CO-DIGESTION OF INDUSTRIAL AND DOMESTIC WASTEWATER

In fulfilment of the Academic requirements of Master of Science Degree in Chemical Engineering in the College of Agriculture, Engineering and Science, University Of Kwazulu-Natal.

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Declaration

I, Jimson Itai Tanyanyiwa, declare that:

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2. This thesis has not been submitted for any degree or examination at any other university.

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As the candidate's supervisor, I have approved this dissertation for submission.

Professor Chris Buckley _____ _____

Name: **Signature:** **Date:**

Dedication

I dedicate this work to my wife, Florence Tinashe.

Acknowledgements

God Almighty – I give thanks to God for his grace and loving-kindness, which gave the opportunity to do this work and the strength and wisdom to complete it.

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My parents: Toendepi and Petronella Tanyanyiwa – Thank you for supporting, encouraging and loving me. Thank you for the sacrifices you made so that I could get a good education.

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Abbreviations

Abbreviation	Description
ACP	Amanzimtoti Co-Digestion Plant
AD	Anaerobic digestion
ACPM	Amanzimtoti Co-Digestion Plant Model
ADM1	Anaerobic Digestion Model no.1
AM	Animal Manure
AnSBR	Anaerobic Sequencing Batch Reactor
AWTP	Amanzimtoti Wastewater Treatment Plant
BPO_DB	Biodegradable Particulate Organics of Dead Biomass
BPO_PS	Biodegradable Particulate Organics of Primary Sludge
C	Elemental Carbon
COD	Chemical Oxygen Demand
DS	Digester Sludge
EC	Electrical Conductivity
EWS	eThekwini Waste and Sanitation
FBSO	Fermentable Readily Biodegradable Soluble Organics
FSA	Free and Saline Ammonia
FVW	Fruit and Vegetable Waste
FW	Fruit/Food Waste
H	Elemental H
HLR	Hydraulic Loading Rate
HRT	Hydraulic Retention Time
ISS	Inorganic Suspended Solids
LBRM	Laboratory Batch Reactor
LBRM	Laboratory Batch Reactor Model
LCFA	Long-Chained Fatty Acid
N	Elemental Nitrogen
O	Elemental Oxygen
OLR	Organic Loading Rate
TAN	Total Ammonia Nitrogen
VFA	Volatile Fatty Acids

Nomenclature

Symbol	Description	Unit
ad	Acidogens/Acidogenesis	
ac	Acetogens/Acetogenesis	
am	Acetoclastic Methanogens/Methanogenesis	
hm	Hydrogenotrophic Methanogens/Methanogenesis	
ks	Half-saturation Constant	mgCOD/L
mu	Maximum Specific Growth Rate	1/day
R	Reaction Rate	g/m^3
S	Substrate Concentration	g
Y	Yield coefficients	gCOD/gCOD
X		
a	Composition subscript for nitrogen in the organic components empirical formula, $C_xH_yO_zNaPb$.	
b	Composition subscript for phosphorous in the organic components empirical formula, $C_xH_yO_zNaPb$.	
x	Composition subscript for carbon in the organic components empirical formula, $C_xH_yO_zNaPb$.	
y	Composition subscript for hydrogen in the organic components empirical formula, $C_xH_yO_zNaPb$.	
z	Composition subscript for oxygen in the organic components empirical formula, $C_xH_yO_zNaPb$.	

Abstract

This study is part of an extensive project studying the possibility of co-digestion of industrial and domestic wastewater at Amanzimtoti Wastewater Treatment Plant in Durban, South Africa. The focus of this study was to develop a model-based procedure to dose the 2 000 m^3 full-scale Amanzimtoti pilot co-digestion plant with expired fruit juice. Modelling and experiments were used to create a six-stage feedback control loop. Experiments were conducted in 6.5 L batch reactors in the laboratory and in the 2 000 m^3 plant that was operated at room temperature with intermittent mixing.

The laboratory reactors were used in the first stage loop for data acquisition at 35°C and 25°C with digester sludge from the 2 000 m^3 plant and expired fruit juice. pH values and biogas flowrate were measured continuously for 24 h during the experiments.

