normal distribution for the data whilst the blue curve identifies the theoretical minimum distribution that can be achieved as per minimum variance control. 40 % of the time, the % DS is outside of specification for the Blackburn site when the offline measurement is recorded. A consequence of the sampling periods; samples extracted at 3-5 days intervals; the variability is of the same order as the standard deviation cannot be reduced due to the low sampling frequency. By sampling at a higher frequency, random process or measurement variations in the % DS could be observed and mechanisms put in place to reduce the level.

On examining the quality metrics of the % DS data from Blackburn, Cp is less than 1 which indicates that there is excessive random variability inherent in the process and Ppk~Cp confirms that this random variability may be reduced by changes to the process such as through improved measurement procedures thereby ensuring % DS is closer to specification. This can be achieved by online % DS analysis as observed for the Mitchell Laithes site, in Figure 5.7b. Montgomery (2005) defines quality as being inversely proportional to variability. The reduction of variability in the process and its outputs enables quality improvement. These are the reasons why a reduction in variability is important for maintaining consistent quality.

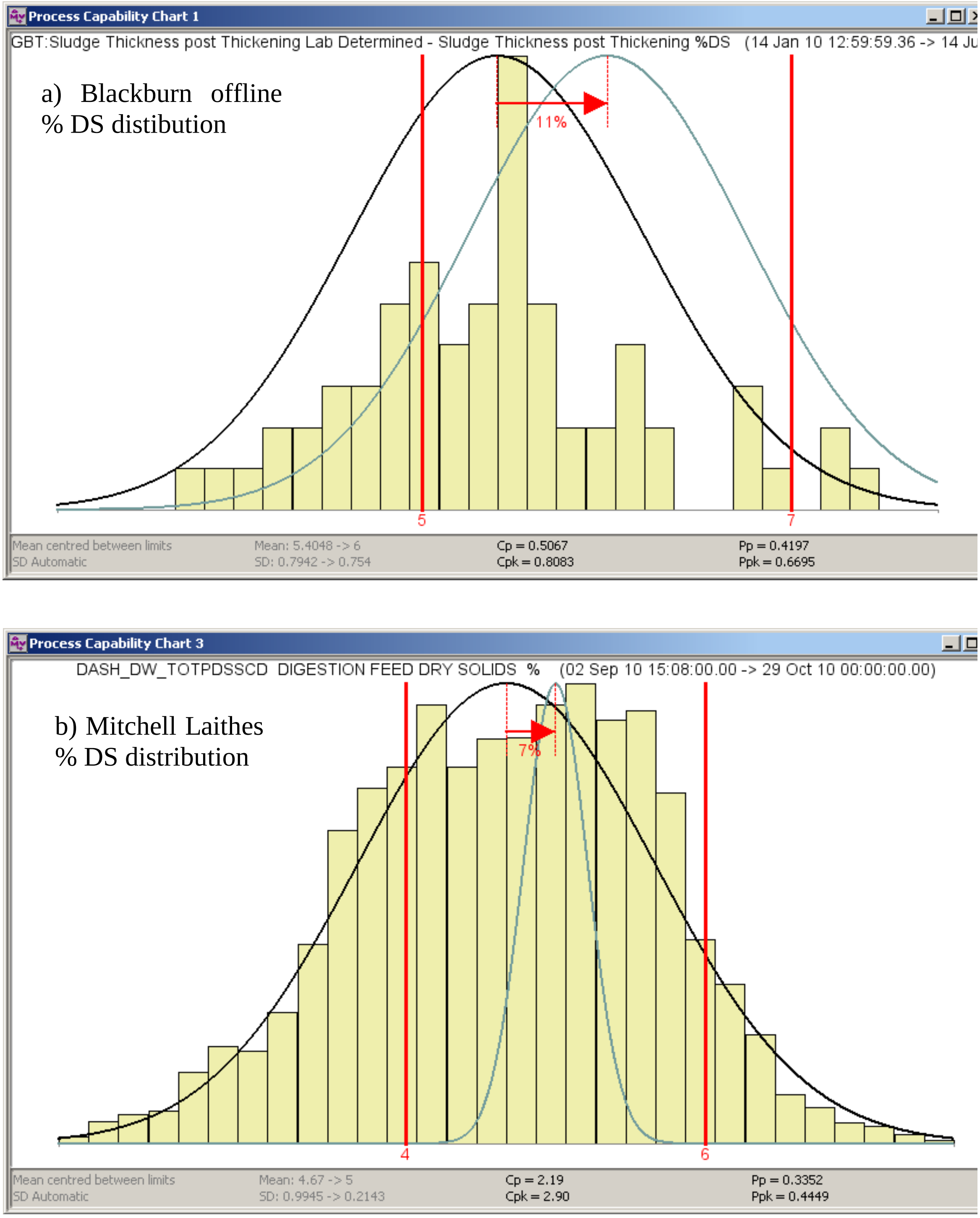
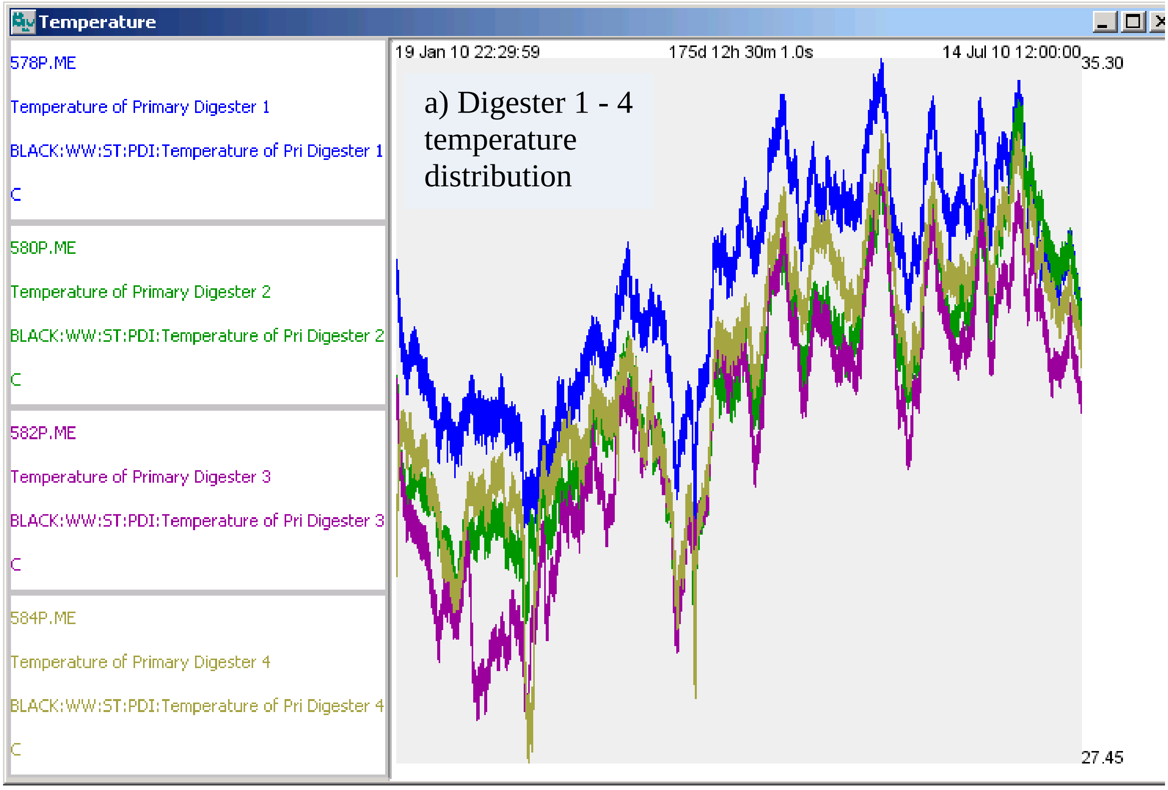


Figure 5.7 Process capability chart for online and offline % DS

The sludge feed % DS to the digester usually does not exceed 10-12 % due to limitations in pumping. High % DS may result in high yields of gas and may give an indication of the contents of nutrients and organics available for the microorganisms to feed on depending on the particular waste. A high % DS is shown to correlate with high yields of biogas (Barber, 2005b). % DS composition is maintained through the addition of polymer, thus justification of the use of polyelectrolyte to increase the % DS content requires an acceptable cost benefit analysis. The benefits include increase gas production, greater quality of solids destroyed and higher capacity within the digester whilst the disadvantages include increased polymer consumption, pumping cost and digester mixing requirements. A study by Baber (2005b) shows that the disadvantages of processing thicker sludge outweigh the advantages of processing at 6 % DS. Polymer addition for increasing sewage sludge % DS is an inefficient route for optimisation and improving cost effectiveness. This study does not take into account the effect of sludge preconditioning systems such as the enzymic hydrolysis or thermal hydrolysis. Previous work by Barber (2005a) has shown that sludge preconditioning systems can reduce sludge viscosity to allow digestion of 9 % DS effectively.

Within the Blackburn AD process, no additional heating is applied to the digesters. Maintaining adequate temperature in the blast cooler is crucial to sustaining the setpoint temperature in the digester. Temperature is measured online and is a key parameter that affects the yield and stability of the process. The four digesters at Blackburn are fed at the same feed rate generally. However there are instances where the feed rate varies for different digesters. This results in slight variations of temperature for the different digesters aside environmental effects on temperature. Figure 5.8a shows a time series plot for the four digesters and Figure 5.8b provides the process capability chart for the temperature for Blackburn digester 1 temperature. The plot shows that a potential improvement of 8.55 % can be achieved. This requires controlling the temperature in the blast cooler to ensure that the digester temperature remains at setpoint or by using supplementary heating and cooling systems on the digesters. The process capability chart gives a value of 1.35 Cp which shows that the process is operating at medium capability and it is evident from Figure 5.8b that there is an opportunity to improve temperature control as the process is operating below specification which is at most times at 35˚C to 30˚C. This is critical as small changes in temperature in the range 35˚C to 30˚C have been shown to reduce the biogas production rate significantly as well methane yield (Chae *et al.*, 2008). Closed loop temperature control could be implemented to reduce the variability and keep the process close to specification as shown in Figure 5.8b, where the standard deviation is reduced by 50 %.



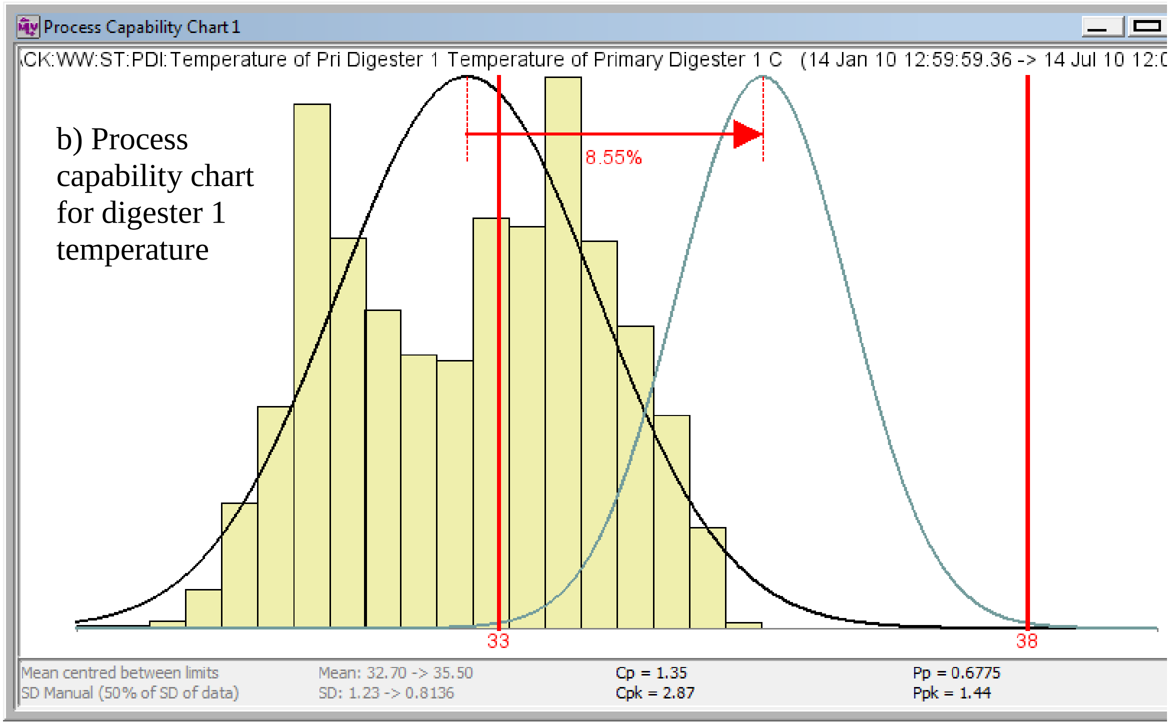


Figure 5.8 Temperature distributions for Blackburn WwTW

Figure 5.9 Digester flow and retention time

The minimum allowable retention time in the primary digesters is 10 days. This retention time, combined with the 2 day retention time in the EEH process, ensures that the digestate sludge is HACCUP compliant. Therefore in theory if the process had no bottlenecks or pH or alkalinity inhibition issues, then the feed rate could be increased by a factor of 1.4 whilst still providing a class A biosolids product.

In the last 10 % of the analysis range, the time to the right hand side of the cursor position in Figure 5.9, the digester feed rate is significantly less with an average feed rate of 620.99 m^3 day^{-1} for the 23 day period, which is a 12 % decrease. Over the same time period, the average retention time was 16.36 days, and the average gas production dropped to 15100 m^3 day^{-1}.

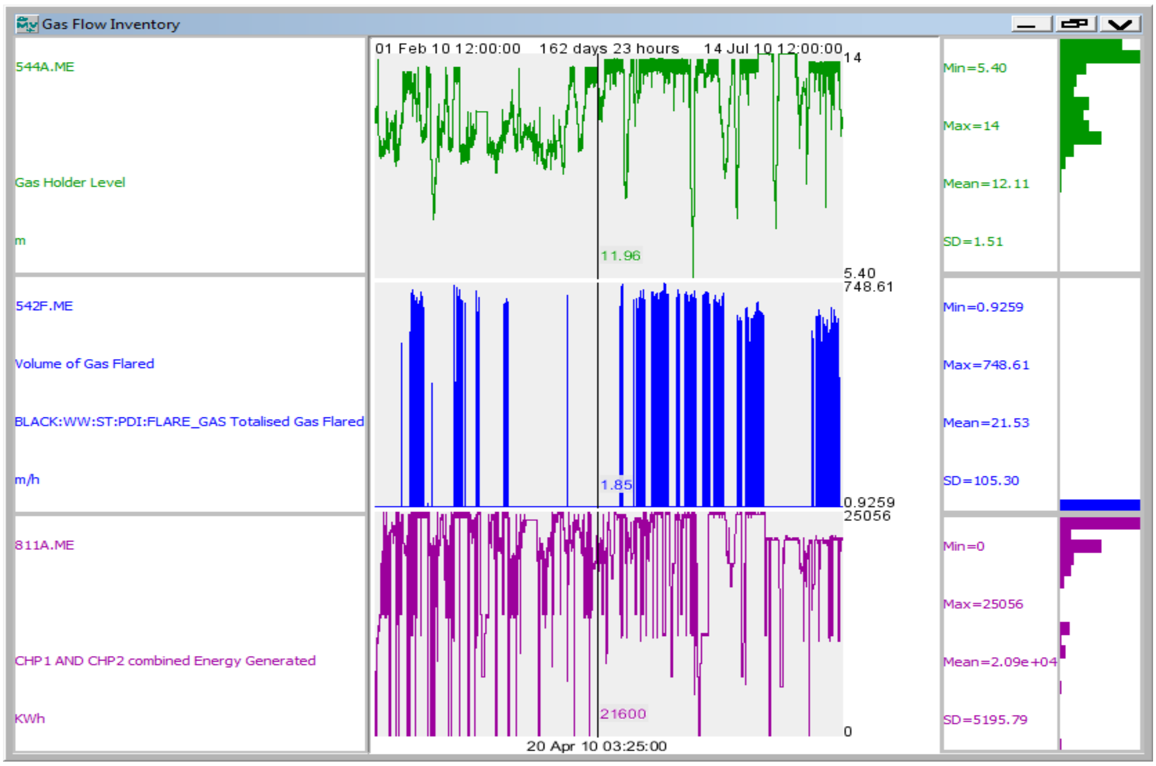


Figure 5.10 Gas holder level, volume of gas flared and energy generated

Figure 5.10 shows trend for gas holder level in the uppermost pane, the middle pane shows the flow to the flare stack, and the lower pane shows the combined electricity generation of the two CHP engines. It was found that for 1.8 % of the time, the gas holder level is full and all engines are working to full power and therefore excess gas at these times require flaring. Therefore the current gas holder and CHPs are unable to efficiently utilise the gas being generated. There is a need for larger engines, which will consume more of the biogas. This will reduce the volume in the gas holder and therefore reduce the instances of gas flaring. CHP2 engine is off when energy generation is below 4000 kWh day^{-1} and this equates to 19.2 % of the time. If the gas holder level is above 13 meters during this time, then is can be assumed that the outage is due to maintenance or an unavoidable incident, rather than simply switching the CHP engine off due to a lack of available biogas. This happens 9.9 % of the time. The remainder of the CHP downtime 9.3 % of the total time of the analysis range considered can be regarded as lost opportunity. In other words, 9.3 % of the time the CHP engines are switched off due to a lack of available biogas, whilst 1.8 % of the time, gas is being flared due to an excess of biogas. This equates to 8885.51 kWh day^{-1} lost on average during these times. The maximum constant level of energy generation for CHP 2 is about 11300kWh day^{-1} and therefore the potential to be gained by having the CHP working at these lost times is

11300 – 8885.51 which gives 2414.49 kWh d^{-1}. Assuming that the average cost of electricity is 6.5p kWh^{-1}, this gives a monetary estimate of the lost opportunity through better gas holder inventory management of about £57283.77 per annum. This clearly shows that the most efficient operation is achieved by maintaining the gas holder level in the range from 13 m to 13.6 m. If the holder level is in this range, then no gas is being wasted through flaring, and the CHP engines are running at their maximum rate. Over the whole analysis range, the gas holder only spends 26.8 % of the time in this ideal range. Figure 5.11 shows a process capability chart of the gas holder level, with the ideal range being entered as high and low specification limits. This chart clearly shows that most of the operating data lies outside of the ideal range and as the flare stack opens on high gas holder levels, the data is clearly not normally distributed, so the process capability analysis can only be considered to be a rough approximation. Even if theoretically 'perfect' minimum variance control were to be achieved, much of the distribution will still exceed the specification limits, so the complete elimination of flaring with the current hardware configuration may be impossible.

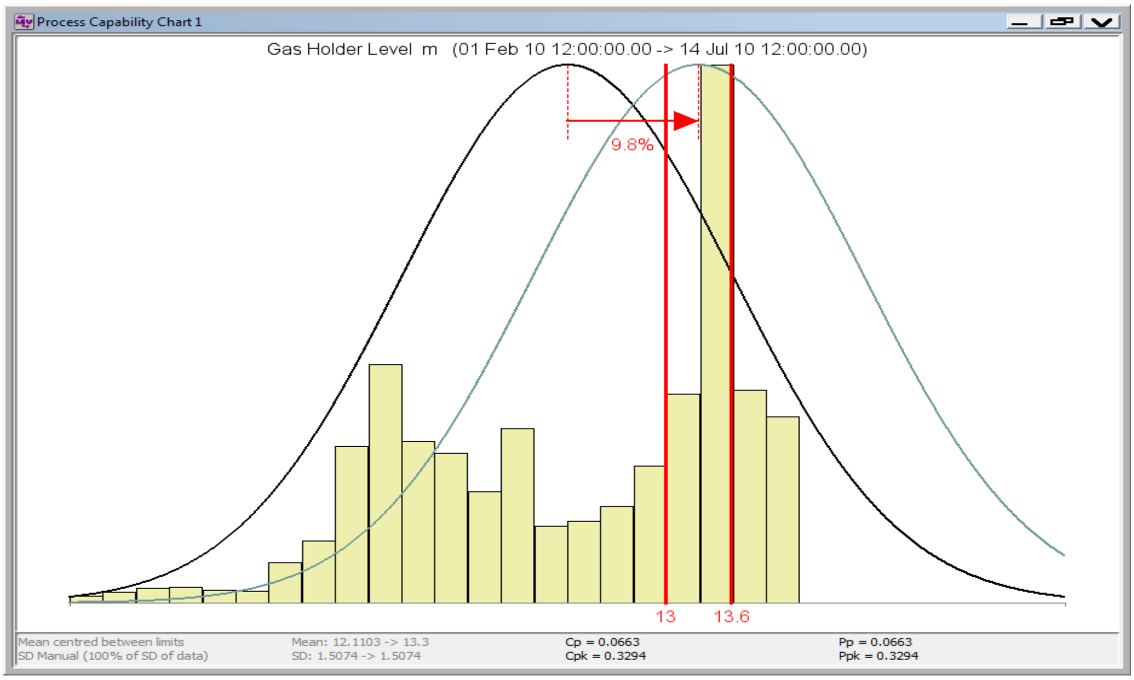
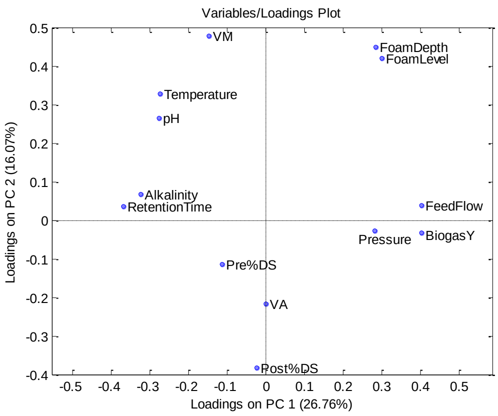


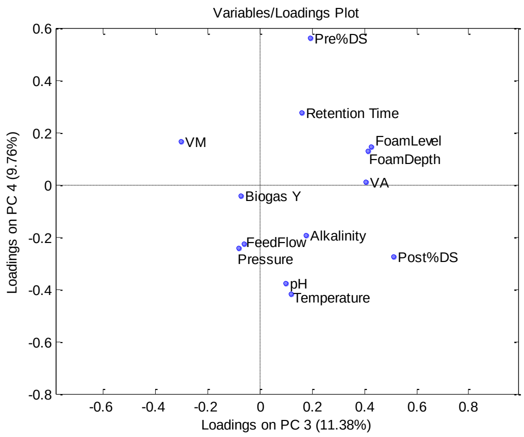
Figure 5.11 Process capability chart of the gas holder level

The majority of the analyses conducted for the Blackburn WwTW site were univariate to fully understand the relationship between the different variables as well as relationships between the observations and variables, principal component analysis (PCA) was conducted using the PLS toolbox in Matlab (Wise *et al.*, 2010). Based on the data available, and KPIs identified in for the Blackburn AD, a total of 13 variables were selected for the PCA. Figure 5.12 provide the loadings plot for the first 4 principal components (PCs). As can be observed, a number of variables are closely related including foam depth and foam level, i.e. as foam level increases, foam depth will increase. pH measurements are sensitive to temperature, and thus pH measurements are temperature dependent.

These analyses allow the confirmation of the theory behind the process and where this is aligned with practice increases the reliability of the data set. Volatile matter (VM) appears to be unrelated to the other variables. VM gives an indication of the quality of the sewage sludge and consequently is expected to correlate with biogas yield. This is not evident from the results. Providing there is a stable digestion process at constant retention time, % DS prior digestion and post digestion will also correlate. This may give an indication of the variability in feed composition. Thus % DS of the digestate may not necessary be controlled by the % DS of the feed. Volatile matter, volatile acids and sewage sludge chemistries may perhaps have greater effect on the digestate quality than % DS.



a) Loadings Plot PC1/PC2



b)Loadings Plot PC3/PC4

Figure 5.12 Loadings plot for PC1-PC4

Investigation of these variables affect the output parameters of biogas yield, post digestion % DS and foam levels, the data generated from Blackburn was undertaken through a DoE analysis in Minitab 16 Statistical Software (Microsoft-cooporation, 2006). It was assumed that the variables are linearly related. Table 5.3 shows the estimated effects and coefficients when gas production is the output parameter. Temperature, feed rate, retention time, feed % DS and their interactions effects on gas production was analysed.

A standard method of assessing the goodness of fit for a statistical model is the coefficient of determination R^2. R^2 is the quotient of the variances of the fitted values and observed values of the independent variable, given by:

$$r^2 = \frac{\sum(\hat{y}_i - \bar{y})^2}{\sum(y_i - \bar{y})^2} \qquad \text{Equation 5.2 (Yau, 2015)}$$

where y is the observed values of the independent variable, $\hat{y}_i$ is the fitted value and $\bar{y}$ is the mean. R^2 lies between 0 and 1 and if R^2 is equal to 1, the model is a perfect fit to the data whereas if R^2 is 0, the model is unsatisfactory or the mean is the best fit. For these reasons the R^2 values observed are very low for the Blackburn analysis crucial variables which affect gas production in a digestion process are not included as the data is unavailable. For example, although the % DS is included, an increase in % DS does not directly correlate to an increase in gas production as it depends more on the quality of the sludge. Measurement of feed sludge composition and quality is thus required with information of sludge age, amount of primary and second sludge, level of biodegradable substrate, and the types of organic material. Other external factors include mixing, volatile fatty acid (VFA) accumulation and pH effects which are also not included.

The final results for estimated effects and coefficients for biogas yield are shown in Table 5.3. These provides that all four factors, temperature, feed flowrate, retention time and % DS have a significant effect on biogas yield. Although this is well understood and the reasons are clear, it provides additional credibility to the data generated from the site in that it captures the linearity theory. The effect of retention time is an interesting finding as it is monitored to generally ensure compliance.

Table 5.3 Final estimated effects and coefficients for gas produced

Term	**Effect**	**Coef**	**SE Coef**	**T**	**P**
Constant		-81.4	60.48	-1.35	0.181
Temperature	576.0	288.0	79.58	3.62	0.000
Feed flow	485.6	242.8	79.58	3.92	0.000
Retention time	-600.2	-300.1	96.97	-3.09	0.002
Feed % DS	857.6	428.8	117.80	3.64	0.000
Temperature x Feed flow	-644.2	-322.1	104.91	-3.07	0.003
Temperature x Retention time	1337.5	668.7	165.28	4.05	0.000
Temperature x Feed % DS	-634.6	-317.3	99.45	-3.19	0.002
Feed flow x Retention time	548.1	274.0	106.58	2.57	0.011
Feed flow x Feed % DS	-1169.9	-584.9	157.85	-3.71	0.000
Retention time x Feed % DS	1165.0	582.5	115.12	3.76	0.000
Temperature x Feed flow x Retention time	-1356.7	-678.3	223.73	-3.03	0.003
Temperature x Retention time x Feed % DS	-959.7	-479.8	124.73	-3.85	0.000
Feed flow x Retention time x Feed % DS	-1506.6	-753.3	201.86	-3.73	0.000
S = 41.1282, PRESS = 248518, R^2 = 38.70 %, R^2 (pred) = 32.79%, R^2 (adj) = 32.75 %					

Figure 5.13 shows four plots demonstrating the effect of various factors on biogas production. The normal plot Figure 5.13a identifies the factors or combination of factors which have the greatest effect on biogas production. The plot shows that the combinations of temperature and retention time have the highest percentage effect on gas production.

Contour plots are used to explore the potential relationship between three variables. The two contour plots in Figure 5.13c and 5.13d explore the 3-dimensional relationship in two dimension of (c) Feed % DS vs gas production and temperature and (d) retention time vs gas production and temperature; where the darker the colour, the higher the feed % DS and retention time (Microsoft-cooporation, 2006). As such high feed % DS is given by temperatures below 32°C and gas production rates between 130 and 200 m^3 d^{-1}. The contour plot in Figure 5.13d for retention time vs gas production and temperature was more scattered as there are two optimums for retention time as such it is difficult to draw conclusions from this. However a positive correlation is expected and the results are inconclusive, as there is a requirement for further validation of this analysis with new robust data. Economical aims for processes such as AD systems aim to produce high yields of products at low energy consumption usage as quickly as possible, thus by improving the efficiency of the process, lower temperature with short retention times resulting in high levels of biogas produced is the ideal economic benefit. The contour plots show that this had not been achieved; there is therefore a strong requirement for monitoring the incoming sludge to better estimate which condition can yield an efficient optimum gas production.

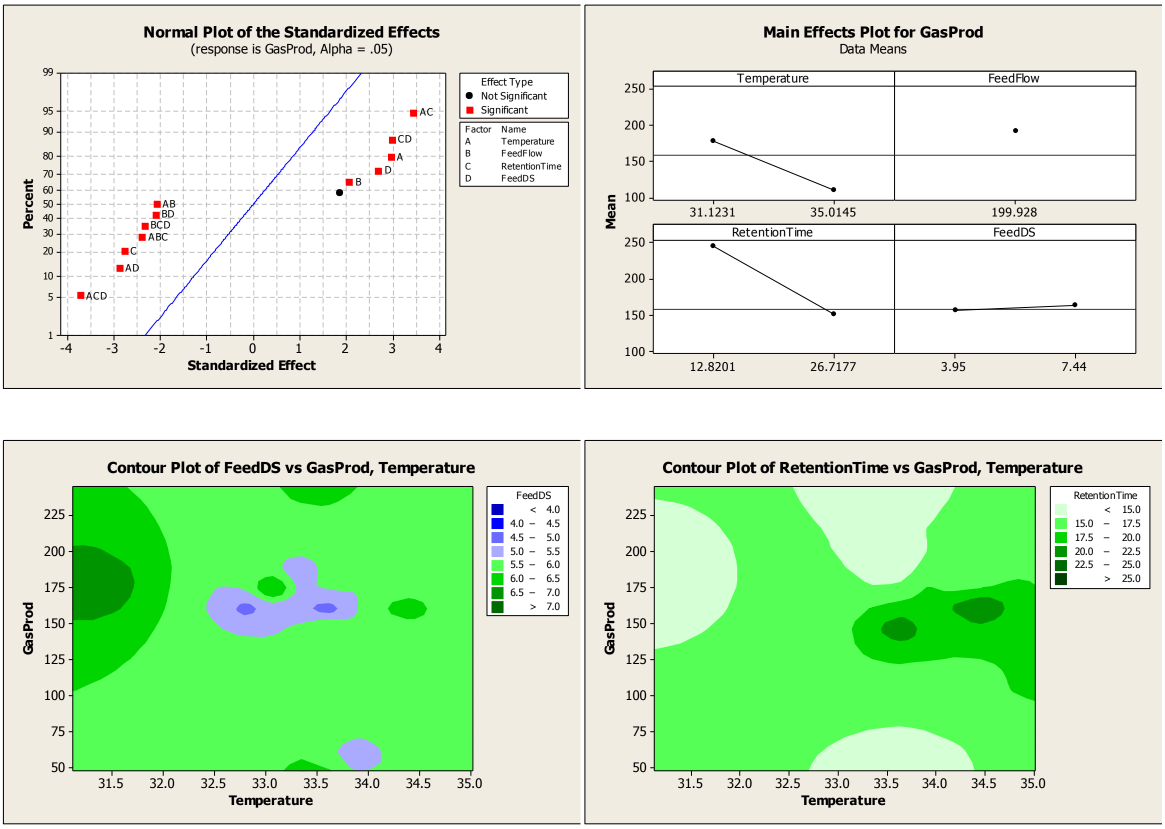


Figure 5.13 Factor effect analyses

Key findings from Blackburn can be summarised as:

1. Significant level of variability in the % DS;
2. Opportunity for digester temperature control;
3. Low gas yield with performance below design specification;
4. Foam level build-up and effects on biogas production on the whole process;
5. Low volatile solids destruction;
6. Digester feed rate limitation due to inventory;
7. CHP engine capacity limitation;
8. Sludge inventory scheduling, cause of large instability within the process;
9. An optimum identified for gas holder level efficiency range;
10. Opportunities for online instrumentation.

These results can be classified into two groups (i) bottlenecks inherent in the process (1-5) and (ii) bottlenecks associated with inventory and instrumentation (6-10). Through discussing with the operators and from the conclusions drawn from the initial findings, it was clear that before optimisation of the actual process can be achieved, in terms of optimising biogas production, and stabilising the process, the bottlenecks in inventory and limitations associated with scheduling and instrumentation capacity need to be reduced or removed.

It was calculated that by increasing the CHP unit capacity for the site to avoid gas flaring, about £45,800 per annum could be generated. A further £57,200 per annum could be generated by aligning the energy production with CHP unit. Furthermore a considerable amount of money could be generated from scheduling of biogas production to align with the CHP capacity. This depends on a constant feed rate to stabilise the digestion process. However operators have little control over imported sludge with respect to frequency, quantity, quality and limited capacity for storage; the feed rate is mainly determined by the buffer tank level. Reducing the variability in these factors could massively reduce the overall variability and instability in the process.

The analyses performed for this site identifies significant bottlenecks which may be improved with increased in instrumentation and robust monitoring to enable control of the process. A summary of the key bottlenecks are:

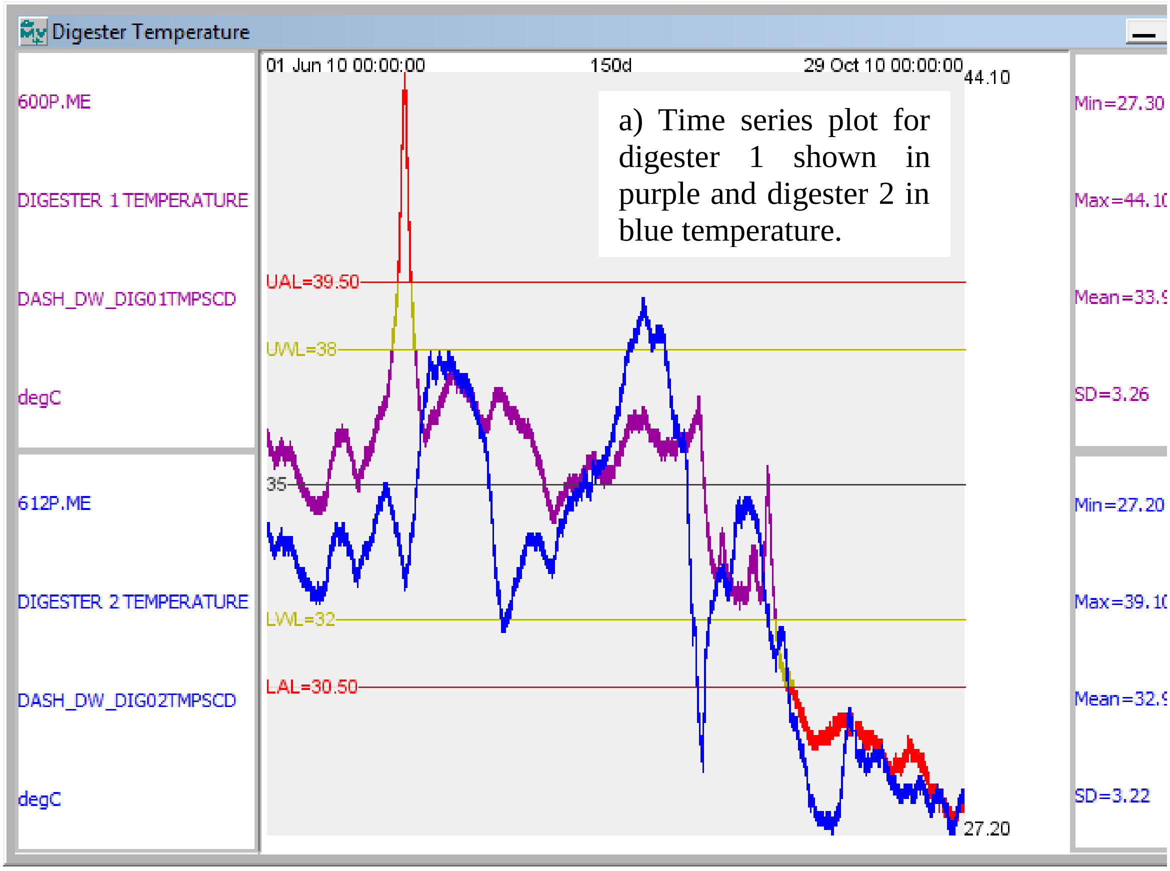
- Infrequent feed % DS monitoring;

- Inefficient heating and recirculation of the enhanced enzymic hydrolysis stage;
- lack of cooler optimisation for ensuring the temperature specification is maintained;
- Feed flow is the only manipulated variable;
- There is very little online measurement of chemical properties inside the digester including VFA, alkalinity and H_2 in the liquid phase;
- Hindrance of inventory control on gas production efficiency.

Hence improved process performance can be achieved through reducing the hindrance of uncontrolled scheduling and inventory impact on the overall process and through improved monitoring. Thus through model development of the process, the model can be used to predict the future state of the process to help reduce the impact of inventory and scheduling and optimise control. However as the complex AD process has large time delays, several control variables (CVs), limited manipulated variables (MV's), nonlinear, oscillatory multistage reactions, and typically large scale in nature with complex dynamics; some quality variables such as H_2 reacts faster and thus has a different time to reach study state in comparison to CH_4 makes the process difficult to model as discussed in Section 2.3.

5.4.2 Mitchell Laithes MAD

At Mitchell Laithes temperature is maintained through heat exchangers and sludge mixers mounted on the digesters. This gives some level of automated control for the operators as they can vary the hot water temperature through the heat exchangers. The variability in the temperature profile for this site is significantly high, deviating considerably from specification and best practice (Horan, 2009) for digestion processes for which low variability of temperature is required; see Section 2.5. Figure 5.14a shows the time series plots for digester 1 (purple) and digester 2 (blue) temperatures. Digester 1 lies between 17 and 44˚C and this is outside the range for mesophilic digestion systems temperature range between 30 to 40˚C. Low temperatures can effect biogas production and quality as temperatures and overheating the digester affects the energy requirement as energy reduction is a key business KPI for the consortium; a simple closed loop temperature control would potentially reduce the variability in it. This is illustrated in the process capability chart plot Figure 5.14b. The Cp is 1.02 with 65 % of the data falling within the temperature specification and hence the process performs close to its specification level. However with Ppk value of 0.4186 results in Ppk << Cp and thus there is an opportunity for improved control of the process to enable plant performance to meet its capability.



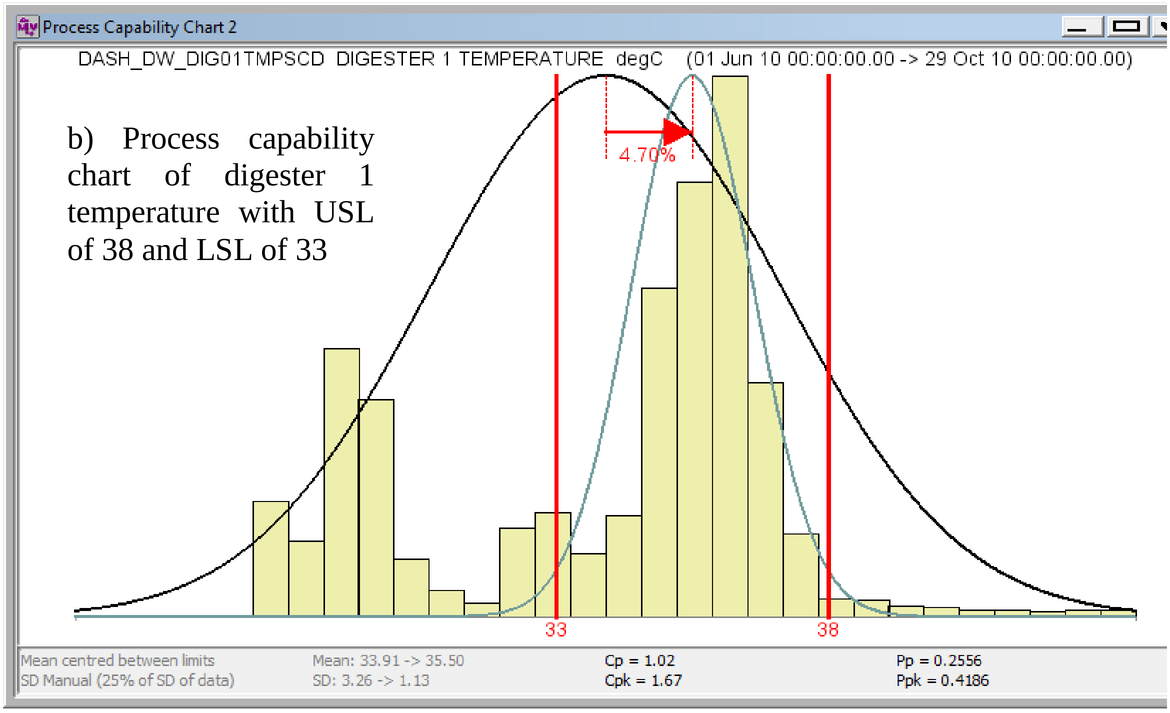


Figure 5.14 Temperature profile for Mitchell Laithes WwTW

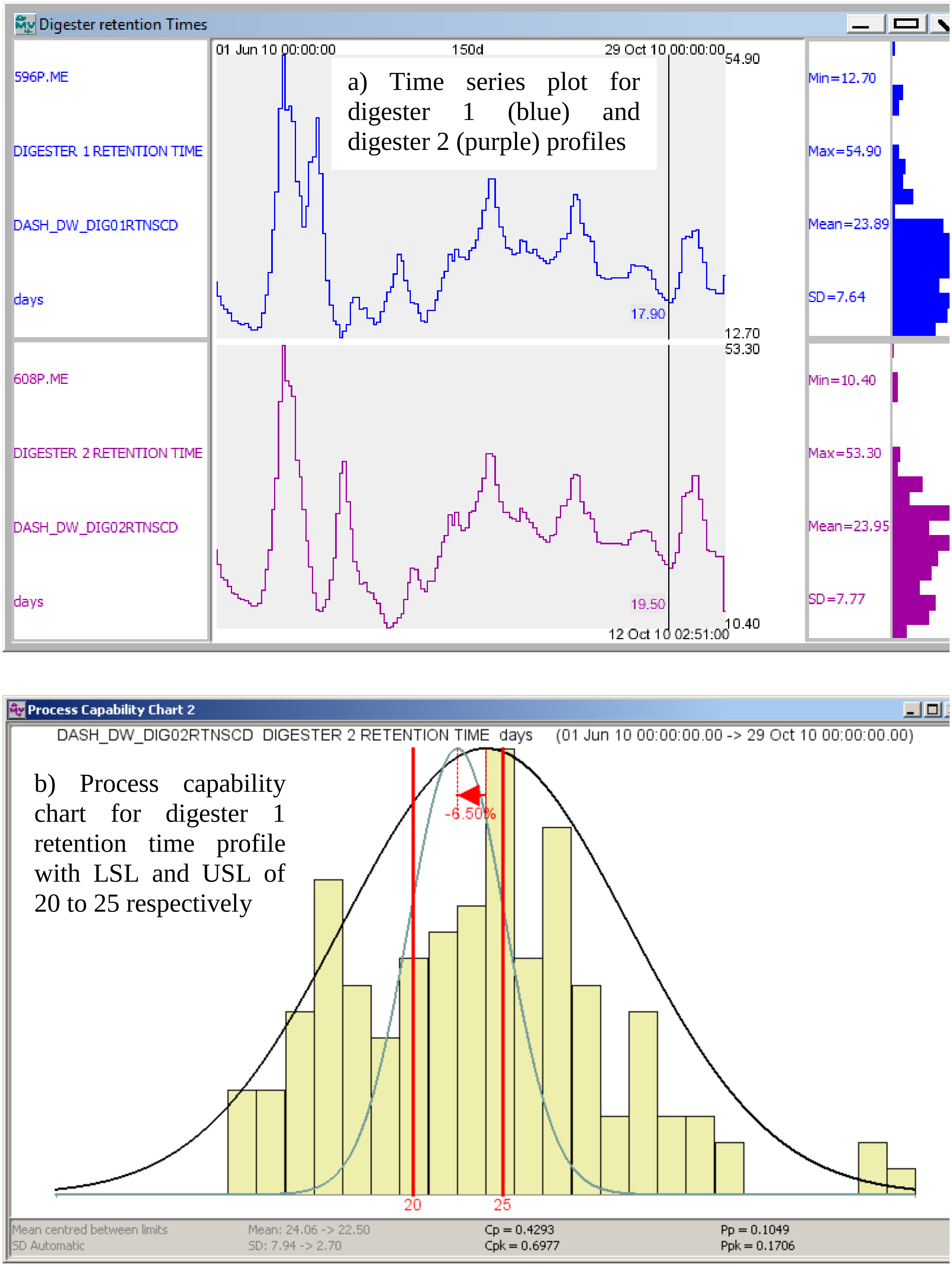


Figure 5.15 Mitchell Laithes digester retention time profiles

Retention time is the length of time required to achieve complete degradation. This is affected by process parameters such as sludge composition and temperature. For MAD systems this generally is at least 20 days (Song *et al.*, 2004). Retention time affects digestate quality and therefore compliance. The sludge is expected to remain in the digester for a minimum time dependent on the temperature of operation and HACCP ensure that the digestate being spread on agricultural land complies with the relevant microbiological standards such as the safe sludge matrix (Davis *et al.*, 2010) as HACCP manage and reduce potential risks to human health and the environment.

Figure 5.15a shows the retention time profiles for the two digesters and Figure 5.15b gives the distribution of retention time for digester 1. The average retention time for digesters 1 and 2 were 23.89 and 23.95 days respectively. The minimum allowable retention time in the primary digesters is 12 days. This retention time, ensures that the digestate sludge meets the requirements for acceptable digestate quality. However, for single stage MAD, the optimum digestate quality and biogas production typically requires over 20 days of retention time. As shown there is significant variability within the data due to changes in the feed and digestate removal rate, with the retention time ranging over 42 days. The specification limits for Mitchell Laithes is set between 20 and 25 days shown in Figure 5.15b and digester 1 (blue plot), the process performs within this specification range for only 27 % of the time. 35.3 % the retention time below 20 days and 37.3 % it is above 25 days offers an opportunity to increase throughput for the process. Hence for a possible 70 % of the time, the sludge produced does not meet specification. By reducing the variability in feed flow into the digester, the variability of retention time may be reduced and the system could be better controlled to specification. There is scope here for optimisation, by balancing the inventory management requirements with the aim to minimise the variability in retention time.

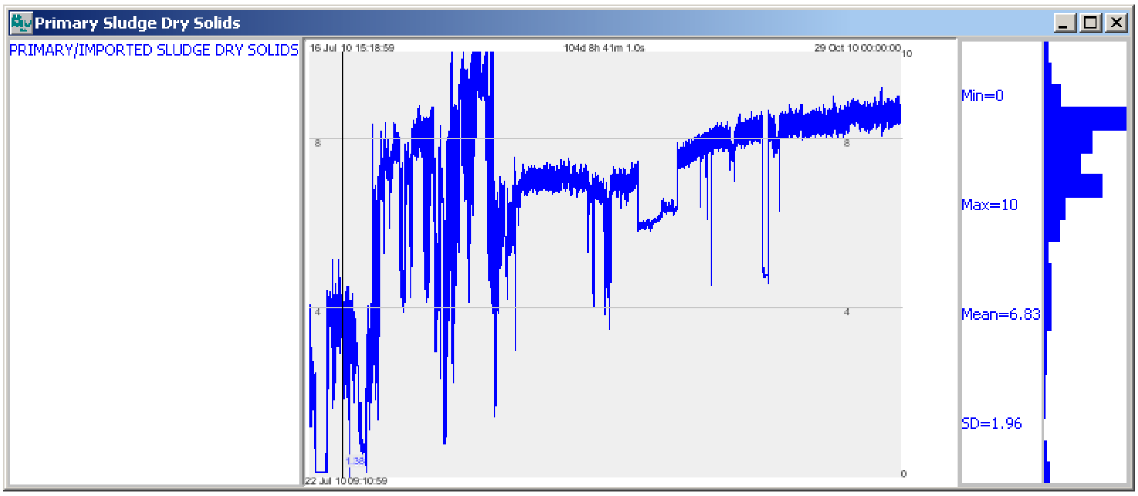


Figure 5.16 Primary and imported % DS

The Mitchell Laithes AD process had a number of Hach Lange online dry solids analysers located at various points in the process. Figure 5.16 shows the signal for the primary imported sludge dry solids and Figure 5.7 showed the process capability chart. The blue 'theoretical' minimum variance distribution is considerably smaller than the black 'actual' variance distribution. In other words, it is theoretically possible to control the % DS much more tightly than it is controlled at the moment. The Figure also shows that 9.9 % of the data is outside the low specification limit of 4 %, and 32.2 % of the data is outside the high specification limit of 8 % with an average % DS was 6.83 %.

Figure 5.17 Sludge buffered stock level and digester feedflow

Figure 5.17 trends show the buffered tank stock level and the digester 1 and 2 feedflow and 12 hour average. Once the buffered stock level drops below approximately 35 %, both the level signal, and the feed to the digesters tends to stop and over the whole analysis range, the stock level was below 35 % for 26.8 % of the time, and was above 80 % for 11.8 % of the time. For all of the observed cases when the buffered stock level was above 80 %, the digester feed rate was running at a reasonably high level. Therefore for smooth disturbance-free operation of the digester, the buffered stock level should be maintained above 35 %.

The effect of the feed rate upon the digester temperature is shown in Figure 5.18. In this figure, before the cursor position, both digester vessels receive almost exactly the same amount of feed, and the two digester temperatures are correlated accordingly. After the cursor marker, almost all of the feed is diverted to digester 2, whilst digester 1 receives very little feed. This immediately causes the digester 2 temperature to drop, whilst the digester 1 temperature increases rapidly. When the feed proportion is swapped later on, the opposite effect happens to the temperature.

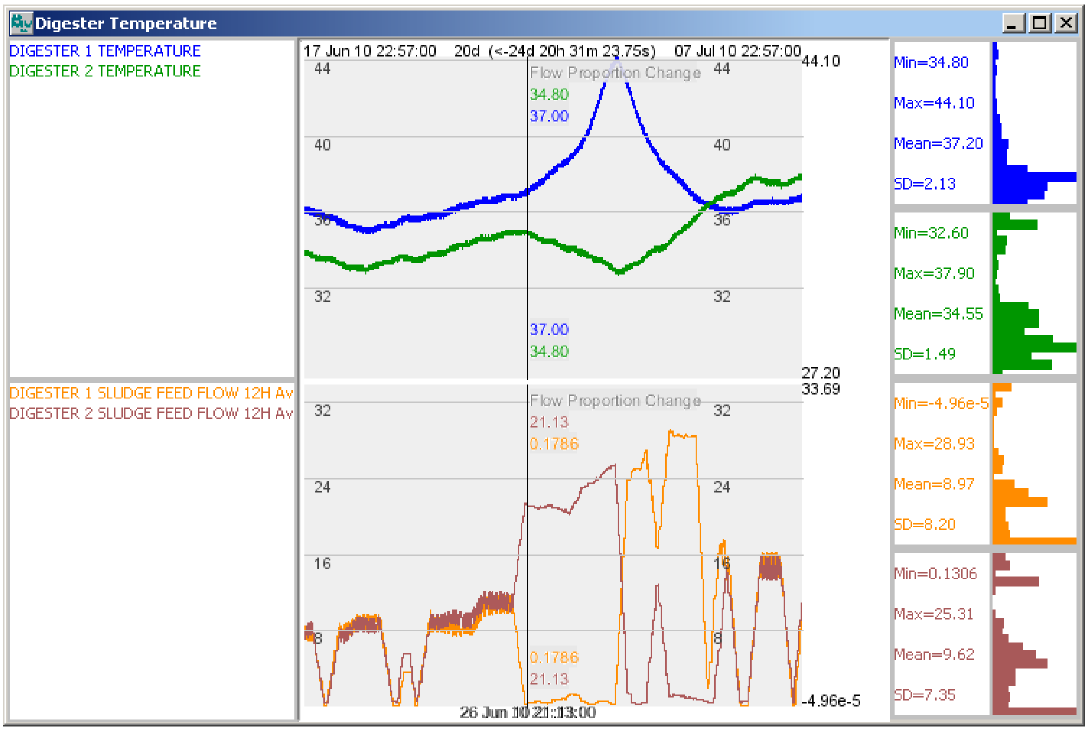


Figure 5.18 Digester feedflow effect on digester temperature

The effect of digester feed rate on the gas production is demonstrated in Figure 5.19. Raw sludge feed rate signals for digester 1 and digester 2 in the uppermost pane of the plot. Twelve-hour averaged versions of the same signals are shown in the middle pane of the trend. The bottom trend shows the gas flows from the digesters 1 and 2, and combined gas flow, and a 12 hour averaged combined flow shown as the black trace. The averaged gas flow is relatively constant whilst the average feed rate is constant, however after the first cursor, the feed is shut off for long periods, and consequently the gas flow drops significantly, ultimately reaching a value of less than half of the original gas flow before the feed is restored.

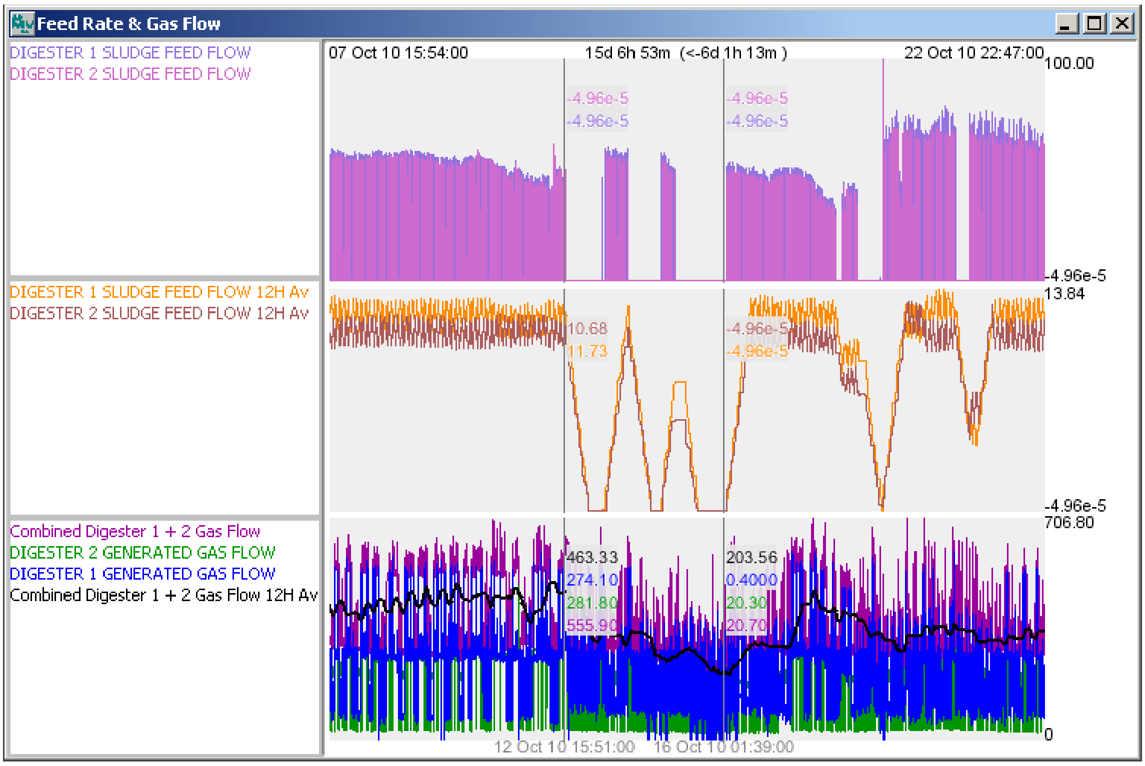


Figure 5.19 Digester feed flow effect on gas production

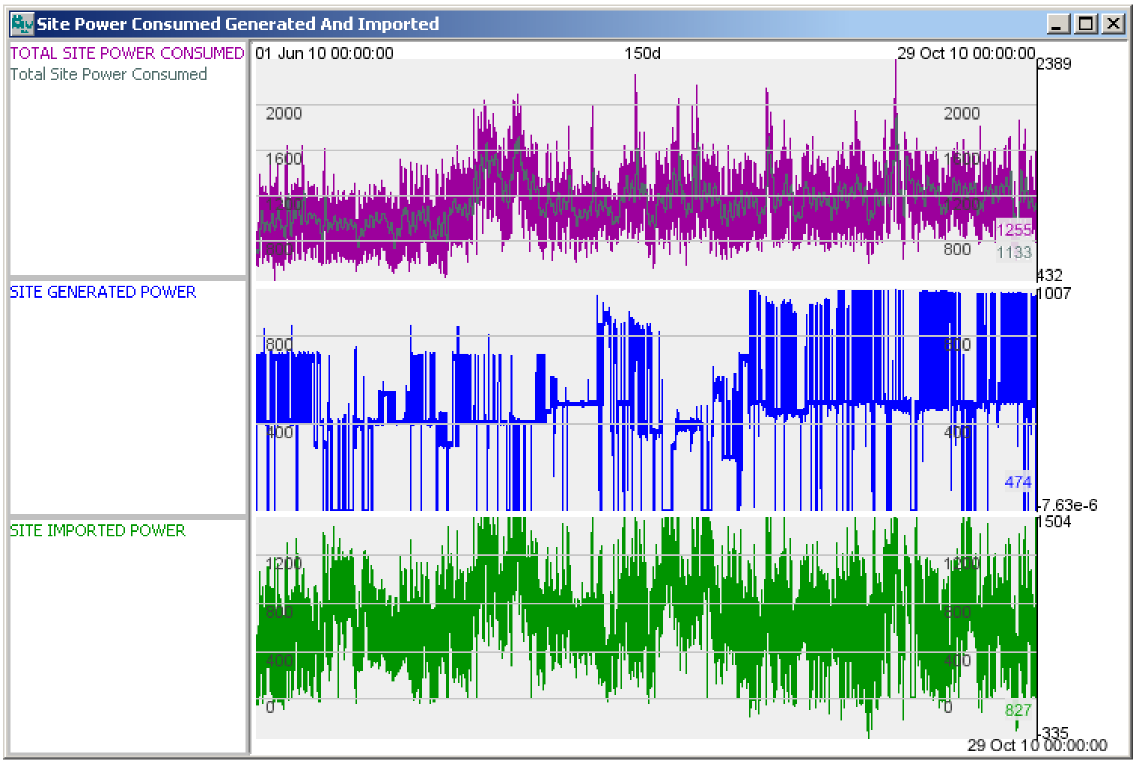


Figure 5.20 Site power consumed, generated and exported

The average total site power consumed is 1117.47 kW, whilst the average site generated power is 505 kW, and the average imported power is 665.85 kW. Figure 5.20 shows plots for the power consumed, generated and imported. The site generated power tends to be either a high, medium or low value depending on the capacity of the CHP's. As the site is almost always importing power, the value of the site generated power can be calculated based on the import tariff price. This tariff price varies from site to site, and on a temporal basis. For the purposes of demonstration we have used the following illustrative figures:

- 00:00 to 07:00: 4.6 p kWh^{-1}
- 07:00 to 16:00: 6.7 p kWh^{-1}
- 16:00 to 19:00: 13.3 p kWh^{-1}
- 19:00 to 24:00: 6.7 p kWh^{-1}

The average value is £813.82 per day equivalent to £297,000 per annum. This value does not include the value of renewables obligation certificates. Clearly the value of the electricity produced is highly temporal, depending on the current tariff, and the number of CHP's running. Assuming that the biogas storage capacity can be adequately managed, it is theoretically possible to increase the value of the power generated to £974.44 per day equivalent to £355,670 per annum simply by aligning the peak tariff with the peak CHP generation. This represents a value increase of £58,626 per annum, or a 19.7 % value improvement.

Key findings from the Mitchell Laithes site are:

- Significantly high variability in the retention time of the process;
- The site produces very little electricity of approximately 0.49 MWh tDS^{-1}, which is below what is observed for similar AD systems 0.8-0.9 MWh tDS^{-1};
- Feedflow limitations imposed by upstream and downstream sludge thickening and dewatering instrumentations (GBTs, Centrifuges, belt thickeners), which affects the availability of thickened sludge;
- Online % DS data analysis showed significant variability in the data and that the process was operating outside specification for a large period;
- The site compares well with generalised MAD systems, producing 297 Nm^3 tDS^{-1} of biogas which fits into the upper range observed for typical MAD's of 200-300 Nm^3 tDS^{-1};

- There is a significant bottleneck with respect to controlling the temperature close to specification as there is large variability observed.

General conclusions from this site are similar to those of Blackburn WwTW. The effect of inventory and scheduling effects on the digestion process were more evident on this site. The opportunity for a predictive controller to reduce the variability in the feed through better prediction of inventory is essential. The efficiencies of systems such as the centrifuges can be greatly improved. There are various sludge thickening devices available such as centrifuges, belt thickeners, thickening drums and other dewatering units. Analysis can be conducted to evaluate the efficiencies of these systems to better inform the water companies on ways to reduce the bottlenecks these instruments impact on the downstream processes of the overall digestion process.

5.4.3 Bran Sands CAMBI MAD

Measurements of temperature within the digester are obtained from three probes. These are placed in the upper, middle and lower levels of the digester. Figure 5.21a shows a plot of the temperature for digester 3, and it can be observed that the average temperature for all three levels is about 41˚C thus considering the 2500m^3 size; digester there appears to be good temperature distribution throughout. This is achieved by a closed loop temperature control system. The variability is further greatly reduced in comparison to Blackburn and Mitchell Laithes; thereby highlighting the potential for reducing variability in temperature through a closed loop control system.

Water content of the sludge is one of the most important factors with regards to the total energy demand of the thermal hydrolysis. The hydrolysis temperature plays a key role in the energy balance. CAMBI recommends 165˚C as the optimised temperature based on experience. Temperatures for the reactors are not available however temperature of the sludge coming out of the flashtank is on average 111˚C. CAMBI states that this temperature (out of the flash tank) should be about 102˚C and ‘practically kept constant’. Figure 5.21b shows the actual temperatures from the flash tanks which fluctuate considerably. By deviating from the design on key parameters such as this, Bran Sands digestion operates below the designed energy balance for the system.

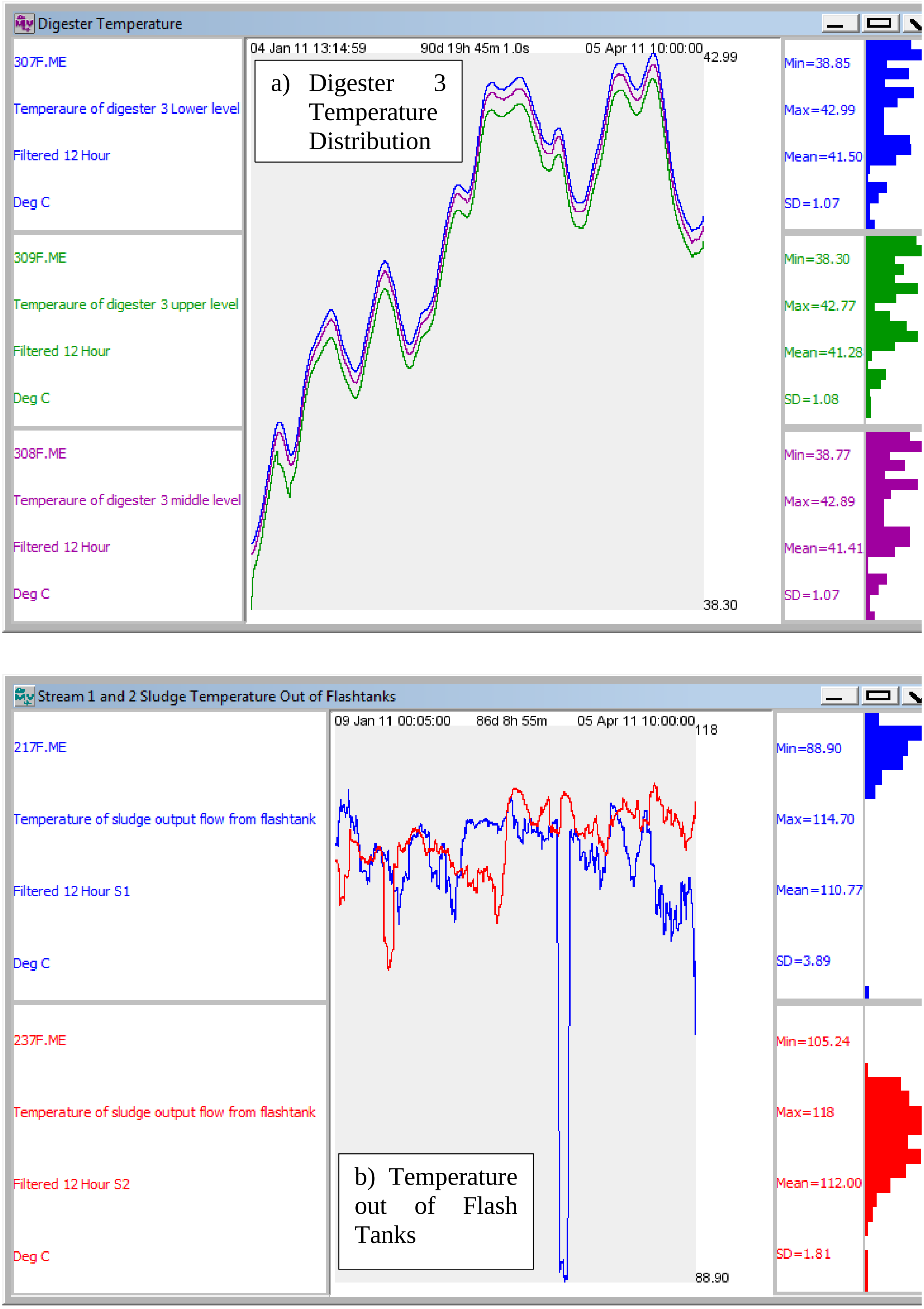
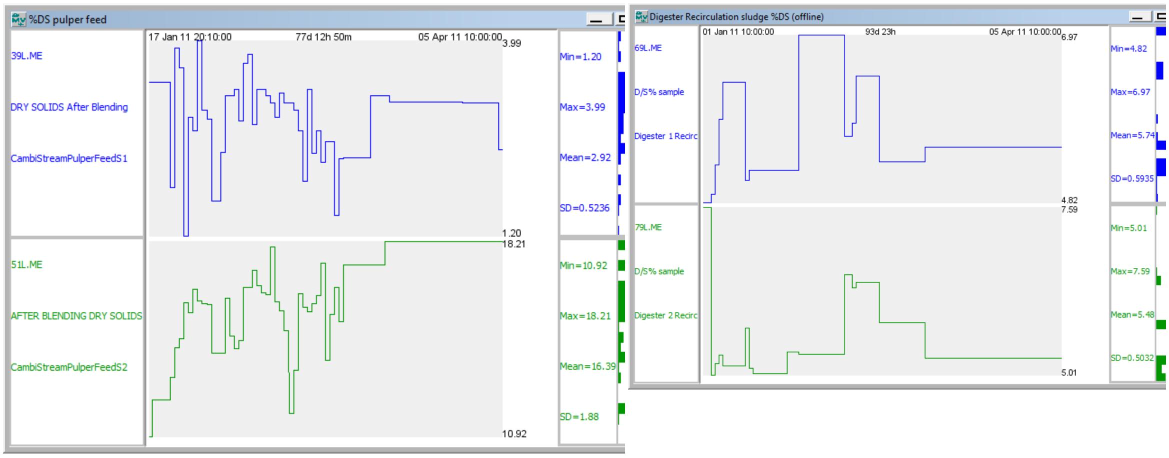


Figure 5.21 Temperature profiles for digester 3 and the flash tanks

The process design states that 12.3 % DS in the reactor as the optimum. The viscosity at 12.3 % DS is low enough to ensure good homogeneity of the sludge and steam mixture. Figure 5.22a gives the offline results for % DS for the two pulpers. The energy balance is based on the sludge feed into the pulper at 15.9 % DS. The injection of recycle steam from the flash tank and the reactor leads to approximately 14 % DS of sludge out of the pulpers. There is considerable variation in the pulper output % DS in Figure 10a. The variation in sludge input to CAMBI is ±1.0 % DS about the hourly average that was set for the design. The % DS from the digester recirculation units is given in Figure 5.22b. The range is between 5 and 7 % DS. This is low for a CAMBI process as one of the key design benefits of the CAMBI technology is that it can handle % DS at a level of 14 %. Thus the process is performing below its capabilities.

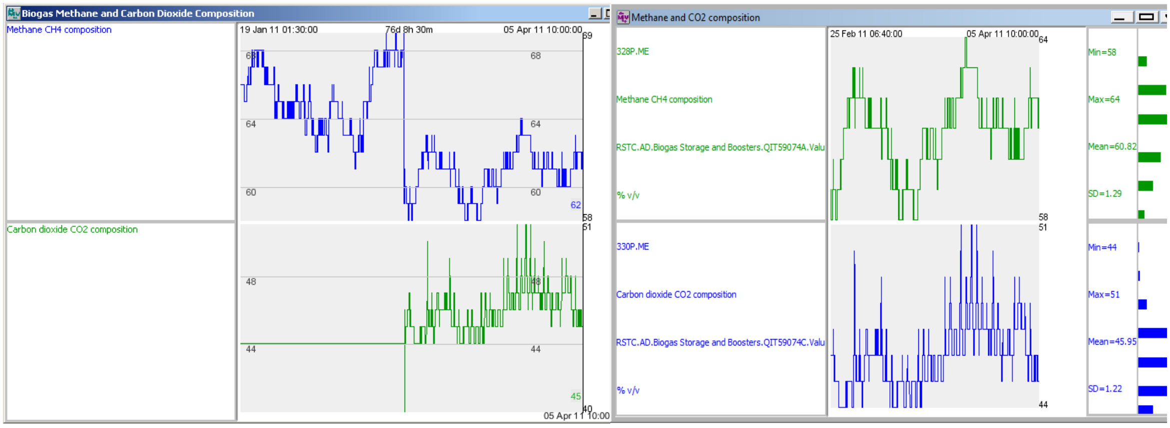


Offline analysis of % DS from the pulpers

Offline analysis of % DS from digester recirculation

Figure 5.22 Analysis of % DS from the pulpers and digester recirculation

For mesophilic digestion, CH_4 is generally in the range between 65-68 % of the gas concentration and 32-35 % for CO_2. Figure 5.23a gives the signal for the whole analysis range and not all of the 94 day analysis range is shown in this trend, additionally, the CO_2 composition measurement only appears to be available from the 24th of February onwards. Figure 5.14b show trend for both signals in the range where there is data for both signals from 01 January 2011 to 05 April 2011 with CH_4 composition between the range 58-64 % and CO_2 between 44-51 %. CH_4 composition is at the low end of the specification resulting in high CO_2 levels in the gas phase. Analysis of the CH_4 signal reveals that the gas component swings through a range of 10 %. Sensitivity analysis conducted using the AD spreadsheet (Redman, 2010) showed that a 1 % increase in CH_4 composition results in an approximately 1.7 % increase in the energy content of the biogas. For this reason, maintaining high CH_4 composition in the gas may have a greater effect on the energy produced than increasing biogas yield.



Plot of actual CH_4 (green) and CO_2 (blue) composition in biogas for the analysis range

Zoomed-in plot of actual CH_4 (green) and CO_2 (blue) composition in biogas for a section of the analysis range

Figure 5.23 CH_4 and CO_2 composition analysis

CH_4 content may be increased through:

- Co-digestion: improving the substrate composition improves CH_4 content (Callaghan *et al.*, 1999; Sosnowski *et al.*, 2003; Lehtomäki *et al.*, 2007; Astals *et al.*, 2011; Zhang *et al.*, 2011). This is however difficult to assess as the different feed streams need to be investigated to assess the CH_4 yield potential;
- Temperature: temperatures between 32-35˚C are deemed to be the most efficient for stable continuous production of CH_4 for mesophilic digestion (Song *et al.*, 2004; Chae *et al.*, 2008; Ward *et al.*, 2008). At low temperatures CH_4 content tends to be higher while biogas yield as a whole is lower;
- CH_4 production may increase with increasing organic loading rate (OLR) (Ince *et al.*, 1995) prior to overloading. As there is significant variability in the CH_4 content for the Bran Sands data, monitoring and control of parameters such as the feed rate may be used to control the CH_4 composition. A study showed that OLR affects the CH_4 composition (Babaee and Shayegan, 2011) and by

modelling the effect of feed rate and CH_4 into the potential controller can help with obtaining highest possible yields for CH_4.

A second interesting observation was seen for CH_4 composition and digester feed rate. Figure 5.24 shows a 12 hour filtered signal for the digester feed rate in blue and a 12 hour filtered signal for CH_4 composition in the gas phase. The data suggests that as the feed rate increases, CH_4 composition decreases. The opposite effect is observed within the benchmark simulation model 2 (BSM2) (Alex *et al.*, 2008a), where an increase in feed rate causes an increase in CH_4 yield. It is possible that a different variable is causing the decrease in CH_4 yield. This may be due to the feed sludge stoichiometry such as sludge age, low % DS and variation in the organic matter which might cause the methanogens reaction step to shift towards the production of increased CO_2 yield instead of CH_4. NWL is keen on exploring co-digestion regimes with wastewater sludge. Analysis of the digestion system with cause effect analysis on changes to sludge composition and effects on KPIs such as CH_4 yield need to be undertaken. This is more important for this site as there is considerable evidence that the digestion process is highly unstable due to foaming issues that affect both upstream and downstream processes.

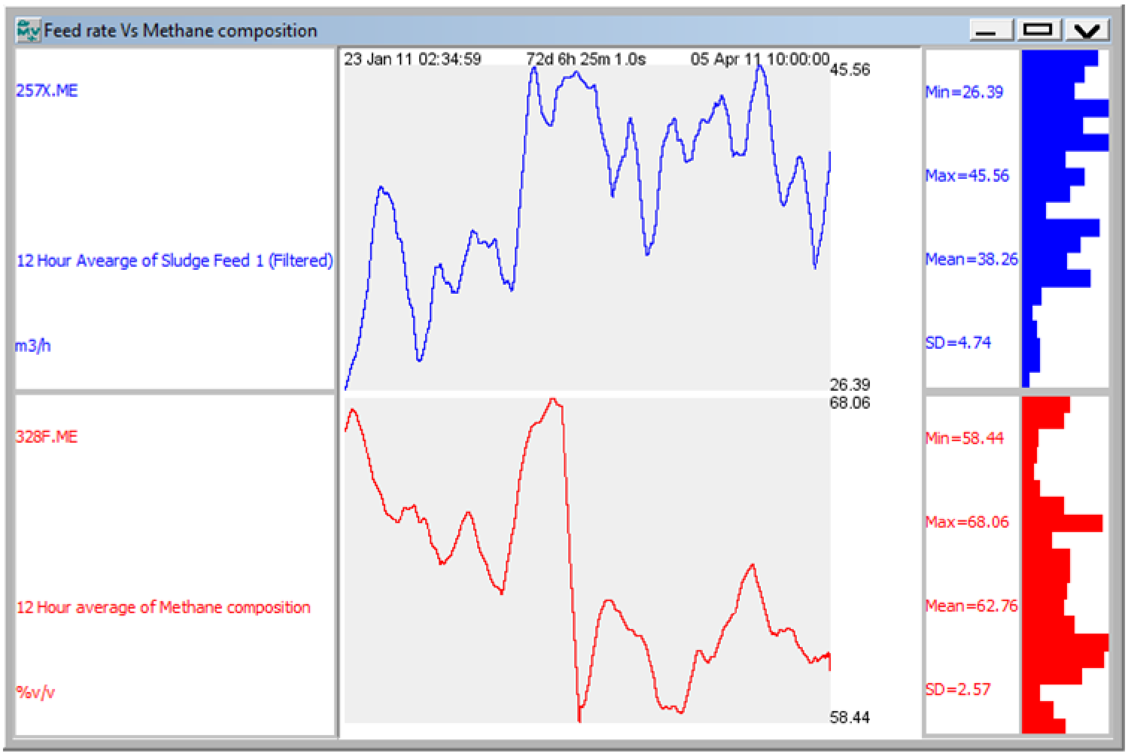


Figure 5.24 Digester feed flow versus CH_4 composition

The Bran Sands AD digesters are fed non-continuously to guarantee a minimum retention time for all of the material entering the digester vessels over 15 minute recording interval of individual data points which is not of a sufficiently high resolution to allow an analysis of the individual hourly 'feeds' to the digesters. A 12-hour moving average filtered version of the sludge feed flow was produced for each digester as shown in Figure 5.25. The filtered signals give a much clearer indication of the actual feed rate behaviour. The relative proportions of the sludge feed to the three digesters are constantly changing, along with the total overall feed rate and the mean flow to digester 1 is 12.29m^3 hr^{-1}, the mean flow rate to digester 2 is 10.46 m^3 hr^{-1} and the mean flow rate to digester 3 is 14.28 m^3 hr^{-1}.

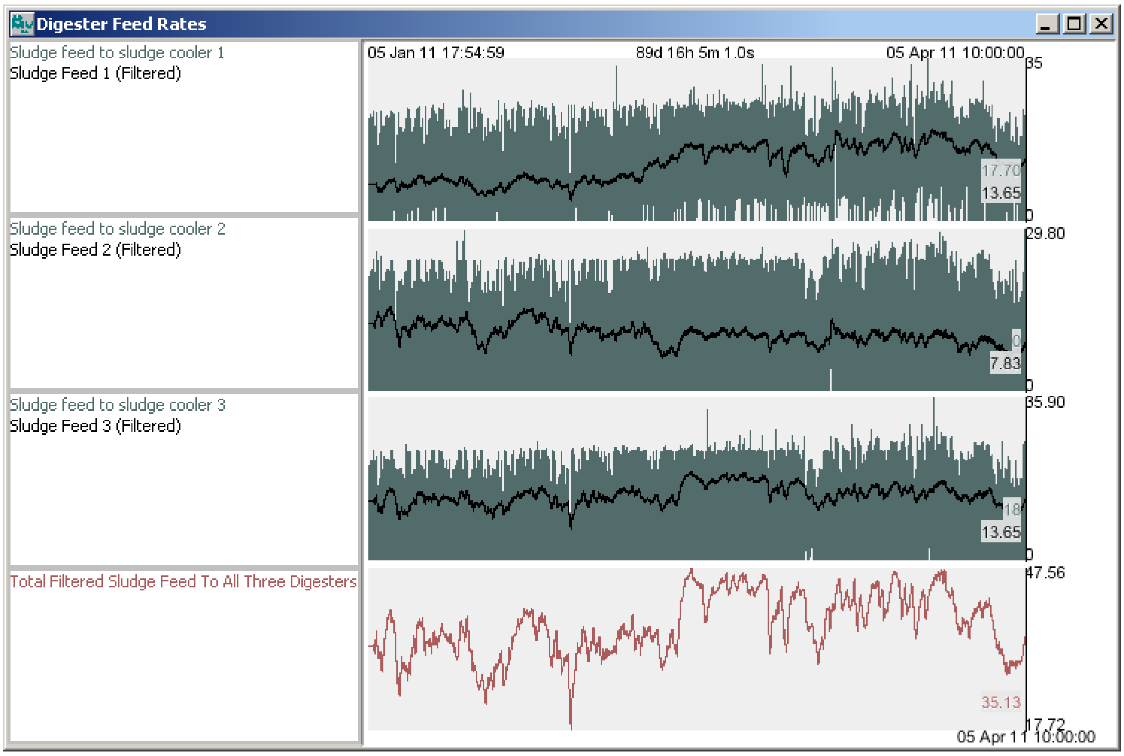


Figure 5.25 Digester feed rates

Figure 5.26 shows that the differences in feed rates are significant, and strongly affect the retention times, along with the likely gas production levels. Given that each digester has a working volume of 6700 m^3, then the retention time in the digester may be calculated from the digester influent flows. The calculated Retention Time was produced using this filtered flow information. Given the flow rate from the coolers (and thus into the digesters) was an average of 294m^3 day^{-1} for Digester 1, 251m^3 day^{-1} for

Digester 2 and $342m^3$ day^{-1} for Digester 3, the retention times in these digesters was calculated as an average of 25.5, 27.5 and 20.5 days respectively.

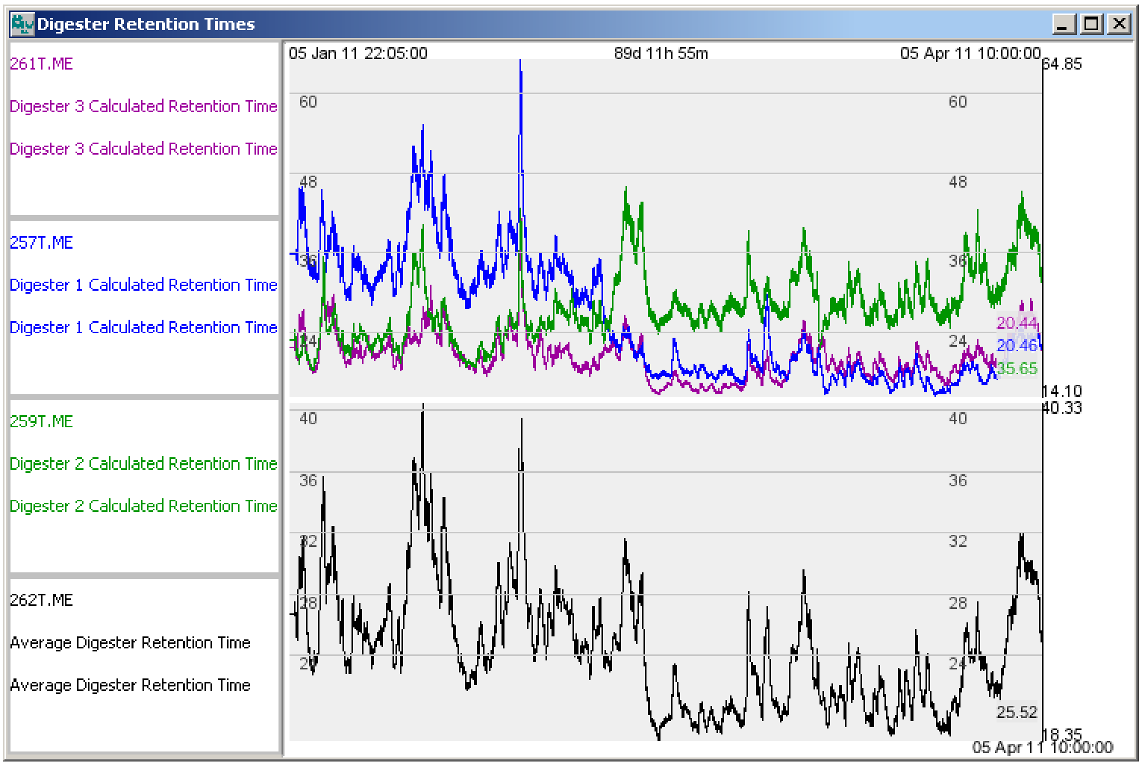


Figure 5.26 Digester retention time

Further inspection of the data leads to an interesting relationship between the retention time in the digesters, and the total energy generated by the gas engines. In this case, the average digester retention time has a correlation coefficient of -0.8 with the energy generated from gas indicating a high level of correlation between these variables. This can be demonstrated visually by comparing the retention time with the inverse of the energy metric, in Figure 5.27a. This implies that in this instance a reduction in the average retention time would provide an increase in the energy produced. This can be further confirmed by inspecting the cumulative sum of the retention time, and of the energy usage in Figure 5.27b.

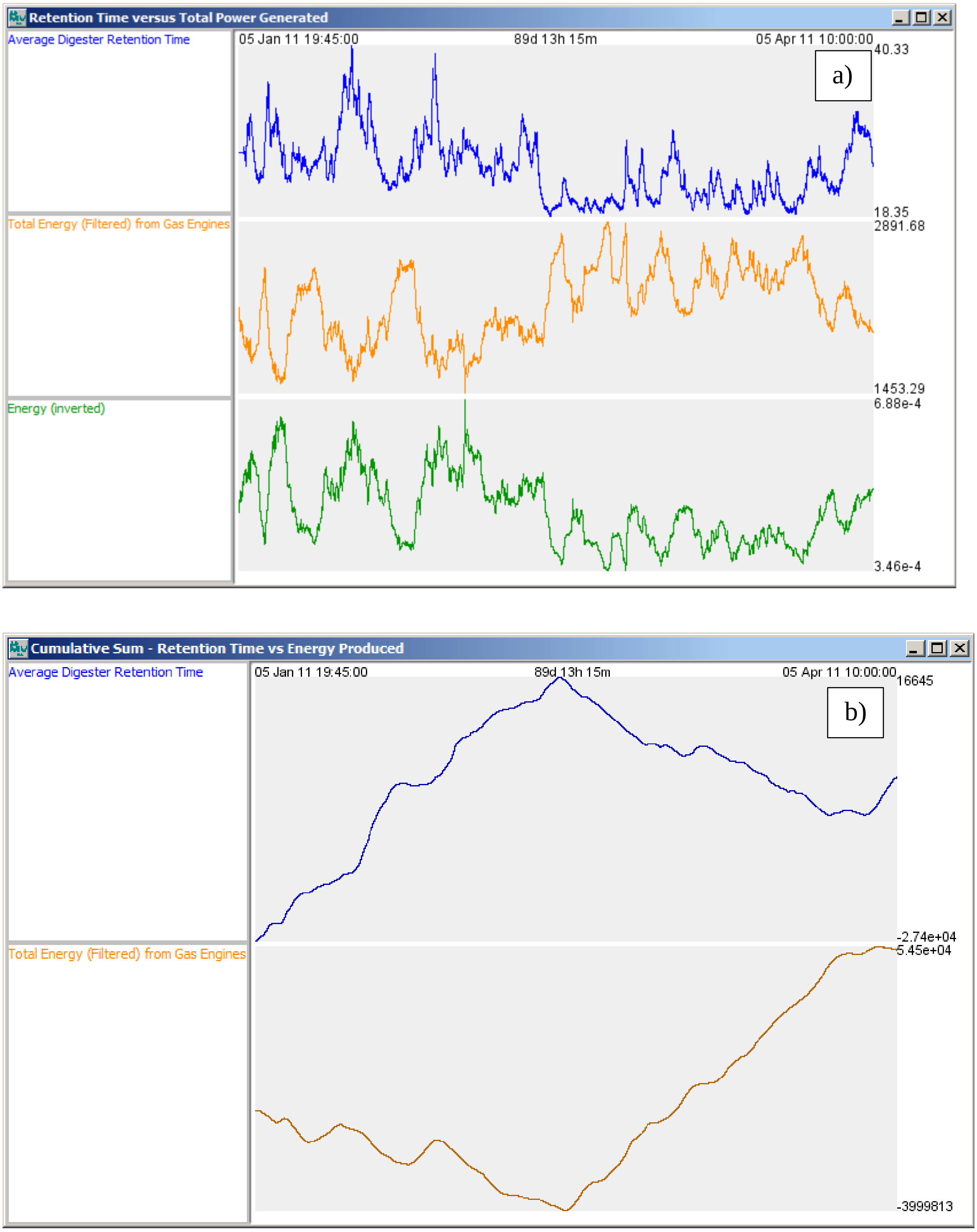


Figure 5.27 Average digester retention time and cumulative sum – retention time vs energy produced

At the time of analysis Bran Sands was undergoing several initiatives to address some of the problems. There are several opportunities which were not revealed from the data generated. Some of these however need to be resolved to improve the overall efficiency at the site. The issue of foaming currently means the digestion process is operating below its capability. Further work and analysis is required to remove or reduce this bottleneck from the process to enable the digestion to reach maximum capability.

The Bran Sands digestion process is fairly new and, as such the level of instrumentation was expected to be quite high in comparison to sites like Mitchell Laithes. The data generated from the site did not allow an efficient evaluation of the site's digestion process. Key signals such as biogas flowrate and % DS feed to digester were unavailable making it difficult to compare results from this site with others.

Key findings from Bran Sands are as follows:

- Gas flow measurements unavailable;
- Inventory and scheduling bottlenecks affecting sludge availability;
- CHP engine capacity limitation;
- The average energy produced is about 0.34MWh tDS^{-1} which is well below typical ranges of 0.8-0.9MWh tDS^{-1};
- Maintaining efficient heat balance and heat availability;
- High % DS variability.

5.4.4 Sensitivity analysis

The data generated from Bran Sands especially had a number of KPI signals missing. To help with the business case, sensitivity analyses were conducted using the AD spreadsheet (Redman, 2010). This is a free publicly available spreadsheet, part of a biogas toolbox designed to assist the AD developer in assessing the viability and optimisation of different options. There are various feed streams available in the toolbox however; wastewater sludge characteristics are not modelled as the project is more aligned with the energy from crops sector.

100 % efficiency is fictional and cannot be achieved as maintenance and repairs are inevitable. Additional limitations of capital, management ability, labour, communication and or instrumentation may cause inefficiencies. A 1 % increase in CHP efficiency may increase income by up to 3 % as indicated by the AD spreadsheet. Various factors may improve efficiency of the whole site such as optimising feedstock throughput, electricity and heat production (utilisation of all energy produced through efficient energy balance for the site), improving the operational efficiency, reducing the feedstock costs and feedstock capacity could potentially significantly improve efficiency.

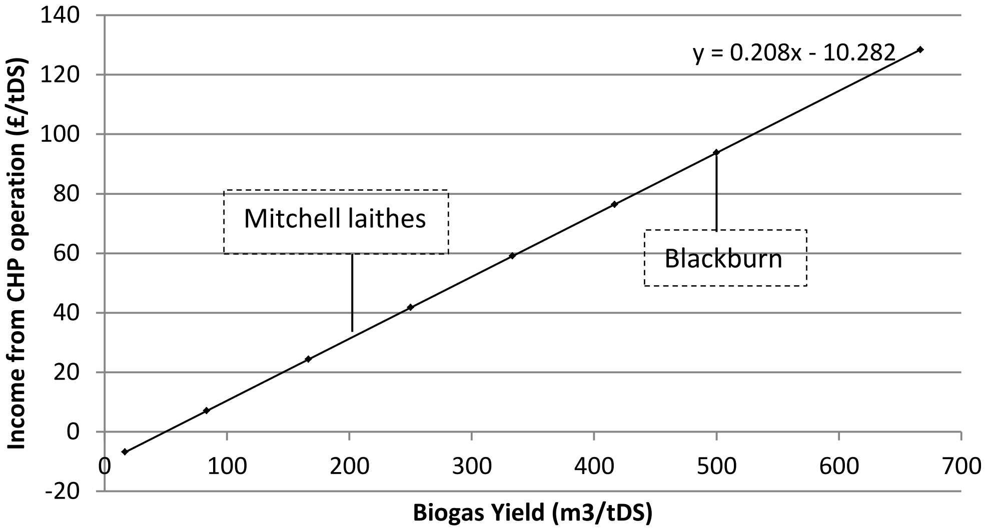


Figure 5.28 Biogas yield efficiency

Figure 5.28 shows a plot of increasing the efficiency of biogas yield against an increase in income generated from the process. This is achieved by means of energy production through CHP units as per the model in the spreadsheet with the value of renewable obligation certificates (ROCs) (ofgem, 2011b) which doubles the unit value of electricity. As expected, there is a strong linear correlation between yield increase and income. The biogas yields from Mitchell Laithes and Blackburn are shown on the plot; however data for Bran Sands site is unavailable to be indicated on the plot. This analysis gives a basis for improving the biogas yield efficiency per tDS fed to the digester. A second analysis was conducted to study the effects of the digester output on the co-digestion of different waste streams. Wastewater sludge characteristics are not included in the model and as such are not used in the analysis. As expected there is a positive increase in value in pig slurry by mixing it with vegetable waste. By knowing the economics of obtaining certain feedstocks, a cost benefit analysis can be conducted with the help of analysis such as this to determine the capability of certain co-digestion regimes.

5.5 Discussions

Due to the level of instrumentation at the three benchmark sites, a comparison between them is limited. Table 5.4 provides a summary of the KPIs available at all three sites. In general, there two stage AD processes at Blackburn and Bran Sands outperforms the single stage MAD at Mitchell Laithes. However, although Bran Sands site is relatively new the Blackburn site outperforms Bran Sands. This is shown by the level of gas production per tonne of dry solids fed into the digester, which is more than 4 times the level gas produced at Mitchell Laithes. This may be due to the quality of the sludge used at this site, thus without significant analysis of the sludge composition at these sites, it is difficult to conclude on the reason for the differing performances apart from the difference in technologies and practices.

Table 5.4 Site comparison of KPI

KPI	**Blackburn**	**Bran Sands**	**Mitchell Laithes**
Gas produced pet tDS of feed ($Nm^3\ tDS^{-1}$)	453	297	106
Electricity produced per tDS of feed	0.53	0.49	0.209
Organic loading rate (mean in kgVS $m^3\ d^{-1}$)	3.50	1.84	1.68
Digester temperature range (˚C)	27 to 35	38 to 43	27 to 44
Retention number average (days)	14 (+2)	24	23
Digester feed rate ($m^3\ h^{-1}$)	29.34	37.04	19.61

The spread of the data from the three sites varies considerable as shown in Table 5.5. Although Mitchell Laithes site has a temperature control, the site has the largest temperature variance.

Table 5.5 Analysis of the spread of temperature data for the benchmark sites

	Mean	**StDev**	**Variance**	**Median**	**Range**
Blackburn	31	2.739	7.5	31	8
Bran Sands	40.5	1.871	3.5	40.5	5
Mitchell Laithes	35.5	5.34	28.5	35.5	17

The feasibility study revealed several opportunities in the process; potential savings can be made by increasing the CHP capacity and aligning energy production with unit electricity cost price. Long term solutions based around this AD project, include enhanced monitoring of the process through soft sensor development and the development of a multi-objective advanced controller to meet the aims of the various control objectives. The aim of the study was firstly to provide a business case for the application of an advanced control system to the AD processes.

The benchmark study was carried out with the aim of applying advanced control such as MPC to improve the process. Significant findings were (1) Inventory and scheduling have an impact on both downstream and upstream processes and form the main bottleneck in the process; (2) There exist lack of online instrumentations; (3) There is limited monitoring of the process in general; (4) Offline analyses results in long sampling intervals; (5) There are quality variables which are not performing at their specification setpoints and (6) Foaming issues with unknown specific cause.

These formed strong evidence for the project to progress to the development phase to develop solutions to improve these AD systems. Being an industrially focussed Engineering Doctorate, the benchmark study is used to evaluate the improvements that can be gained from using MPC on the AD systems. MPC may be beneficial (i) continuous process: the availability of feed and the effects of inventory and scheduling is of high importance. MPC can enable modelling the past feed to allow better prediction of the future inventory. Controlling the inventory both upstream and downstream of the digestion process is crucial to optimising the whole process, advanced control scheme can help with this; (ii) lack of instrumentation: MPC can harness soft sensor capabilities into the control system and make it possible to reduce the need for new instrumentations for measurement. However although these form a strong case for implementation of advanced control system, these cannot be quantified at this stage due to a lack of relevant data for direct cause effect analysis to establish a definitive business case. (iii) MPC offers advantage of repeated online optimisation (feedback) and solving multivariable and constrained with varying objectives and limits of varying uniformity.

Results generated so far successfully demonstrate an opportunity for advanced control structures such as MPC and the SWOT analysis in Table 5.6 demonstrates this. The strengths of the benchmark study lies within the commonalities of the results and the identification of quick fix money saving solutions. There is opportunity to improve inventory and scheduling impacts on the AD process thus phase II activities start with Chapter 6 the inventory simulation which aims to reduce inventory and scheduling bottlenecks. There is also opportunity to improve monitoring on the process and Chapter 7 volatile solids soft sensor development aims to achieve this. Weaknesses identified in the benchmark study results have the potential risks of (i) the necessary minimum and ideal instrumentation may prove to be unreliable or inadequate to provide reliable information; (ii) current AD systems may prove to be uncontrollable, large disturbances or too few adjustable parameters. Difficulty in meeting all or most of the control objectives may increase the complexity of the operation and (iii) real time experimental testing needed to obtain a rich dataset for modelling may be difficult to undertake.

5.6 Conclusions

The benchmark study was successful in highlighting significant opportunities for control and optimisation, implementation of a multi-objective robust advanced controller that satisfies the aims of the project will be challenging. This is due to the high level of uncertainty and unknowns within the system. A lack of robust online or offline instrumentation results in unknown feed composition, uncertainty in the state of the degradation process and quality of the system outputs. As a result, modelling of the process has proven to be difficult. Additional studies are required to investigate feed composition for the various sites, determine potential causes of foaming and digester degradation pathways to better predict the process outputs.

It can be concluded that no single technology outperforms the other and there are several commonalities in the performance of the different systems. Increased monitoring of key parameters and studies into whole plant optimisation such as focus on the energy balance is essential to improving the performance of the plants.