The experimental data collected was used to calibrate a model of the laboratory reactor in the second stage. The WEST modelling platform was used for all modelling activities. The model was a UCT adaptation of the ADM1 model, and it used glucose as a representative of expired fruit juice as indicated in earlier work.

Extensive kinetic parameters from the second stage were used to develop a model of the 2 000 m^3 plant in the third stage.

Expired fruit juice was dosed into the 2 000 m^3 plant, and pH data was collected continuously over 24 h in the fourth stage. The pH data was used in the fifth stage to calibrate the model of the 2000 m^3 plant model to the dosing of expired fruit juice. Extensive kinetic parameters from the fifth stage were used to develop the 6.5 L batch reactor model in the sixth stage.

The 35°C experimental data was successfully used in the development of the 2 000 m^3 plant model. The feedback control loop can be used to guide how much expired fruit juice can be dosed in the 2 000 m^3 plant. Although the feedback control loop was successful, various components of the 2 000 m^3 digester were not functional, which resulted in the feedback control loop being completed only once.

Chapter 1: Introduction

EThekwini Water and Sanitation (EWS) operates 27 wastewater treatment plants which process approximately 460 Ml/day of sewage. This corresponds to 100 tonnes of dry sludge per day produced, which has to be disposed of properly (eThekwini Municipality, 2011). After treatment, the final wastewater effluent is discharged to nearby water sources. In most South African coastal cities, the water resource is sometimes a deep-sea outfall. Treated effluent disposal into any water body is controlled and regulated through a discharge permit from the Department of Water and Sanitation. Organisations that dispose effluent to a marine or surface water source have to pay a fee. (Bailey, 2004).

Sludge disposal into the sea is regulated (Government, 2016); alternative disposal methods are necessary. Disposal on land is also be limited by restrictions due to regulation of metals in the soil (Paul and Liu, 2012). Due to the KwaZulu-Natal Provincial Gazette no. 1763 (Government, 2016) on sea disposal, the EWS plans to cease disposal of sludge into the sea from its Southern Water Treatment Works (eThekwini Municipality, 2011).

Act No. 108 of 1996 of the constitution of South Africa states that water resources management is a national government responsibility. It gives the government mandate to use water, protect and conserve it, as well as to manage it in an equitable and sustainable manner (Mhlanga, 2008, Government, 1996). Sea disposal is economical but because it is illegal according to Government (2016) in the future more options have to be considered. Onsite land disposal is limited by the available land on the treatment works. Off-site land disposal costs approximately R1,200,000 annually as authorised by the Department of Water Affairs, and is unlikely to be authorised again (eThekwini Municipality, 2011).

Due to the above mentioned disposal challenges, new waste management strategies are being considered. More efficient production methods and waste minimization, that prioritize the integration of pre-emptive environmental strategies, have to be investigated. The presence of numerous anaerobic digestion (AD) facilities that are under-utilised in KwaZulu-Natal was a motivation for seeking ways to improve their usage. For example, Amanzimtoti Wastewater Treatment Works has six ADs, and only half are operational. Industrial effluent from the surrounding areas can be treated using the unused digesters. Prospecton industrial area, which is in the vicinity of the wastewater treatment plant supplies 50% its volumetric load (Remigi and Buckley, 2006).

High organic content industrial effluent which when individually digested is toxic to AD archaea can be simultaneously treated with municipal sludge. The simultaneous treatment of two or more wastewater streams with complementary characteristics is called co-digestion. This enables waste streams with inhibitors to be treated without harming the performance of the AD process (Remigi and Buckley, 2006, Logan, 2016). Co-digestion presents the opportunity of integrating the waste management system in an economically and environmentally sustainable manner (Logan, 2016).

Sometimes the characteristics of waste streams may be incompatible, causing fluctuations in the AD process. Nevertheless, some AD processes respond negatively to perturbations; hence although co-digestion has the potential to positively influence the AD process, the limitations

posed by digester instability reduce the range of application of co-digestion. Advanced process control and monitoring are necessary for practical application of co-digestion (Logan, 2016).