Table 5.6 SWOT analysis summary of key findings from the benchmark study

Strengths	**Weaknesses**
• Benchmark of three industrial sites with bottlenecks identified for each • There are several commonalities within the results from the three main sites such as variability in certain measurements • Calculated KPIs compared to other known KPIs for similar digestion processes • Quick fix money saving solutions identified, such as alignment of electricity production or usage with tariff prices	• Unusual observations observed for some KPIs, illustrating inaccuracies in data or unknown observations differ from literature and experience • Lack of data or information to enable cost benefit analysis to be conducted to yield a definitive business case • Inventory and lack of instrumentation hinders evaluation of the chemistries within the AD process
Opportunities	**Threats**
• There is a significant need for improved instrumentation to enable better monitoring and control of the process • For certain parameters such VFA and H_2 in the liquid phase there is an opportunity for soft sensor development • Energy balance at each site requires optimisation; heating and cooling and digester temperature control • Scheduling and inventory improvement through predictive controllers	• The benchmark sites are unique in nature, a generic controller may not be possible • Typical opportunities for advanced control requirements are identified, however further studies required to test out the capability of advanced controller for AD systems • Accuracy and reliability of data, can models built from such data be reliably used in model based control?

6 Inventory simulation

6.1 Introduction

The benchmark study in Chapter 4 identified a number of issues including:

1. Inventory and scheduling have an impact on both downstream and upstream operations and form the main bottleneck in optimising AD processes;
2. There is a significant lack of online instrumentation;
3. There is limited monitoring of the process in general, resulting in a lack of detailed understanding of the process.

The key bottleneck for optimising industrial AD processes is thus related to the sludge scheduling and inventory levels. AD processes are typically downstream processes at wastewater treatment works (WwTW), and therefore the availability of sludge depends on the upstream processes including activated sludge processes (ASPs), aeration and settling tanks. Most AD process sites also import sludge from other WwTW sites and the deliveries are irregular and unpredictable in volume and quality. This was the case for all the benchmark sites and the operators try to reduce the uncertainty in the imported sludge volume, quality and frequency to improve the stability of the AD process. The inventory at any particular site varies considerably and is further impacted by amounts of storage and or buffer tank availability.

Close control of feed is essential for the stability of the process. This is because feed flow rate to the digester which is generally the only manipulated variable is dependent on the level of scheduling and inventory. Constant feed flow is desirable for the stability of the process as large changes in feed affects the process drastically. More specifically, large changes in inventory levels results in large fluctuations in feed rate causing instability in the process. Inventory and feed rate variations act as the main disturbance in the system. It is therefore desirable to feed the digester with as constant a feed as possible.

This issue was explored further by designing a simulation to evaluate the capability of a model predictive controller to control the inventory levels and reduce their disturbance on downstream processes. It is hypothesised that by removing this disturbance, the true capability of implementing an advanced controller for the optimisation of the overall AD system can be identified. A simulation model reflecting the characteristics of the industrial process and the effect of inventory on its operation was designed. A study was then conducted to test the capability of model predictive control to regulate inventory levels and to remove or reduce the effect of inventory on process performance.

6.2 The simulation model

The design and details of the simulation can be found in standard Perceptive functional design specification document titled “Anaerobic Digester Inventory Simulation” giving a detailed overview of the simulation model. The codes are written in the basic programming language within the Perceptive Engineering Ltd (PEL) software solution and this is provided in the disc attached. Perceptive Engineering Ltd has proprietary rights to the simulation model, therefore only a summary of the model is given here.

The schematic of the simulation process in Figure 6.1 provides the human machine interface (HMI) using DAQfactory provided by AzeoTech (AzeoTech, 2012). Figure 6.1 provides a schematic of the simulation process. The simulation model begins with the Gravity Belt Thickener (GBT) where an unknown composition of sludge is thickened. Thickened sludge from the GBT flows into the thickened sludge silo or buffer tank. Sludge flowrate and percentage dry solids (% DS) are the two variables available to the GBT. Dynamic data from Blackburn WwTW is streamed into the GBT. The rate of the streamed data is scaled depending on the time of the week. The streamed flow is multiplied by 1.2 for weekdays and 0.5 for weekends. This is because on observing the inventory levels of sludge at benchmarked sites; inventory levels at the beginning of the week were very high and at weekends there were no deliveries apart from Bran Sands WwTW for which there are considerably low deliveries on weekends. Therefore, the inventory available on these sites reduces considerably on weekends. This is crucial knowledge to add into the simulation as it enables an opportunity for maintaining constant feed to the digester and depicting the important disturbances into the system.

The simulation also contains a heating circuit as depicted in Figure 6.2. Waste heat energy from the CHP is used to heat a hot water circuit with additional heat provided by a backup boiler. Heat is lost from the system either from the main digester vessel through convection, conduction, or from adiabatic coolers. The thermal inertia of the adiabatic cooler is simulated as a first order response with time delay and the setpoint value for the adiabatic coolers is negative, to denote heat flow out of the system; whilst the thermal inertia of the backup boiler is simulated as a first order response with time delay and the setpoint value for the backup boiler is positive, to denote heat flow into the system. The adiabatic coolers and backup boilers are controllable elements in the simulation. This enables an analysis for optimising the energy production and the overall heat balance for the system to address one of the project aims of the overall project for reducing carbon footprint. Cost elements for heating and cooling the system are implemented into the model to enable best operation to be maintained.

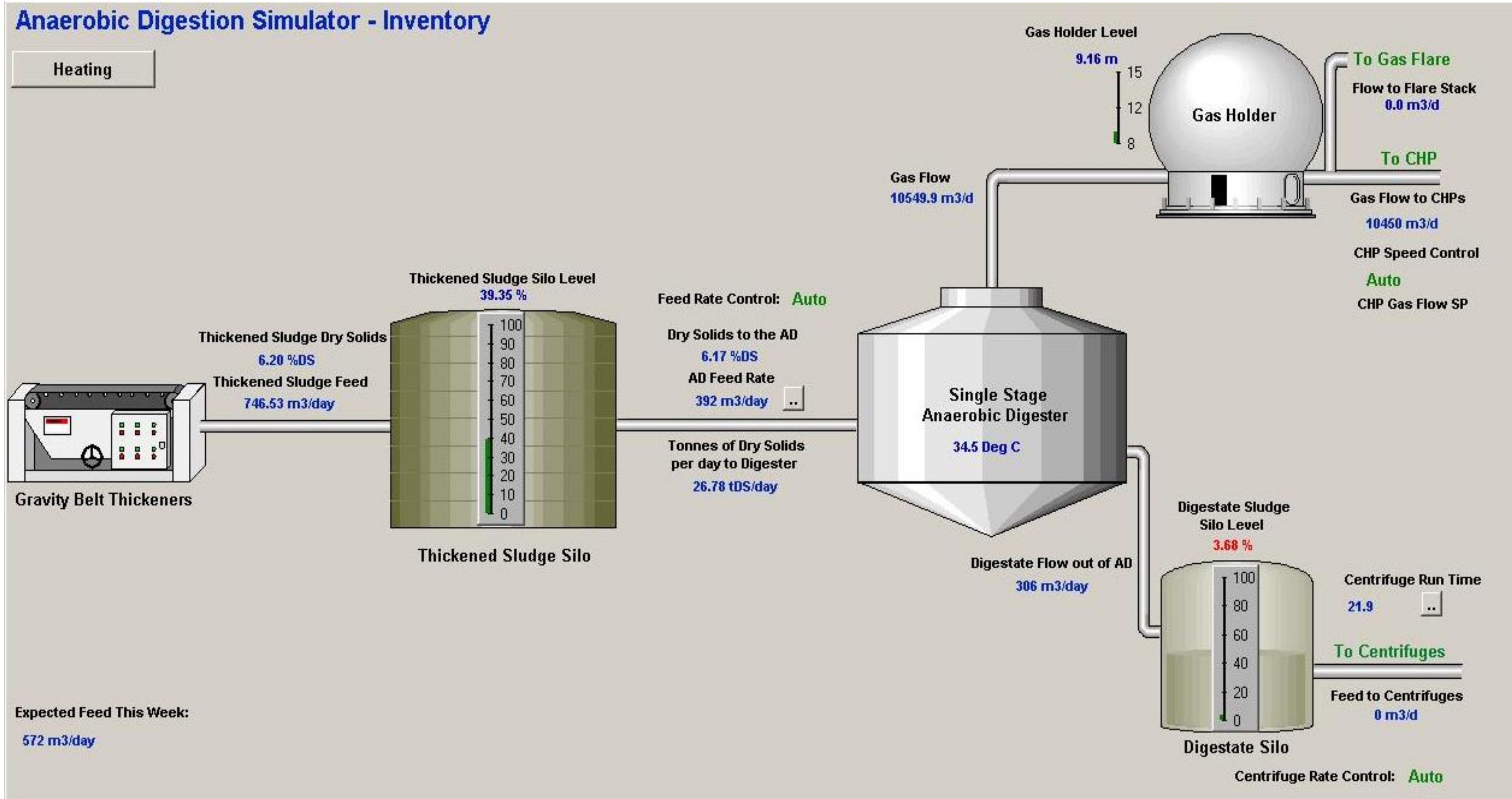


Figure 6.1 Schematic of AD inventory simulation

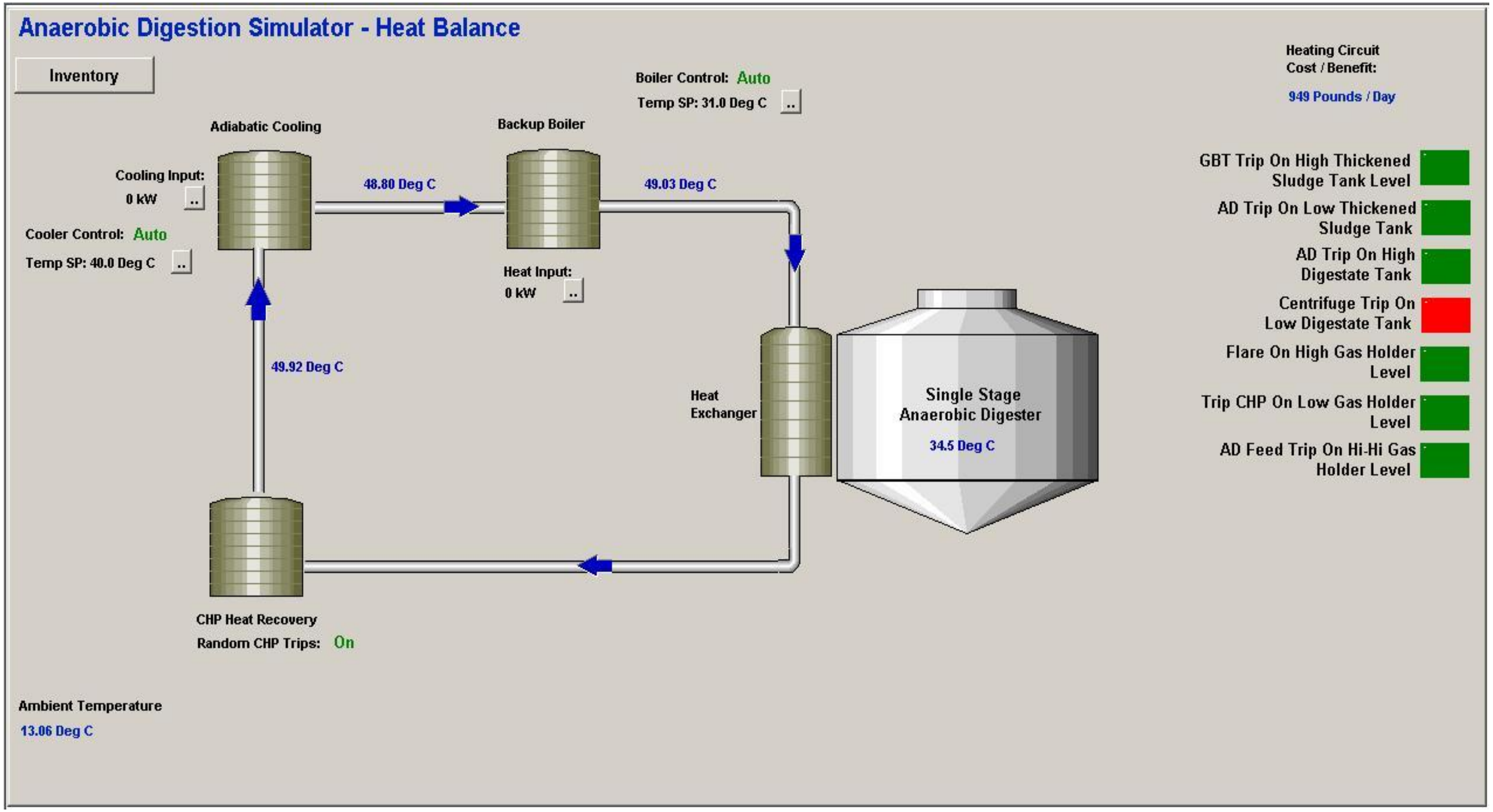
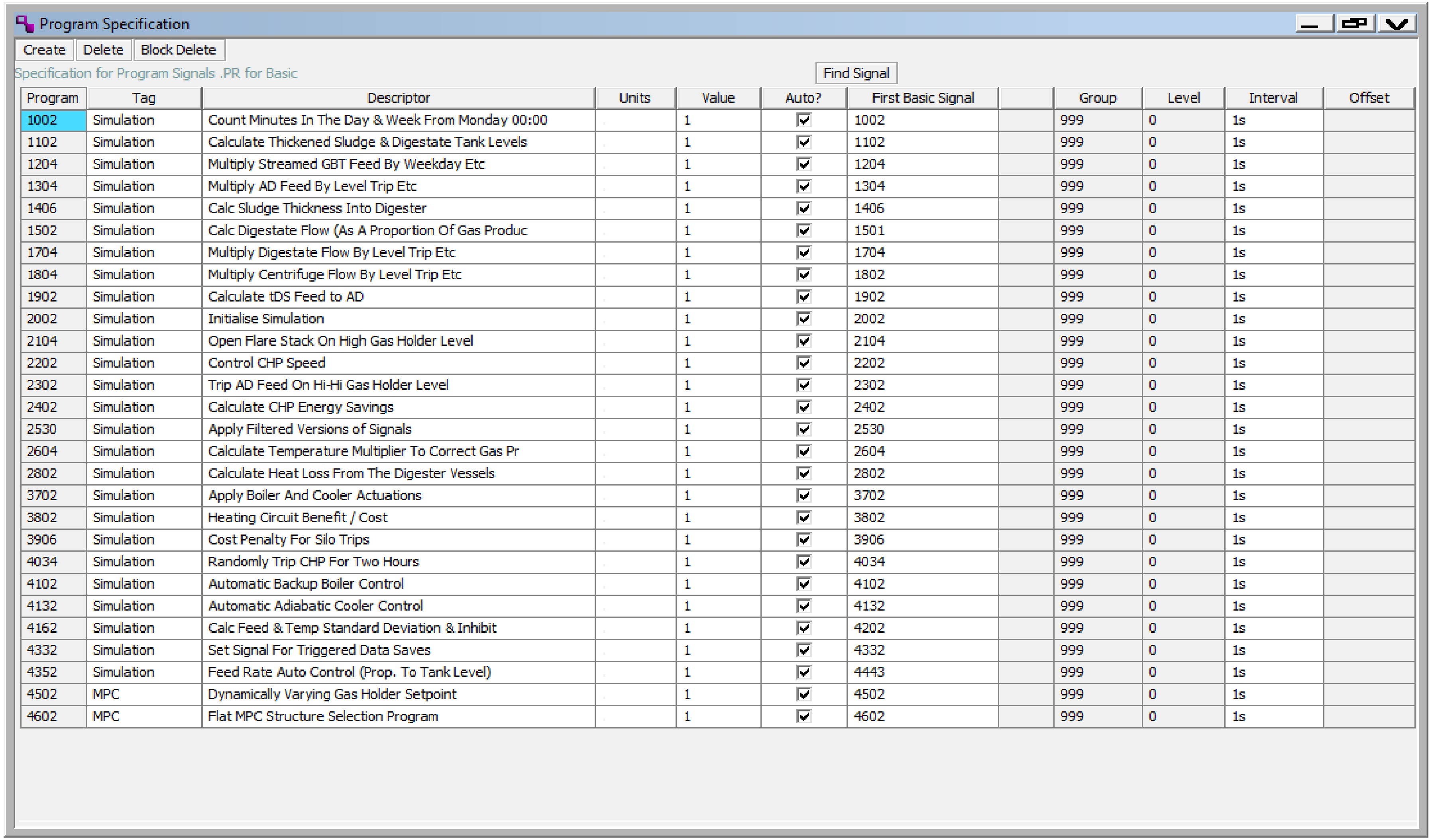


Figure 6.2 AD simulator heating circuit



Program Specification

Create | Delete | Block Delete

Specification for Program Signals .PR for Basic

Find Signal

Program	Tag	Descriptor	Units	Value	Auto?	First Basic Signal		Group	Level	Interval	Offset
1002	Simulation	Count Minutes In The Day & Week From Monday 00:00		1	☑	1002		999	0	1s	
1102	Simulation	Calculate Thickened Sludge & Digestate Tank Levels		1	☑	1102		999	0	1s	
1204	Simulation	Multiply Streamed GBT Feed By Weekday Etc		1	☑	1204		999	0	1s	
1304	Simulation	Multiply AD Feed By Level Trip Etc		1	☑	1304		999	0	1s	
1406	Simulation	Calc Sludge Thickness Into Digester		1	☑	1406		999	0	1s	
1502	Simulation	Calc Digestate Flow (As A Proportion Of Gas Produc		1	☑	1501		999	0	1s	
1704	Simulation	Multiply Digestate Flow By Level Trip Etc		1	☑	1704		999	0	1s	
1804	Simulation	Multiply Centrifuge Flow By Level Trip Etc		1	☑	1802		999	0	1s	
1902	Simulation	Calculate tDS Feed to AD		1	☑	1902		999	0	1s	
2002	Simulation	Initialise Simulation		1	☑	2002		999	0	1s	
2104	Simulation	Open Flare Stack On High Gas Holder Level		1	☑	2104		999	0	1s	
2202	Simulation	Control CHP Speed		1	☑	2202		999	0	1s	
2302	Simulation	Trip AD Feed On Hi-Hi Gas Holder Level		1	☑	2302		999	0	1s	
2402	Simulation	Calculate CHP Energy Savings		1	☑	2402		999	0	1s	
2530	Simulation	Apply Filtered Versions of Signals		1	☑	2530		999	0	1s	
2604	Simulation	Calculate Temperature Multiplier To Correct Gas Pr		1	☑	2604		999	0	1s	
2802	Simulation	Calculate Heat Loss From The Digester Vessels		1	☑	2802		999	0	1s	
3702	Simulation	Apply Boiler And Cooler Actuations		1	☑	3702		999	0	1s	
3802	Simulation	Heating Circuit Benefit / Cost		1	☑	3802		999	0	1s	
3906	Simulation	Cost Penalty For Silo Trips		1	☑	3906		999	0	1s	
4034	Simulation	Randomly Trip CHP For Two Hours		1	☑	4034		999	0	1s	
4102	Simulation	Automatic Backup Boiler Control		1	☑	4102		999	0	1s	
4132	Simulation	Automatic Adiabatic Cooler Control		1	☑	4132		999	0	1s	
4162	Simulation	Calc Feed & Temp Standard Deviation & Inhibit		1	☑	4202		999	0	1s	
4332	Simulation	Set Signal For Triggered Data Saves		1	☑	4332		999	0	1s	
4352	Simulation	Feed Rate Auto Control (Prop. To Tank Level)		1	☑	4443		999	0	1s	
4502	MPC	Dynamically Varying Gas Holder Setpoint		1	☑	4502		999	0	1s	
4602	MPC	Flat MPC Structure Selection Program		1	☑	4602		999	0	1s	

Figure 6.3 Programming signals specification page

6.2.1 Simulator structure model

The model consists of seven auto regressive with exogenous inputs (ARX) model blocks which form the basis of the simulation. These block models relate to:

1. Thickened sludge tank;
2. Heating water temperature after combined heat and power (CHP);
3. Digestate tank;
4. Heating water temperature after coolers;
5. AD gas production;
6. Heating water temperature after backup boilers and;
7. Gas holder level simulation.

The underlying structures of the blocks are recursive least squares (RLS) models. The block models describe the tank levels, gas production, heating and energy usage in the system. The simulator enables models identified within the PerceptiveAPC design system to simulate the AD plant behaviour. The models can be read or fed into the online system to generate simulated data after model development in the design system. In configuring a simulator block several properties are required to be specified. These are:

1. Group level – determines whether the simulator is active or not during online. Default group signal for simulators is 999.GR operations;
2. Level – determines the conditions under which the block can become active, the level of the group signal must be higher than or equal to this level;
3. Update interval – defines the interval of the simulator;
4. Sample interval – interval at which new data samples are read into the simulator algorithm, setting the sample interval smaller than the update interval helps reduce noise.

For a nonlinear system such as the AD process, linear modelling techniques may be ineffective at characterising the cause-effect relationships. However, as the simulator model is simplified to account mainly for heat balance and level control, these factors are easily modelled and therefore linear models are adequate for this system. The use of linear model approach is driven by the use of PerceptiveAPC system. Model extensions of physiochemical and biochemical characteristics of the sludge may require nonlinear modelling techniques such as neural networks which are available in the PerceptiveAPC.

6.2.2 Simulator design

For the understanding of the behaviour of the AD system over time, it is important to understand the time response of the system to be able to predict the systems response and hence, how the ability to implement process control. By understanding the system dynamics, it is possible to determine the speed of response, the level of overshoot before settling, oscillations in the system, process instabilities and how rapidly a step change in a process parameter takes to reach steady state and the rate of change of output parameters. For an AD process, the dynamics differ for each stage of the digestion process and also for parameters within a particular process. Therefore understanding the dynamics at each of the digestion stages and how these affect process parameters is essential for control.

Current data generated from the benchmark sites fails to provide a complete profile of the system dynamics of the AD process, with respect to the effect of inventory on the process. The benchmark data and process understanding resulted in the development of a simulation model for the optimisation of the inventory. The complex characteristic of the AD system results in limitations in the developed models of the process and, consequently, there are inconsistencies between the process model and industrial AD systems. These issues are due to a lack of in depth process knowledge such as:

- Limited number of process interactions being modelled – these are summarised in Figure 6.3 and focus on parameters that directly or indirectly effect inventory of the system;
- Assumptions on the scale of some unmeasured parameters;
- Assumptions on the rate of change of some process effects – the scaling factors for temperature and feed flow effect on biogas production in Tables 6.1 to 6.3 are assumptions based on theoretical understanding;
- Models which do not take into account full indirect effects – for example the biogas production is based upon a univariate simulation model using the dry solids signal to the digester as the cause signal for the model with 16 days as time taken to reach steady state and scale factors for temperature and feed flow rate applied as summarised in Table 6.1, 6.2 and 6.3 showing temperature correction, feed rate standard deviation correction and digester temperature

standard deviation correction for biogas production respectively. This model fails to account for the effect of digester environmental conditions and the biochemical composition of the feed.

The feed rate is scaled according to the temperature in the digester. This reflects the fact that gas is produced at different digester temperatures, based on the same amount of material feed to the digester. The temperature correction scaling factor (varies linearly between the different temperature ranges) implying that for the maximum gas production, the digester temperature should be maintained at a value of between 35 and 40°C. The digester operation is the most stable with maximum gas production when the feed rate to the digester is maintained at a stable value, thus the feed rate standard deviation correction is intended to replicate this effect. The digester temperature standard deviation correction aims to replicate the effect of improved gas production due to reduction in temperature variation.

Table 6.1 Temperature correction for biogas production

Temperature range (°C)	<15	15-20	20-25	25-30	30-32	32-35	35-40	40-42	>42
Scaling factor	0.2625	0.2625-0.42	0.42-0.6	0.6 - 0.84	0.84-1	1-1.167	1.167-1.167	1.167-0.2625	0.05

Table 6.2 Feed rate standard deviation correction for biogas production

Feed rate	<50	50-100	100-250	>250
Correction factor	1	0.98	0.95	0.9

Table 6.3 Digester temperature standard deviation correction for biogas production

Standard deviation	<0.4	0.4-0.8	0.8-1.2	>1.2
Scaling factor	1	0.98	0.95	0.9

The simulation model was validated and verified to compare the model and its behaviour to the benchmark sites. This included an iterative calibration process to make adjustments to the revised model. The objective of the model was to reduce the disturbances in the process as a result of variation in sludge inventory levels through the application of a model predictive advanced controller. The hypothesis was therefore; the model predictive controller can effectively control the sludge inventory levels, thus improving the stability of the process and maximising biogas and energy production. This will be illustrated through a reduction in the level of tank level 'trips' (i.e. the tank level violating the upper and lower limits of tank alarm settings), increasing the energy production and overall site efficiency. The aim of using the simulation in this manner is to gain further understanding from the process and to utilise this during the plant testing or design of experiments on the industrial site. Changes made on the plant will thus be a combination of the results from the simulation results and improved process understanding. This dynamic model provides a platform for testing control and optimisation strategies primarily for assessing the capability of a model predictive control (MPC) controller for removing or reducing the scheduling and inventory bottleneck.

The benchmark data showed that the industrial systems are subject to several level trips from the buffer tanks, gas holders, buffer tanks, digestate tanks and centrifuges. Level trips are incorporated on the buffer tank, thickened sludge silo, digester, digestate silo and gas holder tanks to trip. This is typical of digestion plant operation and there is a cost element associated with overflowing the tanks or starting and restarting instrument. Flow to the buffer tank stops above 99 % full, until the level drops to 90 % full and if the buffer tank level falls below 1 % full, feed to the digester is tripped to stop until the level reaches 10 % full.

Table 6.4 Simulation level trip signals

Signal ID	**Description**	**Values**
100.ME	GBT trip on high thickened sludge tank	0=ok 1=tripped
102.ME	AD feed flow trip on low thickened sludge tank	0=ok 1=tripped
104.ME	AD feed flow trip on high digestate tank	0=ok 1=tripped
106.ME	Centrifuge trip on low digestate tank	0=ok 1=tripped
108.ME	Flare on high gas holder level	0=ok 1=tripped
110.ME	Trip CHP on low gas holder level	0=ok 1=tripped
112.ME	AD feed flow trip on hi-hi gas holder level	0=ok 1=tripped

Table 6.4 and Figure 6.4 provide the level trips occurring for the simulation prior to controller implementation. As can be seen the level trips occur on a frequent basis and the thickened sludge tank level overshadows all other trips. The model objective is therefore to ascertain a way to reduce trips occurring. A base line analysis was initially conducted from the simulation to establish input or output, data availability, model structure, parameter estimation and evaluation of model accuracy.

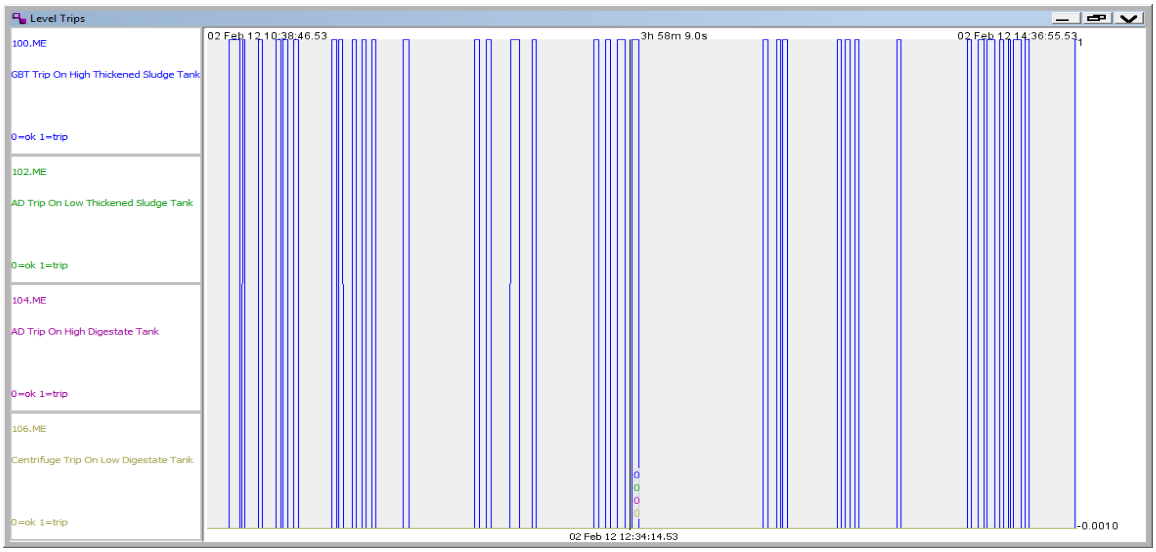


Figure 6.4 Level trips

6.2.3 System understanding

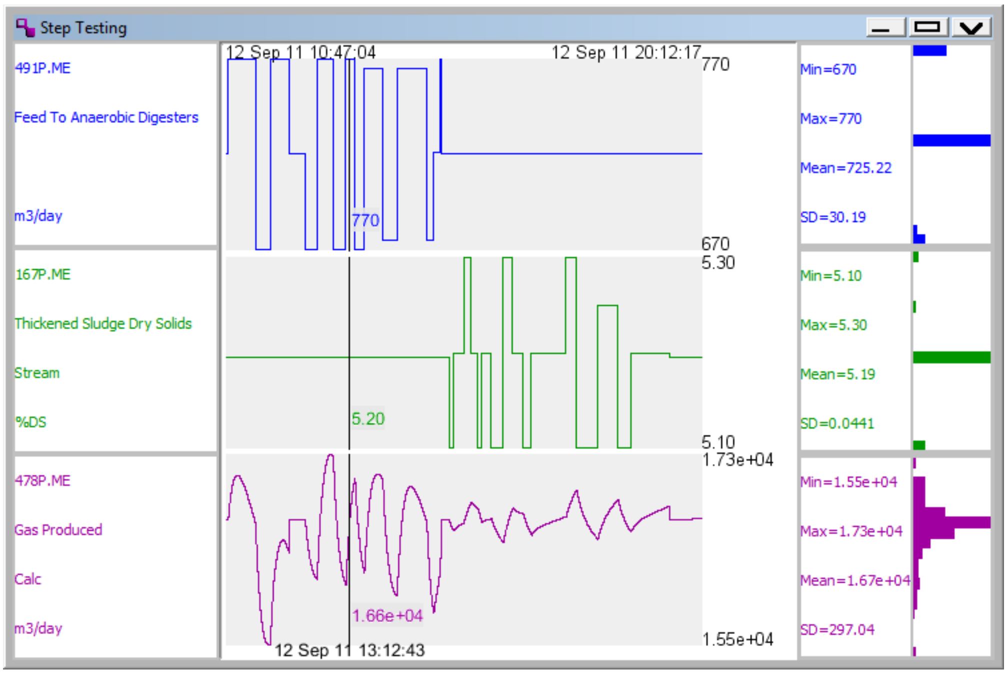


Figure 6.5 Step tests for feed flowrate and % DS and their effect on biogas production

Following the completion of the simulator design, step changes were performed on the manipulated inputs including feed flowrate and % dry solids to observe the changes in measured outputs such as biogas production. These process excitations or step tests were conducted to generate data which captured the dynamics necessary for the modelling. An example of this is shown in Figure 6.5, with step changes of feed flow rate in blue, % dry solids in green and the result of the step changes shown in the gas production plot in purple. As can be seen, the peaks and troughs of the gas produced plot coincide with the step changes of the feed flow rate and % dry solids. The data generated from the step tests were used to establish relationships within the system and comparisons were made to ensure the simulation results fitted with what had been observed or expected to at the industrial sites. This evaluation of system performance led to an iterative method where the model was continuously updated to make it reflect more closely to the performance of the industrial process. Some significant findings from initial simulated outputs were:

- The main bottleneck in the process was identified to be the thickened sludge tank level. The feed to the thickened sludge tank is depicted in Figure 6.6 in blue over a period of four weeks of simulation time shown in the black division lines. The figure shows considerable variation over the 4 week period as a direct result of variation in imported sludge. The tank level has the highest number of level trips and this is shown in Figure 6.4. Knowledge of the scheduling of imported sludge from other AD is crucial to the control and optimisation of the process;

- The simulation also revealed insight into the best initial set points for the system which limits the amounts of level trips. For example the feed to thickened sludge tank peaks at about 2393 $m^3 day^{-1}$ with an average or mean flow of about 620m^3 day^{-1}. These flowrates mean that the tank can fill and empty quite quickly. Feed flow-rate to the digester can therefore be set to the average flow of the thickened sludge tank feed to 620 m^3 day^{-1};
- The digestate feed rate to digestate tank level is dependent on digester feed. The feed flow to digester drastically reduces the digestate tank level; this operates in an on or off batch mode process (at zero or 2200 m^3 day^{-1}). Knowledge of the AD feed rate, digestate flow or digestate tank level is required to manipulate the centrifuge in order not to trip the digestate tank level as this had a great impact on the tank level.

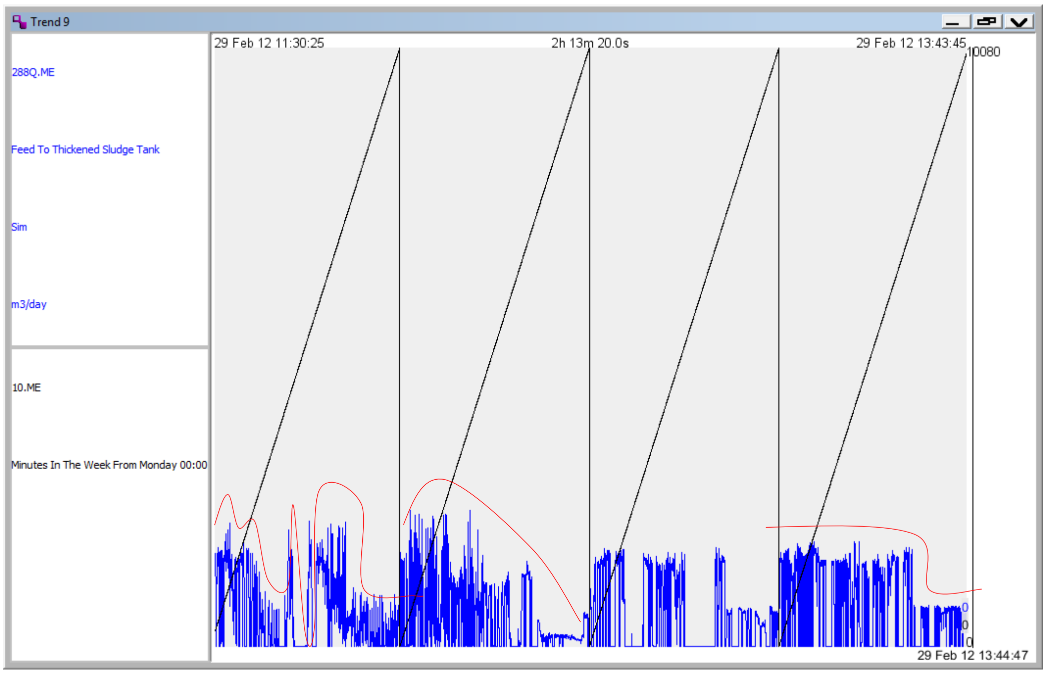


Figure 6.6 Feed to Thickened sludge tank

The MPC controller enables disturbance profile modelling of expected sludge levels over the week and therefore a degree of the disturbance can be predicted. Although the profile varies greatly there is a general drop in the feed to the thickened sludge tank level over the weekend, this increases generally from Monday, and by Wednesday inventory levels are in the high range through to Friday. Figure 6.6 shows the various profiles over four days. Modelling of the disturbance profile into the system will help with reducing disturbances in the system as a whole as the sludge inventory level had a knock on effect for almost every process in the system.

6.3 Modelling

The PerceptiveAPC model development software uses data driven algorithms to develop empirical models instead of using first principle models which require theoretical knowledge of the systems components. The full AD process is too complex for first principle modelling, for the purposes described here, and therefore the use of statistical process models to describe the system is followed. Step tests were conducted to generate an appropriate dataset for the modelling. The training data needed to satisfy various features to include richness, variability and consistency. This ensured that the process moves around throughout the data range; the data included all the operating ranges of the process; to avoid the controller struggling if the process moves to a different region and the dataset is together in sequence. The MPC models are used to test the capability of an advanced controller for controlling the process as a whole, specifically to address the findings from the benchmark study. Two main models were developed:

1. **MPC1**: a 'basic' structure as the standard MPC control structure depicted in Figure 6.7;
2. **MPC2**: a 'split dynamic' model structure depicted in Figure 6.8 where the system dynamics are split into slow and fast characteristics with the aim of improving total control of the system.

MPC1 in Figure 6.7 shows cause signals on the left hand side in brown (measured signals), light and dark blue colours as the actuators with effect signals on the right in light and dark green consisting of set points, state targets and output parameters. The cause signals are linked to their effect signals by the black arrows. For example, the measured signal 491.ME feed rate is linked to the actuator signal 1000.AC AD feed rate which is linked to the effect signals of 332Q.ME Thickened sludge Tank Level (SC), 1000.CT Feed Rate Steady State Target, 478P.ME Biogas Produced By AD (set point), 569P.ME Digestate Tank Level (SC) and 585P.ME Primary Digester Temperature (Set point).

MPC1 and MPC2 both use the same cause and effect signals. MPC2 aims to investigate the potential improvement for MPC control through separation of the different levels of system dynamic. Fast dynamic parameters are for example biogas flow, heating and cooling aspect of the process and slow dynamics are typical parameters contributing to the production of biogas.

Following the selection of model cause and effect signals, the next step was to set the model objectives. The main model objective is to avoid tripping the various levels. The hierarchy of the objectives is summarised in Table 6.5. The lists 9 control objectives and constraints in order of importance, with 10 being the most important and 2 the least important. Brief description of the reasons for the objectives and the order of ranking are also provided in the table. For example, prevention of AD feed stream tripping as a result of high gas holder level is given the highest level of importance of 10. This is caused by low levels of sludge in the buffer tank. Avoidance of this is the main aim of the simulation and ensures constant feed to the system.

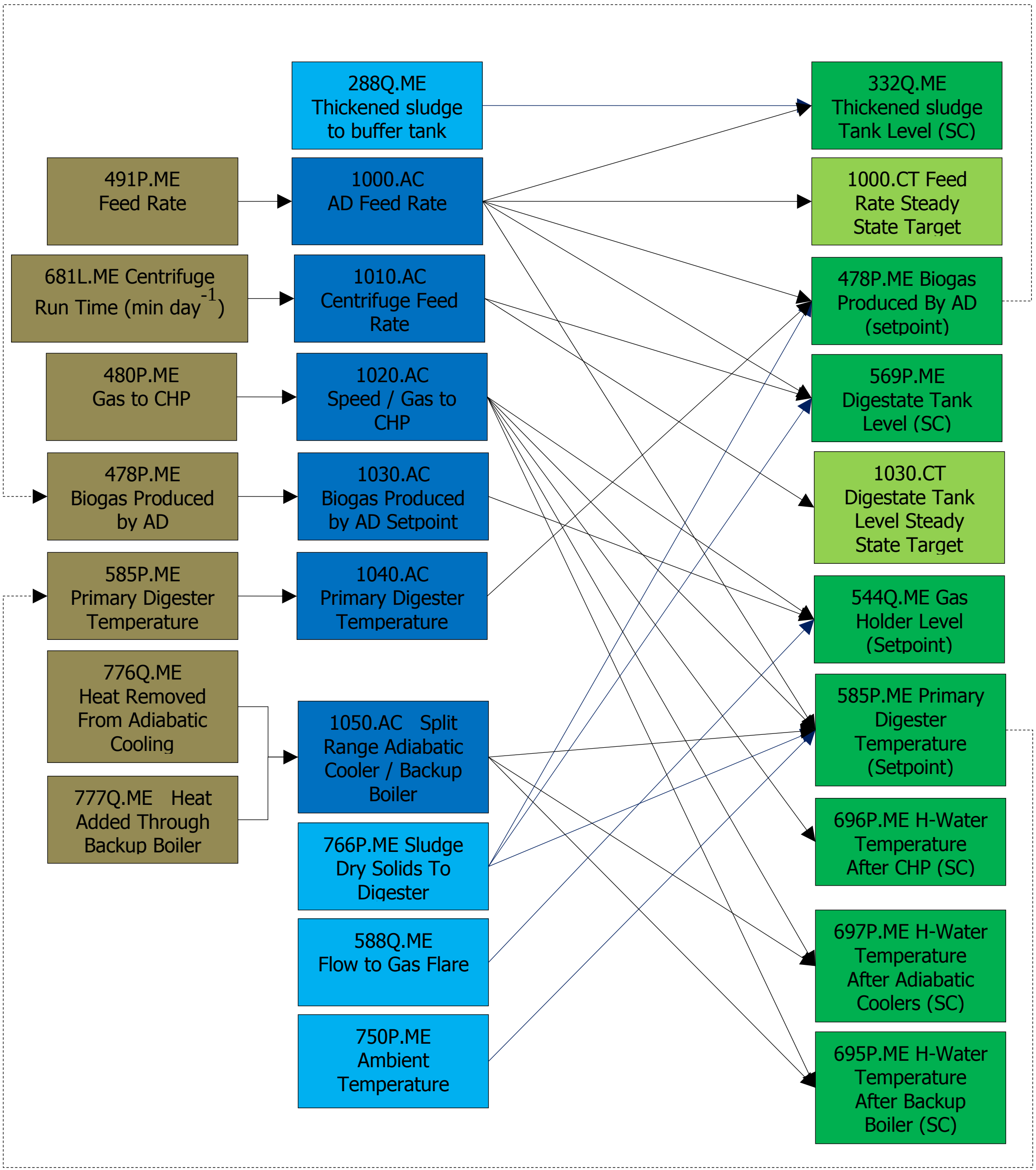


Figure 6.7 MPC1 basic model structure

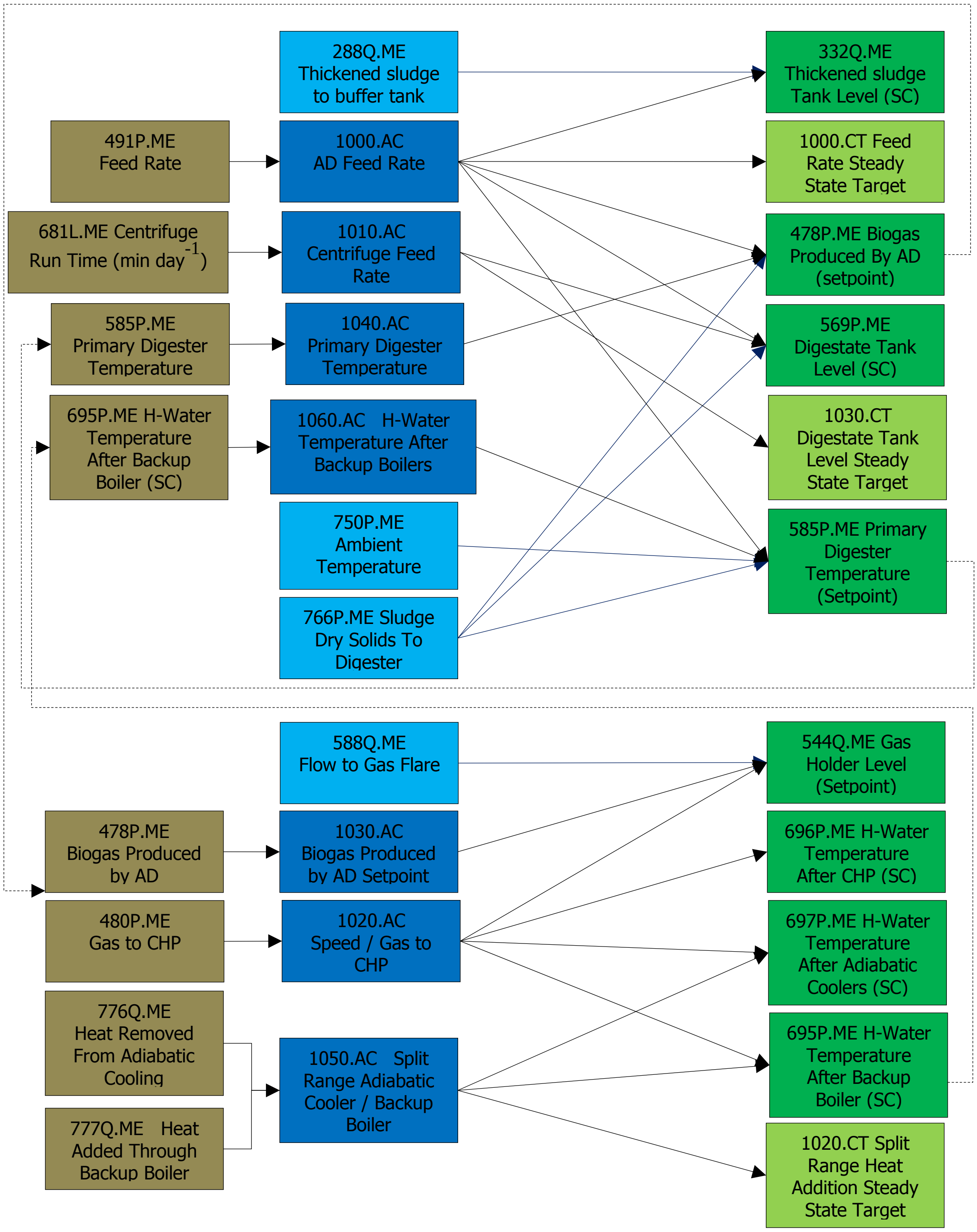


Figure 6.8 MPC2 split dynamic model structure

Table 6.5 Hierarchy of control objectives and constraints

Control objective or constraints	Hierarchy of	Reason
Prevention of AD feed tripping as a result of high gas holder level	10	Causes feed rate instability. Results in flaring of gas and hence affect CHP efficiency and energy production per tDS processed
Prevention of AD feed tripping On high digestate tank level	9	Cause feed rate instability. Increase retention time in the system and hence reduces throughput in the system
Prevention of AD feed flow tripping on low thickened sludge tank level	8	Affects all downstream processes. Cause feed rate instability, limits gas production and results in waste of resources
Prevention of CHP unit tripping on low gas holder level	7	Affects energy production. Scheduling to improve revenue generation through aligning energy produced with triad periods
Prevention of GBT instrument tripping due to high thickened sludge	6	Affects the upstream processes
Prevention of gas flaring due to high gas holder level	5	Waste and environmental issue. Currently regulations permit flaring of gas into the atmosphere. This may change over time with tougher regulations and therefore there is a greater need to prevent this
Reduction of AD feed rate variability	4	This causes instability in the digestion process and may cause foaming
Increasing the average value of CHP energy savings	3	Through alignment of energy production with peak electricity selling price
Prevention of centrifuge instrument tripping on low digestate tank level	2	This affects downstream processes (post digestion)

6.3.1 MPC model building in PerceptiveAPC

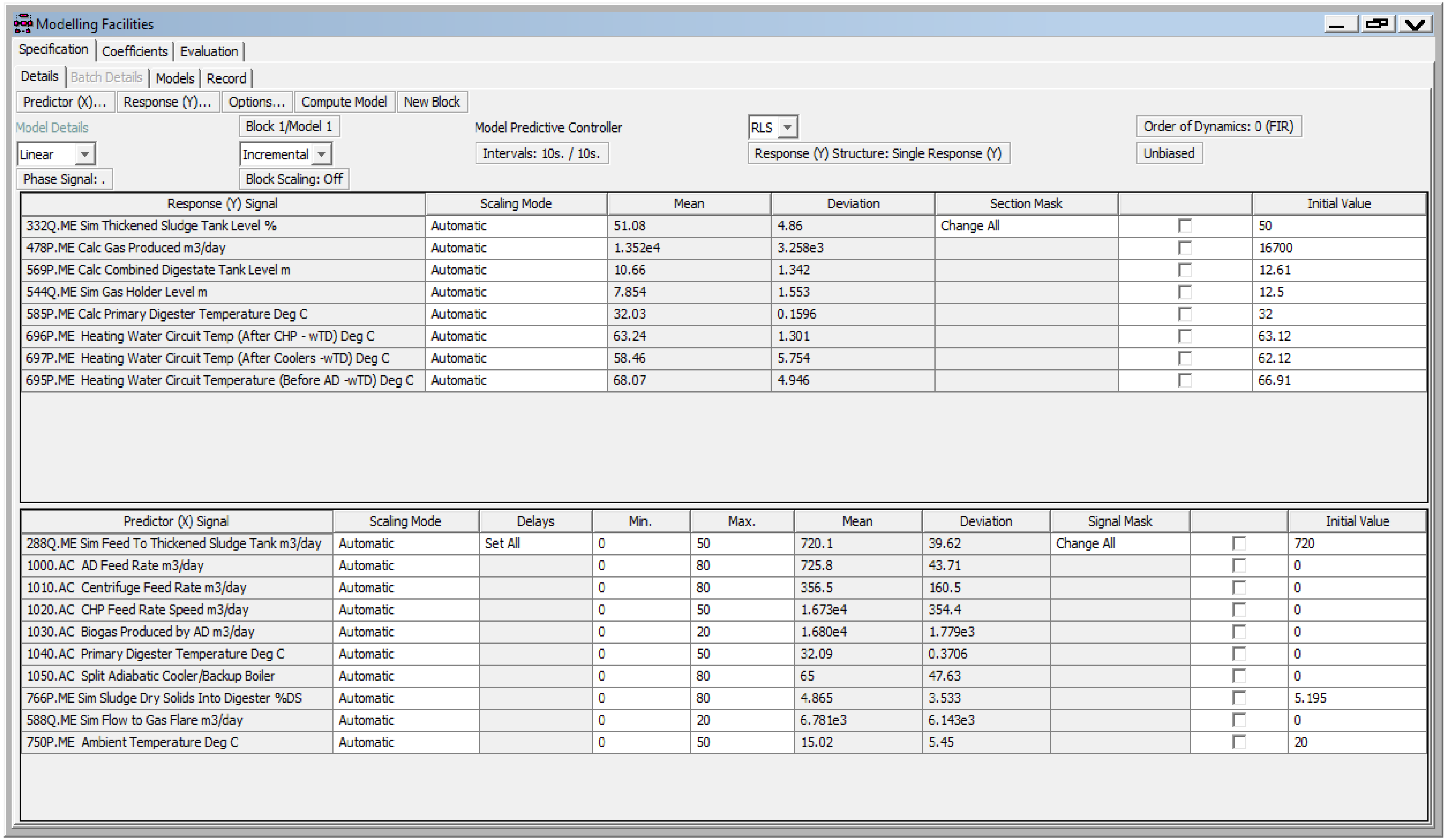
The modelling page in PerceptiveAPC consists of tabs for specification, coefficients and evaluation. The specification tab is where the MPC model attributes or details are specified and this is depicted in Figure 6.9. The coefficients page allows evaluation of model coefficients followed by model evaluation. The steps followed on the modelling page are selection of the model details:

1. **Model cause and effect signals**: the model details begin with the selection of the model cause and effect signals. These are selected as per Figure 6.7 and 6.8;
2. **Block mode**: MPC was selected for the block model as a controller model was required instead of an estimator or simulator model;
3. **Model type**: Within the PerceptiveAPC framework both linear and nonlinear model types can be derived.
4. **Model structure**: the model structure selection enables the user to select absolute or incremental model structure. The basic finite impulse response (FIR) model format is modified to enable the history of incremental changes in the cause signals to be used rather than history of the absolute changes. If a model is nonlinear then the model is also absolute and incremental nonlinear models are not permitted. As a linear model type was constructed, the incremental model is selected to improve the robustness of the model in the presence of unmeasured process drift.
5. **Model format**: There are three options available in PerceptiveAPC including principal component analysis (PCA), partial least squares (PLS) and recursive least squares (RLS). As the linear incremental model type was selected, RLS is the most appropriate computation algorithm as it enables different paths in the model to be identified separately using different sets of data, as all coefficients in the model are changed when the model is identified in PCA and PLS models (Jiang and Zhang, 2004; *Perceptive Engineering Ltd*, 2012). Therefore, linear RLS models allow 'path by path' modelling, which is achieved by masking out other paths, which is required as per Figure 6.7 and 6.8. Modelling each path separately allows different coefficients to be selected and the effectiveness of each path on the overall model can be identified.

   Figure 6.10 illustrates example of four variables affecting temperature prediction. The diagram shows the fastest approach of making changes to temperature is through the changes to the feed rate (A). The cold sludge coming into the digester cools the digester down faster than changes in ambient temperature, cooler or boiler settings and gas flow to the CHP units. Within the simulation, the incoming sludge is of lower temperature, which means the heating of the digester is more difficult or happens slower than the cooling of the digester when cooler sludge is continuously fed into the digester.

The next fastest effect on the digester temperature is the cooler or boiler settings (D), where there is an initial delay to bring the temperature to the set point. This is followed by a faster response, provided that the disturbances are kept to a minimum. Ambient temperature (B) affects is the third effective cause signal, but unlike the other factors, this is an environmental disturbance which cannot be controlled. The CHP speed (C) had the lowest effect. Understanding of the model coefficients enables further understanding on how to control the overall process;

6. **Model response structure**: The choice of multiple or single effect structure model depends on the type of model required. For multiple effect structures, the effect on the prediction of any effect signal involves all other effect signals from the multivariate structure. This allows effect signals to be cross-coupled in the resulting structure. Single effect eliminates the cross-coupling, which is ideal for model based controllers as it can reduce poor effects (through bad data) in the effect signals and, therefore, making the model more robust.
7. **Order of dynamics and Delays**: The order of dynamics specifies how many of the previous samples of the effect signal are used in conjunction with the cause terms to predict the effect signals trajectory. A higher order of dynamics may provide better prediction during unmeasured disturbances and may also yield a model less sensitive to process noise. In this case the order of dynamics was set to one to enable ARX modelling type. For control applications, an order of dynamics of 1-3 is typical. The number of auto regressive nodes is determined by the order of dynamics assigned to the model; for FIR models, the order of dynamics is set to zero and the difference between the min and max delay should be longer than the longest transient time to steady-state of any of the effect signals.



Response (Y) Signal	Scaling Mode	Mean	Deviation	Section Mask		Initial Value
332Q.ME Sim Thickened Sludge Tank Level %	Automatic	51.08	4.86	Change All		50
478P.ME Calc Gas Produced m3/day	Automatic	1.352e4	3.258e3			16700
569P.ME Calc Combined Digestate Tank Level m	Automatic	10.66	1.342			12.61
544Q.ME Sim Gas Holder Level m	Automatic	7.854	1.553			12.5
585P.ME Calc Primary Digester Temperature Deg C	Automatic	32.03	0.1596			32
696P.ME Heating Water Circuit Temp (After CHP - wTD) Deg C	Automatic	63.24	1.301			63.12
697P.ME Heating Water Circuit Temp (After Coolers -wTD) Deg C	Automatic	58.46	5.754			62.12
695P.ME Heating Water Circuit Temperature (Before AD -wTD) Deg C	Automatic	68.07	4.946			66.91

Predictor (X) Signal	Scaling Mode	Delays	Min.	Max.	Mean	Deviation	Signal Mask		Initial Value
288Q.ME Sim Feed To Thickened Sludge Tank m3/day	Automatic	Set All	0	50	720.1	39.62	Change All		720
1000.AC AD Feed Rate m3/day	Automatic		0	80	725.8	43.71			0
1010.AC Centrifuge Feed Rate m3/day	Automatic		0	80	356.5	160.5			0
1020.AC CHP Feed Rate Speed m3/day	Automatic		0	50	1.673e4	354.4			0
1030.AC Biogas Produced by AD m3/day	Automatic		0	20	1.680e4	1.779e3			0
1040.AC Primary Digester Temperature Deg C	Automatic		0	50	32.09	0.3706			0
1050.AC Split Adiabatic Cooler/Backup Boiler	Automatic		0	80	65	47.63			0
766P.ME Sim Sludge Dry Solids Into Digester %DS	Automatic		0	80	4.865	3.533			5.195
588Q.ME Sim Flow to Gas Flare m3/day	Automatic		0	20	6.781e3	6.143e3			0
750P.ME Ambient Temperature Deg C	Automatic		0	50	15.02	5.45			20

Figure 6.9 PerceptiveAPC V4.1 modelling page

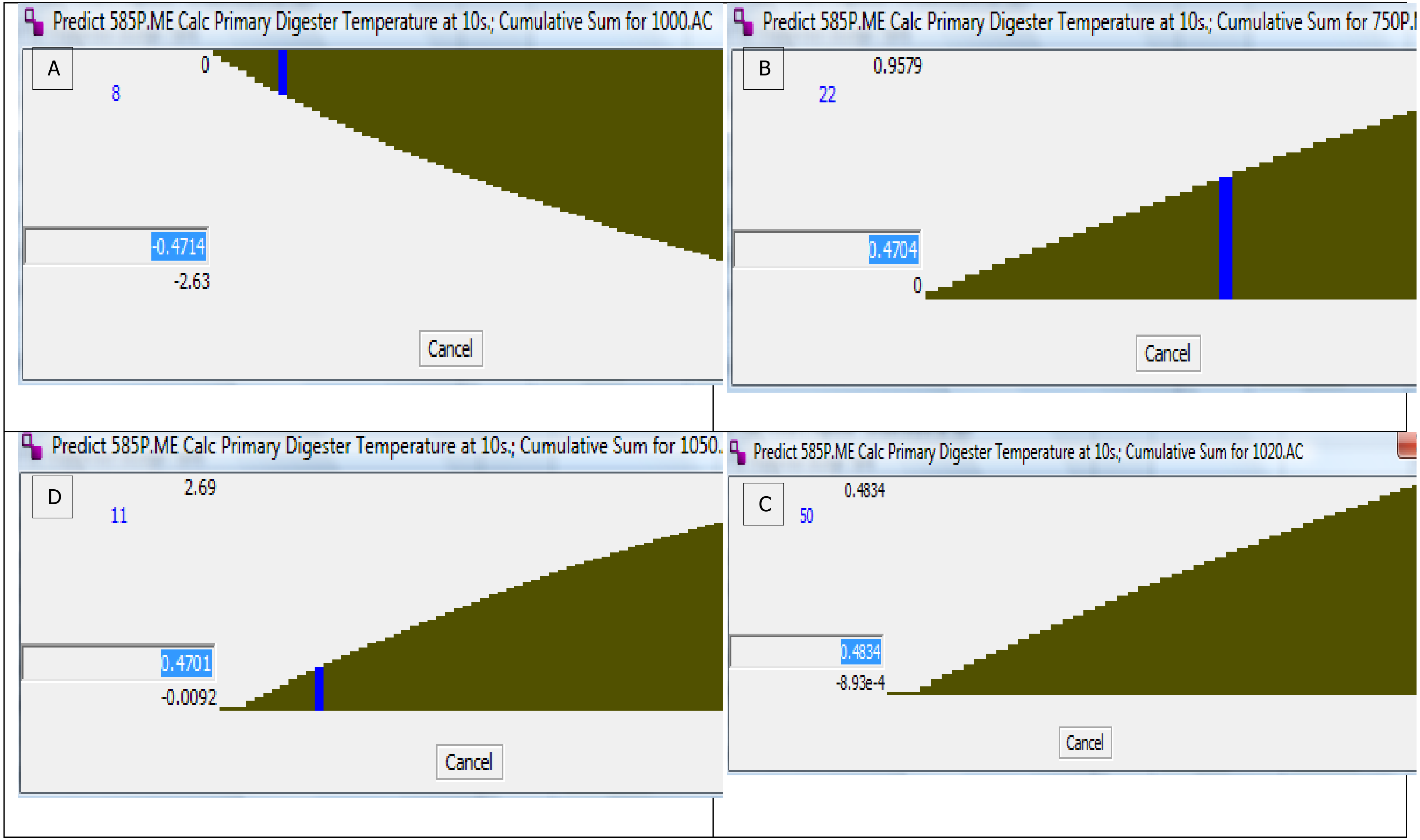


Figure 6.10 Temperature prediction coefficients

6.3.2 PID model

A PID controller was designed in PerceptiveAPC using basic code. The code is included in the disc attached. The PID model was designed to control temperature by manipulating the feed rate. Detail analysis of the model has not been conducted due to software licence expiration of the PerceptiveAPC, however the PID model was evaluated at 33°C setpoint and the results is compared with MPC1, MPC2, split dynamic model and the optimiser model.

6.4 Controller testing

Following the development of the MPC controller in Section 6.3, the next step was to evaluate the controller performance through a series of scenario evaluation tests. There were:

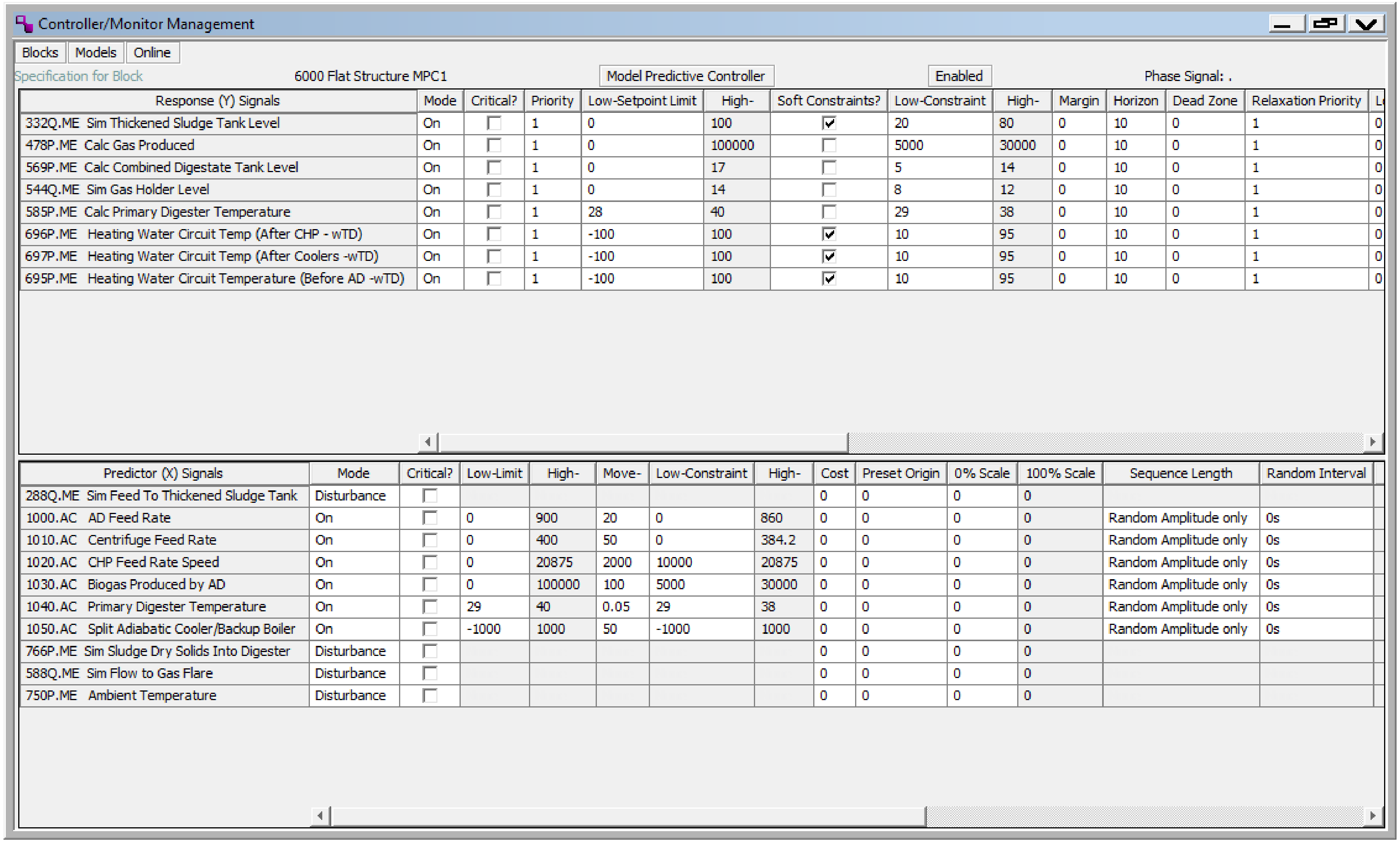
- Evaluating the MPC1 controller structure in Figure 6.7, this forms the standard controller for the inventory simulation;
- Evaluation of the MPC2 'dynamic' two level structure in Figure 6.8 to test the impact of splitting the system dynamics into 2 models of fast and slow dynamics on controller performance;
- Alternative controller comparison with a conventional controller such a PID. A PID controller is developed and simulated to compare results with MPC1 and MPC2 and evaluate the performance between traditional and advance controllers;
- In addition, an optimiser was developed to test and evaluate the performance of MPC1, MPC2 and the PID controller scenarios with an optimiser to test for controller performance with the optimiser.

These four evaluation scenarios helped to assess the need for an advanced controller, and were compared to the design benchmark system where there is 'no control'. This forms the general status of the benchmarked sites in Chapter 5.

6.4.1 MPC1: the benchmark structure system evaluation

The benchmark structure MPC1 was evaluated to understand the capabilities of MPC. MPC1 model was loaded into PharmaMV Real-Time environment as depicted in Figure 6.11. The Real-Time environment allows models developed in the development environment to be deployed in real time. The figure shows the specification page for the response signals (the top section of the figure) and cause or predictor signals at the bottom of the figure.

The Real-Time environment has a controller monitor management framework where the model specification can be set. The specification for MPC1 can be set to include the order of priority, hard and soft constraints, and high or low set point settings for the different signals. A series of overnight runs of the simulation was conducted to iteratively change the settings to tune the controller to yield optimum performance. Five examples are provided in this section which includes obtaining the optimum setpoint for feed rate, adiabatic cooler, back-up boiler setting, digestate tank level, CHP feed rate and ambient temperature effect on digester temperature.



Controller/Monitor Management

Blocks | Models | Online

Specification for Block 6000 Flat Structure MPC1 Model Predictive Controller Enabled Phase Signal: .

Response (Y) Signals	Mode	Critical?	Priority	Low-Setpoint Limit	High-	Soft Constraints?	Low-Constraint	High-	Margin	Horizon	Dead Zone	Relaxation Priority	L
332Q.ME Sim Thickened Sludge Tank Level	On	☐	1	0	100	☑	20	80	0	10	0	1	0
478P.ME Calc Gas Produced	On	☐	1	0	100000	☐	5000	30000	0	10	0	1	0
569P.ME Calc Combined Digestate Tank Level	On	☐	1	0	17	☐	5	14	0	10	0	1	0
544Q.ME Sim Gas Holder Level	On	☐	1	0	14	☐	8	12	0	10	0	1	0
585P.ME Calc Primary Digester Temperature	On	☐	1	28	40	☐	29	38	0	10	0	1	0
696P.ME Heating Water Circuit Temp (After CHP - wTD)	On	☐	1	-100	100	☑	10	95	0	10	0	1	0
697P.ME Heating Water Circuit Temp (After Coolers -wTD)	On	☐	1	-100	100	☑	10	95	0	10	0	1	0
695P.ME Heating Water Circuit Temperature (Before AD -wTD)	On	☐	1	-100	100	☑	10	95	0	10	0	1	0

Predictor (X) Signals	Mode	Critical?	Low-Limit	High-	Move-	Low-Constraint	High-	Cost	Preset Origin	0% Scale	100% Scale	Sequence Length	Random Interval
288Q.ME Sim Feed To Thickened Sludge Tank	Disturbance	☐						0	0	0	0		
1000.AC AD Feed Rate	On	☐	0	900	20	0	860	0	0	0	0	Random Amplitude only	0s
1010.AC Centrifuge Feed Rate	On	☐	0	400	50	0	384.2	0	0	0	0	Random Amplitude only	0s
1020.AC CHP Feed Rate Speed	On	☐	0	20875	2000	10000	20875	0	0	0	0	Random Amplitude only	0s
1030.AC Biogas Produced by AD	On	☐	0	100000	100	5000	30000	0	0	0	0	Random Amplitude only	0s
1040.AC Primary Digester Temperature	On	☐	29	40	0.05	29	38	0	0	0	0	Random Amplitude only	0s
1050.AC Split Adiabatic Cooler/Backup Boiler	On	☐	-1000	1000	50	-1000	1000	0	0	0	0	Random Amplitude only	0s
766P.ME Sim Sludge Dry Solids Into Digester	Disturbance	☐						0	0	0	0		
588Q.ME Sim Flow to Gas Flare	Disturbance	☐						0	0	0	0		
750P.ME Ambient Temperature	Disturbance	☐						0	0	0	0		

Figure 6.11 PharmaMV 4.1 Controller Monitor management screen

Digester feed rate: to gain an understanding of the best setpoint for the feed rate, it was necessary to generate the average flow to the thickened sludge tank as shown in Figure 6.13; the feed to the thickened sludge tank is shown in black and the feed rate to the digester in red. In this case the mean flow to the thickened sludge tank is of the order of 611 m^3 day^{-1}. The feed rate to the digester must have a maximum flow of 860 m^3 day^{-1}, to enable sufficient organic loading rate (OLR). Therefore the median value of 611 m^3 day^{-1} was set as the setpoint to ensure constant flow to the digester. The distribution is skewed and therefore the median (625 m^3 day^{-1}) may be more appropriate estimate for the setpoint and, therefore, the setpoint for the feed rate within this simulation was set to 625 m^3 day^{-1}. The feed rate had a more dominant effect on the digester temperature. In order to control the setpoint effectively, the constraints on digester feed must be tighter.

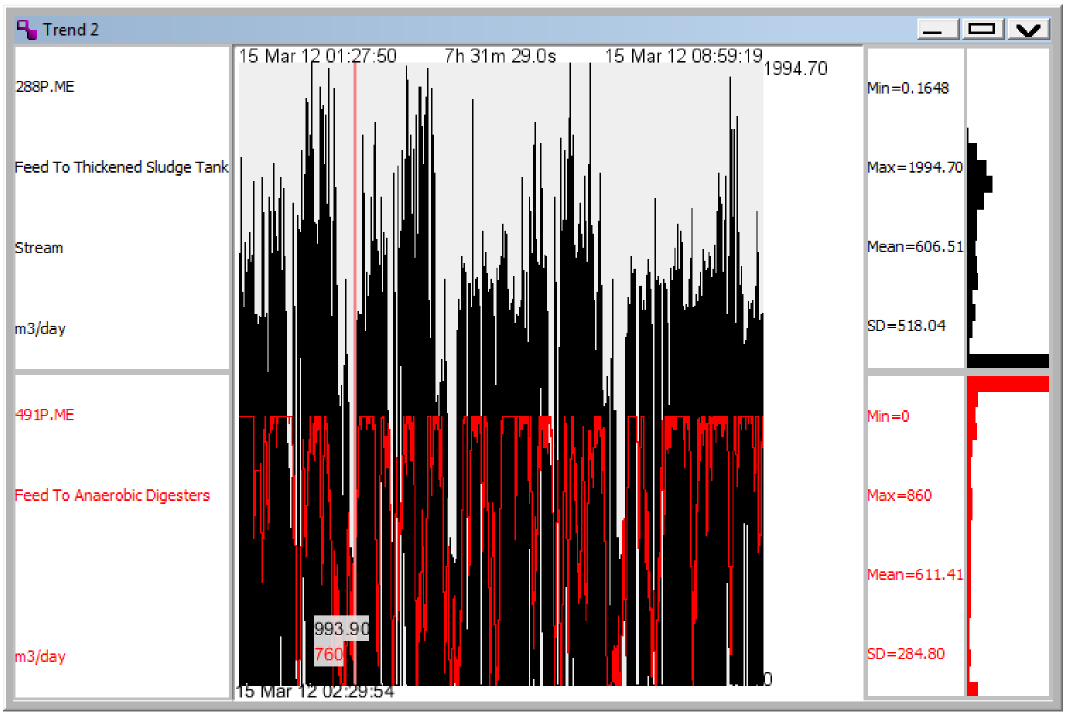


Figure 6.12 Feed to Thickened sludge tank and feed flowrate plot

Adiabatic cooler and backup boiler split: the settings for the adiabatic cooler and backup boiler split (1050.AC) signals are crucial to maintaining not just the digester temperature but also the feed rate setting. Figure 6.13 shows the MPC controller overview page. The first half of the plot (left hand side) shows the past profile of the plots and the right hand side shows the future prediction of the MPC. This is split by the black line in the middle which shows the current status of the plots. The plots show (from top-down) the MPC block status in black, which is in 'auto' mode which means the controller is active. This is followed by the actual digester temperature in green and the MPC prediction of digester temperature in brown. The 1050.AC is shown in blue, with its target setpoint in pink with the red lines showing the high and low constraint levels. AD feed rate is given in light purple and CHP feed rate, sludge dry solids, flow to gas flare and ambient temperature are given in purple. The rate at which heating or cooling is available to the digester is essential for establishing the rate at which the digester heats and cools. At low 1050.AC splitting, the digester takes a long time to cool and heat and the 1050.AC signal almost acts in an on or off mode, violating the low and high constraint setpoints. The -100:100 kW split appears to be too low for heating and cooling the system, looking at the process data obtained; a setting of -1000:1000 kW for 1050.AC was used. This enables faster heating or cooling and also appears to behave in a similar way to observations in the process data.

Digestate tank: Figure 6.14 illustrates the digestate tank level in red, the centrifuge demand multiplier in green, centrifuge feed rate in black, digestate flow from the digesters in blue and AD feed rate in Pink. There was an initial difficulty in controlling the digestate tank level by centrifuge run time alone as the major influence on the tank level is the digestate feed rate from the digesters which determines the flow of sludge from the digesters to digestate tank. By modelling the tank with feedforward information of the digestate feed rate, the model was greatly improved.

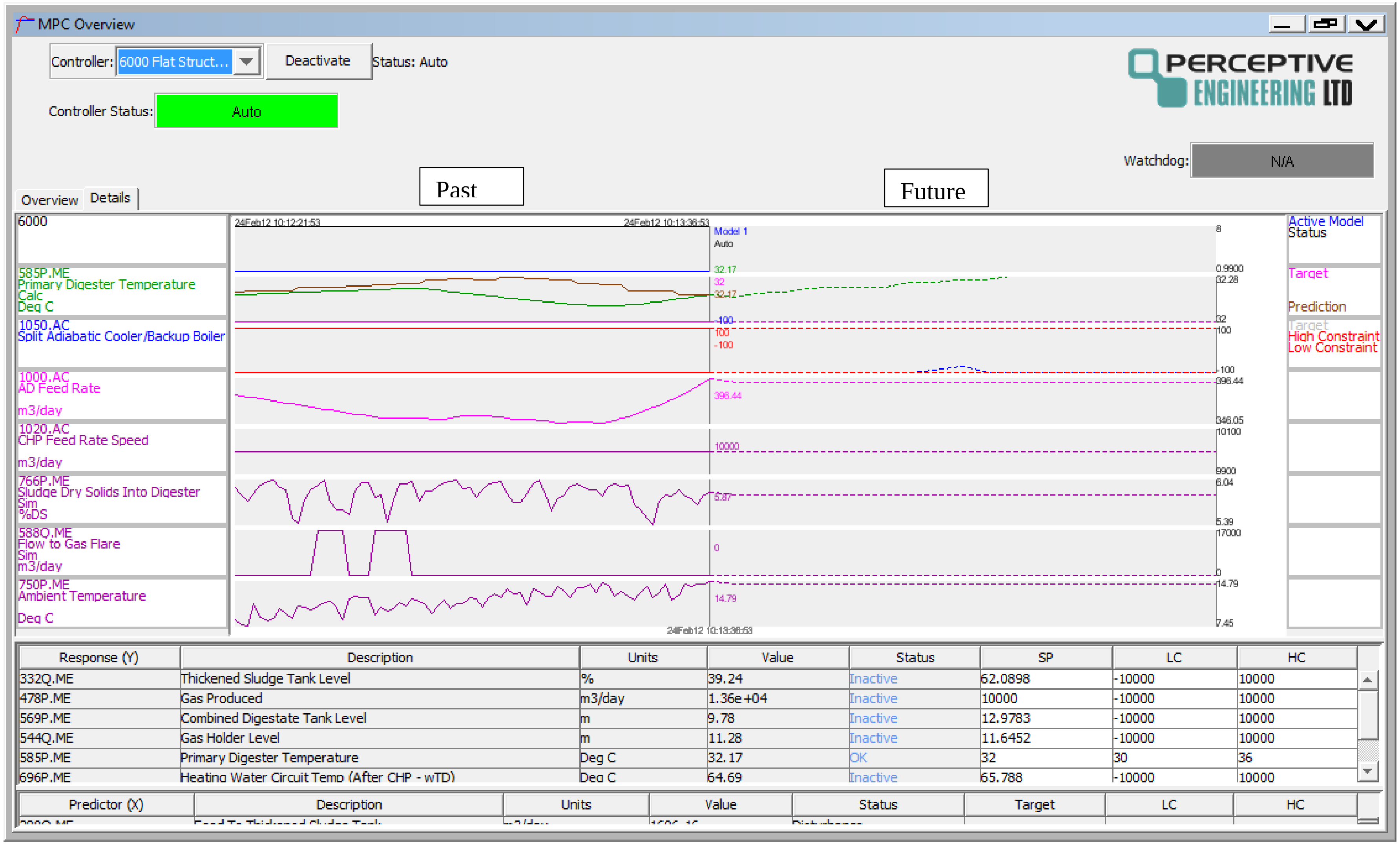


Figure 6.13 Signal 1050.AC controller setting

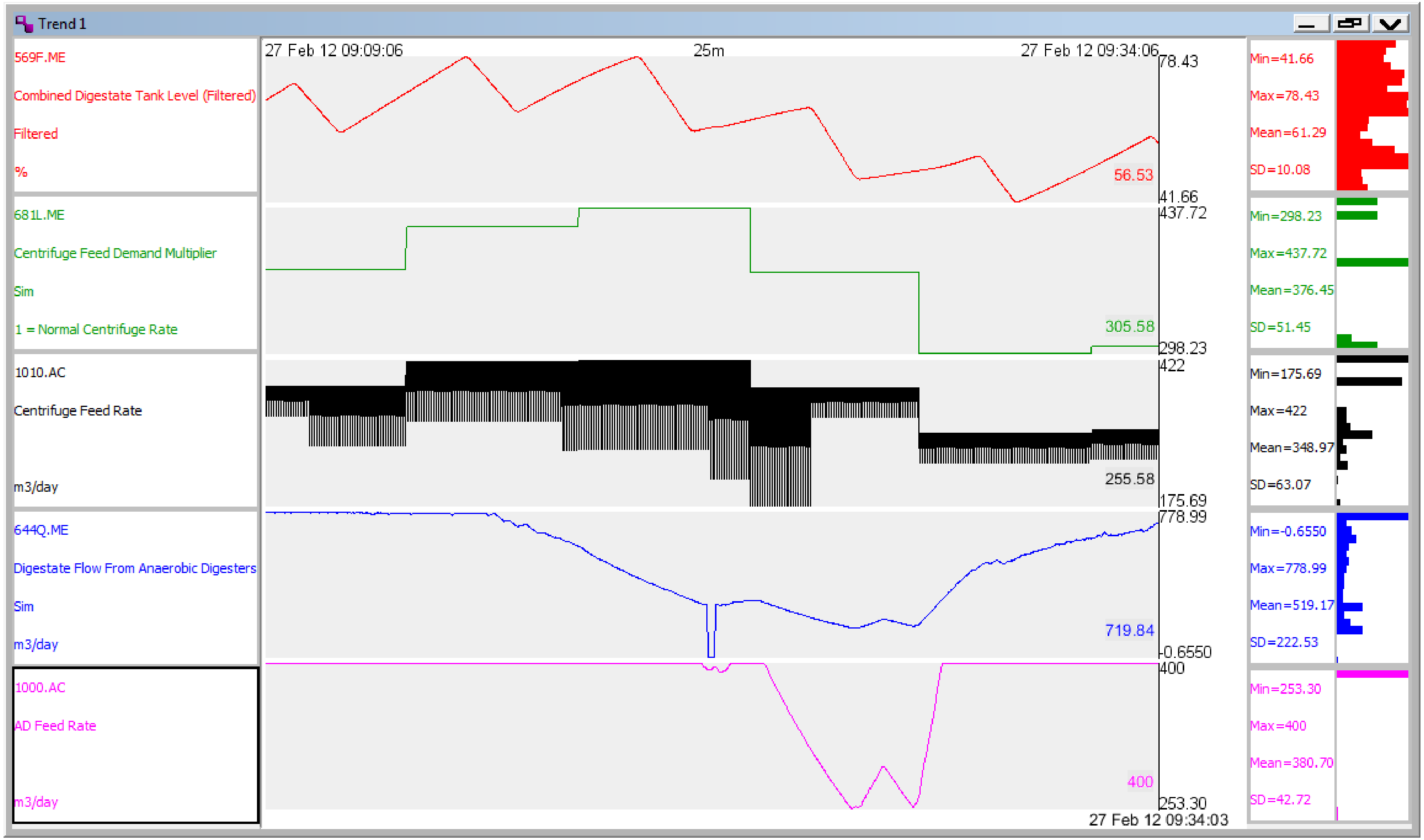


Figure 6.14 Digestate tank cause and effect analysis

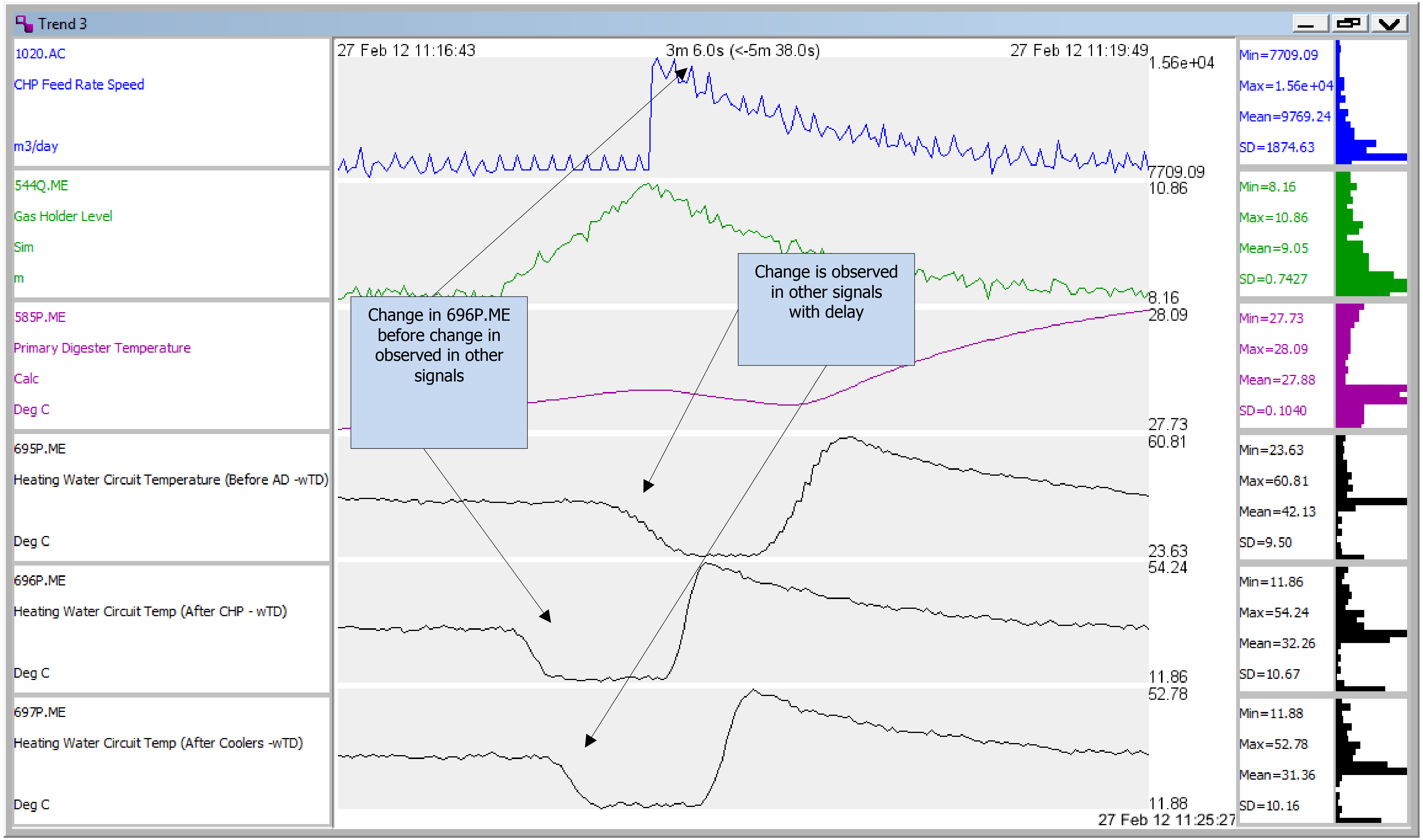


Figure 6.15 CHP feed rate cause and effect analysis

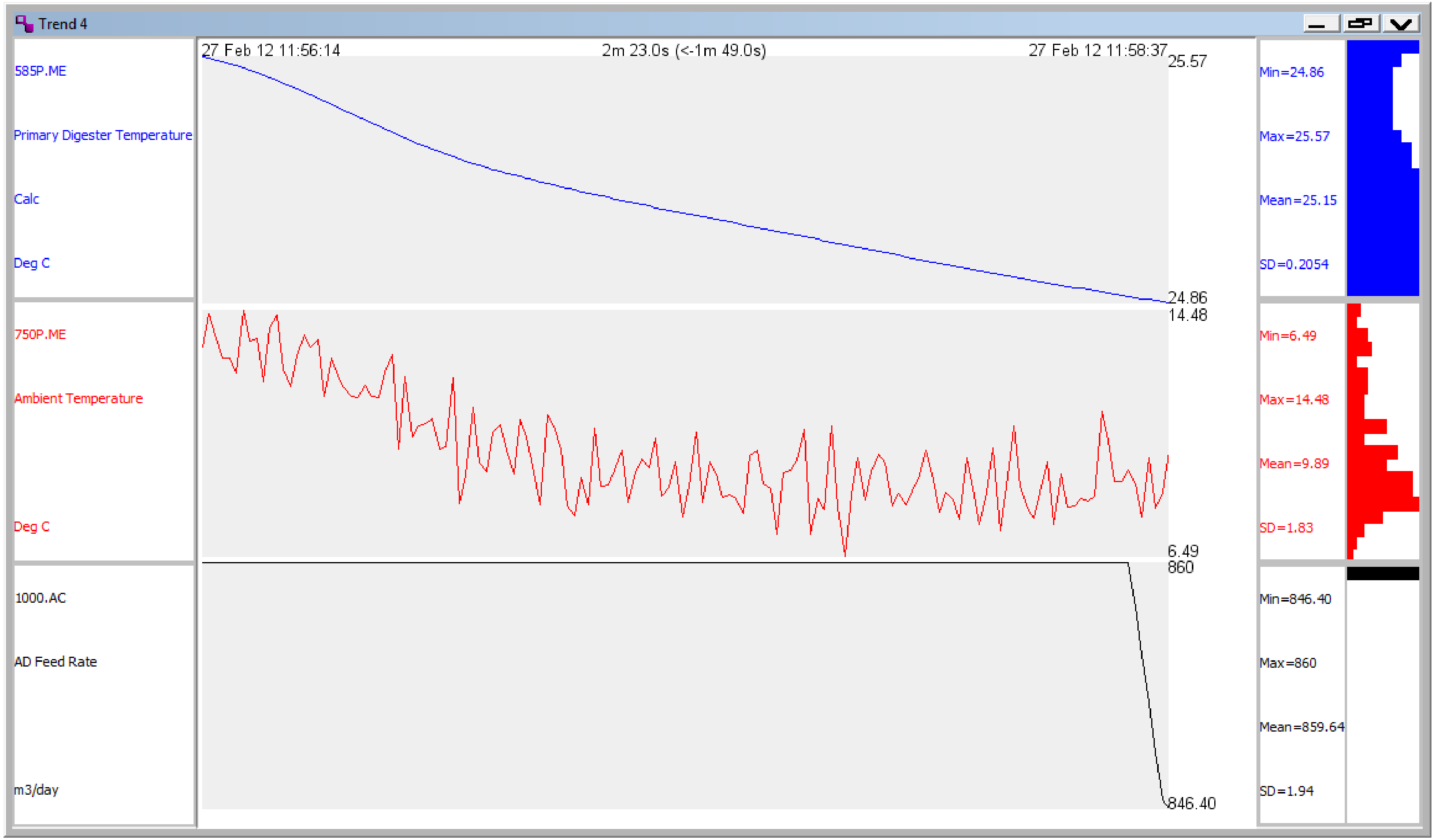


Figure 6.16 Ambient temperature effect on digester temperature

CHP feed rate: Figure 6.15 shows plots of CHP feed rate speed in blue top plot, followed by the gas holder level in green, digester temperature in purple and the heating water circuit temperatures (before the AD, after CHP and after the coolers) in black. The plot shows that changes in CHP feed rate do not correspond well with setpoint changes. Due to the high priority set for the controller objective and constraints to avoid flaring biogas (shown in Table 6.5), as the gas holder level rises to its high constraint level, the setpoint of the CHP feed rate is override to increase the flow to reduce the level in the gas holder. Comparison with other related signals shows it corresponds to a drop in the heating water circuit temperatures affecting the CHP feed rate. Understanding of these cause and effect relationships has enabled better control implementation to be achieved.

Ambient temperature: ambient temperature effect on digester temperature is considerable as illustrated in Figure 6.16, with digester temperature in blue, ambient temperature in red and digester feed rate in black. An increase of one degree in ambient temperature increases the digester temperature by 0.089˚C. Ambient temperature is set as a disturbance in the controller specification due to it being an environmental effect which cannot be controlled or predicted. However by understanding an increase or decrease change in ambient temperature effect the digester temperature, the digester temperature can be controlled better by factoring in the effects of ambient temperature with manipulated variables effecting temperature.

6.4.2 Bottleneck shift

Bottlenecks are defined in the simulation as processing steps which hinder optimum digestion of sludge to high yields of biogas. Depending on what the hierarchy of control objectives are, the bottle neck in the process shifts to different processing steps. However the main bottleneck in the process is the thickened sludge tank. The level of thickened sludge available for digestion determines the variability in AD feed rate and, therefore, affects the downstream processes. This is a result of the main controller objective set to prevent the AD feed flow tripping as a result of high gas holder level, which means the AD feed flow is more dependent on the biogas level than the thickened sludge level. By setting the main controller objective to avoid tripping the thickened sludge flow to the AD, the bottleneck shift to the gas holder level. This is a typical situation observed on all of the benchmarked sites as sludge inventory are generally high which result in optimum digester feed flows yielding high levels of biogas. Due to finite levels of CHP units, this result in biogas being flared when CHP units run at optimum levels. This issue may be only resolved through increasing the capacity of tanks as this is the approach taken at Blackburn to increase CHP capacity through an additional an CHP unit. Nevertheless the optimisation question remains as to whether it is possible to process the high sludge inventory without flaring gas or tripping the CHP units at this capacity. At present, this does not appear to be possible due to the high inventory levels and constraint on tank volumes, still there is a considerable reduction in gas flaring for which the cost will be beneficial to operate in this manner and flare little gas, rather than invest in increased tank capacity to the site such as additional CHP units. This is of course subject to environmental regulations, as tighter control on gas flaring will inevitably occur and increase the importance of avoiding gas flaring objective in the system.

6.5 Controller results

Following an iterative approach to tuning and tightening the MPC controller, a series of seven hour simulation runs were conducted to evaluate the system. Seven hours of simulation time equates to about twelve weeks of 'real-time'. The seven hour runs were conducted for the series of scenario evaluation tests outlined in Section 6.5 which includes:

- Evaluating the MPC1 controller structure, results for this is given in sections 6.5.1 and 6.5.2;
- Evaluation of the MPC2, results for this is given in Section 6.5.3 ;
- Evaluating the optimiser on MPC1 controller, results for this given in Section 6.5.4;
- PID controller evaluation and 'uncontrolled' scenario analysis is provided in Section 6.5.5.

6.5.1 MPC1

The simulation process is bottlenecked in capacity just like the industrial processes benchmarked in the feasibility study. Therefore for a given design and capacity availability, optimum setpoints can be identified and only then can the process be fully optimised. Due to the process continuing to be inhibited by capacity, the level of feed into thickened sludge tank has to be reduced or the tank sizes increased to enable the process to be optimised. Therefore the simulation can serve as a test bed for designing new plants.

Through setting and tightening constraints on the thickened sludge tank level, the tank level is maintained without tripping. The tanks increase AD feed rate to keep the tank at the low level resulting in increased biogas production and led to the bottleneck moving to the gas holder. As CHP units are run at maximum speed, increase of gas flaring occurs.

The mean of the thickened sludge tank and the digester feed rate plot shown in Figure 6.12 are close to each other; 606 and 611 for the sludge tank feed and the digester feed respectively considering the large ranges as indicated by the standard deviation which, is 581.16 and 181.19 for 288Q.ME and 491P.ME respectively. The digester feed rate for the purpose of stability and control needs to have minimum standard deviation. To limit this gas holder level setpoint is kept to a minimum of 9 to avoid hitting the low constraint setpoint of 8 which is required for maximum efficiency of the CHP operation.

Tighter control is required on the thickened sludge tank level due to the large disturbance of incoming sludge to the site. Giving the tank lots of head room enables it to accommodate variation when sludge availability increases and reduces as the changes are very rapid over a large range. For this reason the tank level 332Q.ME is set as a soft constraint with high and low constraint limits as 60 and 40 %, respectively. The tight constraint limits enable the tank to adjust without hitting the levels where trips occur. These tight constraint limits are required for ideal control of the industrial process.

The digestate tank level and centrifuge operation can be controlled fairly easily due to the feed forward information from AD feed rate. Temperature is controlled very well and this was expected as most industrial sites have reliable temperature control.

The key findings from the simulation assessment can be summarised as follows:

- The feed to thickened sludge tank level i.e. the sludge inventory on site changes quickly and is unpredictable, therefore prediction of incoming feed is not possible. The aim was to implement disturbance profile modelling into the controller design to help the controller better predict changes;
- Temperature is best controlled by the feed rate for cooling with cold sludge feed making heating more difficult as cold sludge is continuously added. The next factor affecting temperature is the cooler or boiler settings followed by ambient temperature and CHP speed respectively;

- The best setpoints are identified to best control the process with constraints settings based on system dynamics and process understanding.

With respect to the aims of this study, it is evident that an advanced controller such as MPC can reduce the limitations of inventory for a constraint optimisation problem such as this. This can be carried out through measurement accuracy, speed of response, stability and relative stability and sensitivity. Process prediction is only as good as the underlying model, then knowledge and account of eventualities and variability is essential to maintaining effective control. Disturbances can be a result of change in process dynamics, measurement noise or external factors.

In summary, the model predictive controller has been shown to significantly improve the process. Best temperature settings for various scenarios are identified. An advanced controller such as MPC can be used to effectively control the multi-constraint, nonlinear characteristic of the process. The MPC calculates a future set of moves to avoid the constraint violation. This has been shown to improve the process in a simulation environment as shown in Figure 6.17; where about 40 % increase in biogas production can be achieved at 13 % lower average temperatures.