According to Ekama (2009), the history of process control in AD systems is poor; hence before co-digestion is even considered a rigorous AD control system has to be adopted. Using a model-based control strategy for anaerobic co-digestion has the potential of assisting the development of eco-friendly sustainable technology. Models allow the anaerobic digestion process to be optimized and also mitigate risk to digester stability by using mathematical processes as a foundation for high-level process control as well as allow an understanding of process dynamics. A model of the co-digestion process was key to design, implementation and control of the co-digestion process. Nevertheless, a model's capacity to provide useful information is related to how accurately the mathematical equations are able to represent the intricacies of the various physicochemical and biological interactions describing the co-digestion process and the information used in its validation and calibration (Logan, 2016).

The potential of using co-digestion as an economical and sustainable waste treatment method as well as the challenges of its widespread application, motivated the eThekwini Municipality through its department of Water and Sanitation, to develop a 2 000 m^3 pilot project to study the possibility of co-digestion of concentrated industrial effluent with sewage sludge at Amanzimtoti Wastewater Treatment Works. The Amanzimtoti Co-digestion Project (ACP) was commissioned to develop an engineering system for the co-digestion of concentrate industrial wastewater with sewage sludge to be employed at the plants run by the municipality (Logan, 2016).

Figure 0-1: Amanzimtoti Wastewater Treatment Works 2 000 m^3 pilot digester

Figure 0-2: Amanzimtoti Wastewater Treatment Works 2 000 m^3 pilot digester control panel

A Memorandum of Understanding (MOU) between PRG and the EWS gave PRG the responsibility of offering scientific support in various water and sanitation projects. This study was part of the MOU in which the possibility of co-digesting concentrated industrial effluent and sewage sludge was investigated. The main purpose of this study was to find a scientific solution to the management and control of anaerobic co-digestion with concentrated industrial wastewater by using an anaerobic co-digestion model.

1.1 Purpose of the study

The study is a continuation of the work done by Logan (2016). Logan (2016) continued on the Water Research Commission project K5/2001 on Co-digestion of Sewage with Industrial Concentrates done (PRG, 2001). In the project, a 2 000 m^3 digester was refurbished by the EThekwini Municipality, and a dual nozzle tank mixing system was added to it. Storage tanks

for industrial concentrate storage were also built. The storage tanks had a pumping system, valves, flow meters and level sensors.

Figure 0-3: Storage tanks with pumping system used to store 5 m^3 industrial wastewater each for the Amanzitoti Pilot digester

The combination of storage tanks and digester was monitored and controlled using a computerised system.