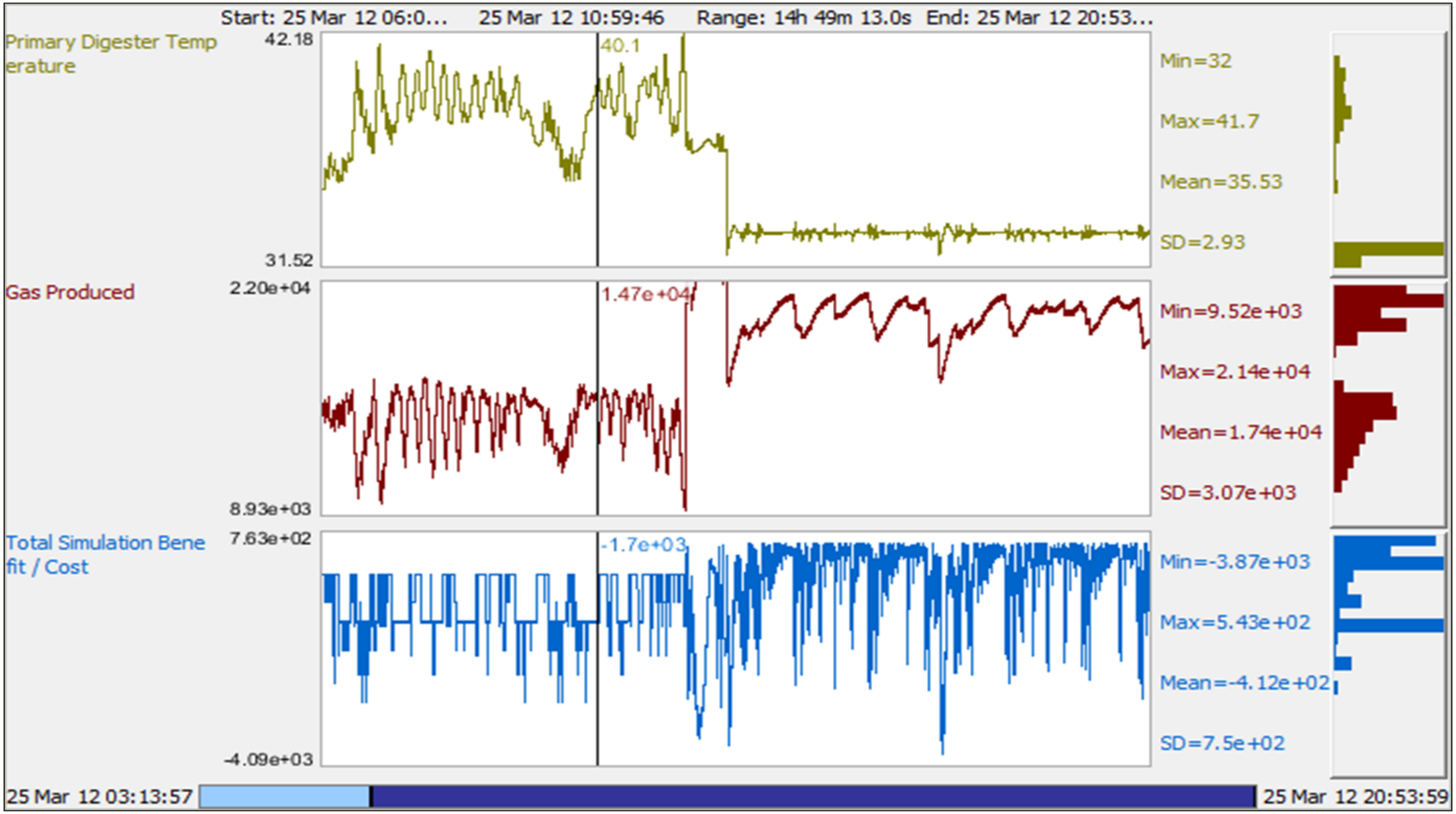


Figure 6.17 Inventory improvement results

6.5.2 Cost benefit analysis of MPC1

The MPC1 model is further evaluated on cost benefit basis to quantify the financial gain from the controller. There are costs benefit elements associated with several parameters which are calculated by the simulation. These cost and benefit elements were modelled into the simulation as shown in Figure 6.18 to yield the total simulation cost benefit signal shown at the bottom of the plot in black. The cost and benefit elements are:

1. Savings associated with CHP electricity generation, the benefit is calculated based on the following energy tariffs, shown in the blue (top) in Figure 6.18. 4.6 p kWh^{-1} - before 07:00, 13.3 p kWh^{-1} - between 16:00 and 19:00 and 6.7 p kWh^{-1} - any other time.
2. Cost associated with the thickened sludge silo tripping on a high level, resulting in no sludge being imported onto site until the 'backlog' is cleared, therefore a cost penalty of £1000 day^{-1} for 24 hours is applied. This is shown in green in Figure 6.18.
3. Cost associated with the thickened sludge silo tripping on a low level is shown purple in Figure 6.18. This requires the operator to do some work to clear the trip and reset the plant, therefore a cost penalty is applied with the penalty of £600 day^{-1} for four hours.
4. Cost of the digestate silo tripping on a high level leading to the operator having to clear the trip and reset the plant, therefore a cost penalty of £600 day^{-1} for eight hours is applied. This is shown in dark yellow in Figure 6.18.
5. £600 day^{-1} for six hours is applied to the gas holder tripping on a high level, resulting in the operator doing some work to clear the trip and reset the plant. This is shown in light purple in Figure 6.18.
6. £600 day^{-1} for six hours is applied the digestate silo trips on a low level. This is shown in orange in Figure 6.18, with all the cost penalty elements tripping the tanks acting in on or off mode.
7. Electrical energy cost associated with running the adiabatic coolers is shown red in Figure 6.18. The conversion efficiency between electrical energy and thermal energy is assumed to be 50 % and the benefit is calculated based on the energy tariffs of 4.6 p kWh^{-1} - before 07:00, 13.3 p kWh^{-1} - between 16:00 and 19:00 and 6.7 p kWh^{-1} - any other time.

8. There is a fuel energy cost associated with running the backup boiler is shown in blue (bottom) of Figure 6.18. The boiler running on distillate fuel oil.

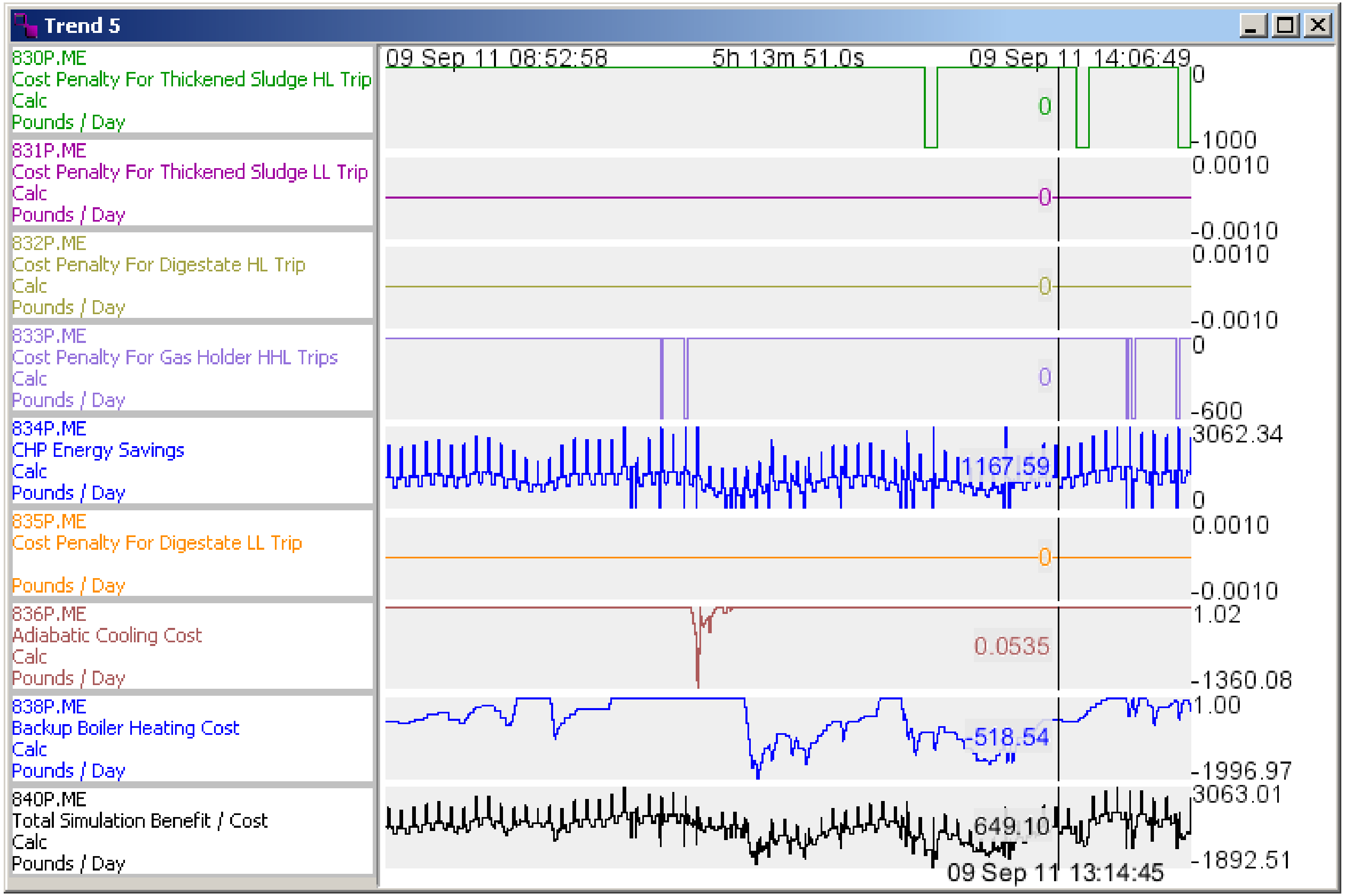


Figure 6.18 Signals associated with ‘real time’ cost calculations

The cost and benefit elements of the system are evaluated through changes in the temperature setpoint. This is because temperature crucially effects the benefits of the system, namely biogas production as this is modelled with the biogas correction factors shown in Table 6.1, 6.2 and 6.3 in Section 6.2.2 and also the cost elements associated with cooling and controlling the system.

Mesophilic digesters generally operate around 35˚C with a range between 25-45˚C. The optimum temperature varies depending on the feedstock composition (Monnet, 2003). Overnight runs (7 hours of simulation time, equivalent to about 3 months of 'real life' time) of the simulation were conducted at temperatures between 25-40˚C. The aim was to evaluate best temperature condition for the operation of the simulation at set conditions with the hypothesis that the optimum is around 35˚C.

Table 6.6 shows a summary of results from 14 overnight runs showing the effect of temperature variation on the number of trips as previously listed in Table 6.4, CHP energy savings and total simulation cost benefit analysis. The analysis of the trips included:

1. The number of trips occurring – calculated from number of times any of the level trips occur;
2. % of time trips occur – this is calculated as the % time taken to reset the level trips;
3. GBT trip on high thickened sludge tank level (H TsT);
4. AD trip on low thickened sludge tank level (L TsT);
5. AD trip on high digestate tank level (H DigestT);
6. Centrifuge trip on low digestate tank level (L DigestT);
7. Flare on high gas holder level (H GHL);
8. CHP trip on low gas holder level (L GHL);
9. AD feed trip on high gas holder level (H GHL).

Together these 9 analyses of the trips together with the savings achieved by the CHP unit yield the total simulation cost benefit analysis on the basis of the hierarchy of control objectives and constraints set in Table 6.5.

Table 6.6 shows that lower temperature settings i.e. below 28˚C operate at a cost and higher temperatures produce benefit for the system and therefore the digester should be run 35 and 38˚C. This reflect the temperature effect on biogas production modelled with a biogas correction factors shown in Table 6.1, 6.2 and 6.3 in Section 6.2.2, and follows a parabola distribution as shown in Figure 6.20.

Table 6.6 Cost benefit associated with temperature

	Temperature (˚C)	No. of trips	% time of trips occurring	CHP energy savings	Total simulation cost benefit	GBT Trip on H TsT	AD Trip on L TsT	AD trip on H DigestT	Centrifuge Trip on L DigestT	Flare on H GHL	CHP trip on L GHL	AD feed trip on H
Run 1	25	513	101.7	538.6	-2297.17	197	0	88	0	0	228	0
Run 2	26	483	94.9	582.03	-2445.9	199	0	87	0	0	193	0
Run 3	27	425	86.3	643.6	-2379.14	203	0	88	0	0	134	0
Run 4	28	362	78.2	696.1	-2364.27	203	0	87	0	0	70	0
Run 5	29	322	75.9	740.56	-2340.86	207	0	90	0	2	30	0
Run 6	30	293	72.9	799.93	-2319.04	202	0	88	0	1	0	0
Run 7	31	395	49.9	1307.9	-255.56	347	0	0	0	32	0	16
Run 8	32	395	50.8	1413.32	-11.38	338	0	0	0	35	0	22
Run 9	33	430	54.1	1449.15	-27	354	0	0	0	44	0	32
Run	34	455	60.8	1441.74	-193.7	332	0	0	0	84	0	39
Run	35	691	65.8	1440.63	-391.87	350	0	0	0	291	0	50
Run	36	1533	77	1452.89	-483.05	383	0	0	0	1073	0	77
Run	37	1529	75.7	1465.67	-910.59	365	0	0	0	1092	0	72
Run	38	1101	70.9	1465.61	-2732.98	327	0	0	0	738	0	46

Analysis of the baseline analysis of the simulation performance without the controller showed an average biogas production of 13,500m^3 day^{-1} as shown in Figure 6.19, a CHP energy saving of £973 day^{-1} and all the seven level trips shown in Table 6.4 tripping. With the controller active, CHP energy saving is increased to £1,465 day^{-1} and the lower levels of the baseline only show low temperatures below 30˚C. If this average is maintained throughout the year, there is a saving of £492 day^{-1}, equating to approximately £179k a year. The cost to implement a control project at Perceptive Engineering Ltd had two elements, the software and the engineering services. The software generally cost around £12,000 for a "small" site, and £18,000 for a "large" site, although this varies between projects. The cost for engineering services varies also and generally the more manipulated variables, the greater the estimated cost. For a site similar in size to the simulation, this would be of the cost of £45k; making the total cost of the controller £63k. For this cost, the payback time for installing the controller would be less than 6 months.

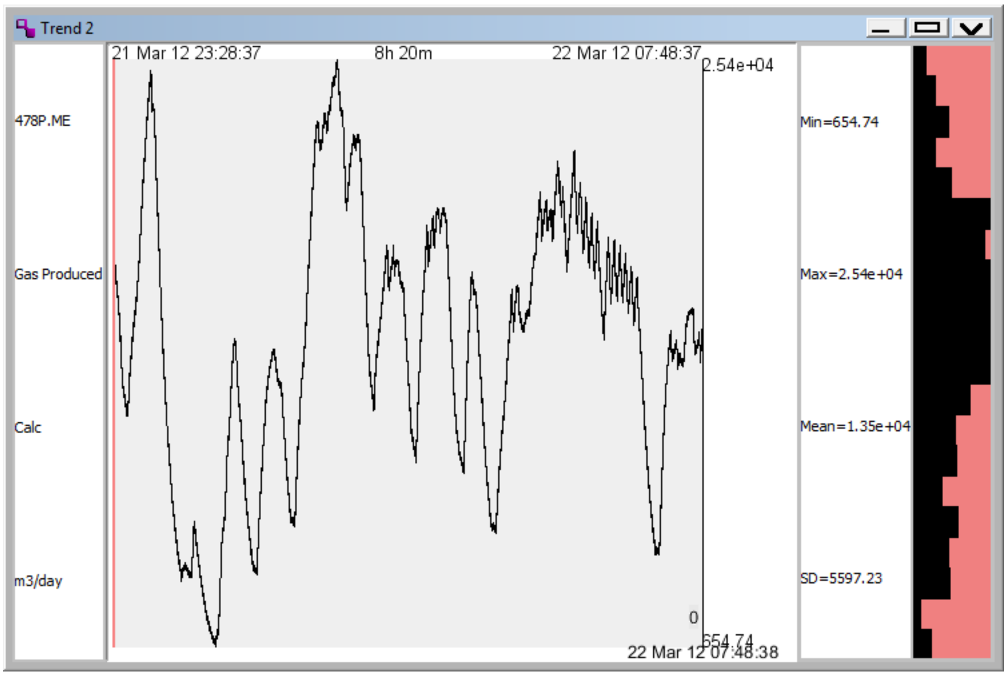


Figure 6.19 Biogas produced

Although the controller is shown to increase CHP energy savings by up to 33 %, real-time optimisation and multivariable control systems typically add 6-10 % value to process (Cutler and Perry, 1983). This is therefore a large saving on the CHP units. The total cost benefit monetary value achieved for the simulation gave negative cost values as shown in blue in Figure 6.20. The plot shows the cost benefit value achieved for temperatures between 25 and 30°C is constant. The shape of the plot between 30 and

38°C however shows a bell curve or normal distribution plot with a peak at 33°C. The negative values indicate that the plant cost money and made no profit with the controller. However the negative values were a result of high cost penalties associated with tripping the tank levels. The baseline simulation without the controller resulted in a total cost of £2,135 day^{-1}. By setting the baseline as a zero cost benefit value and the shifting the actual cost benefit values up by £2,135; Figure 6.20 also shows the shifted total simulation cost benefit in red. This therefore gave highest cost benefit value for the system at about £2,100 day^{-1}.

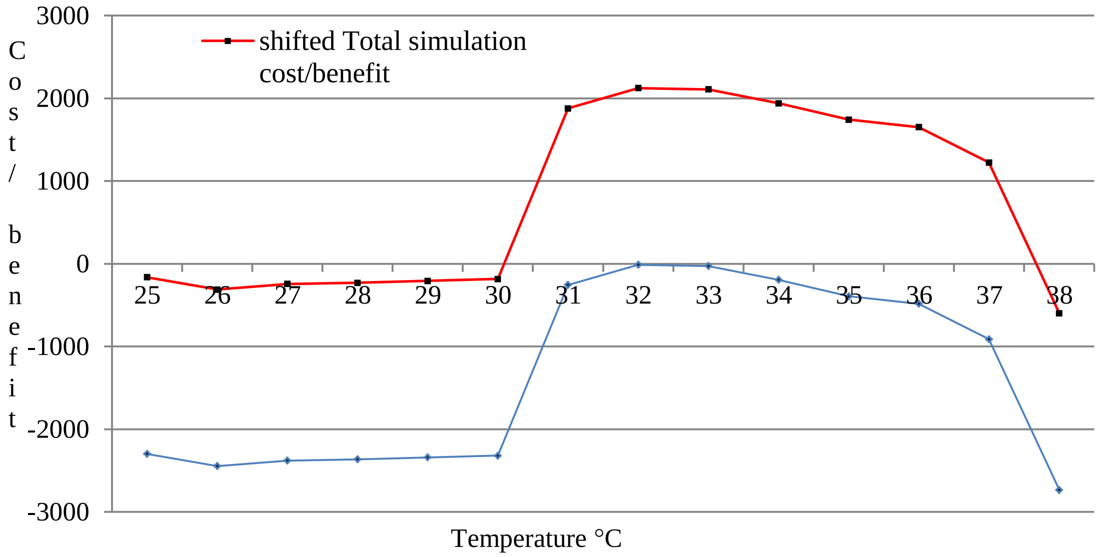


Figure 6.20 Total simulation cost benefit

There is constant benefit up to 30˚C before a large positive increase at 31˚C as shown in Figure 6.20. The plot shows the optimum cost benefit gain to be around 32 to 33˚C. This is again at the lower end of the mesophilic specification. The plot also shows total benefit in £ day^{-1} to be below zero at all temperature settings. From the industrial data, this is not true of AD systems as the process generates positive revenue. This is a result of the cost elements built into the simulation design, where the balance of energy produced revenue and cost associated with tank trips are not at the correct settings, though the shape of the curve is valid for AD systems and changes in the cost values will only shift the plot up. The revenue calculation does not also take into account ROCs (renewable obligation certificate), which doubles the value of energy produced on ADs.

Figure 6.21 illustrates the various trips occurring for the overnight runs at different temperatures. From the results it is clear that for the temperature range of 25 to 38°C studied using MPC1, the trips on the AD for the low thickened sludge tank level and the centrifuge trip on high digestate tank is totally eliminated by the controller. Therefore, the main issues for the overnight runs are the trips on high thickened sludge tank level and the AD trip on high digestate tank level. This means that the level of inventory coming into the site may be higher than what the plant is capable of processing. The other level trips reflect the temperature effects on gas production as at low temperatures, the CHP trip on low gas holder level occurs whilst at high temperatures; gas is flared and the AD trip on high gas holder level occurs. This is expected due to the temperature effect on biogas production modelled with a biogas correction factors shown in Table 6.1, 6.2 and 6.3 in Section 6.2.2. However the level of trips is greater at high temperatures and should be avoided as the trips occurring at high temperatures may be of greater cost due to gas flaring and tripping the CHP.

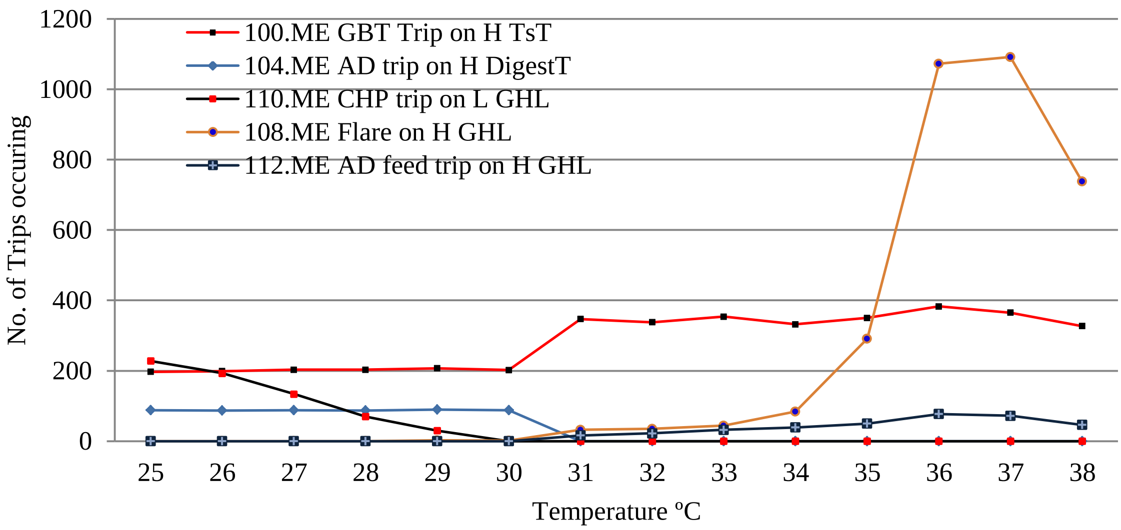


Figure 6.21 Number of trips

Figure 6.22 shows a plot of CHP energy savings against temperature settings between 25 to 38˚C. This shows a steady linear increase between 25 and 30˚C followed by a large increase in CHP energy savings between 30 and 31˚C of about £510. The plot illustrates that the peak energy saving is at 33˚C and this temperature setpoint was related to the gas flaring at high temperatures and therefore increasing the temperature above 33°C does not significantly increase CHP energy savings.

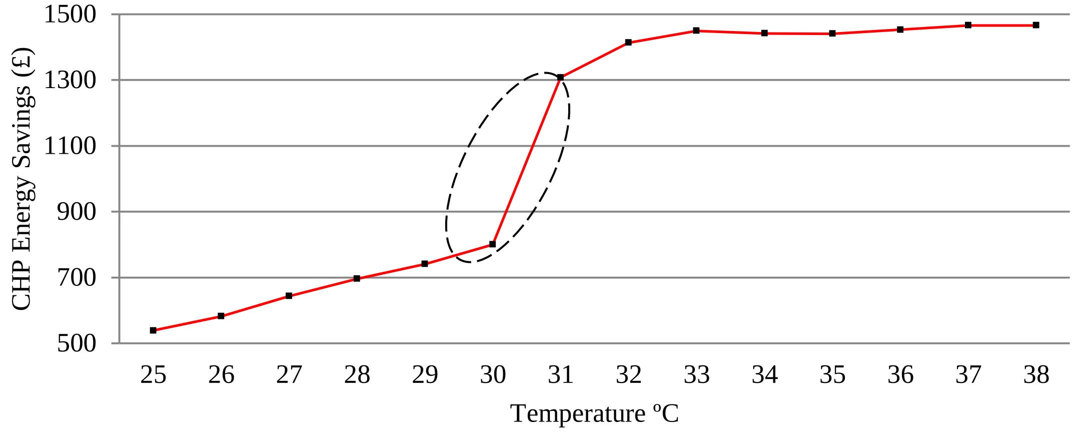


Figure 6.22 CHP energy savings against temperature

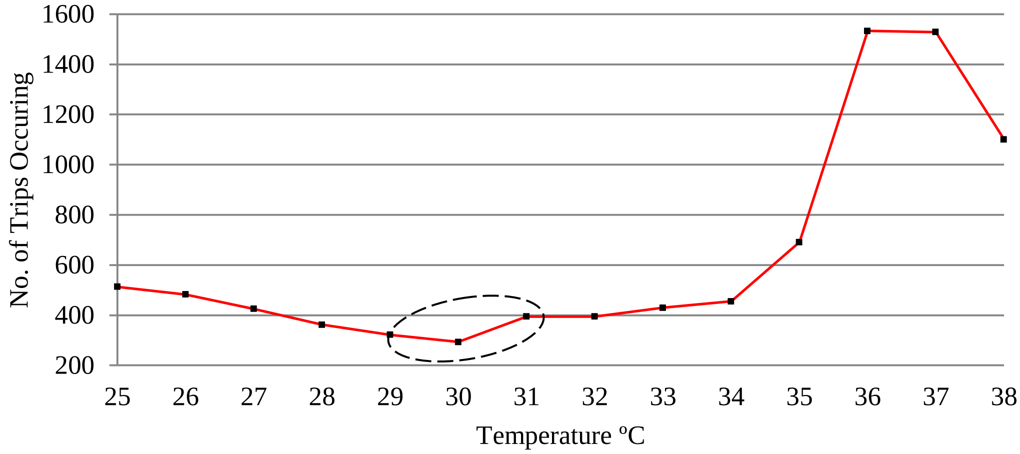


Figure 6.23 Number of trips occurring versus temperature

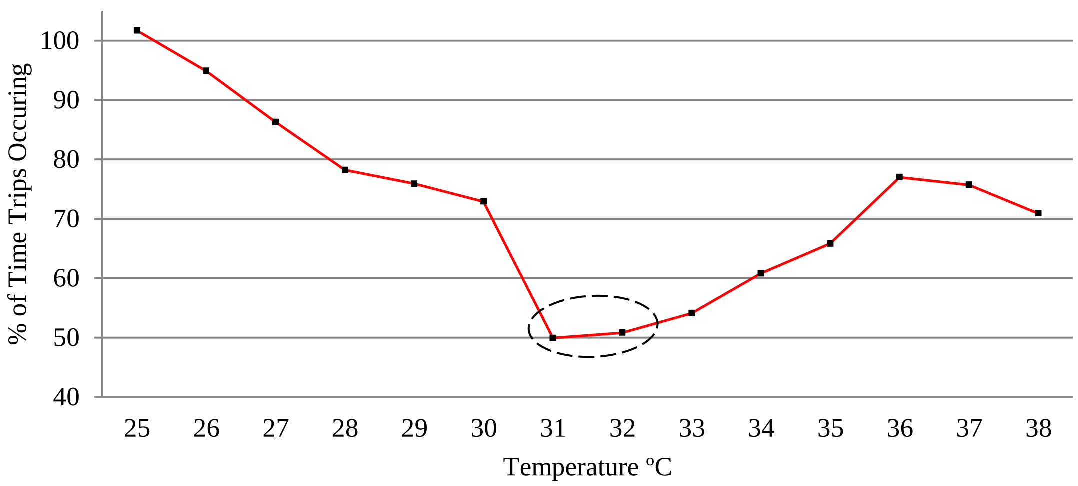


Figure 6.24 % of times trips occur

Figure 6.23 and Figure 6.24 shows the give number of trips occurring and the % of time trips occur. There is high level of trips occurring around 36 to 37˚C resulting from trips in the gas holder leading to gas flaring. This is due to the increase in high gas production resulting from the high temperatures. The gas is being flared because the CHP units have reached their maximum capacity. Figure 6.23 also show the temperature settings where minimum trips occur. This is highlighted by the black circle between 31 and 32°C setpoints. The % of time the trips occur shown in Figure 6.24 is also lowest at these setpoint. This is, therefore, the best setpoints for achieving lower levels of trips occurring at the lowest amount of time.

The key findings from the simulation assessment can be summarised as follows:

- Significant reduction in level trips, with total elimination of AD trip on low thickened sludge tank level and centrifuge trip on low digestate tank level;
- A key setpoint in the process is around 31˚C, where the level trips are at zero, or stable. Total simulation cost benefit and CHP energy savings increase significantly above 31˚C;
- Optimum temperature for total simulation cost benefit gain was found to be around 33˚C instead of the predicted optimum of 35˚C. This is specific to the simulation conditions, as sludge inventory is high, high temperature operations incur more trips and the cost element associated with these within the simulation makes operation at high temperatures not cost effective. The optimum is therefore process dependent as at different capacities and operational constraints, the optimum will vary.

6.5.3 MPC2: System dynamics

This section reviews the results for the MPC2 controller depicted in Figure 6.8. This controller was designed to investigate the benefits of separating the slow and fast dynamic parameters in the simulation as AD system has varying dynamics.

On observing the controller in the simulation, it became evident that the slow dynamic structure was too slow to react to the changes in the fast dynamics structure and effected the rate of response in meeting the controller objectives. This can be demonstrated in Figure 6.25. The plot show gas holder level (purple) has fast dynamics and is affected by biogas production which is affected by digester temperature (blue) and feed rate (green). As the gas holder level increase to the point of tripping the level, the feed rate and or temperature should reduce dependent on the state of those values. In this scenario, the temperature continues to increase, which maintains the gas holder level at high and therefore tripping and feed rate changes gradually. The lack of reduction in the feed rate at a faster rate is supported by the thickened sludge tank level, which is at its high levels and also tripping and therefore the high thickened sludge tank level requires the feed rate to increase. This is an example of the controller struggling to meet the hierarchy of control objectives and constraints shown in Table 6.5. The gas holder tank and thickened sludge tank tripping are the top two objectives the controller is aiming to avoid. For this type of scenario assessment, the controller appears to struggle to meet the various objectives set. This may be due to inaccurate dynamics splitting.

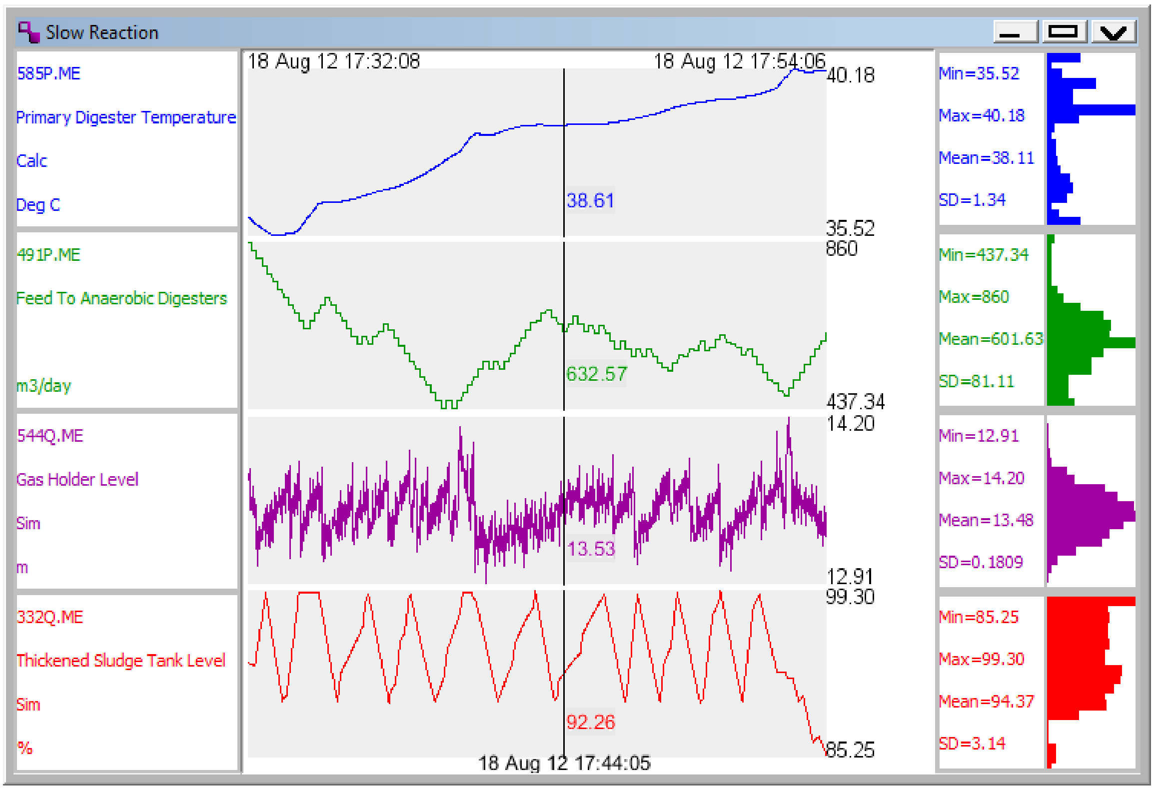


Figure 6.25 Slow and fast dynamics

The findings from MPC2 assessment can be summarised as:

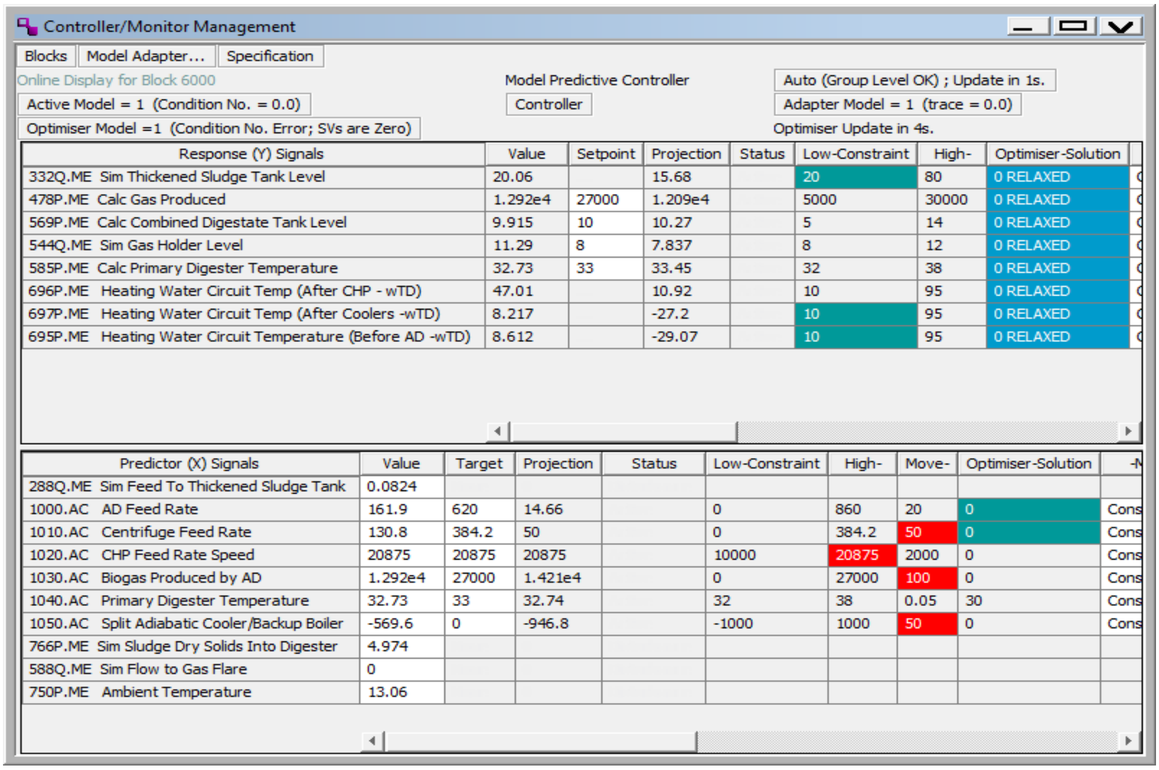
- Reduction in the number of level trips in general and % of time trips occurring;
- Temperature setpoint is less controlled;
- Process more erratic and therefore further tuning may be required to smooth the controller;

- Gravity belt thicker trip on high thickened sludge tank tripped above 197 times for all MPC1 simulation runs, however for the MPC2 model; this is reduced to 77. Which is over a 60 % reduction in the number of trips occurring for the GBT system;
- The overall simulation cost benefit did not improved for the settings.

Although the findings show that the MPC2 simulation system is less controlled smoothly in comparison to the MPC1 structure, there is a significant reduction in the number of level trips occurring in the system. Further assessment can be conducted on this model to ascertain whether any further improvements can be made.

6.5.4 Optimisation

A quadratic programming (QP) optimiser discussed in Section 4.3.1 and 4.3.3 is applied to the MPC1 structure in Figure 6.7 and evaluated. The first objective of the QP optimiser is to keep the process within the bounds of its constraints followed by cost minimisation.


Controller/Monitor Management

Blocks | Model Adapter... | Specification

Online Display for Block 6000

Model Predictive Controller

Auto (Group Level OK) ; Update in 1s.

Active Model = 1 (Condition No. = 0.0)

Controller

Adapter Model = 1 (trace = 0.0)

Optimiser Model =1 (Condition No. Error; SVs are Zero)

Optimiser Update in 4s.

Response (Y) Signals	Value	Setpoint	Projection	Status	Low-Constraint	High-	Optimiser-Solution
332Q.ME Sim Thickened Sludge Tank Level	20.06		15.68		20	80	0 RELAXED
478P.ME Calc Gas Produced	1.292e4	27000	1.209e4		5000	30000	0 RELAXED
569P.ME Calc Combined Digestate Tank Level	9.915	10	10.27		5	14	0 RELAXED
544Q.ME Sim Gas Holder Level	11.29	8	7.837		8	12	0 RELAXED
585P.ME Calc Primary Digester Temperature	32.73	33	33.45		32	38	0 RELAXED
696P.ME Heating Water Circuit Temp (After CHP - wTD)	47.01		10.92		10	95	0 RELAXED
697P.ME Heating Water Circuit Temp (After Coolers -wTD)	8.217		-27.2		10	95	0 RELAXED
695P.ME Heating Water Circuit Temperature (Before AD -wTD)	8.612		-29.07		10	95	0 RELAXED

Predictor (X) Signals	Value	Target	Projection	Status	Low-Constraint	High-	Move-	Optimiser-Solution	-N
288Q.ME Sim Feed To Thickened Sludge Tank	0.0824								
1000.AC AD Feed Rate	161.9	620	14.66		0	860	20	0	Cons
1010.AC Centrifuge Feed Rate	130.8	384.2	50		0	384.2	50	0	Cons
1020.AC CHP Feed Rate Speed	20875	20875	20875		10000	20875	2000	0	Cons
1030.AC Biogas Produced by AD	1.292e4	27000	1.421e4		0	27000	100	0	Cons
1040.AC Primary Digester Temperature	32.73	33	32.74		32	38	0.05	30	Cons
1050.AC Split Adiabatic Cooler/Backup Boiler	-569.6	0	-946.8		-1000	1000	50	0	Cons
766P.ME Sim Sludge Dry Solids Into Digester	4.974								
588Q.ME Sim Flow to Gas Flare	0								
750P.ME Ambient Temperature	13.06								

Figure 6.26 Controller Management page of flat structure with optimiser

For comparison purpose; all optimum settings for the MPC1 structure were kept as shown in Figure 6.26, depicting the controller management page with the optimiser switched on. When the QP optimiser is active, the solution is 'relaxed' in most cases. This happens when the QP cannot find a feasible solution within the defined constraint limits, therefore the constraint limits are allowed to be 'relaxed' according to the priority settings that have been provided (*Perceptive Engineering Ltd*, 2012). This means the solution provided is not the optimum operating point of the process but a best attempt was carried out to satisfy the constraints and priorities. QP 'relaxed' output or infeasible solution may be due to model errors or incorrect model set-up.

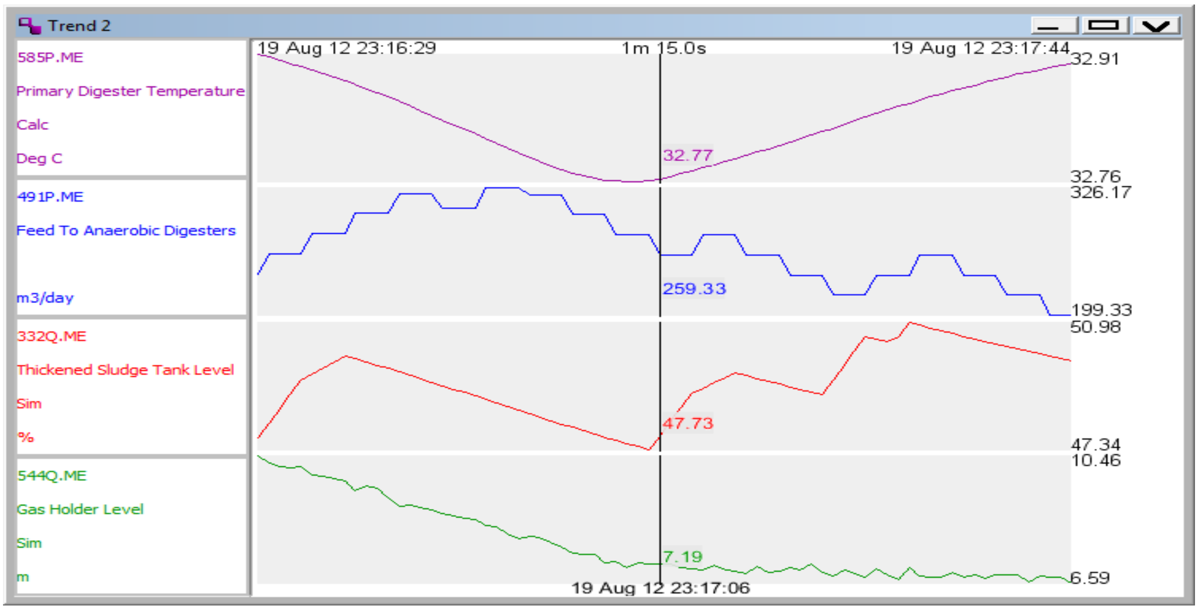


Figure 6.27 Tighter control achieved with optimiser

The result from the optimiser showed tighter control is obtained with temperature values deviating less than 0.5˚C. Although constraints were violated at some reduced instances, the optimiser appears to control the process well as shown in Figure 6.27. The figure shows primary digester temperature (purple), feed rate (blue), thickened sludge tank level (red) and gas holder level (green). As the thickened sludge tank reduces close to its low limit level trip, the feed to the AD gradually reduces to enable the thickened sludge tank level to increase. A decrease in feed rate cause the gas holder level to reduce further due to the low feed rate and this causes the temperature to increase to enable more gas production.

6.5.5 Controller performance comparison

This section compares MPC1, MPC2 and the MPC1 with the optimiser PID controller and the base model without controller. The best performing temperature setpoint for the simulation was at 33°C and thus the simulated results were at 33ºC. Figure 6.28 depicts the CHP energy savings and total simulation cost benefit in £ per day. The results favour the benchmark MPC1 controller shown in dark blue, which yields highest CHP energy savings for the system and high total simulation cost benefit value. This is followed closely by the MPC1 with the optimiser controller shown in light blue and then the MPC2 (purple). The performance with a 'no controller' shown in red performs better than the PID controller and although the 'no controller' yields £0 of total simulation benefit to the system, the PID controller results in £510 cost.

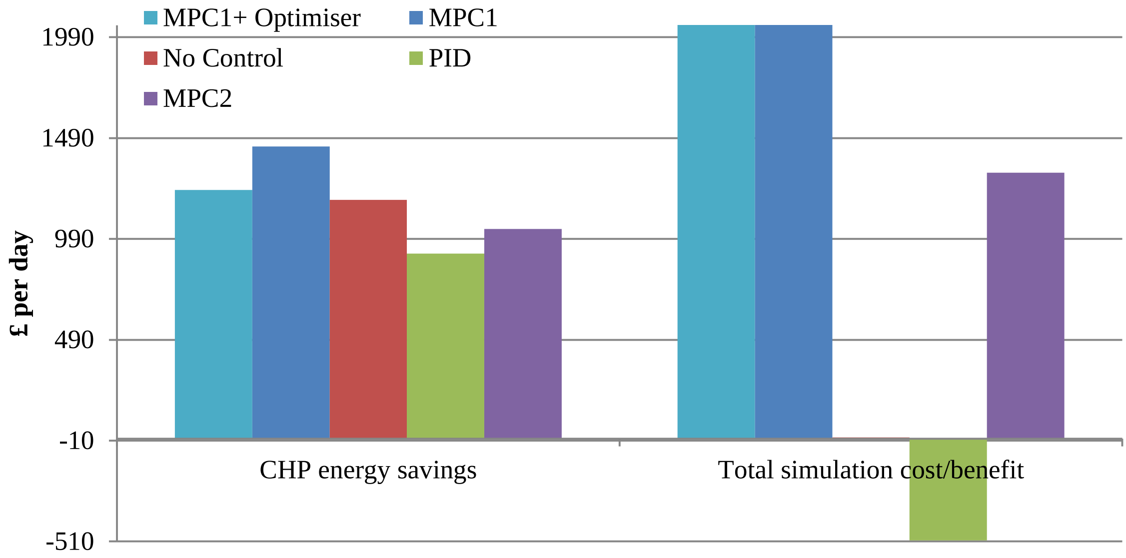


Figure 6.28 Controller evaluation comparisons: CHP energy savings and total simulation cost benefit

The benefit of the optimiser on MPC1 was evident on comparing the number of trips and the % time of time the trips occur. There appears to be a significant reduction in the number of level trips occurring with the MPC1 and optimiser as shown in Figure 6.29 in dark blue. The figure shows a reduction in trips with the optimiser for up to 92 % less from the 'no control' benchmark simulation system. This is a significant finding and may help formulate the case for implementing an optimised solution for the actual industrial application for the project.

MPC2 plotted in red is shown to outperform MPC1. This is a significant finding as MPC2 was shown to have 60 % and 63 % reduction in level trips and % of time the trips occur respectively, whilst MPC1 was shown to have 38 % and 49 % reduction in level trips and % of time the trips occur respectively. There separating the various dynamics in the simulation enables reduction in level of trips. However MPC2 yields lower energy savings and total benefit than MPC1.

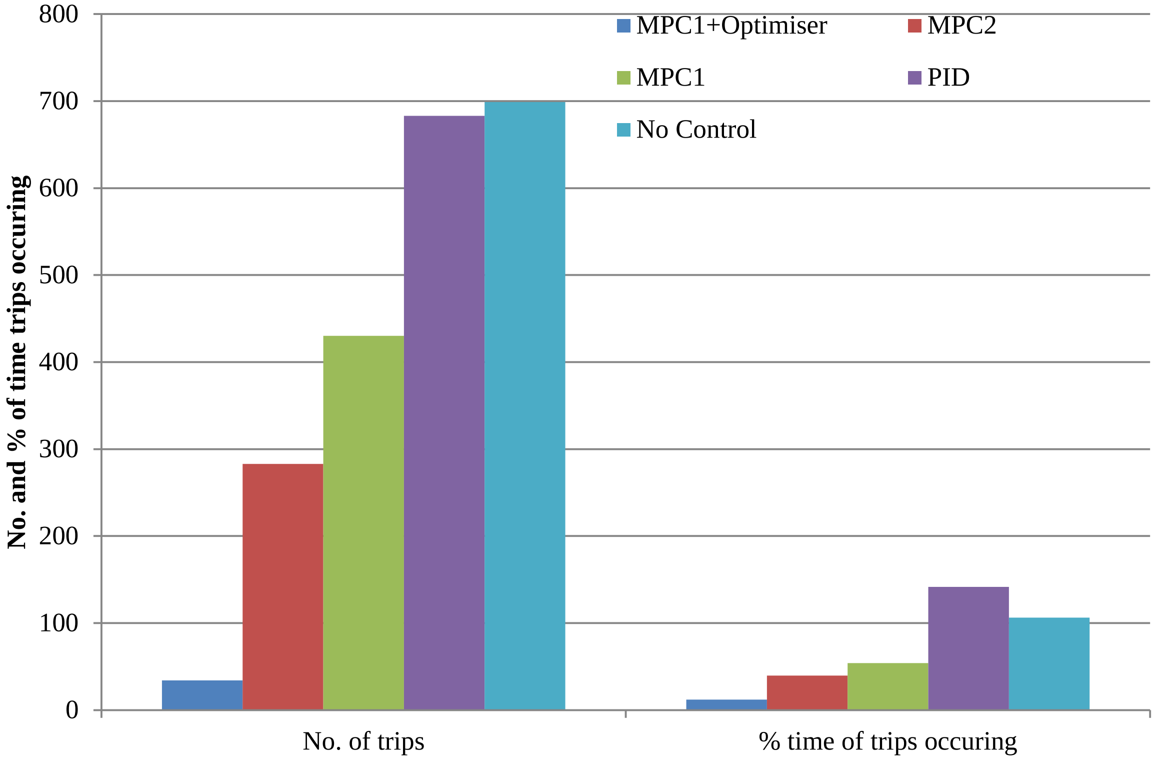


Figure 6.29 Controller evaluation comparisons: No. of trips and % time of trips occurring

Although the PID controller yields 2 % reduction in level trips than the ‘no controller’, the PID controller takes longer to reset itself as shown in Figure 6.29 purple with the longest % of time the trips occur. The 2 % in level trips can potentially increase by developing multiple PID controllers on the system. However the reduction in level trips did not reflect the CHP energy savings and the overall cost benefit of the system. This may be due to the values given to certain cost elements within the model. For example, priority settings and actuator move weights were tuned to ensure low levels of trips occur as the primary aim of the simulator. Therefore the simulator aims to limit the level of tank trips before optimising CHP energy savings and biogas production to improve the overall cost benefit of the simulator.

6.6 Discussions and conclusions

The inventory simulation was subject to several assumptions and therefore the results presented here have to be treated with caution. There is however significant evidence that an advanced controller such as MPC can significantly reduce the number of level trips; as per the scenarios tested in the analysis.

The simulation results illustrate that the multi-objective control problem of AD can be controlled with respect to scheduling and inventory. The simulation also highlights the problems associated with the system dynamics. The large variability in the system means variables such as temperature settings take a considerable time to heat or cool down with the boiler cooler settings whilst the cooling effect on increased feed is more instantaneous. Therefore the benefit of separating the dynamics in MPC2 has been shown to significantly reduce the number of level trips occurring.

There remain significant trips still occurring in the system, especially for the MPC1, which were mainly due to the system capacity to cope with the high sludge inventory. The degree of improvement with respect to control and efficiency of the process controllability is subject to the design. Capacity plays a detrimental role, as findings from all benchmarked sites showed a bottleneck resulting from the inventory. This had led to AD systems being historically designed at larger scales than operational intent. In spite of this, these processes are still subject to capacity limitations. With respect to the AD consortium for this project, this was an area where better understanding is required for future designs. The design limitation issue cannot easily be removed and companies cannot continue to design larger plants than needed for operation to enable better flexibility for inventory and scheduling due to economic factors. The aim therefore is to apply better control and optimisation solutions to improve the process and reduce the limitation of capacity. This will be achievable not just through better monitoring but increased and combined understanding of the various areas of the process. Strong integration of microbial, bio-physiochemical and engineering for improving the economics of the process will yield better improvement of the control of AD processes.

The existing control system at Blackburn WwTW is reduced to temperature and level controls. The benchmark study showed that this level of control was not efficient for controlling the process; however the data available lacked capturing of the system dynamics for modelling for control implementation. The simulation here is used as a basis to evaluate the specific dynamics, correlations and relationships needed to design controllers for a potential system. This would require plant testing or formally DoE to yield robust data for modelling. Future activities following on from the assessment conducted so far therefore includes plant testing to generate data robust enough for constructing models as per the simulation to evaluate the MPC1, MPC2, MPC1 plus optimiser and PID controllers for controlling inventory and optimising the AD system as a whole.

Generating robust data for modelling requires instruments that can measure the required parameters capturing the dynamics, correlations and relationships within the system. In some such cases robust instrumentation was unavailable and as such opportunities for inferential measurements were investigated. Chapter 7 is an example of such investigation which aimed to test the capability of building volatile solids inferential sensor model.

7 Volatile solids model

7.1 Introduction

Lack of instrumentation is the main control bottleneck in the AD process. Sensors and analysers are necessary to reduce the variability related to changes in the initial conditions, uncertain kinetics and input concentrations of the process. Without knowledge of the process conditions, the process is inevitably difficult to control.

Inferential measurement is a powerful and increasingly popular methodology that allows process quality and difficult to measure process parameters to be inferred from other easily measurable parameters such as temperature, flows and pressures. This study investigates the opportunities for developing inferential sensor for volatile solids (VS).

7.2 Digestate

Traditionally, the objective of AD in wastewater treatment plants (WwTP) has been that of sludge stabilisation and odour reduction. Biogas production, solids destruction and pathogen reduction are now key areas of interest with biogas being the main product. The second by-product, digestate, is the solid component that remains after digestion, and is typically used for agricultural purposes or sent to landfill. Digestate quality is thus becoming more important with industry exploiting it as a valuable end-product. The availability of instrumentation for the monitoring of digestate quality is limited and generally offline. Risk-based management and control procedures are in place to manage digestate quality, in particular where the intended use is agricultural land. The quality of the digestate must comply with appropriate microbiological standards, including the safe sludge matrix (SSM) (Davis et al., 2010). Digestate quality attributes as defined by the Publicly-Available Specification 110 (PAS110) (WRAP, 2010) and the SSM include the level of VS, volatile fatty acids (VFA), residual biomass potential (RBP), animal by-product (ABP) and hazard analysis and critical control points (HACCP) for compliance with declarations of pH, total nutrients (Nitrogen, Phosphorus, Potassium), total solids (TS), and loss on ignition (WRAP, 2010) required. PAS110 ensures that the AD system uses suitable input materials, which are effectively processed to produce digestate product in sufficient time. The process must also be managed and monitored to meet both market needs and for the protection of the environment. The specification offers digestate producers guidelines for the AD process, as industry accepted specifications for digestate and ADs are unavailable.

Process monitoring in the fermentation industry is well advanced and established. The similarities of such processes are aligned with AD and therefore technological developments in this area are interest to AD researchers. Process Analytical Technology (PAT) enables monitoring of complex biological processes using electrochemical and spectroscopic instruments. By applying PAT with chemometric multivariate data analysis to the AD process, it could ensure the optimum potential of the AD process to reach new levels of stability, robustness, reliability and effectiveness (Madsen *et al.*, 2011).

Chapter 2 and 3 demonstrated the strong requirement for increased robust instrumentation, for the AD process, which is the main bottleneck in process control improvement. There is a strong interest to characterise the quality of digestate but to date, there is no set specification for digestate quality. SSM and PAS110 are used as guidelines to meet HACCP compliance. Therefore the availability of an online digestate quality attribute through the use of PAT and chemometric multivariate analysis would enhance the control of digestate quality and could potentially increase the value of the digestate.

Biosolids is the term used to describe the treated solids fraction of the digestate or stabilised sewage sludge (Lawrence K; Wang *et al.*, 2008). The safe sludge matrix (Chambers *et al.*, 2001) governs the regulation for applying sewage sludge on agricultural land. This is supported with processing requirements, storage and application procedures to reduce the risk to human health and the environment. The stability of the digestate is defined by several factors such as the level of pathogens, odour and reduction in further decomposition of the organic materials involved (Gomez *et al.*, 2005). There is no single accepted analytical method to measure this multi-attribute stability factor. However there are several individual tests to define the degree of stabilisation. Digestate as a quality output measurement of the digestion process is dependent mainly on feed sludge composition, digestion temperature and retention time. The process greatly depends on influent feed composition and therefore in order to model digestate quality, knowledge of the feed composition is required. The quality test for digestate is based on test for stability, test for compliance and declaration of other quality variables. These are:

- VS;

- VFA (0.43g COD gVS^{-1});
- Residual biomass potential (RBP) 0.25l gVS^{-1};
- Animal by product (ABP) and HACCP compliance;
- Declaration of pH, total nutrients (Nitrogen, Phosphorus, Potassium), TS, loss on ignition.

The compliance element is based on the digestion conditions of temperature and retention time and is the main aim during digestion to meet the HACCP requirement. This requires digesting the sludge for a set period of time at a set temperature dependent on the characteristic of the feed stream.

Total solids (TS) measure the solids in the digestate and are composed of insoluble suspended solids (SS) and soluble compounds. Volatile solids is the main organic fraction which can be burnt off from the SS (Alturkmani, 2010). The quality of digestate is defined by the organic and inorganic matter present, in the absence of phytotoxicity and weed seeds.

The key parameters affecting digestate quality are temperature and retention time (Seadi and Holm-Nielsen, 2010). However due to the highly variable feed compositions in the feed and feed flow, these parameters may affect digestate quality immensely. The digestion process offers valuable nutrient source as the process generally enhances the availability of nutrients. Characterisation of digestate quality requires the stability factors and declaration of the pH and nutrients to be modelled. Analysis of the nutrient content is very important, as it affects the price for selling digestate. This is calculated from the sum of nutrients (N, P_2O_5 and K_2O) available to plants for land application. Provided there are measurements for these variables, the digestate quality can be calculated. Chapters 2 and 3 demonstrated current methods for measuring digestate are limited to irregular, infrequent and offline measurements of % DS and volatile matter.

Instrumentation for measuring digestate quality parameters as determined by pH are readily available and implement on industrial scale AD systems. Control of nitrogen removal rate and phosphate precipitation are measured (Ingildsen, 2002), where N, P and K nutrient values are measured offline. VFA sensors are available on pilot scale and information for industrial scale application is not available. Residual biomass potential can also be calculated offline. There are testing procedures for all these variables as part of the PAS110 criteria (WRAP, 2010). Table 7.1 highlights the test procedures and requirements for digestate quality measurements.

Table 7.1 Digestate quality test procedures

Test	Method	Test period	Accuracy or reproducibility
RBP	Measure of stability by measuring the total biogas production within a specified period of time, at 35˚C	28 days	Affected by high VFA concentrations
VFA	Online instrumentation available for AnaSense, Capilex etc. methods include wet chemistry methods of distillation, colorimetric technique, titration and gas chromatography such as the Shimadzu GC-2010 (Shimadzu, 2012).	Minutes	Weak concentrations are difficult to detect, accuracy increases with high concentrations.
VS	Commonly two step drying method by heating the sample to about 105˚C to dry off the water, the weighted dry cooled sample is then dried further at 550˚C to dry off the VS	About 7 hours	Affected mainly by the temperature and drying time.

7.2.1 Volatile solids

Volatile solids are organic compounds found in animals and plants. The biological digestion process of AD breaks these solids down and converts into CH_4, CO_2 and H_2 etc. Volatile solids in the digestate is determined by the % DS fed into the digester, the sludge composition, digestion temperature and the % DS of the digestate. VS is analysed by drying a sample of the digestate in high temperature ovens. This is an important digestate quality output test for stability and the % VS remaining in the digestate will eventually break down post digestion and potentially pollute the environment (through land application as biosolids). High VS content in the digestate means fewer solids are converted into biogas during digestion and therefore results in a waste of resources. There is therefore an economic and environmental reason for reducing the level of VS in digestate. Measurement of VS enables a quantitative measure of the organic matter but fails to account for biodegradability of the solids in the digestion process. Therefore high VS (low degradation) levels post digestion may indicate process inefficiency or the presence of organic matter like lignin which are not biodegradable (Schievano *et al.*, 2011). VS destruction rate is inevitably affected by many factors to including level of polymer added, digester operating temperature, mixing efficiency, retention time, characteristic of the microorganisms available, composition of sludge etc. These factors make the VS measure difficult in both prediction and estimation.

VS provide an indication of the stability of the digestate and hence the stability of the process can be inferred. Online instrumentation for VS is not available and, although offline analysis can be conducted, the sampling rate is typically low and irregular. VS may potentially provide a better indication of the sludge quality (biochemistry) than other measurements such as % DS (Dry Solids Percentage). It is expected that VS will negatively correlate with biogas production, as an increase in biogas corresponds to an increase in the breakdown of organic molecules and therefore lower VS. The effect of temperature on VS may be more complex due to the non-linear relationship between temperature overall process performance. In general an increase in temperature from mesophilic to thermophilic increases the reaction rate and efficiency at which the organic solids are destroyed resulting in a lower VS (Buhr and Andrews, 1977). A negative correlation can be expected between VS and retention time, with VS having been shown to decrease with increasing retention time (Moen *et al.*, 2003). Measurement test procedures for VS are also simpler than those conducted offline for VFA or RBP, as the test for VS does not require wet chemistry techniques such as titration, colorimetric and chromatography techniques as required for VFA (Palacio-Barco *et al.*, 2010). For these reasons, VS is an important digestate quality attribute and the use of VS for online monitoring and control will potentially result in a tighter control on digestate quality.

7.2.2 Soft sensor use in AD systems

The behaviour of a process is indicated by the measurements made and are related to the state of the process. Information contained in many secondary variables reflects the behaviour of the primary variables. Therefore, the aim of this study is to investigate whether secondary variables such as VS can be inferred from primary state variables such as temperature and feed flow. Figure 7.1 depicts a soft sensor application model; where the primary output measured is also connected to the estimator parameter. The estimator updates the soft sensor model or estimator. This is essential for the errors between estimated and measured primary outputs to be used by the estimator parameter to drive the parameters of the soft sensor model to yield a more representative value. Therefore the adaptive soft sensor is typically multi-rate systems with the estimation of the primary outputs are produced at a faster sampling rate of the inputs and secondary outputs.

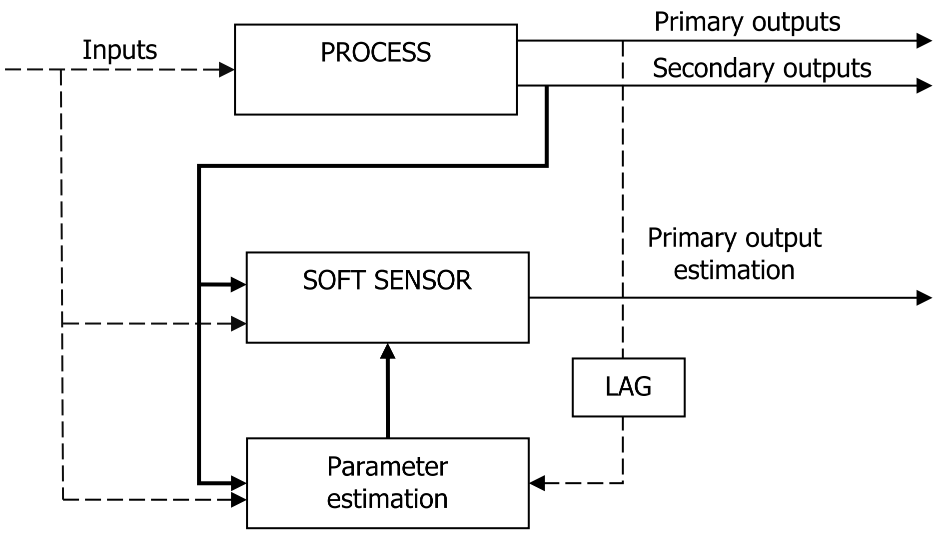


Figure 7.1 Soft sensor implementation

7.2.3 Volatile solids soft sensor

Soft sensors develop a relationship between a hardware sensor for a measurable variable and an estimation algorithm (software) to provide an online estimate of an ummeasurable variable (Chéruy, 1997). Due to the difficulty and the uncertainty in the modelling of an AD system, a data driven approach will be used for the monitoring of VS for the control of process stability and to meet compliance requirements.

Volatile solids provide an indication of the stability of the digestate and may infer the stability of the process. Online instrumentation for VS is not available and, although offline analysis can be conducted, this often has low and irregular rates of sampling. VS may provide a better indication of the sludge quality (biochemistry) than other measurements such as % DS (Dry Solids Percentage). It is, in theory, positively correlated with feed rate and negatively correlated with temperature, retention time and gas production.

VS are affected by a number of factors that are important to consider for modelling purpose:

- A higher temperature is shown to increase the speed of degradation and hence higher temperatures may result in lower VS levels;
- The digester feed rate determines the retention time, and organic loading rate (OLR). By increasing the feed rate, the retention time is reduced and therefore the sludge spends less time in the digester resulting in higher VS levels potentially (Ponsá et al., 2008);
- Feed composition is the main disturbance affecting VS levels, as digester biogas and digestate depend on the composition of the incoming sludge. This includes the level of VS entering the digester and the composition of the organic compounds and microorganisms, and is therefore the primary source of variability and the main disturbance (Ashekuzzaman and Poulsen, 2011);
- Environmental factors such as pH, mixing and microorganism population also affect VS. Antagonism (the suppression of some species of micro-organisms by others), acclimation (adaptation to a new environment or a change to the old environment) and synergisms (micro-organisms acting together for mutual benefit) together can affect the level of VS that remains after digestion (Chen *et al.*, 2008).

Assuming linear relationships exist, these factors can be captured by the Equation VS = Ax + By + e; where A is the OLR of the system, B is the temperature, x are the unmeasured disturbances entering the system, y are the environmental factors including pH and mixing and e is the error. Challenges faced in the development of a VS soft sensor are associated with the unmeasured disturbances and the other unknown environmental factors associated with microorganism activity.

To date there is no evidence of the application of a VS soft sensor. The reasons for lack of studies into VS soft sensor development and commercial availability of robust online instrumentation for VS are the same for other parameters such as VFA and % DS. These reasons can be grouped into two (1) reasons within the industry (specifically water industry where AD systems are more common) and (2) difficulty in designing of robust instruments for treating bio-products such as digestate.

7.3 Blackburn AD volatile solids soft sensor development

Data from Blackburn WwTW anaerobic digestion process is used as the industrial data for use in the VS soft sensor development study. The soft sensor development procedure is outlined in Figure 4.6. These steps are common to most data based modelling techniques with steps 2, 3, and 4 being the most important stages for getting a good model. The availability of 'good data' is dependent on:

- Sensor availability: The 'right' parameters being measured, having the right instruments available to get the required data;
- Accuracy and validity of the measurement systems: for evaluation of systematic errors;
- Precision and reliability of the measurement systems: to account for random errors;
- Sensitivity and dead band of measurement systems.
- Sampled at the right rate and or frequency to capture the dynamics within the process.

These make the selection of 'right' data a key step to obtaining a good model. Furthermore 'good data' is about process coverage also. This needs more thought coming up with more science and appropriate what constitutes 'good data'. If the initial data going into the modelling procedure is not robust enough, then inevitably, it will be difficult to obtain a robust predictive model using such data.

7.3.1 Data selection

The Blackburn dataset contains approximately 396 signals, collected within the time range of 14 January 2010 13:00 to 14 July 2010 12:00, i.e. about 188 days. The data is time-aligned with a sampling interval of five minutes. Screening of all 396 signals was conducted to select both online and offline signals which may have effect on the VS of the digestate. There are signals which may affect VS from the start of the process in the primary settlement tanks where offline measurement such as chemical oxygen demand (COD), ammonia and soluble solids to digestate analysis of % DS and volatile acids (VA). Current data from Blackburn WwTW provide offline information for digestate volatile matter (VS), pH, alkalinity, volatile acids (VA), and percentage dry solids (%

DS). These are laboratory data extracted approximately twice per week. These fail to meet the requirements of the PAS110 directive and general assessment of digestate value, which includes: digestate stability measurement for residual biomass potential (RBP), data for the log kill (HACCP), and nutrient levels for Nitrogen (N), Phosphorus (P) and Potassium (K). These are important for setting the price for the digestate, as per the AD calculator.

The offline VS, VA, pH, and % DS may be used to estimate the quality of the digestate. Modelling of all these parameters will require a multiple-input multiple-output (MIMO) system that will be difficult to assess the quality of the digestate. In such cases, experience indicates that, multiple multiple-input single-output (MISO) models are preferable. The plan is therefore to develop a MISO system for modelling VS, pH or VA. From the data provided there are several signals available for the development of a possible soft-sensor. However most of these signals are only available offline. Online signals that may be useful in developing the soft sensor include:

- Digester liquid and foam levels and flows;
- Polyelectrolyte usage;
- EH hydrolyse stage temperature in and out;
- Pasteurisation stage temperature in and out;
- Digester gas produced and pressure;
- Digester temperature.

There are different levels of measurements for the different processing units as depicted in Table 7.2. There are mixing and buffering tanks before or after each stage. The sampling time at each point therefore reflects the measure of the variable at the time and therefore temperature in the hydrolysis phase, is not a measure of the same sample in the digester at any particular point. Thus the measurements need to be time aligned. The sludge preparation area has few online signals but some useful offline signals regarding sludge composition. Data from this area will be excluded as all the feed stream is entered into the buffer tanks and continuous feed of the mixed sludge is fed to the thickening phase. Although there are good online data for the thickening stage, as a means of reducing variability in the system, the thickened sludge is entered into a buffer tank before feeding into the EEH, thus the tanks act as filters as well as delays. Without any details of the lag time for the thickening stage, the data cannot be time shifted to reflect the digestion process. This is true for the other processing steps except the EEH stage which is known to take 1.5-2 days and therefore can be shifted to match VS. For this reason data selected for the modelling are extracted from the EEH and digestion phase alone. However the sludge flows from the EEH is split into the 4 digesters and there are irregularities as at times the total flow is directed towards one single digester. For these reasons, the EEH data is also excluded from the analysis. This leaves only variables during the digestion phase, for which due to limited instrumentation, most of the key parameters needed to characterise VS are unavailable, these include pH, alkalinity, VFA and sludge composition.

Table 7.2 Signal availability for different processing units

	Sludge	Thickening	EEH	Digestion	Digestate
Process function	mixing imported food and sewage sludge with sites own sludge	Removal of excess water and polymer addition to yield % DS between 6-8 %	Separates hydrolysis and acidogenic stages from methanogenic stage. Inactivates pathogen, optimise process and reduce RT.	Stabilisation of sludge, gas production and pathogen reduction	Digestate cake preparation process.
Main Processing units	BAFF, sumps, grit removal, storage units	Gravity belt thickener, polymer dosing unit, air mixing and thickened sludge buffer tank	3 serial CSTR's at 42˚C, 3 serial batch tanks at 55˚C and 2 water sludge or water HEX	Adiabatic cooler, 4 digesters	Polymer dosing unit, centrifuge, 3 buffer centrate balancing tanks
Online signals	Flows	Sludge fed through thickener, poly usage. Unthickened sludge, buffer tank level, energy cost or usage and volume	Thickened sludge flow in or out, tank level, boiler circuit temperature, hydrolyser or pasteurisation stage sludge temperature in or out, foam levels, energy cost and usage	temperature, pressure, temperature, sludge flow, gas produced, foam depth and liquid level	Levels, flow, cake pile level, centrate speed, poly dosing flow or usage
Offline signals	Ammonia, BOD, COD, SS. 16 tank levels	Ammonia, BOD, COD, pH, VS, % DS	None	None	H_2S, % DS, SS, alkalinity, pH, VA, VM
Average process duration	Continuous	Continuous	2 days	14 days	continuous
Mode of operation	Continuous	Continuous	Batch or Continuous	Continuous	Continuous
Processing effects on VS	Feed composition and sludge age	Concentration of polymer, initial VS and % DS will have significant effect on final VS	Temperature, hydraulic residence time, feed rate, and mixing will significantly affect VS	Temperature, feed rate, retention time and mixing will significantly affect VS	Not applicable

7.3.2 Data Pre-processing

The process data generated is generally very noisy; as it contained a lot of errors, missing data and outliers it therefore required various pre-processing techniques to refine the data. The systematic pre-processing procedure is:

- Handle missing data;
- Outlier detection;
- Data alignment;
- VS offline data pre-processing to reflect the online data;
- PCA.

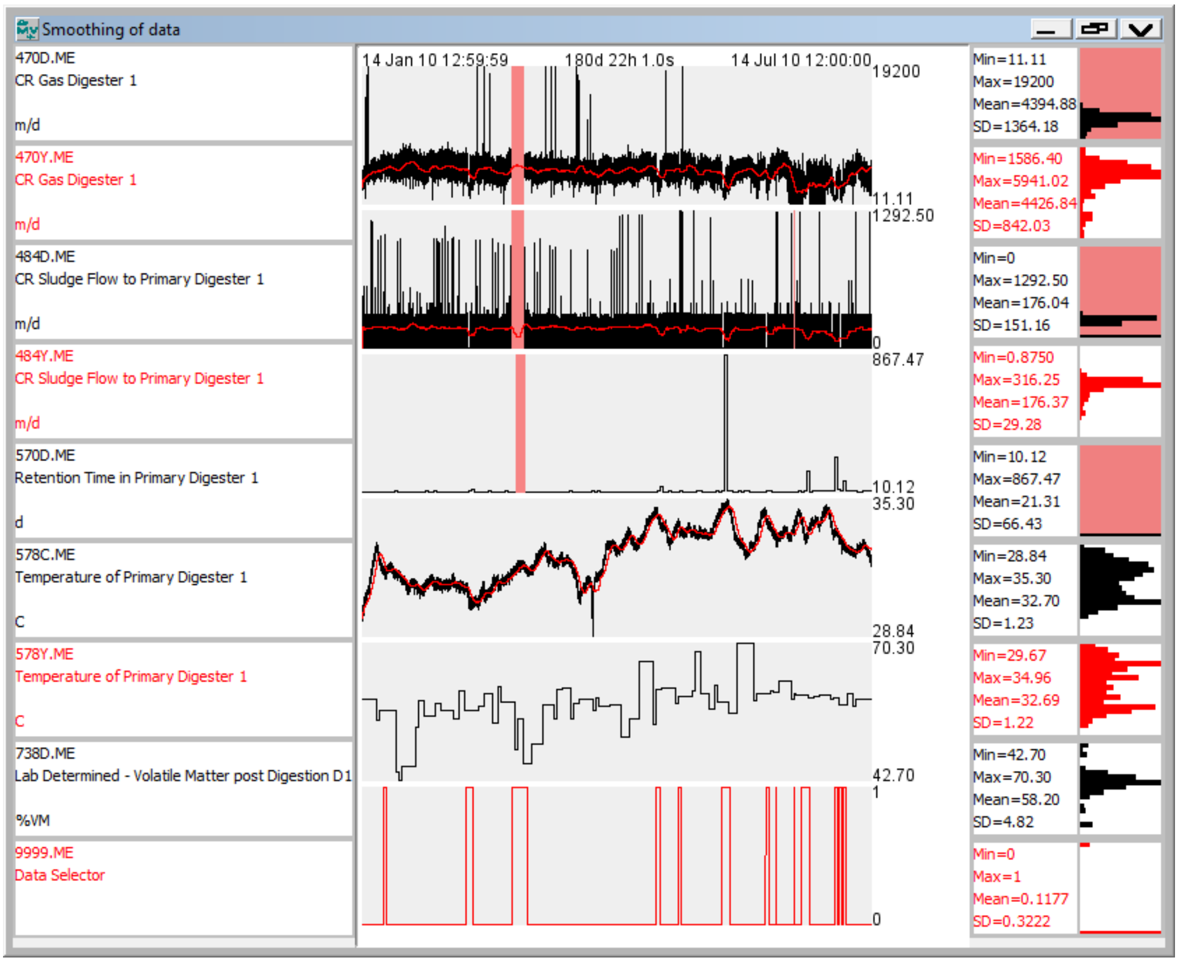


Figure 7.2 Data selector use to remove missing data

There are large sections of data missing in the signals due to a possible power or operational failure as shown in pink on Figure 7.2. Due to the large level of missing data, the data selector was used to remove the data completely from the analysis. On visual inspection of time series plot of the missing data, it was evident that some of the samples were outliers or errors. In Figure 7.3, plot of retention time for primary digester 1 is shown as 570D.ME. On the plot there is a signal peaking at 867.47 days for retention time. This is a clear error as normal operating range for retention time is between 20 to 25 days or less for EEH digesters. Removal of the missing data and extreme outliers resulted in selection of 88.2 % of the data for analysis (these are signals that equal 1 on the data selector signal) with 11.8 % of the data removed.

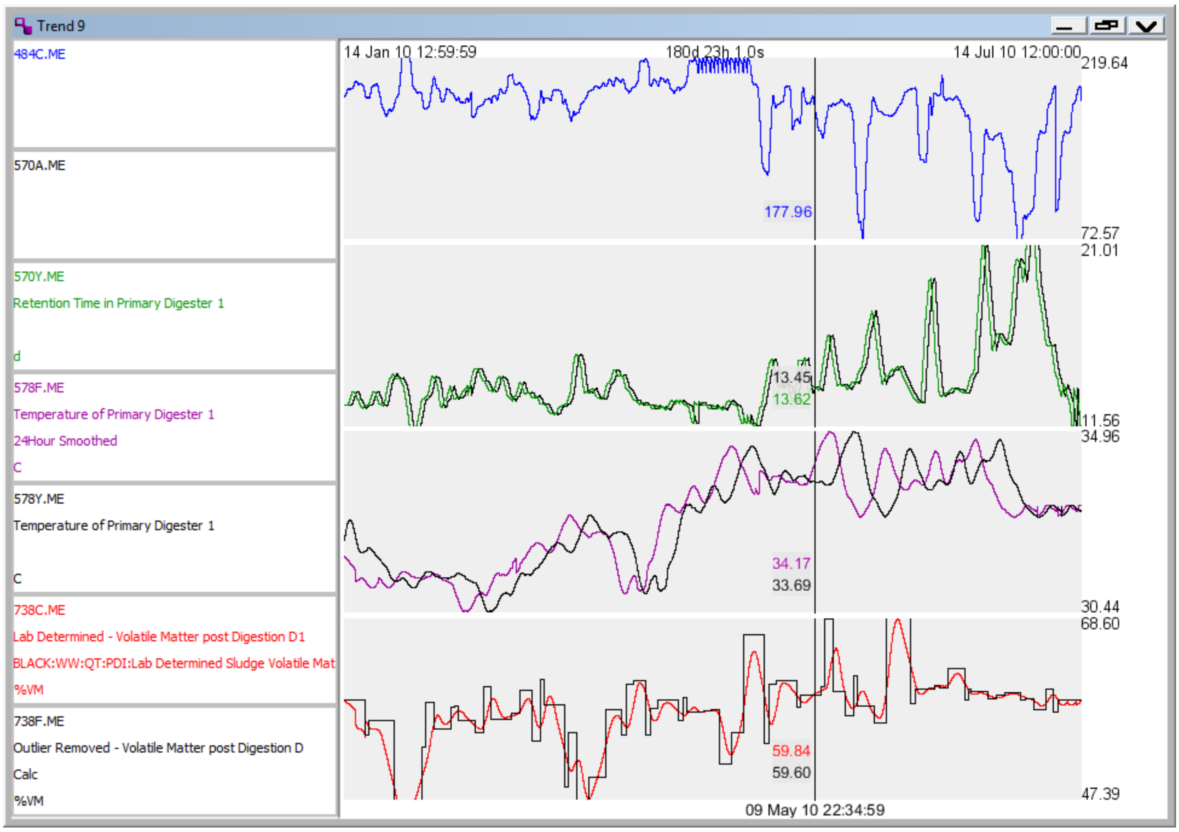


Figure 7.3 Signals post data cleaning and signal shifts

Outlier detection is one of the initial steps in data analysis for obtaining a coherent data set. It is common that what may be seen through visual inspection as noise or error may not be necessarily bad data and that these outliers can carry important information about the process. As such removal of what may be deemed to be as outliers can lead to a model giving incorrect results, misspecification and biased parameter estimation (Ben-Gal, 2005). The univariate hampel filter (Hampel, 1971; Hampel, 1974) addresses the issue outliers have on the robustness of an estimator. The hampel filter approach was then used to remove further outliers such as the spikes in feed and gas data.

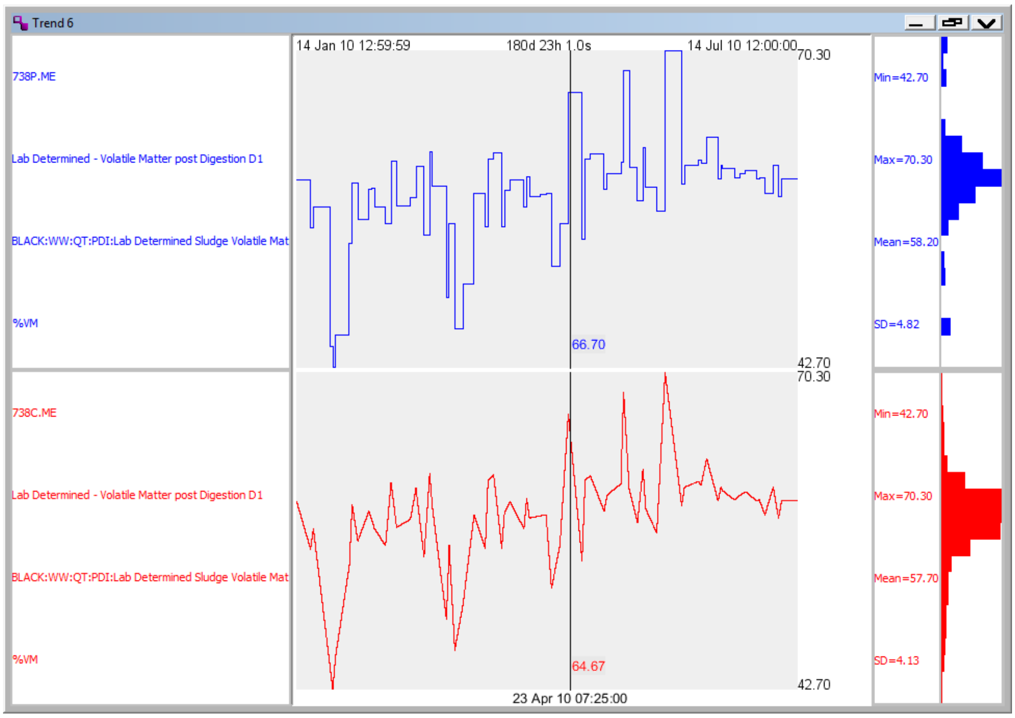


Figure 7.4 Volatile solids signal from process data showing actual and pre-processed signals

Figure 7.4 depicts plot of the VS signal from the process data where the top blue plot is the actual signal and bottom red is the pre-processed signal. The offline VS data has 50 samples over the whole 6 months period of data collected compared to 17280 samples for the online signals. The offline signals are extracted 2 to 3 times per week and there are various factors affecting the sampling and analysis which needs to be taken into consideration, such as:

- Multiple sampling points: the sample can be extracted from different points dependent on which pump is in use;
- Sampled amount for analysis varies: an accurate measure of the analysis sample is not conducted but judged from experience. The initial weight is noted and the final weight is taken from it to give the loss in weight due to VS. It is evident that drying times effect VS values, the variation in weight can effect the drying time and therefore yields inaccurate measurement of VS;
- Operator variation;
- Data entry: the calculated VS values are entered into the PI historian system from which there can be errors, especially in matching the time stamped against the time the sample is taken;

- Control: there is little evidence of operator retraining or management systems to ensure tests are carried out correctly.

These sampling and analysis issues suggest a poor level of accuracy in the VS data. As a consequence the data may not capture the dynamics or give a full of account of VS in the digester.

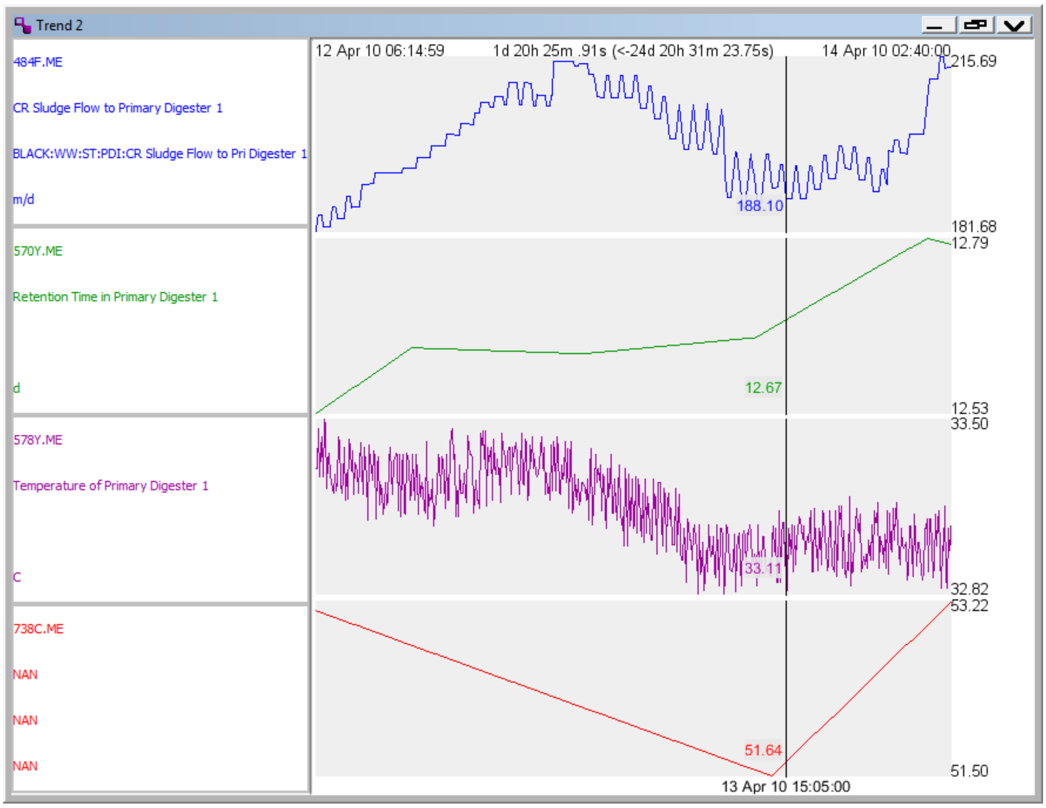


Figure 7.5 Observation of effects of sludge flow on retention time and temperature

Volatile solids are affected by temperature and the retention time. Both these parameters are controlled by the digester feed. This makes the digester feed the most important cause attribute. The feed controls the process in general; however the signal operates in an on or off mode and as such required averaging of the data over a 12 hour period. The correlation between the variables is useful to consider. Increase in temperature causes a reduction in VS levels yielding a negative correlation, however the observed correlation in Figure 7.5 is the opposite, as there is a positive correlation. This arises due to problems in time alignment. The data is shifted to align the observations, in order to capture the uncertainties in the lag times such as the time taken for an increase in temperature to take an effect on volatile solids. This was conducted through visual inspection of the data to identify patterns which may identify the cause-effect characteristics of the process. Misalignment in the data also resulted in cause signals to act as effect signals with respect to VS and therefore data alignment was key to the model building.

Table 7.3 Initial correlation analysis

Peak correlations	VS	Temperature	RT	Feed flow
VS	1	-0.543	-0.557	0.547
Temperature	-0.543	1	-0.548	-0.416
RT	-0.557	-0.548	1	-0.285
Feed flow	0.547	-0.416	-0.285	1

In a theoretical sense, temperature, retention time and feed flow depicted in Figure 7.5 should have significant effect on VS and therefore should be highly correlated with VS. Table 7.3 summarises initial peak correlation analysis of VS against these parameters conducted in PerceptiveAPC. By shifting the data sets and aligning the signals, the expected peak correlation is achieved. From this initial analysis, the signs (±) of the correlations are as expected; negative correlations for temperature and retention time as increase in these factors reduces the level of VS and positive correlation for feed flow as increases in the feed flow increases the VS levels. However the values of the correlation values are weak, which may be because of the dynamic impact.

7.4 Modelling

A good quality model relies on the quantity and quality of the data used for the modelling. It has been suggested that the input data must have minimum of 5 measured changes with 5 times larger than the noise associated with the input (Boudreau and McMillan, 2007). The historical data generated for the VS prediction model lacked this characteristic and therefore a possible DoE may be required for improvement of the quality of the data. Such a procedure involves conducting step or pseudo random binary sequence (PRBS). The generation of such data may take months to years for a bioreactor system such as the AD.

Chemometric methods of PCA and PLS are used in the modelling stage for obtaining predictive model for VS. Given a set of data consisting of a large number of interrelated variables, PCA aims reduce the dimensionality of the data set whilst retaining the variation in the data set as much as possible (Jolliffe, 2005). Principal component analysis (PCA) was developed in 1901 by Pearson (Pearson, 1901) with the geometric optimisation explanation and later Hotelling in 1933 (Hotelling, 1933) with the algebraic derivation of PCA. Principal component analysis (PCA) is popular procedure for reducing the dimensionality of the variable space. The inferential sensor study uses the PCA technique for examining the relationships within the AD process data. This has a large number of measured quality variables of which most are highly correlated therefore reducing the dimensionality of the multivariate data to a few manageable dimensions. Importantly the original variables are retained as each principal component is a linear combination of the original variables. This enables the representation of the original data set containing correlated variables, in a new ordinate system that is characterised by uncorrelated variables called principal components (PCs).

The procedure was carried out using Matlab software with the PLS toolbox (Wise *et al.*, 2010). The data was first autoscaled before applying PCA since the variables have different units. As PCA aims to capture variation, autoscaling enables all variables to be treated on an equal basis in the analysis and therefore variables that have greater variation due to the magnitude of the variable do not dominate variables with smaller order of magnitude of variation.

7.4.1 Correlation analysis

Correlation analysis on both offline and online signals which may have an effect on VS was conducted, and the results shown in Figure 9. However most do not reflect the impact on the sludge within the digester due to the different process stages. Most of the signals showed have little or no correlation with VS, which could be due to time delays within the processes. The opportunity to have VS predicted online within a short time period is essential for control of the AD process. Therefore there was a need to establish the time delays for the various cause signals. The effects of these parameters on VS is not well established from first principles and as a result, the time taken for VS variable to settle to steady state after a step change for parameters such as temperature, feed rate, retention time or gas production cannot be determined theoretically. As a result an iterative search was conducted to establish an appropriate min or max delays for the model, and therefore the data shifted to align the cause and effect variables.

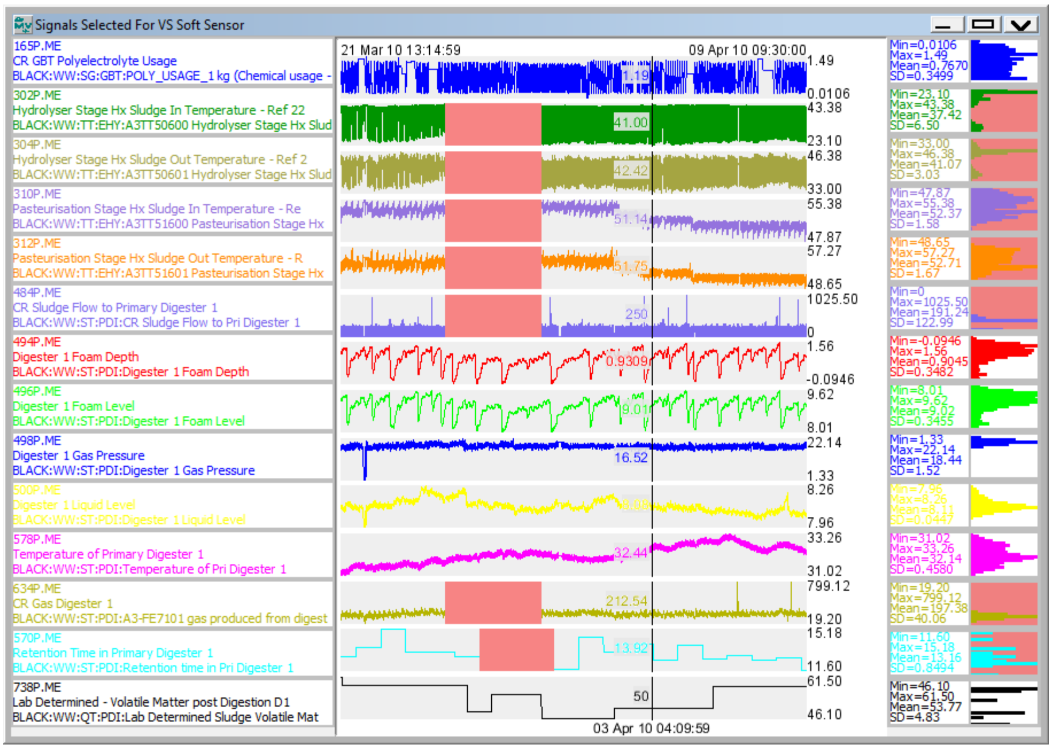


Figure 7.6 Signals Selected For Modelling

Figure 7.6 lists the signals available for modelling required for the VS soft sensor. These are online signals that may affect digested sludge VS. This constitutes of 14 signals which required pre-processing before analysis to remove bad data caused by missing values. The missing data approach is to replace bad values by the last good value.

The data in general contained a lot of spikes and the measurement of the flow was contaminated by opening and closing the valve, resulting in a repetitive irregular pattern. To reduce this, spike removal analysis was conducted on the gas produced, and the feed flow signal was averaged over an hour to reduce the on or off pattern in the data.

The development of the soft sensor was conducted in two phases. Phase 1 required analysis of the data to investigate which of the variables selected have a statistically significant effect on the digested sludge VS. This was conducted using PCA and response surface regression analysis in Minitab 16 Statistical Software. Phase 2 required the use of the PerceptiveAPC PLS modelling solution to formulate a prediction model.

The online signals formed a large dataset which was too large for analysis in Minitab 16 Statistical Software. The VS offline signal holds the same data point for about 2-3 days. The data was therefore reduced in size to reflect the changing VS data points only. The 46945 samples were therefore reduced to 67 samples. This considerable reduction in the sample size will effect the results considerably but will allow better estimation of the effects on VS.

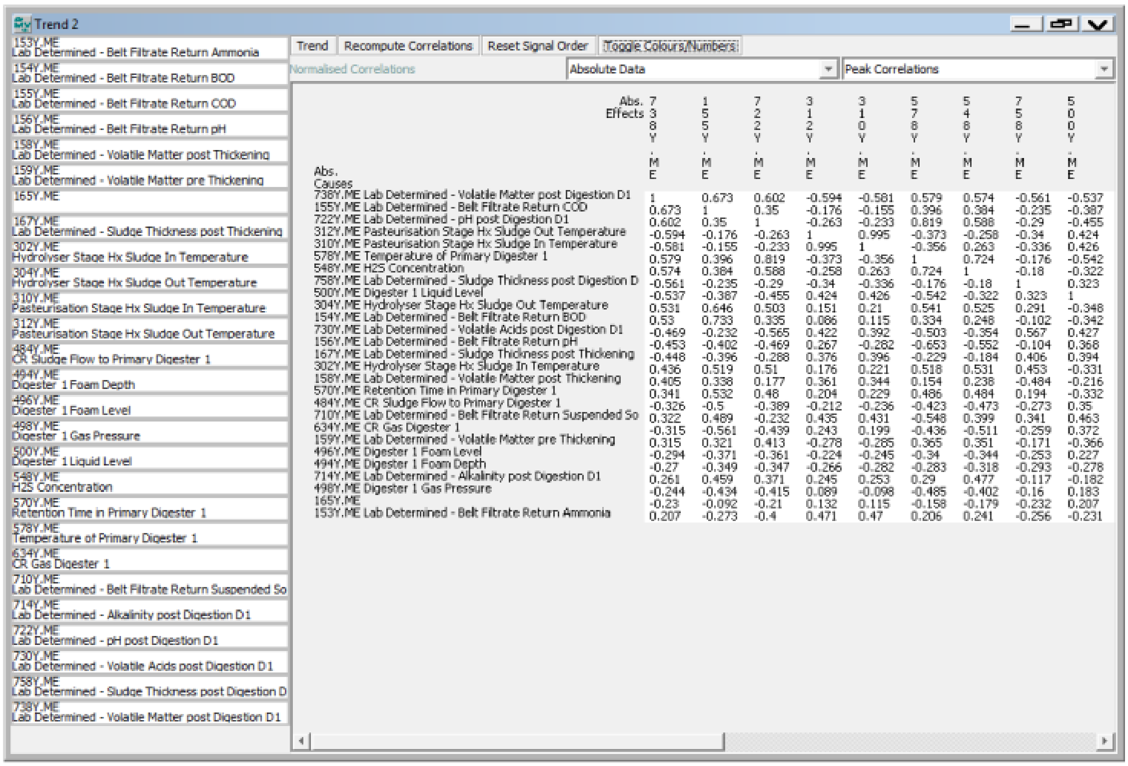


Figure 7.7 Correlation analysis on various signals

The correlation analysis results in Figure 7.7 indicate overall weak correlations for all the cause signals. These are peak correlations and some of the cause signals selected do not just have little theoretical justification but also the delays and changes in the various stages of the process mean that these cannot be used as direct effects. There were several variables which were shown to correlate strongly with VS, such as foaming and liquid levels. These variables may be related to other variables, for which the relationship or correlation may be caused by another factor in the system such as the sludge composition. Variables deemed to have a causation relationship with VS include temperature and feed rate which also determines the retention time, but the correlation values for these are much weaker than expected. The results here are therefore insufficient for selecting these as cause signals for the prediction model and therefore further analysis is required to select variables that can aid with building a theoretically and industrially robust prediction model.