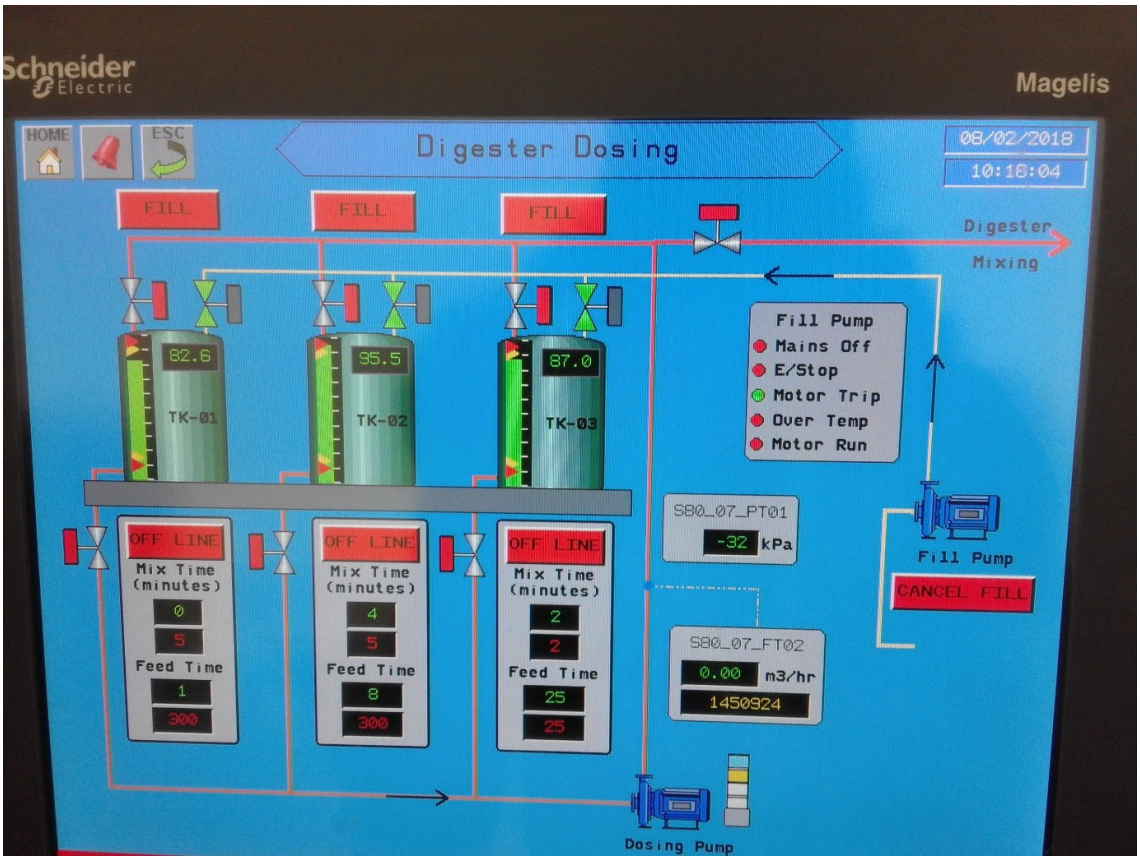


Figure 0-4: Storage tanks control panel showing the three storage tanks, valves, pumps and piping system

Logan (2016) developed a laboratory-based system composed of two 6.5 L batch reactors for screening industrial concentrates. He also developed models for both the 2 000 m^3 digester and the 6.5 L.

Figure 0-5: Laboratory at Amanzimtoti Wastewater Treatment works where screening experiments are conducted using 6.5 L batch reactors

Figure 0-6: shows two 6.5 L batch reactors for screening industrial wastewater

The purpose of the current study was to build on the work by Logan (2016) and (PRG, 2001) and develop a complete feedback control loop cycle for use in controlling the dosing of industrial wastewater in the Amanzimtoti Co-digestion Project. Logan (2016) used expired fruit juice as the concentrated industrial effluent.

Table 0-1: Water Research Commission Co-digestion project plan, a timeline and completion rate

Activity	***By who***	***Date of completion***
Installation of Anaerobic digester mixing system	*EThekwini Municipality*	*Completed in 2011*
Installation of Industrial wastewater storage, dosing and control system	*EThekwini Municipality*	*Completed in 2011*
Installation of Wastewater screening laboratory	*EThekwini Municipality*	*Completed in 2011*
Development of the University Of Cape Town Model	*Osborne et al. (2012b)*	*Completed in 2012*
Laboratory wastewater screening tests and modelling	*Logan (2016)*	*Completed in 2016*
Anaerobic digester testing and modelling	*Logan (2016)*	*Completed in 2016*
Co-digestion digester testing and modelling		*Not done*
Testing the effect of temperature variation on digester kinetics		*Not done*

The Pollution Research Group provided scientific support at all stages of the project. The six STAGES had to be done to complete the feedback control loop cycle for it to be completed. The most important STAGE in the cycle was conducting operations at full scale in the Amanzimtoti Co-digestion Project plant. Osborne et al. (2012b) and Osborne et al. (2012a) developed the UCT ADM2 model, which was the foundation for the modelling done by Logan (2016). Logan (2016) went through STAGE 1, STAGE 2 and STAGE 3, which are the laboratory screening tests in 24 h. He also conducted a test on the 2 000m^3 digester without dosing any industrial wastewater and then developed a model for it. He did not go through STAGES 4, 5 and 6, hence he did not complete the feedback control loop.

Logan (2016) managed to operate STAGE 1, STAGE 2 and STAGE 3 in 24Expired fruit juice was used in the current project was composed of is a simple sugars (glucose and fructose) as well as fermented simple sugars, making it highly degradable and benign. A simple co-substrate was necessary because it would be easy for the biomass to digest simple sugars. The purpose of the study was to establish a system for dosing industrial effluent into the Amanzimtoti pilot digester hence a simple effluent in the form of expired fruit juice was

selected to. In the future, it was anticipated that more complex industrial effluents would be considered for the pilot digester.

1.2 Significance of the study

The study is critical because it will lay a foundation for the integration of industrial effluent and municipal waste management through co-digestion in an eco-friendly and sustainable way. If implemented successfully, co-digestion has the prospect of decreasing the financial and

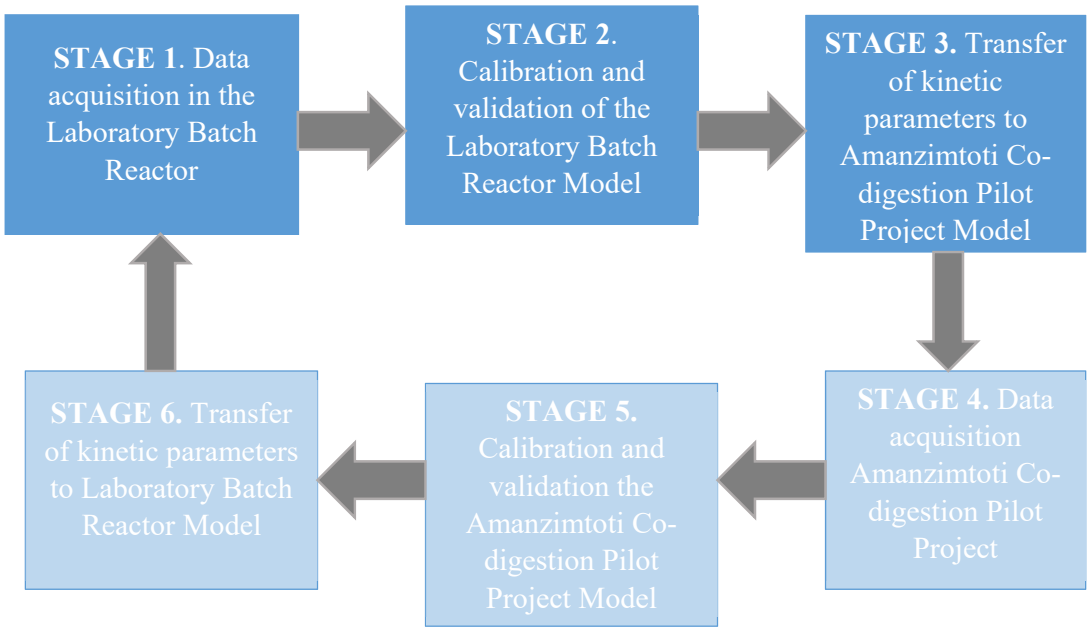


Figure 0-7: Feedback control loop cycle for the Amanzimtoti Co-digestion Pilot Project developed by Logan (2016)

environmental burden of treating municipal and industrial wastes, while also increasing biogas production and detoxifying harmful compounds (Logan, 2016).

The operation of a co-digestion plant using a feedback control loop system based on a model improves knowledge of the system while also improving process control and system optimization. This method also provides operators and researchers with a means to evaluate co-digestion of different industrial effluents by qualifying and quantifying their effect on digester performance with no risk to the digester. For consistency of composition, source-separated effluent was used as a co-substrate.

The eThekwini municipality does not have an extensive industrial-scale application of co-digestion. Logan (2016) conducted similar experiments, but the key difference between his work and this study was that he did not do any actual co-digestion experiments on the Amanzimtoti C-digestion Pilot Project. It took him 24 h to conduct STAGE 1 to STAGE 3. The co-digestion trials were necessary to complete the feedback control loop cycle. The study also details the engineering challenges that the municipality faced during co-digestion trials.

1.3 Delimitations of the study

The investigations done in this study were restricted to developing a complete feedback control loop cycle. The steps taken to complete the cycle were:

a) Collecting experimental data from the Laboratory Batch Reactor (LBR)
b) Using the collected data to calibrate and validate a model of the Laboratory Batch Reactor Model (LBRM).
c) Transferring of kinetic parameters from the LBRM to a model of the ACP.
d) Data collection from the ACP
e) Calibration and validation of the ACPM.
f) Transfer of the kinetic parameters from the ACPM to the LBRM.

The same equipment, sewage sludge source and industrial effluent source that was used by Logan (2016) were used in this study. Moreover, the same period of 24 H for STAGE 1 to STAGE 3 had to at least be maintained or reduced.