7.4.2 Parallel coordinates

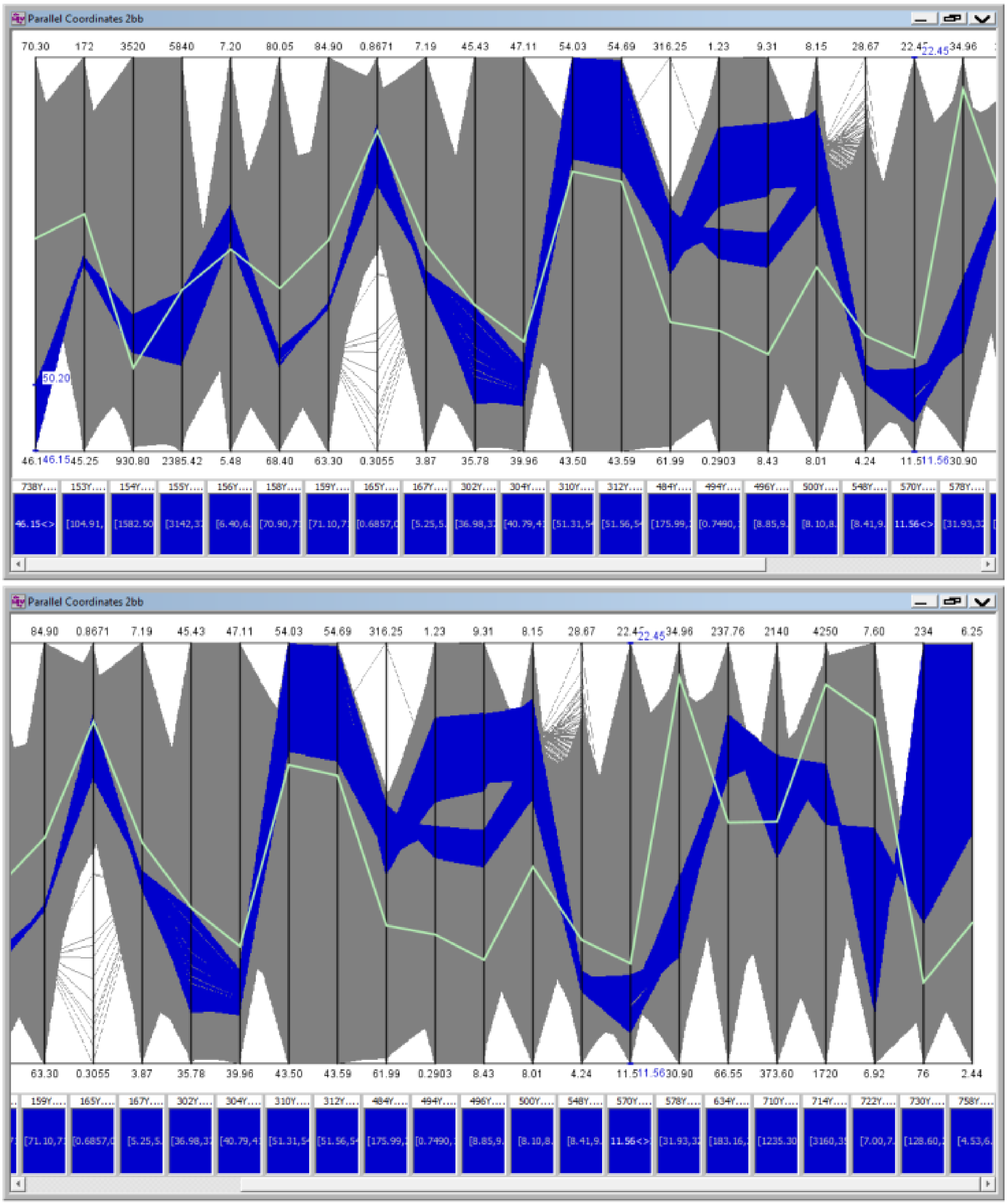


Figure 7.8 Parallel coordinates plot A and B

Parallel coordinates plots conducted to explore relationships between different signals. This is robust method for visualising and analysing multivariate data. The results given in Figure 7.8 showed that high pasteurisation temperatures in and out of the EEH stage correlate with low VS levels. This is a significant finding as high pasteurisation temperature means the initial pre-treatment stage in the EEH has significant effect on the level of VS. However the relationship is not a direct linear function as the pre-treated sludge goes into a buffer unit before entering the digester. High levels of % DS also infer high levels of VS, which is expected. Low levels of pH post digestion is shown to yield low level of VS as digester pH is not available it can be assumed that by keeping the digestion pH low, VS destruction rate may increase resulting in the low levels of VS observed. However the range of pH post digestion is quite small between 6.9 and 7.6 and although most of the lower level of pH is observed for low VS, there are high pH values for low VS as well. BSM2 simulation environment may give further insight into pH effect on VS and this is to be investigated further.

7.4.3 Minitab 16 Statistical Software response surface regression analysis

Hypothesis test analyses were conducted here to determine whether there is enough evidence to reject or accept the null hypothesis. This was conducted using Minitab 16 Statistical Software (Microsoft-cooporation, 2006) and background to be covered in the methodology section of the thesis.

Table 7.4 Estimated regression coefficients for VMPD

Term	Coef	SE Coef	T	P
Constant	56.353	0.8117	69.425	0.000
Foam Level	-3.079	1.1942	-2.578	0.012
Liquid Level	-5.680	1.6086	-3.531	0.001
Dig1Temp	2.104	1.0257	2.052	0.044

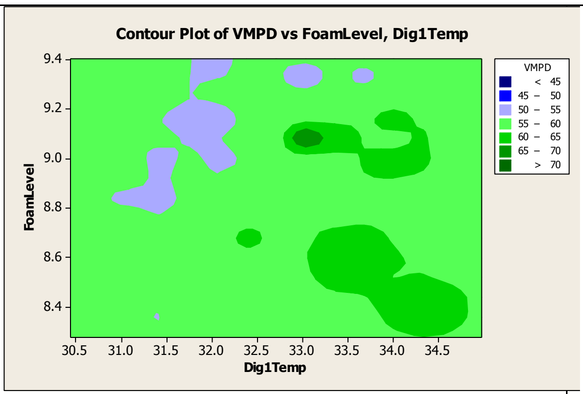
The final results from this analysis showed the factors that have statistical significance to VS were foam level, liquid level and temperature in the digester. These factors have P-value <0.05 and are shown in Table 7.5. P-value is an estimate of the probability that the results occurred by accident. That is there is lee than 5 % chance that the results were by chance. Temperature is expected to have significant effect on VS as high temperature may increase the VS destruction rate. Foam and liquid level significance is unexpected as there is no example of this scenario in literature. However foam level may give an indication of the characteristic of the sludge, such as level of surfactants, polymer usage etc. while the digester liquid level may give an indication of the amount of solids in the digester. This is essential as digester output flowrate signal is not available and % DS going into and out of the digester is measured offline. Therefore these findings may have some scientific backing.

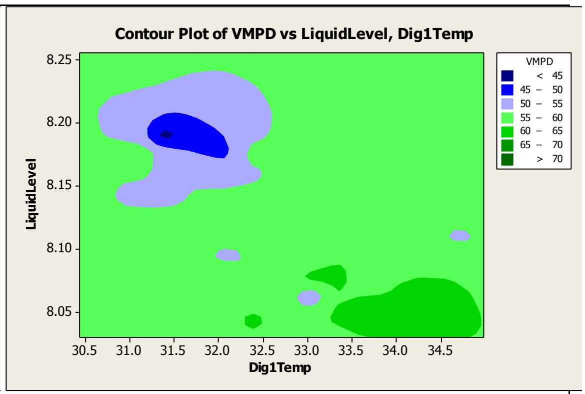
The response surface regression results for the Minitab model is shown Table 7.10. The P-values for liquid level has greater significance than digester temperature. There may be other parameters such % DS, pH, VS fed in that may have greater significance, but this results only reflect the characteristic of available online signals. These however generates very low R^2 values = 29.20 % R^2(pred) = 16.35 % R^2(adj) = 25.83 % and this may be yet again a result of limited available online data. Thus the low predictive characteristic of the model can be inferred as although these factors have significant effect on VS, the models generated are not as robust.

Table 7.5 Estimated regression coefficients

Term	Coef
Constant	459.138
Foam Level	-5.40100
Liquid Level	-47.3333
Dig1Temp	0.925014

The standard error of regression (S) has value of 4.12750. This gives an indication of the level of prediction of the response value to the equation; the lower the value the better the prediction. The estimated regression coefficients for VS are given in Table 7.6. This is the equation for calculating VS from the factors of foam level, liquid level and digester temperature.





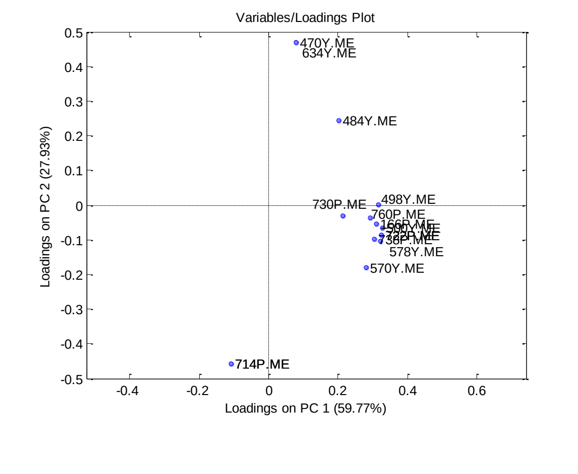
A	B

Figure 7.9 Contour Plots for VS against Foam Level, Liquid Level and Digester Temperature

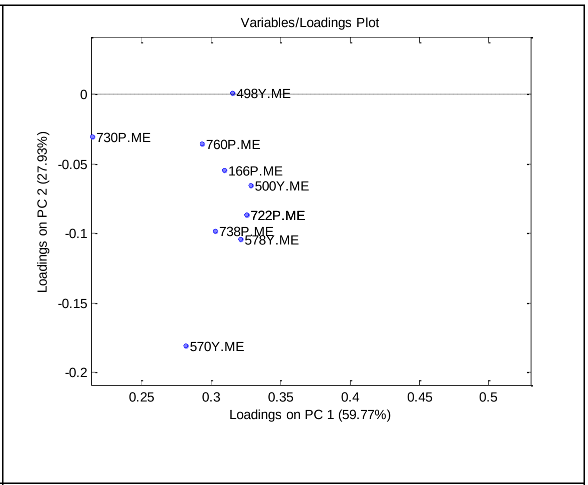
The contour plots depicted in Figure 7.9 shows that from the design high levels of foam and liquid level is required to obtain low VS levels at low temperatures. High liquid levels may mean that the level of solids may be low in the digester and therefore lower VS. This may be the reason for the strong statistical significance. Correlation with foam level is not so strong. From the contour plots in Figure 7.9, there is not a clear best operating domain by which the 3 factors of temperature, foam and liquid level can be operated to ensure low VS and therefore high gas production etc. From Figure 7.9a, low VS level at most is associated with low temperatures, although temperature spread is quite wide and high foam levels. The rise in foam level may be due to increase VS destruction rate and therefore increase in reaction increase may constitute high foam level and therefore low VS output. From plot B, low temperature effects on VS are more visible and correspond with high liquid levels. In theoretical sense and therefore the hypothesis expect high temperatures to correspond with low VS rather than low temperatures. For these reasons, along with the weak predictive model generated, the model has little scientific and process knowledge justification and therefore deem unsuitable.

PCA was used here to establish the relationships between the data and samples or identifying patterns within the data as shown in the 6 diagrams in Figure 7.10. The final zoomed in plots in figure 13E and 13F reveal that feed rate, temperature and gas produced show to be similar, closely grouped with VS and therefore related to the VS.

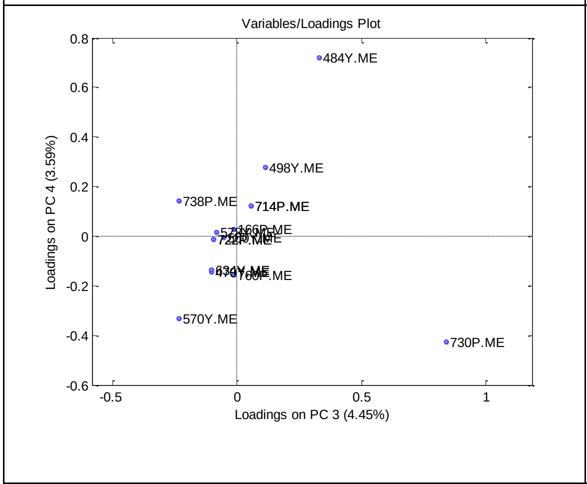
7.4.4 Principal component analysis



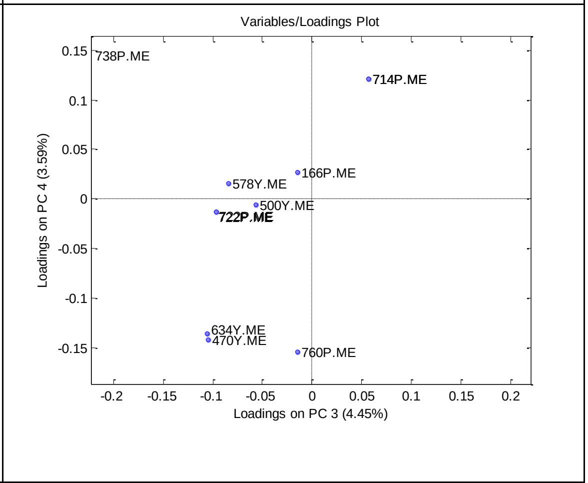
PC1:PC2 plot



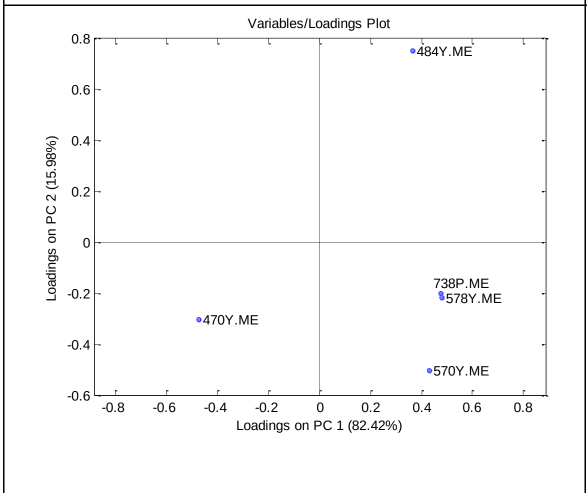
B: zoomed in view



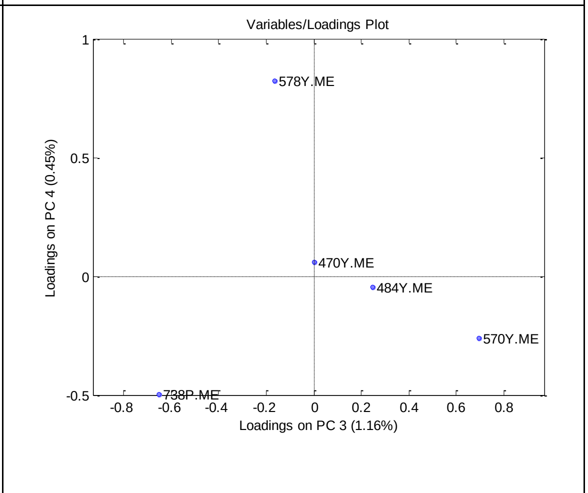
C:PCe:PC4 plot



D: Zoomed in PC3:PC4 plot



E: PC1:PC2 Final



F: final PC3:PC4 plot

Figure 7.10 PCA results of available signals

7.4.5 Estimator modelling in PerceptiveAPC solution

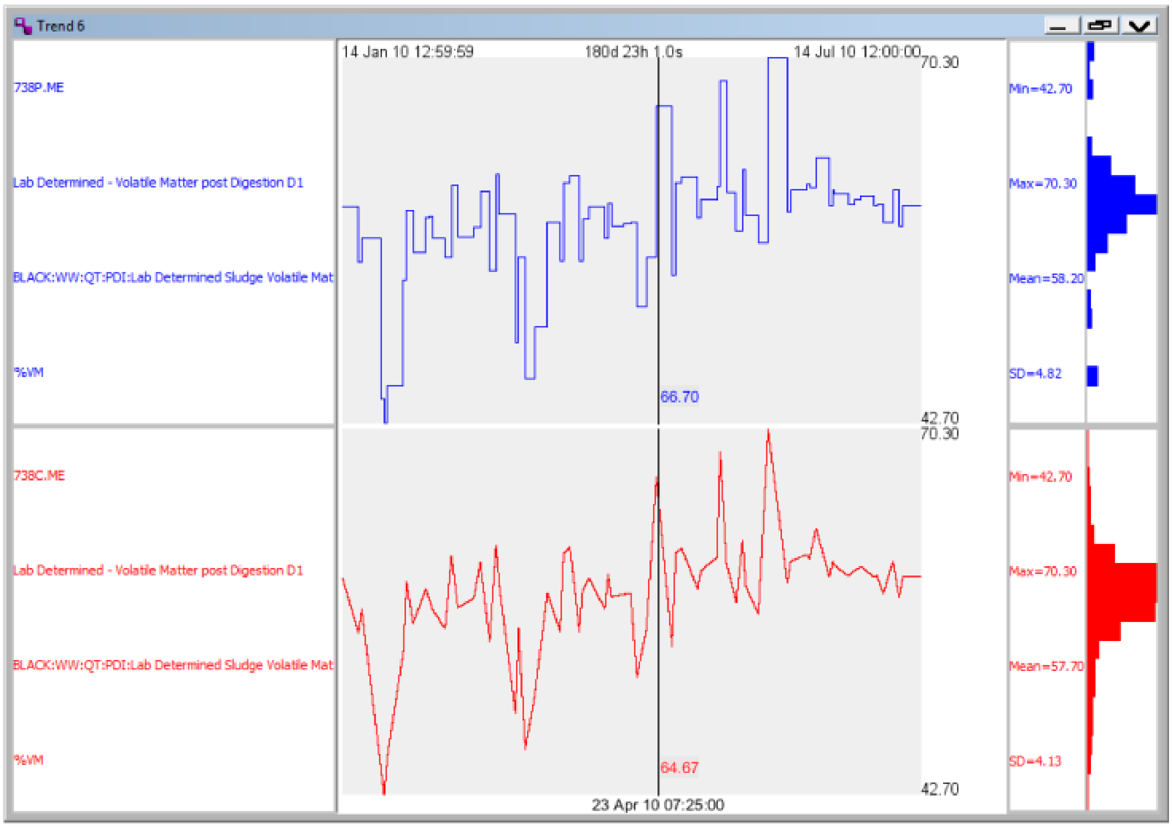


Figure 7.11 Actual and pre-processed VS signal

Figure 7.11 shows actual VS signal in blue and pre-processed signal in red. Due to low number of samples and the VS values being held until a new sample value is available, peak position filtering was conducted on the data. This gives the best approach of filling in the gaps in sampling. About 50 samples over the whole 6 months of data collected compared to over 17280 for online data. Offline samples are extracted 2-3 times per week from multiple points of sampling. Sample amount for analysis varies with focus only in the loss of weight as the difference between the initial sample weight and final weight after testing. Quality control of the analysis procedure is difficult to determine as there is no documentation of re-training, or management system in place to ensure all tests are carried out in similar manner. The values generated from the offline tests are entered into the PI historian system; there is a chance of possible errors on inserting the data back in the data historian. All analysis conducted are also subject to operator variation, for these various reasons, the accuracy, precision and significance of the offline VS data is difficult to determine. The data however covers a wide range of values; with minimum and maximum value of 42.70 and 70.30 respectively, these give acceptable VS and unacceptable VS results as per the PAS110.

Table 7.7 give the results for correlation analysis conducted in Matlab (Mathsworks, 2012). These values are very low and fail to provide quantify significant relationship between the factors of feed rate, feed VS, temperature, pH and gas produced. With such low correlation value, a weak predictive model will inevitable be resulted from these value. The signs (±) of the correlation values fail to make scientific sense. Theoretically as the feed rate increases, digestate VS should increases and therefore yield a strong positive correlation as the sludge spends less time in the digester and thus lower degradation process generated. However a weak negative correlation is observed. High temperatures are expected to increase the degradation process and therefore more organics are broken down, thus low VS resulting. Giving a strong negative correlation instead of the weak positive correlation observed. This infers that as you increase the temperature, VS values increases. Although this confirms the results from the Minitab study, there is no scientific justification for it. This is also true for the gas production effect on VS. As VS decreases, inferring that there is high degradation rate, this should result in high gas production. Unexpectedly a positive correlation is observed where a strong negative is presumed.

Table 7.6 Blackburn digestate VS correlation values

Digestate VS correlation values	Feed rate	Feed VS	Temperature	pH	Gas produced
Blackburn process data	-0.2839	0.2884	0.4096	0.3247	-0.1663

Figure 7.12 shows the loading plot after shifting VS data for 1 day to correspond with feed rate and temperature effects. 738X.ME is VS. Feed rate (484X.ME) positively correlates with VS and Temperature (578X.ME) negatively correlates with VS. This pre-processing helps to obtain the expected signage of correlation and higher correlation values. Provided the dynamics in the system observed is correct and thus justification for shifting the online data forward one day, then this shift in data may result in a better predictive model which makes scientific sense to some degree.

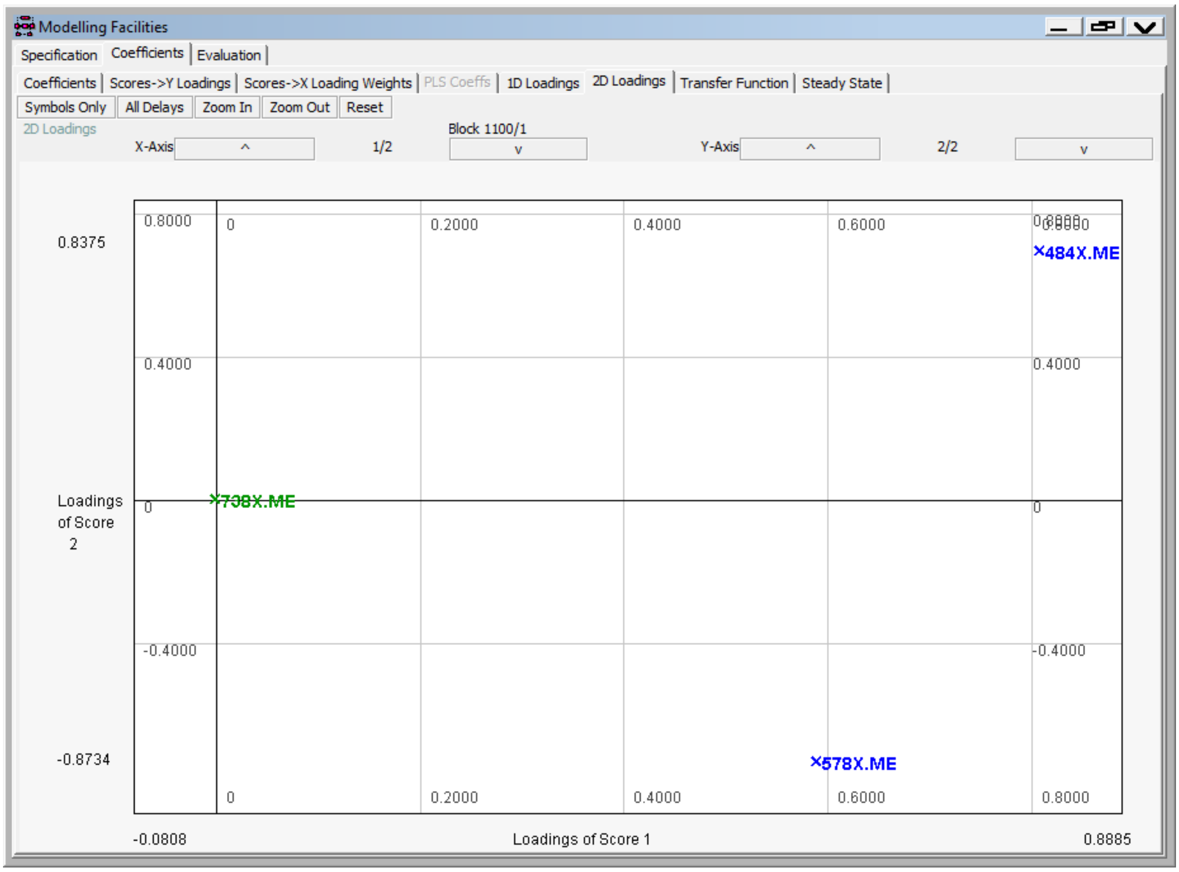


Figure 7.12 Loading plot of Blackburn process model

As the correlation analysis fail to identify factors that have significant relationship with VS, temperature and feed rate were selected to build a model in PerceptiveAPC (*Perceptive Engineering Ltd*, 2012). Figure 7.13 give the results for model errors obtained for the final VS model using Blackburn data. The lowest model prediction errors, within a range of about 10 % VS is shown. This is quite considerable as the range of VS data used is between 51-68 % of about 17 % range. There errors are too high to justify a robust predictive model and therefore the BSM2 simulation will be use further to see if a predictive model can be conducted for VS.

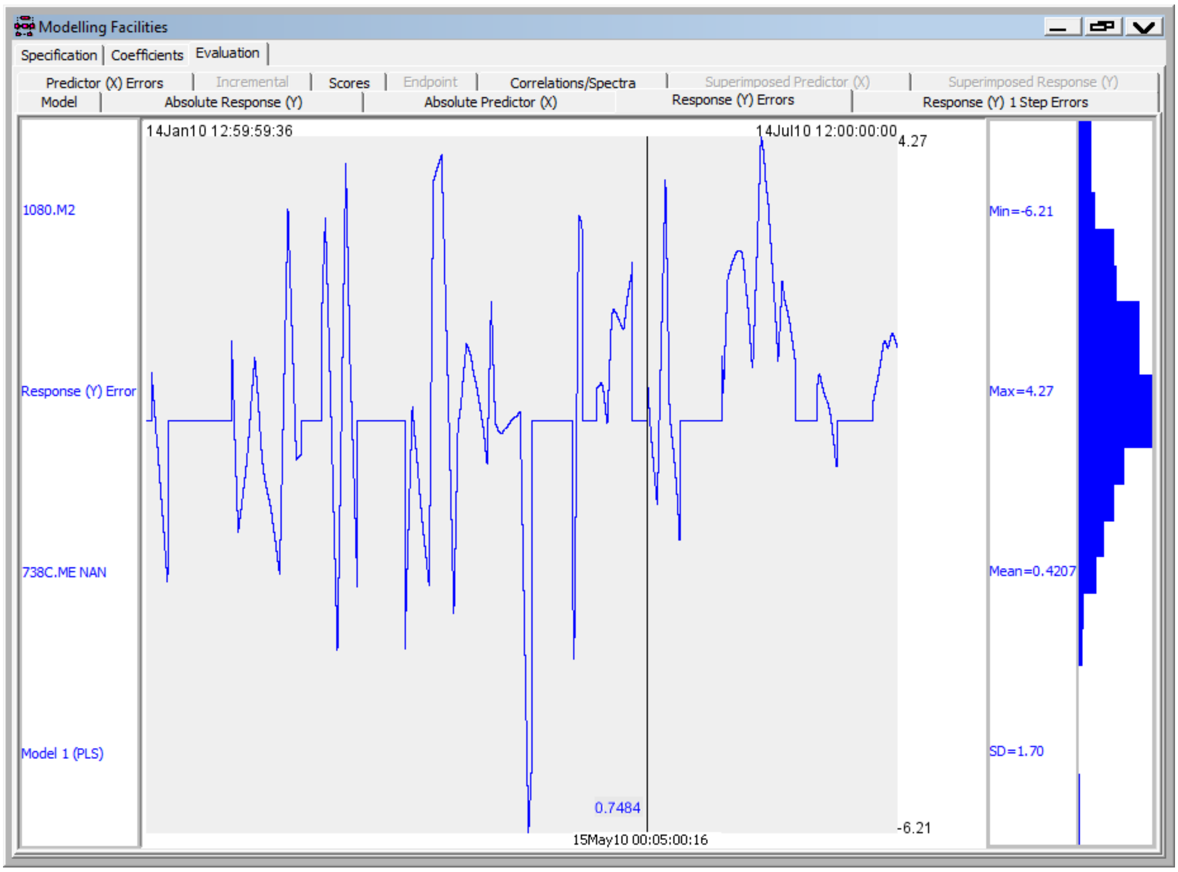


Figure 7.13 Final process model errors

7.5 Volatile solids soft sensor development in ADMI

Benchmark systems are popular for the assessment of process performance i.e. biogas yield, control system evaluation and comparison of similar purposes are common in defining the best possible approach to take before implementation for cost reduction. A wastewater treatment plant (WwTP) should be considered as a single completely integrated system. This would enable primary and secondary clarification units, activated sludge reactors, anaerobic digesters, thickeners, dewatering systems and other sub-processes to be combined, operated and controlled by local and supervisory control systems taking into account he interactions between the processes (Henze *et al.*, 2008).

The European cooperation in science and technology (COST) Action 682 and 624 which ended in 2004 was set up with the aim of developing benchmark tools for simulation based evaluation of control strategies for activated sludge plants. This work is now continued under the framework of the IWA Task Group on Benchmarking of Control Strategies for WwTPs. Together the group have developed:

- Benchmark simulation model no.1 (BSM1) is based on an activated sludge process (Alex *et al.*, 2008b) is based on the activated sludge model no.1 (ASM1) (Jeppsson, 1996);
- ADM1 model (Batstone *et al.*, 2002b) is deemed adequate for predictions with enough accuracy to be useful in process development, optimisation, and control. It is a standard benchmark for developing operational strategies and evaluating controllers;
- Benchmark simulation model no. 2 (BSM2) combines BSM1 and ADM1 (Alex *et al.*, 2008a).

These models are used by over 50 groups worldwide with over 100 publications at international conferences, journals and several PhD theses relating to the benchmark models. The BSM1 and BSM2 simulation environments define plant layout, influent loads, test procedures and evaluation criteria.

BSM2 is a detailed procedure for implementing, analysing and evaluating the impact and performance for existing and novel control strategies applied to wastewater treatment plants (WwTPs). The protocol includes a completely generalised WwTP model that is suitable for a benchmarking procedure and evaluation criteria. The system includes the IWA ADM1 with several modifications (Rosen *et al.*, 2006). Through its integration biological transformations, liquid-gas transfers, and gas production are feasible. The model includes slow and fast dynamics; the range of time constants in ADM1 is large (from seconds to months) and therefore constitutes a stiff system. Stiff solvers are implemented for pH and the dynamic state variable characteristic for hydrogen (Sh2) for speed enhancement by a factor of 100. Model interfaces are included to combining ASM1 and ADM1. ADM1 section of the BSM2 is used to study the effects of VS. This is possible because the solids going into the digester can be controlled and more importantly their composition can be changed and effects studied.

Mathematical models of the digestion process generally aim to achieve the following:

- Calculate estimates of the reactor volume, biogas production and its compositions, and to estimate the retention time to determine the performance of a specific system;
- Allow sensitivity analysis to be conducted for various process parameters;

- The cross-checking of simulation study results with actual plant performance gives added knowledge about the model, and can identify gaps in the predictive capability of the model;
- Use in whole plant optimisation studies, as they can predict how the digestion process is affected by upstream processes, and how the digestion process can impact on downstream processes (Appels *et al.*, 2008).

The ADM1 model is used here to compare and cross-check the result of the process data VS model. As ADM1 is entirely theoretical, theoretical assessment of the process model can be achieved.

7.5.1 Parameter evaluation in ADM1

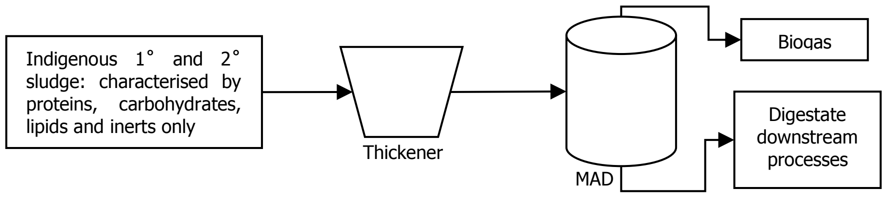


Figure 7.14 Schematic of the simulation process

The schematic for the simulation process is shown in Figure 7.14. ADM1 is composed of many several key measurement parameters such as VFA's and sludge composition. However there are several limitations within the model, such as:

- Sludge characterized by proteins, carbohydrates and lipids only. This over simplifies actual sludge characteristics;
- Temperature effects considered for physiochemical parameters but not for the biochemical reactions, temperature effects are not fully modelled;
- Temperature cannot be varied within the simulation but able to conduct single runs at different temperature settings between 0-60˚C;

Over simplification of the model and lack of temperature dependence means the model greatly defers from actual AD processes. The complexities and nonlinearities within AD processes are a mainly impacted by the feed composition and environmental factors of temperature. ADM1 however offer several opportunities to include:

- The organic compounds and inerts make-up the total solids. Therefore able to add VS signal as a % of the organic compounds and the inert;

- Opportunity to monitor VFA accumulation;
- Opportunity to explore gas composition effects on changes to feed and VS.

With these opportunities, step tests can be conducted to generate data for modelling the VS. although there are more key signals available in the simulation such as gas composition and measure of the various VFA's these are not available in the process data and therefore, for model 'like for like' comparisons, these useful variables were eliminated from the model. Thus an alternative model investigating the various parameters available for modelling will be conducted to illustrate if with improve in measurement; a better model can be generated with more variables.

$$TSS = 0.75(X_S + X_I + X_{B,H} + X_{B,A} + X_P$$

Where X_S is the slowly biodegradable substrate, X_I is particulate inert organic matter, $X_{B,H}$ as active heterotrophic biomass, $X_{B,A}$ as active autotrophic biomass and X_P as particulate products arising from biomass decay. These are the components measured in the ASM1 domain to constitute solids going into the digester.

Table 7.7 COD Equivalent of polymer

Polymer	Equivalent to COD
1g carbohydrates	1.07g COD
1g lipid	2.91g COD
1g protein	1.5g COD

The digester interface has these parameters converted to 3 main organic forms of proteins, carbohydrates and lipids which make up the level of volatile solids measured in kg COD m^{3-1}. The chemical oxygen demand (COD) is the amount of oxygen required to oxidise the organic carbon completely to CO_2 and water. COD contains both biodegradable and non-biodegradable solids. COD measurements were converted into VS through the following estimations for the simulation as shown in Table 7.8.

Table 7.8 Percentage of organic constituents in primary and secondary sludge (Horan, 2009)

	Primary	secondary
Proteins (%)	60	70
Lipids (%)	25	20
Carbohydrates (%)	15	10

Protein comprises the largest fraction of wastewater organic material, and as such, its destruction is intimately linked to desirable increases in volatile solids destruction. Typical protein content in wastewater sludge is given in Table 7.8 along with average value for lipids and carbohydrates.

Initial system evaluation of ADM1 was conducted and findings were:

- % VS in post digestion sludge may be higher in primary sludge than in secondary sludge;
- Temperature effects gas production and pH considerably. While its effect on VS is less effective;
- Temperature effects on biogas production is greatest at high temperature (above 35˚C) than lower temperatures (below 30˚C);
- VFA accumulation effects greatest between 25-40˚C;
- Feed rate and biogas production have higher effect on VS_out than VS_in and temperature;
- Correlation of VS_out with temperature is very low and can be deemed insignificant;
- Modelling of feed rate and gas production yields good prediction of VS_out, however the same is not observed using Blackburn data. This is possibly due to the sampling regime for VS_out at Blackburn and therefore better sampling may

provide data that can effectively illustrate the correlation of gas production and feed rate on VS_out.

Step Testing

Step tests were carried out to test the system dynamics within BSM2. Some of these results are depicted in Figure 7.15. There are mainly 4 signals going into the digester of mainly the organic matter and inert. The total organic matter going into the digester is assumed to undergo full disintegration with low residues. Therefore the volatile solids are assumed to be the three polymers of carbohydrates, lipids and proteins. The polymers plus the inert give the total solids going into the digester.

Table 7.9 Correlations analysis results for variables in ADM1

VS_out	Feed rate	VS_in	Temperature	pH	Gas produced
1.0000	0.8945	0.7054	-0.0964	-0.4127	0.9306
1.0000	0.9440	0.7380	-0.0829	-0.4419	0.9713

Correlation coefficients of VS out against the 5 components selected and results are shown in Table 7.9. First row for all data and second row data shows data for when the process is in a stable state. As can be seen feed rate, VS_in, and gas produced all form strong positive correlation with VS_out, while temperature and pH form weak negative correlations with VS_out. The weak negative correlation with temperature is a significant finding, as it demonstrates that initial assumption of VS_out being mostly affected by the retention time and temperature mainly does not hold. And therefore VS may be affected greatest by the feed rate, gas produced and the characteristic of the incoming sludge i.e. the VS in. As feed rate and gas produced measurements are easily available, makes these variables ideal for soft sensor model for VS_out. Correlation coefficients values for gas flow and feed rate with VS_out:

Gas flow and feed rate both yields weak negative correlation with VS_out; this is the opposite of what is observed in BSM2 where a strong positive correlation is observed;

This illustrates the weakness in the process data as it deviates strongly from what is expected; however in theory VS_out should decrease with increasing gas production and therefore the negative correlation is expected, but the value of the correlation is very weak and therefore deemed insignificant to yield and accurate or reliable model.

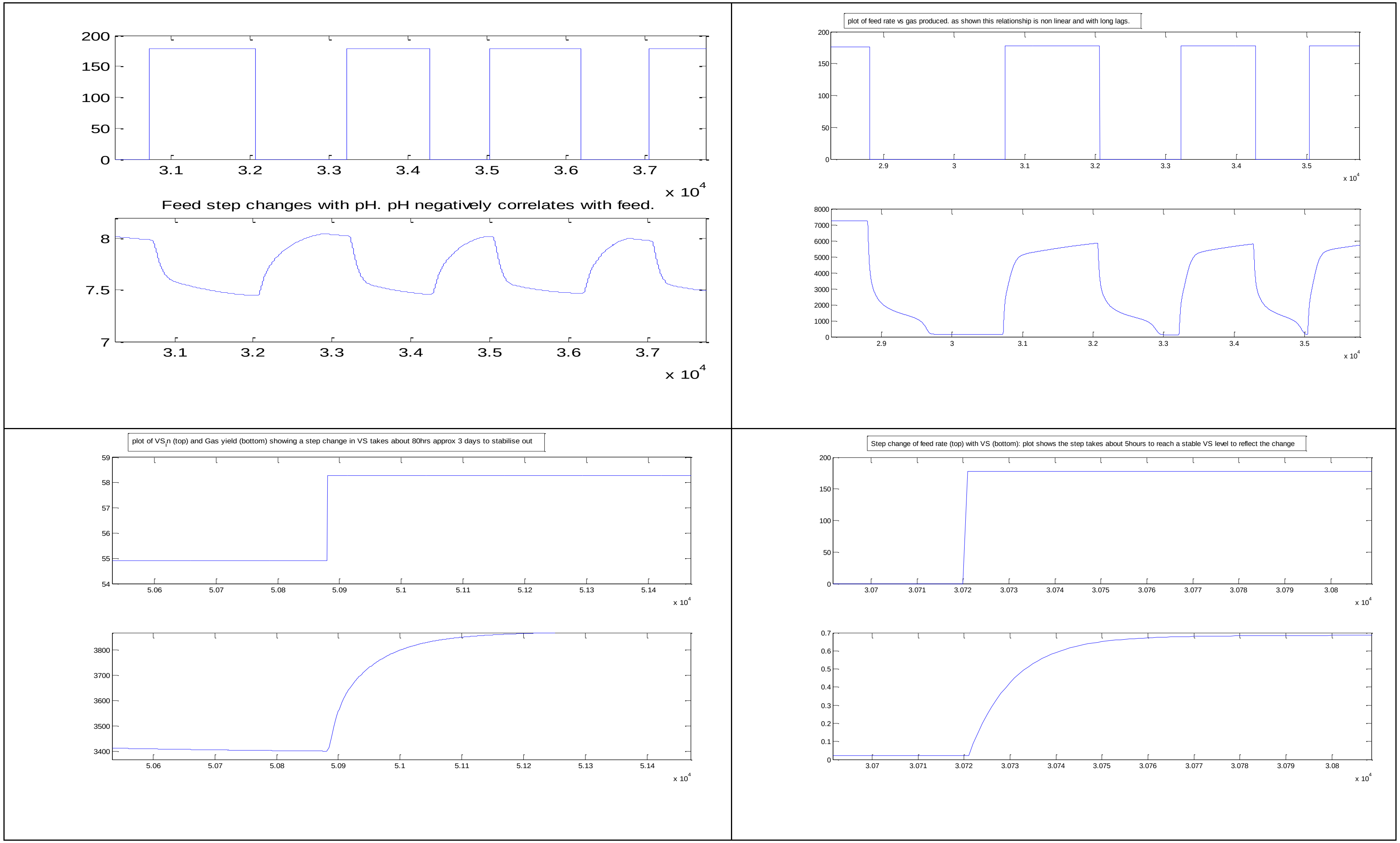


Figure 7.15 Step testing for model generation data

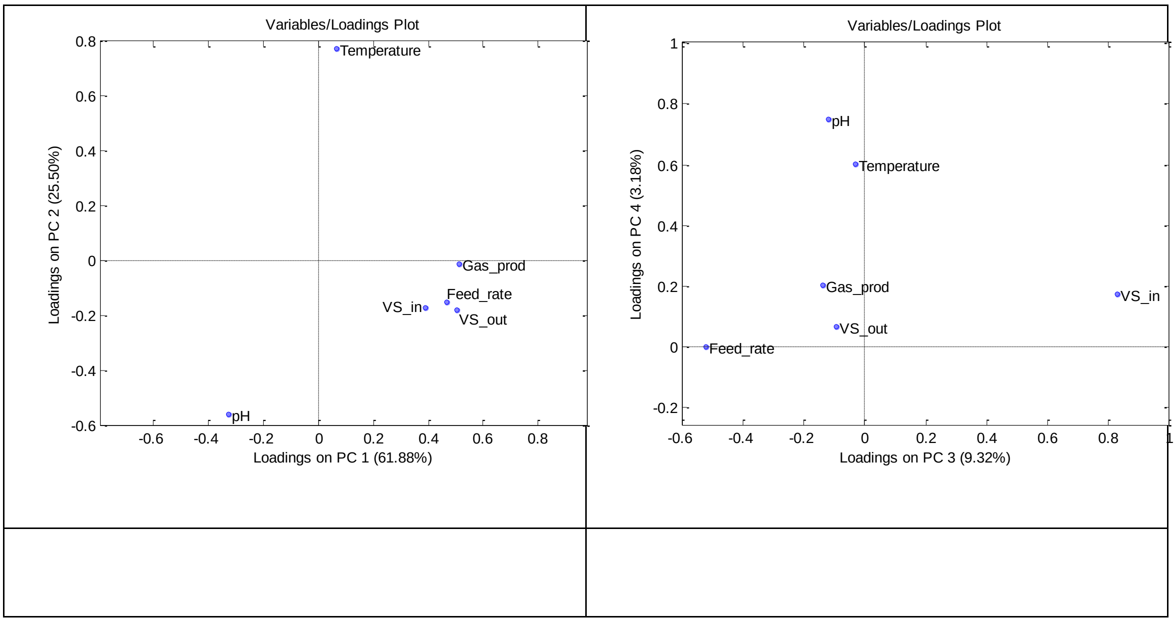


Figure 7.16 ADM1 PCA loadings plots

The PCA loadings plot of the simulated data in Figure 7.16 shows that gas produced rate and feed rate are similar to digestate VS. This is because on the loadings plot, variables 'sitting together', grouped closely infer similar behaviour between variable and thus maybe statically related. This analysis along with the correlation results indicates that a good predictive model can be generated for VS with feed and biogas flowrate alone. The benefits of selecting these two variables include:

- Feed flow and biogas flowrate measurements available online;
- Instrumentation for these are robust and readily available;
- Use off primary input (feed flow) and primary output variables;
- Feed flow is the main disturbance into the system and biogas flowrate a good monitoring parameter.

The structure of the final model is therefore depicted in Figure 7.17. However a successful model with feed and biogas flowrate alone will refute the understanding of the multivariate characteristic of the process. However the various model assumptions, over simplification of the process and the lack of temperature dependency inclusion in the model may simply linearize the model and thus the process and therefore reducing the multivariate characteristic of the process.

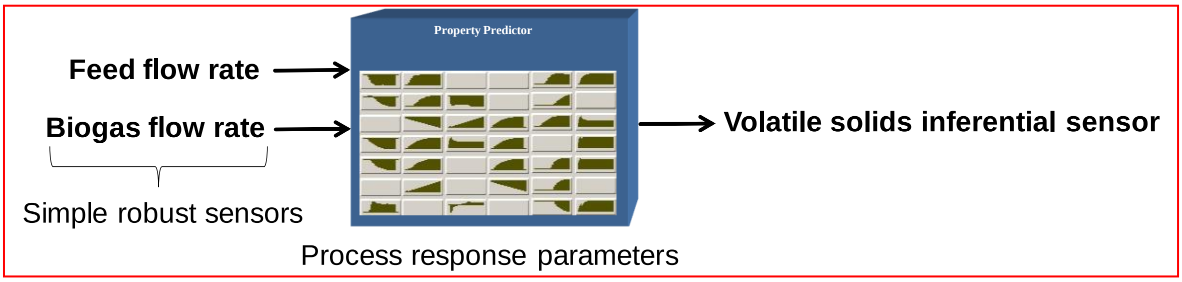


Figure 7.17 VS model

The results from the final model using feed and biogas flowrate to predictive VS is shown in Figure 7.18. The first depict the results for the model in red and model errors in blue. The model errors are very small and therefore a good predictive model is generated.

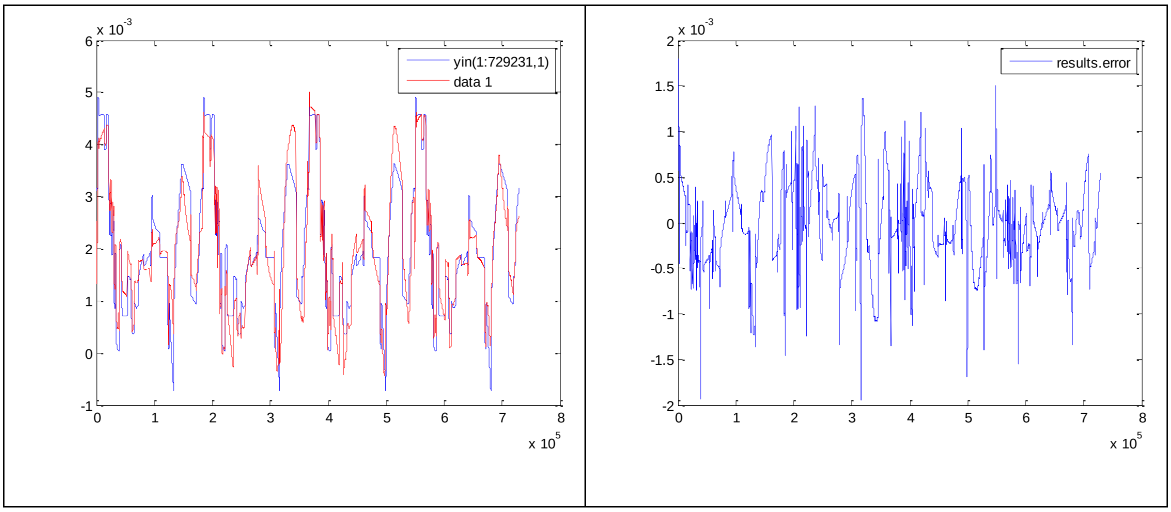


Figure 7.18 VS predictive model from ADM1 results

7.6 Conclusions

The correlations of the variables with digestate VS in the industrial data are all very low and not sufficient to yield a reliable process model. Gas flow and feed flowrate both display a weak negative correlation with digestate VS. This result illustrates the limitations of the process data as it deviates strongly from theory and the simulation study. The low correlations observed may be a result of disturbances in the process which are unmeasured and therefore not included in the model. This may include the feed composition for which there is no measure and the environmental conditions in the digester.

Utilizing the simulation data for the modelling of feed rate and gas production yields a good prediction of digestate VS, however the same is not observed using the process data. This is possibly due to the sampling regime at this site for digestate VS, sampled approximately 2-3 times per week. Better sampling may provide data that demonstrates a correlation between gas production and feed rate, and digestate VS. Analysis of the simulation data revealed that variations in concentrations of VS in the range of 30˚C and 35˚C are very low. In the industrial data, the temperature ranged between 29˚C to 36˚C, indicating that the range measured may be too limited to reveal the effects of temperature on VS.

There is very little studies on digestate and measure of stability with respect to VS. Initially analysis conducted confirms the digester environmental conditions of temperature, levels of liquid and foam have statistical significant effect on VS of digestate. The signals that may be better at characterising the digestate quality includes with respect to VS include online data for:

- % DS;
- Feed type or composition;
- pH;
- Retention time.

However these signals are not available online. The model may improve significantly provided there is possible online analysis for % DS and pH. The data available along with the ADM1 simulation environment give the following findings:

- Good prediction obtained with simulated data;
- The relationships of process variables illustrated with PCA, VS more similar to feed rate and gas production than temperature;
- Deviation of correlation in process data from theoretical expectation, possibly due to various unmeasured overshadowing effects;
- The complexity of the underlying non-linearity in the system evident.

The correlation analysis of variables with digestate VS in the industrial data are all very low and insufficient to yield a reliable process model. Gas flow and feed flowrate both display a weak negative correlation with digestate VS. This result illustrates the weakness in the process data available as it deviates strongly from theory and simulation. The low correlations observed may indicate disturbances in the process which are unmeasured and therefore not included in the model. This may include the feed composition for which there is no measure of and the environmental conditions in the digester.