Notwithstanding the extensive application of AD, designing, operating and controlling the process for sewage sludge treatment is mainly done through empirical guidelines or experience. Mathematical models offer a quantitative description of a system under consideration which enables prediction of its performance and response (Demitry, 2016). Since the study was a continuation of the work done by Logan (2016) and because the equipment used was the same, the variables and parameters used were similar, and work was done to assess the predictive capability of the model he developed under similar conditions. The manipulation of parameters used was also similar to verify reproducibility of results before they were applied to the ACPM.

Logan (2016) also conducted co-digestion experiments at 35^{o}C, but the data was never used in the development of the ACPM. The ACP is not heated and operates at ambient temperature. The impact of transferring kinetic data obtained at a constant temperature to a model that operates at a variable temperature was unknown hence; assessing the potential impact of using data obtained at room temperature in the ACPM was necessary. Temperature coefficients were used to investigate the conversion of data at 35^{o}C to data at 25^{o}C. The STAGES in **Figure 0-7** experiments, the LBR experiments and the simulations in the LBRM were done at 35^{o}C while in the ACP and the ACPM the ambient temperature was used. This difference in temperature has an unknown impact on the results of the study; hence experiments were conducted at 25^{o}C to test whether they can yield the same results as the data obtained at 35^{o}C.

1.4 Scope of the study

The main goal of the project was to find a scientific solution to the management and control of anaerobic co-digestion of a concentrated and consistent industrial wastewater by using an anaerobic co-digestion model. This was done by developing and completing a feedback control loop. All models were calibrated using data collected through experiments that determine the stoichiometric and kinetic parameters of the AD process.

1.5 Aim

To develop simplified computation models of the co-digestion process and apply them to the monitoring and control of the demonstration project at Amanzimtoti.

1.6 Objectives

1. To assess the predictive capability of the model updated through a feedback control loop
    - pH values and gas flowrate to be compared with model predictions.
    - Model initial values to be adjusted to fit the Amanzimtoti Co-digestion Pilot Project data.
    - Additional measurements to be considered if the model significantly deviates from Amanzimtoti Co-digestion Pilot Project data.
2. To develop temperature coefficients using the Laboratory Batch Reactor Model
    - To use the temperature coefficients to correlate Laboratory Batch Reactor Model kinetic data at a higher temperature to match data at a lower temperature.
3. To dose the Amanzimtoti Co-digestion Pilot Project plant and collect gas flowrate and pH data and use it to calibrate the Amanzimtoti Co-digestion Pilot Project Model.
    - pH values will be used to evaluate the model's use in process control, and gas flow rate will be used to do a mass balance to test
    - To capture effluent characteristics by fitting model parameters with kinetic data.
    - To apply the captured characteristics in developing a modelling control iteration loop.
    - To use the control iteration to demonstrate the model's prediction of the dosage limits.

Chapter 2: Literature Survey

A review of the literature is presented in this chapter. **Section 2.1** introduces the anaerobic digestion process; section **2.2** presents the co-digestion process, **section 2.3** summarises some co-digestion case studies, **section 2.4** introduces the history of the co-digestion process at Amanzimtoti Wastewater Treatment works, **section 2.5** introduces anaerobic digestion models, **section 2.6** details the parameter acquisition procedure and **section 2.7** details sensitivity analysis procedures, **section 2.8** details the conclusion to the literature survey**, section 2.9** summarises the overall conclusion **section 2.10** explains why the model needed to be simplified **section 2.11** presents the parameters selected for the regression **section 2.12** details the ***Temperature hypothesis*** **section 2.13** details the ***Feedback control loop hypothesis*** **section 2.14** describes the modelling approach and **section 2.15** gives a summary of the literature review.

2.1 Anaerobic digestion

Anaerobic digestion is the conversion of organic matter by several anaerobic microorganisms in a multistage process that results in the production of mainly methane and carbon dioxide, with composition ranging from 60-70% for methane and 20-30% for carbon dioxide (Tortora et al., 2004). According to (McCarty, 1964, Demitry, 2016) anaerobic digestion is a good way of producing renewable energy. The process has numerous major benefits over other current wastewater treatment methods. Anaerobic digestion can reduce particulate material by up to 50-60% (Bailey and Ollis, 1985). The positive outlook for the future of AD has been hampered by insufficient understanding of the fundamental concepts governing the process necessary to explain and regulate the disturbances that occur in the process and expand the process to for the treatment of various industrial wastes (Labatut and Gooch, 2012).