Utilizing the simulation data in the modelling of feed rate and gas production yields a good prediction of digestate VS, however the same is not observed using the process data. This is possibly due to the sampling regime at this site for digestate VS, sampled approximately 2-3 times per week. Better sampling may provide data that demonstrates a correlation between gas production and feed rate, and digestate VS. Analysis of the simulation data revealed that variations in concentrations of VS in the range of 30˚C and 35˚C are very low. In the industrial data, the temperature ranged between 29˚C to 36˚C, indicating that the range measured may be too limited to reveal the effects of temperature on VS.

The process data in this case study was unable to produce a model suitable for the prediction of VS. The use of the BSM2 model however provided useful information on the dynamics of the anaerobic digestion process. The next stage of this study will use this knowledge to conduct a DoE study on the industrial process. The objective of this DoE study will be the generation of data that covers the wide-ranging dynamics of the system to help build an industrial VS soft sensor.

8 Conclusions

8.1 Introduction

This chapter concludes the thesis by returning to the research questions stated in Chapter 1:

Can an advanced control system improve the efficiency, stability and robustness of an AD process?, what is the minimum instrumentation requirement to achieve the aims identified in the feasibility assessment? and *what is the level of improvement to be gained from advanced control*?

Subsequently contributions and conclusions are summarised, followed by a perspective for future work.

8.2 Discussions

This thesis has encompassed a feasibility study into the use of MPC on industrial AD systems. This has included the benchmark study of four industrial processes, literature search and instrumentation review identifying minimum, essential and '*nice to have*' instrumentation, which formed the completion of phase I activities as set out in Figure 1.1.

The phase I activities aimed to address the first question "*Can an advanced control system improve the efficiency, stability and robustness of an AD process?*" The literature and instrumentation reviews identified the strengths, weaknesses opportunities and threats for an advanced control such as MPC on industrial AD systems. These findings along with the benchmark study formed the basis for the hypothesis that "*advanced control system can improve the efficiency, stability and robustness of an AD process".* The thesis then progressed to demonstrate how an advanced control system can improve the efficiency, stability and robustness of an AD process. The first step for demonstrating the hypothesis was to identify the minimum instrumentation required to for an MPC controller to fulfil the aims identified in the feasibility study. The instrumentation review and the benchmark study identified key instrumentation requirement. Parameters with readily unavailable instrumentation to monitor them online were investigated further through the development of inferential sensor models to predict parameters.

Chapter 7 investigated the VS soft sensor development activities respectively. This chapter concluded that although there were significant improvements to be made with regards to online instrumentation for industrial AD systems, soft sensor models offer possible solutions that negate the need for expensive and potentially problematic online measurements.

Following on from this the simulation study in Chapter 6 has shown the level of improvements that are to be made with MPC. Through the inventory simulation analysis, the hypothesis that significant improvements in the efficiency, stability and robustness of the AD process can be made with MPC was proven true. This was demonstrated at simulation level and not industrial scale. Therefore, it was deemed necessary that the findings from the simulation and soft sensor models underwent further investigation at industrial scale.

The industrial data used for the models in this thesis were not intended for MPC modelling and the data provided have several limitations. The data used were taken from systems where controllability and control model development approaches were not considered at the design stages. Failure to adequately consider controllability and control at the design stage means that any proposed control scheme is restricted by the design. The AD system is subject to considerable uncertainties and disturbances that affect the operating conditions and product qualities such as biogas and sludge composition. To help achieve optimum dynamic performances and economic profits, assessment of the performance with respect to controllability is required at the design phase (Ekawati and Bahri, 2003). Measurements such as separation of the different process phases for the digestion technology help improve the stability and controllability. This reduces the degree of non-linearity in the system yet there still remains an opportunity for improved control.

Although the inventory simulation demonstrated the level of improvements to be made with MPC, there still remained analysis of the potential improvements that could be made on real AD systems. The benchmark study data was shown to be insufficient for modelling the effect of MPC using industrial data and as such various data sets from different AD systems were analysed to test their usefulness for model development for soft sensors and or MPC. A case study was conducted to show the use of sludge composition data for VFA modelling. The case study focused on an analysis of data generated in the School of Civil Engineering and Geosciences, Newcastle University. The data relates to an experimental study of various feed compositions and includes an analysis of the microbial population which provided an insight into the effects of feed composition on the microbial and environmental conditions within a digester. The objective of this case study was to combine the use of multivariate techniques with the process knowledge developed through phase I and II activities and develop an inferential sensor for predicting molecular species population changes to infer stability of the AD process. A second case study was also conducted for the analysis of two datasets obtained from (1) a laboratory for the treatment of wastewater from the starch industry and (2) a pilot plant set-up for the treatment of waste water from the production of bioethanol. The datasets were obtained from the Leibniz University of Hanover at the Institute for Sanitary Engineering and Waste Management. The aim of this case study was to compare different experimental setups of varying feedstocks and use of the data for potential soft sensor or MPC models. A third case study was a comparison of two datasets from different reactor design systems treating the same waste. The reactors were the same size and are fed with same feedstock over a three month period. The objective of this case study was to investigate the impact of different reactor systems. These case studies combined the aims to investigate the impact of varying feedstocks, reactor systems and experimental set-ups to understand how these changes effect the dynamics within the AD process and where possible inferential sensor development was conducted with case study datasets. However due to the limited results obtained from these three case studies, they have not been included in the thesis.

8.3 Conclusion

In summary the main conclusions of this thesis are as follows:

1. MPC controller on a simulated AD system has yielded significant improvements for controlling inventory, yielding:

    - 40 % increase in biogas production can be achieved at 13 % lower average temperatures;
    - £179k a year of CHP energy savings can be achieved, equating to 33 % increase in CHP energy savings using MPC1. This could contribute to the cost of installing the controller with payback period of 6 months maximum;
    - A significant reduction in the number of trips with the optimiser of up to 92 % less trips in comparison with the 'no control' benchmark simulation system;
    - A reduced number in level of trips by separating the various dynamics in the simulation. MPC2 was shown to have 60 % and 63 % reduction in

level trips and % of time the trips occur respectively, whilst MPC1 was shown to have 38 % and 49 % reduction in level trips and % of time the trips occur respectively;

2. A volatile solids inferential sensor was developed yielding good prediction with simulated data;
3. A VFA inferential model is developed with pilot-scale data yielding a degree of prediction;
4. Benchmark analysis of three industrial AD processes has been conducted highlighting the key strengths, weaknesses, opportunities and threats of industrial AD systems
5. '*Minimum*', '*essential*' and '*nice to have*' instrumentation requirements for the AD process was identified.

The phase II activities of prototype development have yielded offline simulation (Chapter 6) and the development of a VS soft sensor (Chapter 7). The difference in results from Chapter 7 regarding the industrial and simulation data has demonstrated the importance of the need for better quality monitoring of the AD process. The process data in this case study was unable to produce a model suitable for the prediction of VS. The use of the BSM2 model however provided useful information on the dynamics of the AD process.

The activities carried out in this thesis has supported the development of ADvisorMV (Perceptiveapc.com, 2015), which is now part of the Perceptive Engineering suite of products.

Research activities from this thesis were conducted in 2011 and 2012 with publications in 2012 and 2013. There are several related publications in 2013 with projects looking into the use of MPC for the AD process. However these tend to focus on small scale systems (Lovett, 2013) and pilot-scale ADs (Haugen, 2014). This thesis is the first known collaborative project between three water companies, a University and a technology provider at industrial scale. Further collaborative research on the AD process should aim to include multidiscipline academics, industrialist to include technology and instrumentation providers.

8.4 Future work

The future work can be summarised as follows:

- Development of an initial DoE to apply step changes on key AD parameters on industrial scale systems to generate data which covers the dynamics present in the system. The objective of the DoE study would be the generation of data that covers the wide-ranging dynamics of the system to help build an industrial VS soft sensor. Increasing the data size for modelling is also essential as the process has long varying dynamics and therefore data that accounts for a long period of the process is essential. The DoE would require the minimum and essential AD instrumentation identified in Chapter 3 to generate the necessary data for modelling;
- Completion of the vendor review and questionnaire: although this has been attempted as part of phase 1 activities, the approach has been unsuccessful. There are now various AD focused networks and groups such as the BBSRC NIBB Anaerobic Digestion (AD) Network (Anaerobicdigestionnet.com, 2015) and these networks can be used as platforms to reach out to the AD community more effectively;
- Validation of the VS model and VFA models on industrial process: the DoE could potentially generate data robust enough to build improved VS and VFA models with industrial data. These models would then require validation on industrial process where the models can be trialled online;
- Development of the functional design specification: validation of the VS and VFA models would increase further understanding of the AD system to enable the final development of the AD-Master's functional design specification as part of the phase II activities set out in Figure 1.1;
- Installation and testing prototypes: completion of phase III activities and this will consists of testing the AD-Master prototype on an industrial process and would include further DoE to generate further data to enable full evaluation and market assessment of the system as phase IV activities.

These future activities were set out prior April 2013 during the period with industrial sponsor's involvement in the thesis. As such, a number of the future activities listed in Section 8.4 may have already taken place as Perceptive Engineering Ltd currently has AD controller product as part of their suit of products (Perceptiveapc.com, 2015).

9 Bibliography

Ahmad, M. and Benson, R. (1999) *Benchmarking in the process industries*. Institution of Chemical Engineers.

Alex, J., Benedetti, L., Copp, J., Gernaey, K. V., Jeppsson, U., Nopens, I., Pons, M. N., Rosen, C., Steyer, J.-P. and vanrolleghem, P. A. (2008a) *Benchmark Simulation Model no. 2 (BSM2)*.

Alex, J., Benedetti, L., Copp, J., Gernaey, K. V., Jeppsson, U., Nopens, I., Pons, M. N., Steyer, J.-P. and vanrolleghem, P. A. (2008b) *Benchmark Simulation Model no. 1 (BSM1)*.

Alturkmani, A. (2010) 'Industrial wastewater', p. 32 [Online]. Available at: www.4enveng.com.

Alvarez, R. and Lidén, G. (2008) 'The effect of temperature variation on biomethanation at high altitude', *Bioresource Technology*, 99(15), pp. 7278-7284.

Anaerobicdigestionnet.com (2015) *Welcome to BBSRC ADNetwork*. Available at: http://www.anaerobicdigestionnet.com/.

Andrews, J. F. (1974) 'Dynamic models and control strategies for wastewater treatment processes', *Water Research*, 8(5), pp. 261-289.

Andrews, J. F. and Graef, S. P. (1971) 'Dynamic modeling and simulation of the anaerobic digestion process', in R.F, G. (ed.) *Anaerobic Biological Treatment Processes*. Washington D.C: American chemical society, pp. 126-162.

Angelonidi, E. and Smith, S. R. (2014) *2nd International conference on Sustainable Solid waste Management*. Athens, Greece. Available at: http://www.athens2014.biowaste.gr/pdf/Angelonidi_Smith.pdf.

Appels, L., Baeyens, J., Degrève, J. and Dewil, R. (2008) 'Principles and potential of the anaerobic digestion of waste-activated sludge', *Progress in Energy and Combustion Science*, 34(6), pp. 755-781.

AppliTek (2009) 'AnaSense: Online monitoring of anaerobic digester and wastewater treatment', p. 8 [Online].

Arnold, M. and Kajolinna, T. (2010) 'Development of on-line measurement techniques for siloxanes and other trace compounds in biogas', *Waste Management*, 30(6), pp. 1011-1017.

Ashekuzzaman, S. M. and Poulsen, T. G. (2011) 'Optimizing feed composition for improved methane yield during anaerobic digestion of cow manure based waste mixtures', *Bioresource Technology*, 102(3), pp. 2213-2218.

Astals, S., Ariso, M., Galí, A. and Mata-Alvarez, J. (2011) 'Co-digestion of pig manure and glycerine: Experimental and modelling study', *Journal of Environmental Management*, 92(4), pp. 1091-1096.

Astals, S., Batstone, D. J., Mata-Alvarez, J. and Jensen, P. D. (2014) 'Identification of synergistic impacts during anaerobic co-digestion of organic wastes', *Bioresource Technology*, 169, pp. 421-427.

Astals, S., Musenze, R. S., Bai, X., Tannock, S., Tait, S., Pratt, S. and Jensen, P. D. (2015) 'Anaerobic co-digestion of pig manure and algae: impact of intracellular algal products recovery on co-digestion performance', *Bioresource Technology*, 181, pp. 97-104.

AzeoTech (2012) *DAQFactory* (Version 5) [Computer program]. AzeoTech Inc. Available at: http://www.azeotech.com/downloads.php.

Babaee, A. and Shayegan, J. (2011) 'Anaerobic Digestion of Vegetable Waste', *ICheaP - 10 The tenth International Conference on Chemical and Process Engineering*. Florence, Italy, 8/5/2011. http://www.aidic.it/icheap10/webpapers/207Babaee.pdf: ICheaP - 10. Available at: http://www.aidic.it/icheap10/webpapers/207Babaee.pdf.

Balsam, J. (2002) 'Anaerobic Digestion of Animal Wastes: Factors to Consider', ATTRA - National Sustainable Agriculture Information Service, p. 12 [Online]. Available at: http://www.bse.vt.edu/green/Documents/ATTRA_AD%20Considerations.pdf.

Barber, W. P. (2005a) 'THE EFFECTS OF IMPROVING SEWAGE SLUDGE DIGESTION', *Water and Environment Journal*, 19(3), p. 11.

Barber, W. P. (2005b) 'THE EFFECTS OF IMPROVING SEWAGE SLUDGE DIGESTION', *Water and Environment Journal*, 19(3), pp. 214-224.

Batstone, D. J., Keler, J., Angelidaki, I., Kalyuzhnyi, S. V., Pavlostathis, S. G., Rozzi, A., Sanders, W. T. M., Seigrist, H. and Vavilin, V. A. (2002a) *Anaerobic digestion model No.1 (ADM1)*. Cornwall: IWA publishing.

Batstone, D. J., Keler, J., Angelidaki, I., Kalyuzhnyi, S. V., Pavlostathis, S. G., Rozzi, A., Sanders, W. T. M., Seigrist, H. and Vavilin, V. A. (2002b) 'The IWA Anaerobic Digestion Model No 1 (ADM1) ', *IWA water science and technology*, 45(10), pp. 65-73.

Batstone, D. J., Keller, J. and Steyer, J. P. (2006) 'A review of ADM1 extensions, applications, and analysis: 2002-2005', *Water science and technology : a journal of the International Association on Water Pollution Research*, 54(4), pp. 1-10.

Batstone, D. J., Torrijos, M., Ruiz, C. and Schmidt, J. E. (2004) 'Use of an anaerobic sequencing batch reactor for parameter estimation in modelling of anaerobic digestion', *Water science and technology : a journal of the International Association on Water Pollution Research*, 50(10), pp. 295-303.

Beck, M. B. (1986) 'Identification, estimation and control of biological waste-water treatment processes', *Control Theory and Applications, IEE Proceedings D*, 133(5), pp. 254-264.

Ben-Gal, I. (2005) 'Outlier Detection', *Data Mining and Knowledge Discovery Handbook: A Complete Guide for Practitioners and Researchers*, p. 16 [Online]. Available at: http://www.eng.tau.ac.il/~bengal/outlier.pdf (Accessed: 02/11/2012).

Bernard, O. and Bastin, G. (2005a) 'Identification of reaction networks for bioprocesses: determination of a partially unknown pseudo-stoichiometric matrix', *Bioprocess and Biosystems Engineering*, 27, p. 9.

Bernard, O. and Bastin, G. (2005b) 'On the estimation of the pseudo-stoichiometric matrix for macroscopic mass balance modelling of biotechnology processes', *Mathematical Biosciences*, 193, p. 27.

Bernard, O., Chachuat, B., Helias, A., Le Dantec, B., Sialve, B., Steyer, J. P., Lardon, L., Neveu, P., Lambert, S., Gallop, J. and Dixon, M. (2004) *10th IWA world congress on Anaerobic Digestion (AD10)*. Montreal, Canada, 29 August-2 september 2004.

Bernard, O., Hadj-Sadok, Z., Dochain, D., Genovesi, A. and Steyer, J. P. (2001) 'Dynamical Model Development and Parameter Identification for an Anaerobic wastewater Treatment Process', *Biotechnology and Bioengineering*, 75(4), p. 15.

Boe, K., Batstone, D. J., Steyer, J.-P. and Angelidaki, I. (2010) 'State indicators for monitoring the anaerobic digestion process', *Water Research*, 44(20), pp. 5973-5980.

Booth, J. (2009) *Feasibility Study for a Central Anaerobic Digestion Plant in Aberdeenshire*. Ltd, S.

Boudreau, M. A. and McMillan, G. K. (2007) *New Directions In Bioprocess Modelling And Control: Maximising Process Analytical Technology Benefits*. ISA.

Bouvier, J. C., Steyer, J. P. and Delgenes, J. P. (2002) 'On-line titrimetric sensor for the control of VFA and/or alkalinity in anaerobic digestion processes treating industrial vinasses ', [Online].

Bowen, J. E., Dolfing, J., Devenport, J. R., Read, L. F. and Curtis, P. T. (2014) 'Low-temperature limitation of bioreactor sludge in anaerobic treatment of domestic wastewater', *Water Science & Technology*, 69(5), p. 1004.

Budiyono, Widiasa, I. N., Johari, S. and Sunarso (2010) 'The Influence of Total Solid Contents on Biogas Yield from Cattle Manure Using Rumen Fluid Inoculum', *Energy Research Journal*, 1(1), p. 6.

Buhr, H. O. and Andrews, J. F. (1977) 'The thermophilic anaerobic digestion process', *Water Research*, 11(2), pp. 129-143.

Cadena-Pereda, R. O., Rivera-Muñoz, E. M., Herrera-Ruiz, G., Gomez-Melendez, D. J. and Anaya-Rivera, E. K. (2012) 'Automatic carbon dioxide-methane gas sensor based on the solubility of gases in water', *Sensors (Basel, Switzerland)*, 12(8), pp. 10742-10758.

Callaghan, F. J., Wase, D. A. J., Thayanithy, K. and Forster, C. F. (1999) 'Co-digestion of waste organic solids: batch studies', *Bioresource Technology*, 67(2), pp. 117-122.

CAMBI (2011) 'CAMBI PLant Locations Worldwide', *Plant Locations*. Available at: http://www.cambi.no/wip4/location.epl?cat=10650 (Accessed: 20/05/2011).

Chae, K. J., Jang, A., Yim, S. K. and Kim, I. S. (2008) 'The effects of digestion temperature and temperature shock on the biogas yields from the mesophilic anaerobic digestion of swine manure', *Bioresource Technology*, 99(1), pp. 1-6.

Chambers, B., Hickman, G. and Aitken, M. (2001) 'The safe sludge matrix : Guidlines for the application of sewage sludge to agricultural land', p. 4 [Online].

Chen, Y., Cheng, J. J. and Creamer, K. S. (2008) 'Inhibition of anaerobic digestion process: A review', *Bioresource Technology*, 99(10), pp. 4044-4064.

Chéruy, A. (1997) 'Software sensors in bioprocess engineering', *Journal of Biotechnology*, 52(3), pp. 193-199.

Cioabla, A. E., Ionel, I., Dumitrel, G.-A. and Popescu, F. (2012) 'Comparative study on factors affecting anaerobic digestion of agricultural vegetal residues', *Biotechnology for Biofuels*, 5(39), Journal, p. 9 [Online]. Available at: http://www.biotechnologyforbiofuels.com/content/5/1/39.

Cleve, M. (2004) 'Least Squares', in The MathWorks, I. (ed.) *Numerical Computing with MATLAB*. the Society for Industrial and Applied Mathematics. Available at: http://www.mathworks.com/moler.

Climate Change Act (2011). Available at: http://www.theccc.org.uk/ (Accessed: 30/07/2011).

Cutler, C. R. and Perry, R. T. (1983) 'Real time optimization with multivariable control is required to maximize profits', *Computers & Chemical Engineering*, 7(5), pp. 663-667.

Dalmau, J., Comas, J., Rodríguez-Roda, I., Pagilla, K. and Steyer, J.-P. (2010) 'Model development and simulation for predicting risk of foaming in anaerobic digestion systems', *Bioresource Technology*, 101(12), pp. 4306-4314.

Davis, B., Hobson, J., Palfrey, R., Pitchers, R., Rumsby, P., Carlton-Smith, C. and Middleton, J. (2010) *Environmental, economic and social impacts of the use of sewage sludge on land*

Derbal, K., Bencheikh-lehocine, M., Cecchi, F., Meniai, A. H. and Pavan, P. (2009) 'Application of the IWA ADM1 model to simulate anaerobic co-digestion of organic waste with waste activated sludge in mesophilic condition', *Bioresource Technology*, 100(4), pp. 1539-1543.

Dimitry, G. (2005) 'Model Identification', *EE392m: Control Engineering in Industry*, p. 23 [Online]. Available at: www.stanford.edu/class/ee392m/.

Dochain, D. and Vanrolleghem, P. A. (2001) *Dynamical Modelling and Estimation in Wastewater Treatment Processes*. Cornwall, UK: IWA Publishing.

Donoso-Bravo, A., Mailier, J., Martin, C., Rodríguez, J., Aceves-Lara, C. A. and Wouwer, A. V. (2011) 'Model selection, identification and validation in anaerobic digestion: A review', *Water Research*, 45(17), pp. 5347-5364.

Ekawati, E. and Bahri, P. A. (2003) 'The integration of the output controllability index within the dynamic operability framework in process system design', *Journal of Process Control*, 13(8), pp. 717-727.

Ericksson, L., Johansson, E., Kettaneh-Wold, N., Trygg, J., Wikstrom, C. and Wold, S. (2006) *Multi- and Megavariate Data Analysis*. Umetrics Academy training in multivariate technology.

Feitkenhauer, H., von Sachs, J. and Meyer, U. (2002) 'On-line titration of volatile fatty acids for the process control of anaerobic digestion plants', *Water Research*, 36(1), pp. 212-218.

Foss, B. A., Lohmann, B. and Marquardt, W. (1998) 'A field study of the industrial modeling process', *Journal of Process Control*, 8(5–6), pp. 325-338.

García-Diéguez, C., Bernard, O. and Roca, E. (2013) 'Reducing the Anaerobic Digestion Model No.1 for its application to an industrial wastewater treatment plant treating winery effluent wastewater', *Bioresource Technology*, 132, p. 9.

García-Diéguez, C., Molina, F. and Roca, E. (2011) 'Multi-objective cascade controller for an anaerobic digester', *Process Biochemistry*, In Press, Corrected Proof.

'GIR5000 series - Biogas & Landfill analysers - Multiparameter analysers for biogas applications', (2016) *Technical datasheet*, p. 2, *mtl-inst.com/images/uploads/datasheets/GIR5000* [Online]. Available at: https://www.mtl-inst.com/images/uploads/datasheets/GIR5000.pdf (Accessed: 25 May 2016).

Gomez, X., Cuetos, M. J., Garcia, A. I. and Moran, A. (2005) 'Evaluation of digestate stability from anaerobic process by thermogravimetric analysis', *Thermochimica Acta*, 426(1-2), pp. 179-184.

Graef, S. P. and Andrews, J. F. (1974a) 'Stability and Control of Anaerobic Digestion', *Journal (Water Pollution Control Federation)*, 46(4), pp. 666-683.

Graef, S. P. and Andrews, J. F. (1974b) 'Stability and Control of Anaerobic Digestion', *water pollution control federation*, 46(4), pp. 666-683.

Guo, J., Peng, Y., Ni, B.-J. J., Han, X., Fan, L. and Yuan, Z. (2015) 'Dissecting microbial community structure and methane-producing pathways of a full-scale anaerobic reactor digesting activated sludge from wastewater treatment by metagenomic sequencing', *Microbial cell factories*, 14(1), p. 33.

Guwy, A. J., Hawkes, D. L. and Hawkes, F. R. (1995) 'On-line low flow high-precision gas metering systems', *Water Research*, 29(3), pp. 977-979.

Hampel, F. R. (1971) 'A general qualitative definition of robustness', *The Annals of Mathematical Statistics*, 42(6), pp. 1887-1896.

Hampel, F. R. (1974) 'The influence curve and its role in robust estimation', *Journal of the American Statistical Association*, 69(346), pp. 383-393.

Hassam, S., Cherki, B., Ficara, E. and Harmand, J. (2012) 'Towards A systematic approach to reduce complex bioprocess models - Application to the ADM1', *20th Mediterranean Conference on Control and Automation (MED)*. 573. IEEE, p. 6.

Haugen, F. A. (2014) *Optimal Design, Operation and Control of an Anaerobic Digestion Reactor*. Telemark University College [Online]. Available at: http://home.hit.no/~finnh/phd/thesis/phd_dissertation_finn_haugen.pdf.

Heinzle, E., Dunn, I. J. and Ryhiner, G. B. (1993) *Modeling and control for anaerobic wastewater treatment*. Springer.

Henze, M., Loosdrecht, M. C. M., Ekama, G. A. and Brdjanovic, D. (2008) *Biological Wastewater Treatment: Principles, Modelling and Design*. London: IWA publishing.

Hill, D. T. (1982) 'A Comprehensive Dynamic Model for Animal Waste Methanogenesis', *American Society of Agricultural and Biological Engineers*, 25(5), p. 7.

Hinken, L., Gasso, P. M., Weichgrebe, D. and Rosenwinkel, H. K. (2013) 'Implementation of Sulphate Reduction and Sulphide Inhibition in ADM1 for Modelling of a Pilot Plant Treating Bioethanol Wastewater', *AD13:13th World Congress on Anaerobic Digestion – Recovering (bio) Resources for the World*. Santiago de Compostela, Spain.

Holm-Nielsen, J. B., Al Seadi, T. and Oleskowicz-Popiel, P. (2009) 'The future of anaerobic digestion and biogas utilization', *Bioresource Technology*, 100(22), pp. 5478-5484.

Horan, N. J. (2009) *Anaerobic digestion training course*. Aqua Enviro.

Hotelling, H. (1933) 'Analysis of a complex of statistical variables into principal components', *J. Educ. Psych.*, 24.

Hse.gov.uk (2015) *ATEX and explosive atmospheres - Fire and explosion*. Available at: http://www.hse.gov.uk/fireandexplosion/atex.htm (Accessed: 15/05/2015).

Ince, O., Anderson, G. K. and Kasapgil, B. (1995) 'Control of organic loading rate using the specific methanogenic activity test during start-up of an anaerobic digestion system', *Water Research*, 29(1), pp. 349-355.

Ingildsen, P. (2002) *Realising Full-Scale Control in Wastewater Treatment Systems Using In Situ Nutrient Sensors*. Lund University [Online]. Available at: http://www.iea.lth.se/publications/Theses/LTH-IEA-1030.pdf.

Iso.org (2015) *ISO 15839:2003 - Water quality -- On-line sensors/analysing equipment for water -- Specifications and performance tests*. Available at: http://www.iso.org/iso/catalogue_detail.htm?csnumber=28740 (Accessed: 16/05/2015).

Jensen, P. D., Astals, S., Lu, Y., Devadas, M. and Batstone, D. J. (2014) 'Anaerobic codigestion of sewage sludge and glycerol, focusing on process kinetics, microbial dynamics and sludge dewaterability', *Water Research*, 67, pp. 355-366.

Jeppsson, U. (1996) *A General Description of the Activated Sludge Model No. 1 (ASM1)*. Lund institute of technology.

Jiang, J. and Zhang, Y. (2004) 'A revisit to block and recursive least squares for parameter estimation', *Computers & Electrical Engineering*, 30(5), pp. 403-416.

Jolliffe, I. T. (2002) *Principal Component Analysis*. second edn. New York: Springer.

Jolliffe, I. T. (2005) 'Principal Component Analysis' *Encyclopedia of Statistics in Behavioral Science*. John Wiley & Sons, Ltd.

Kadlec, P. (2009) *On robust and adaptive soft sensors*. University of Bournmouth.

Kanokwan, B., Damien John, B. and Irini, A. (2007) 'An innovative online VFA monitoring system for the anerobic process, based on headspace gas chromatography', *Biotechnology and Bioengineering*, 96(4), pp. 712-721.

Karray, R., Hamza, M. and Sayadi, S. (2015) 'Evaluation of ultrasonic, acid, thermo-alkaline and enzymatic pre-treatments on anaerobic digestion of Ulva rigida for biogas production', *Bioresource Technology*, 187, pp. 205-213.

Kowalski, R., Gerlach, R. and Wold, H. (1982) 'Chemical Systems under Indirect Observation', in Joreskog, K. and Wold, H. (eds.) *Systems under indirect observations*. Amsterdam, pp. 191-209.

Kugelman, I. J. and McCarty, P. L. (1965) 'Cation Toxicity and Stimulation in Anaerobic Waste Treatment', *Water pollution control federation*, 37(1), p. 21.

Lehtomäki, A., Huttunen, S. and Rintala, J. A. (2007) 'Laboratory investigations on co-digestion of energy crops and crop residues with cow manure for methane production: Effect of crop to manure ratio', *Resources, Conservation and Recycling*, 51(3), pp. 591-609.

Lennart, L. (1999) *System Identification Theory for the User*. Second edn. United States of America: Prentice Hall.

Level, flow, pressure, temperature measurement | Endress+Hauser (2016) 'Uk.endress.com. (2016). Level, flow, pressure, temperature measurement | Endress+Hauser. '. Available at: http://www.uk.endress.com/en [(Accessed: 25 May 2016).

Li, L., He, Q., Ma, Y., Wang, X. and Peng, X. (2015) 'Dynamics of microbial community in a mesophilic anaerobic digester treating food waste: Relationship between community structure and process stability', *Bioresource Technology*, 189, pp. 113-120.

Lidholm, O. and Ossiansson, E. (2008) *Modeling Anaerobic Digestion -Validation and calibration of the Siegrist model with uncertainty and sensitivity analysis*. Lunds Universitet.

Liu, J., Olsson, G. and Mattiasson, B. (2004) 'On-line monitoring of a two-stage anaerobic digestion process using a BOD analyzer', *Journal of Biotechnology*, 109(3), pp. 263-275.

Lokshina, L., Vavilin, V. A., Kettunen, H., Rintala, J. A., Holliger, C. and Nozhevnikova, A. (2001) 'Evaluation of Kinetic coefficients using integrated Monod and Haldane Models for low temperature acetoclastic methanogenesis', *Water Research*, 35(12), p. 10.

Lovett, D. (2013) 'Optimisation of small-scale AD – a computerised control system', p. 30 [Online]. Available at: http://www.wrap.org.uk/sites/files/wrap/Perceptive%20Engineering%20-%20DIAD%202%20feasibility%20study.pdf.

Lyberatos, G. and Skiadas, I. V. (1999) 'Modelling of anaerobic digestion - a review', *Global Nest*, 1(2), pp. 63-76.

Madsen, M., Holm-Nielsen, J. B. and Esbensen, K. H. (2011) 'Monitoring of anaerobic digestion processes: A review perspective', *Renewable and Sustainable Energy Reviews*, 15(6), pp. 3141-3155.

Mairet, F., Bernard, O., Ras, M., Lardon, L. and steyer, J. P. (2011) 'Testing the ability of ADM1 to represent the anaerobic digestion of microalgae', *8th IWA Symposium on Systems Analysis and Integrated Assessment*. Watermatex 2011, p. 8. Available at: http://www.prodinra.inra.fr/prodinra/pinra/data/2011/06/PROD2011d7235293_20110628044829675.pdf.

Marsh, G. (2008) 'Rise of the Anaerobic Digester', *Renewable Energy Focus*, 9(6), pp. 28-30, 32, 34.

Martin, E. B. (2010) *Principal Component Analysis*. Lecture notes. Newcastle University.

Mathsworks (2012) *MATLAB* [Computer program]. Mathsworks. Available at: http://www.mathworks.co.uk/products/matlab/.

Mendez-Acosta, H. O., Palacios-Ruiz, B., Alcaraz-Gonzalez, V., Gonzalez-Alvarez, V. and Garcia-Sandoval, J. P. (2010) 'A robust control scheme to improve the stability of anaerobic digestion processes', *Journal of Process Control*, 20(4), pp. 375-383.

Microsoft-cooporation (2006) *Minitab 15* [Computer program]. Minitab Ltd. Available at: http://www.minitab.com/en-GB/company/contact-us/default.aspx.

Moen, G., Stensel, H. D., Lepistö, R. and Ferguson, J. F. (2003) 'Effect of Solids Retention Time on the Performance of Thermophilic and Mesophilic Digestion of Combined Municipal Wastewater Sludges', *Water Environment Research*, 75(6), pp. 539-548.

Moletta, R. (1998) 'Anaerobic Digestion Monitoring and Control', p. 8 [Online]. Available at: http://rene.moletta.perso.sfr.fr/articles/commande/commande%20automatique%2098.pdf (Accessed: 22/02/2011).

Molina, F., Ruiz, G., Roca, E. and Lema, J. M. (2004) 'Report on full-scale performance of the sensors within TELEMAC', *Deliverable 2.7*, p. 30 [Online]. Available at: http://www.ercim.eu/telemac/del/D2.7_Public.pdf (Accessed: 20/01/2011).

Monnet, F. (2003) *An Introduction to Anaerobic Digestion of Organic Wastes*. Scotland, R. [Online]. Available at:

http://www.biogasmax.co.uk/media/introanaerobicdigestion__073323000_1011_24042007.pdf.

Monsal (2011) 'monsal Advanced Digestion technology', *Advanced Digestion*. Available at: http://www.monsal.com/Biowaste/Advanced_Digestion.asp (Accessed: 22/06/2011).

Montgomery, D. C. (2005) *Introduction to Statistical Quality Control*. 5 edn. New York: John wiley and sons, Inc.

Noone, G. P. (2006) 'A Review of Mesophilic Anaerobic Digestion Technology and the Drivers for Process Changes', *Aqua Enviro Advances in Technology for the anaerobic digestion of municipal sludge*, p. 12 [Online]. Available at: http://www.monsal.com/Documents/Microsoft%20Word%20-%20Technical%20Paper%20-%20No%2038%20PDF.pdf (Accessed: 22/06/2011).

Nounou, M. N. and Nounou, H. N. (2007) 'Improving the prediction and parsimony of ARX models using multiscale estimation', *Applied Soft Computing*, 7(3), pp. 711-721.

Nova analytical systems, i. (2010) 'Nova analytical inc catalog', *Continuous Process Methane Gas Analyzer by Infrared Detector - 470 Series*. Available at: http://catalog.nova-gas.com/viewitems/inuous-methane-analyzers-continuous-ch4-analyzers-/thane-gas-analyzer-by-infrared-detector-470-series (Accessed: 20/02/2011).

O'Brien, M., Mack, J., Lennox, B., Lovett, D. and Wall, A. (2011) 'Model predictive control of an activated sludge process: A case study', *Control Engineering Practice*, 19(1), pp. 54-61.

ofgem (2011a) *Feed-in Tariffs: Guidance for renewable installations*. London: ofgem/ofgem E-Serve. [Online]. Available at: http://www.ofgem.gov.uk/Sustainability/Environment/fits/Documents1/FIT%20generator%20guidance_final.pdf.

ofgem (2011b) *Renewables Obligation: Guidance for generators* London: ofgem. [Online]. Available at: http://www.ofgem.gov.uk/Sustainability/Environment/RenewablObl/Documents1/RO%20Generator%20Guidance%20May%202011%20final.pdf.

Olsson, G., Nielsen, M., Jensen, L. A. and Yuan, Z. (2005) *Instrumentation, Control and Automation in Wastewater systems*. IWA publishing.

Organic-farmers-and-Growers (2011) *First AD plant achieves digestate certification*. Available at: http://www.organicfarmers.org.uk/news/news_more.php?id=217 (Accessed: 16/06/2011).

Palacio-Barco, E., Robert-Peillard, F., Boudenne, J.-L. and Coulomb, B. (2010) 'On-line analysis of volatile fatty acids in anaerobic treatment processes', *Analytica Chimica Acta*, 668(1), pp. 74-79.

Pavlostathis, S. G. and Gossett, J. M. (1986) 'A kinetic model for anaerobic digestion of biological sludge', *Biotechnology and Bioengineering*, 28(10), pp. 1519-1530.

Pearson, K. (1901) 'On lines and planes of closest fit to systems of points in space', *Philosophical Magazine*, 2, pp. 559-572.

Perceptive Engineering Ltd (2012) (Version PerceptiveAPC V4.1) [Computer program]. Perceptive Engineering Ltd.

Perceptiveapc.com (2015) *Perceptive Engineering Products*. Available at: http://www.perceptiveapc.com/products/ (Accessed: 16 May 2015).

pH / ORP transmitters - Analytical Measurement | ABB (2016) 'New.abb.com. (2016). pH / ORP transmitters - Analytical Measurement | ABB'. Available at: http://new.abb.com/products/measurement-products/analytical/continuous-liquid-analyzer/ph-orp-measurement/ph-orp-transmitters (Accessed: 25 May 2016).

Pind, P., Angelidaki, I., Ahring, B., Stamatelatou, K. and Lyberatos, G. (2003) 'Monitoring and Control of Anaerobic Reactors', in *Biomethanation II*. pp. 135-182.

Polit, M., Estaben, M. and Labat, P. (2002) 'A fuzzy model for an anaerobic digester, comparison with experimental results', *Engineering Applications of Artificial Intelligence*, 15(5), pp. 385-390.

Premier, G. C., Dinsdale, R., Guwy, A. J., Hawkes, F. R., Hawkes, D. L. and Wilcox, S. J. (1999) 'A comparison of the ability of black box and neural network models of ARX structure to represent a fluidized bed anaerobic digestion process', *Water Research*, 33(4), pp. 1027-1037.

Products | Bioprocess Control (2016). Available at: http://www.bioprocesscontrol.com/products/ (Accessed: 25 May 2016).

Products Archive - Geotechnical Instruments (UK) Ltd (2016). Available at: http://www.geotechuk.com/products/ (Accessed: 25 May 2016).

Pullammanapallil, P. O., Svoronos, J. M., LYBERATOS, G. and Chynoweth, D. P. (1991) 'Dynamic model for conventionally mixed anaerobic digestion reactors', *AIChE Annual Meeting*. Los Angeles. AIChE.

Qin, J. S. (1998) 'Recursive PLS algorithms for adaptive data modeling', *Computers & Chemical Engineering*, 22(4–5), pp. 503-514.

Qin, J. S. and Badgwell, T. A. (2003) 'A survey of industrial model predictive control technology', *Control Engineering Practice*, 11(7), pp. 733-764.

Ramirez, I., Volcke, E. I. P., Rajinikanth, R. and Steyer, J.-P. (2009) 'Modeling microbial diversity in anaerobic digestion through an extended ADM1 model', *Water Research*, 43(11), pp. 2787-2800.

Redman, G. (2010) *A detailed economic assessment of Anaerobic Digestion technology and its Suitability to UK farming and waste systems* NNFCC, M. b. t.

Rodriguez, J., Roca, E., Lema, J. M. and Bernard, O. (2008) 'Detremination of the adequate minimum model complexity required in anaerobic bioprocessess using experimental data', *Journal of Chemical Technology and Biotechnology*, 83, p. 9.

Rosen, C., Vrecko, D., Gernaey, K. V., Pons, M. N. and Jeppsson, U. (2006) 'Implementing ADM1 for plant-wide benchmark simulations in Matlab/Simulink', *Water Science & Technology: IWA Publishing 2*, 54(4), pp. 11-19.

Ruffino, B., Campo, G., Genon, G., Lorenzi, E., Novarino, D., Scibilia, G. and Zanetti, M. (2014) 'Improvement of anaerobic digestion of sewage sludge in a wastewater treatment plant by means of mechanical and thermal pre-treatments: Performance, energy and economical assessment', *Bioresource Technology*, 175C, pp. 298-308.

Rui, H. (2010) *Nonlinear model predictive control and dynamic real time optimisation for large-scale processes*. Piitsburgh. [Online]. Available at: http://numero.cheme.cmu.edu/uploads/Huangthesis.pdf.

Sandoz, D. J., Desforges, M. J., Lennox, B. and Goulding, P. R. (2000) 'Algorithms for industrial model predictive control', *Computing & Control Engineering Journal*, (June 2000), p. 10.

Saravanan, V. and Sreekrishnan, T. R. (2006) 'Modelling anaerobic biofilm reactors - A review', *Journal of Environmental Management*, 81(1), p. 10.

SCAN (2011) 'spectrolyser for wastewater ', *spectrolyser*. Available at: http://www.s-can.at/text.php?kat=5&id=21&langcode= (Accessed: 22/02/2011).

Schievano, A., D'Imporzano, G., Orzi, V. and Adani, F. (2011) 'On-field study of anaerobic digestion full-scale plants (Part II): New approaches in monitoring and evaluating process efficiency', *Bioresource Technology*, 102(19), pp. 8814-8819.

Seadi, T. A. and Holm-Nielsen, J. B. (2010) *Good practice in Quality managment of AD residues fro biogas production*. Esbjerg: Bioenergy, I.

Shimadzu (2012) 'Product description', *GC-2010 Plus*. Available at: http://www.shimadzu.com/an/gc/2010plus.html (Accessed: 01/11/12).

Shunta, J. P. (1997) *Achieving World Class Manufacturing through Process Control* Prentice Hall PTR.

Siegrist, H., Vogt, D., Garcia-Heras, J. L. and Gujer, W. (2002) 'Mathematical Model for Meso- and Thermophilic Anaerobic Sewage Sludge Digestion', *Environmental Science & Technology*, 36(5), pp. 1113-1123.

Smith, P. H., Bordeaux, F. M., Goto, M., Shiralipour, A., Andrews, J. F., Ide, S. and Barnett, M. W. (1988) 'Biological production of methane from biomass', in R, F. J. (ed.) *Methane from biomass*. W H Smith, p. pp. 44.

Song, Y.-C., Kwon, S.-J. and Woo, J.-H. (2004) 'Mesophilic and thermophilic temperature co-phase anaerobic digestion compared with single-stage mesophilic- and thermophilic digestion of sewage sludge', *Water Research*, 38(7), pp. 1653-1662.

Sosnowski, P., Wieczorek, A. and Ledakowicz, S. (2003) 'Anaerobic co-digestion of sewage sludge and organic fraction of municipal solid wastes', *Advances in Environmental Research*, 7(3), pp. 609-616.

Stephen, B. (2008) 'Least-squares', *Linear Systems and Optimization: Introduction to Linear Dynamical Systems* p. 23 [Online]. Available at: http://see.stanford.edu/see/courseinfo.aspx?coll=17005383-19c6-49ed-9497-2ba8bfcfe5f6.

Steyer, J.-P., Bernard, O., Batstone, D. J. and Angelidaki, I. (2006) 'Lessons learnt from 15 years of ICA in anaerobic digesters', *Water Science & Technology: IWA Publishing 2006*, 53(4-5), pp. 25-33.

Steyer, J. P., Bouvier, J. C., Conte, T., Gras, P., Harmand, J. and Delgenes, J. P. (2002) 'On-line measurements of COD, TOC, VFA, total and partial alkalinity in anaerobic digestion processes using infra-red spectrometry', *water science technology*, 45(10), p. 6.

Su, W. S., Jietae, L. and Ln-Beum, L. (2009) *Process Identification and PID control*. Wiley and Sons.

Supaphol, S., Jenkins, S. N., Intomo, P., Waite, I. S. and O'Donnell, A. G. (2011) 'Microbial community dynamics in mesophilic anaerobic co-digestion of mixed waste', *Bioresource Technology*, 102(5), pp. 4021-4027.

Switzenbaum, M. S., Giraldo-Gomez, E. and Hickey, R. F. (1990) 'Monitoring of the anaerobic methane fermentation process', *Enzyme and Microbial Technology*, 12(10), pp. 722-730.

Theilliol, D., Ponsart, J.-C., Harmand, J., Join, C. and Gras, P. (2003) 'On-line estimation of unmeasured inputs for anaerobic wastewater treatment processes', *Control Engineering Practice*, 11(9), pp. 1007-1019.

Tobias, R. D. (1995) 'An Introduction to Partial Least Squares regression', p. 8 [Online]. Available at: http://support.sas.com/techsup/technote/ts509.pdf (Accessed: 12/10/2012).

UK, P. I. (2011) 'online product description for HK - Dry solids', *Dry solids*. Available at: http://www.processinstruments.net/products/dry-solids.php (Accessed: 23/02/2011).

Vanrolleghem, P. A. and Lee, D. S. (2003) 'On-line monitoring equipment from wastewater treatment processes: state of the art', *Water Science & Technology*, 47(2), p. 34.

Vanwonterghem, I., Jensen, P. D., Rabaey, K. and Tyson, G. W. (2015) 'Temperature and solids retention time control microbial population dynamics and volatile fatty acid production in replicated anaerobic digesters', *Scientific reports*, 5, p. 8496.

Wahab, N. A., Katebi, M. R. and Balderud, J. (2007) *Proceedings of the 15th Mediterranean Confrence on Control and Automation*. Athens, Greece, 27-29 July 2007. http://www.advantech.gr/med07/papers/T04-012-160.pdf: http://www.advantech.gr/med07/papers/T04-012-160.pdf. Available at: http://www.advantech.gr/med07/papers/T04-012-160.pdf.

Wang, L. K., Shammas, N. K. and Hung, Y.-T. (2008) *Biosolids Engineering and Management* [Online]. Available at: www.springerlink.com.

Wang, X. Z. (1999) *Data Mining and Knowledge Discovery for Process Monitoring and Control*. Springer, London.

Ward, A. J., Bruni, E., Lykkegaard, M. K., Feilberg, A., Adamsen, A. P. S., Jensen, A. P. and Poulsen, A. K. (2011) 'Real time monitoring of a biogas digester with gas chromatography, near-infrared spectroscopy, and membrane-inlet mass spectrometry', *Bioresource Technology*, 102(5), pp. 4098-4103.

Ward, A. J., Hobbs, P. J., Holliman, P. J. and Jones, D. L. (2008) 'Optimisation of the anaerobic digestion of agricultural resources', *Bioresource Technology*, 99(17), pp. 7928-7940.

Warthmann, R. and Baier, U. (2013) 'Optimization of anaerobic digestion by pretreatment, additives and process engineering', *http://www.iea-biogas.net/files/daten-redaktion/download/publications/workshop/12/5_Optimisation%20by%20pre-treatment_Warthmann.pdf* [Online].

Wett, B., Eladawy, A. and Ogurek, M. (2006) 'Description of nitrogen incorporation and release in ADM1', *Water science and technology : a journal of the International Association on Water Pollution Research*, 54(4), pp. 67-76.

Wiese, J. and Ralf, K. (2007) 'Laboratory analysis & process analysis biogas plant monitoring', *Application Report*, p. 12 [Online]. Available at: http://www.hach-lange.co.uk/shop/action_q/download%3Bdocument/DOK_ID/14782553/type/pdf/lkz/GB/spkz/en/TOKEN/6u1Aofpp0QTqgeig-dHqhmL2R5I/M/smmpJQ.

Wise, B. M., Gallagher, N. B., Bro, R., Shaver, J. M., Windig, W. and Koch, R. S. (2006) *Chemometrics Tutorial for PLS_Toolbox and Solo*. Wenatchee: Eigenvector Research, I.

Wise, B. M., Shaver, J. M., Gallagher, N. B., Bro, R. and Windig, W. (2010) *PLS toolbox* [Computer program]. Eigenvector Research Incoporated. Available at: http://www.eigenvector.com/software/pls_toolbox.htm.

Wold, H. (1966) 'Nonlinear estimation by iterative least squares procedures', in David, F. N. (ed.) *Research papers in Statistics*. New York: Wiley.

Wold, H. (2004) 'Partial Least Squares', in *Encyclopedia of Statistical Sciences*. John Wiley & Sons, Inc.

Wold, H., Patrick Suppes, L. H. A. J. and Gr, C. M. (1973) 'Cause-Effect Relationships: Operative Aspects', in *Studies in Logic and the Foundations of Mathematics*. Elsevier, pp. 789-801.

Wold, S., Esbensen, K. and Geladi, P. (1987) 'Principal component analysis', *Chemometrics and Intelligent Laboratory Systems*, 2(1-3), pp. 37-52.

Wold, S. and Sjostrom, M. (1998) 'Chemometrics, present and future success', *Chemometrics and Intelligent Laboratory Systems*, 44, pp. 3-14.

PAS 110: 2010 Specification for whole digestate, separated liquor and separated fibre derived from the anaerobic digestion of source-segregated biodegradable material.

Yau, C. (2015) *R Tutorial - An R Introduction to Statistics - Coefficient of Determination*. Available at: http://www.r-tutor.com/elementary-statistics/simple-linear-regression/coefficient-determination.

Zaher, U. E.-S. (2005) *Modelling and monitoring the anaerobic digestion process in view of optimisation and smooth operation of WWTP's*. University of Ghent.

Zhang, L., Lee, Y.-W. and Jahng, D. (2011) 'Anaerobic co-digestion of food waste and piggery wastewater: focusing on the role of trace elements', *Bioresource Technology*, In Press, Accepted Manuscript.