2.1.1 Biochemical processes

AD proceeds in four inter-related phases, namely hydrolysis, acidogenesis, acetogenesis and methanogenesis.

Biochemical processes are determined by the process configuration, the nature of the substrate the organic loading rate (OLR) and the temperature. According to Sötemann et al. (2005a), the hydrolysis and acidogenesis phases represent the slowest step in the AD process (Sötemann et al., 2005a).

Other industrial wastewaters may have lipid and grease degradation as the rate-controlling step. When the temperatures drops below 20°C methanogenesis may continue at a slower rate, but grease and lipid degradation stops, according to Speece (1983).

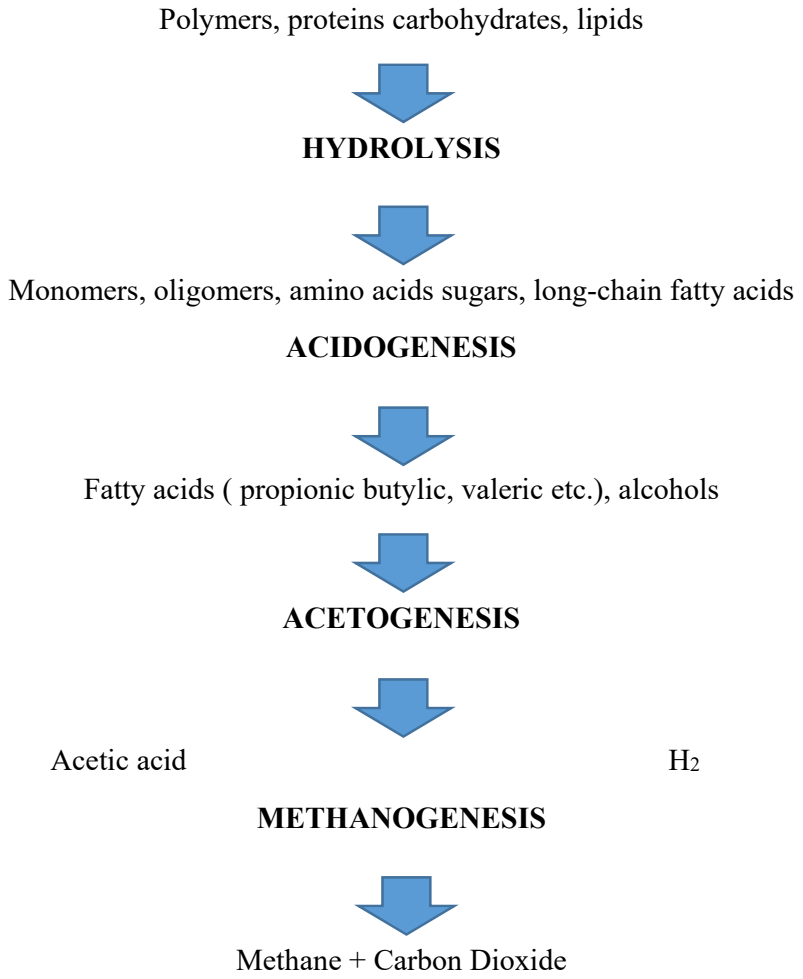


Figure 0-8: Fermentation stages in methane production adapted from Ziemiński and Frąc (2012). CO_2 is produced at each stage after hydrolysis. Some of it is used to produce methane, while the other portion of CO_2 is a by-product of methanogenesis.

The growth rate of each microbial species in the bioprocesses in **Figure 0-8** is determined by the Monod kinetic equation given below (Batstone et al., 2002):

$$R = mu[X] \times \frac{[S]}{k_s + [S]} \qquad \textbf{0-1}$$

Where:

R (g/day) is the reaction rate

mu (1/day) is the maximum specific growth rate

k_s (g/m^3) is the half-saturation constant

[X] (g) is the biomass concentration

[S] (g/m^3) is the substrate concentration

2.1.1.1 Hydrolysis

According to Ziemiński and Frąc (2012), organic polymers and other insoluble organic materials such as fats, proteins and carbohydrates are degraded to fatty acids, amino acids and mono-sugars. Extracellular enzymes called hydrolases are responsible for the hydrolysis. Cellulose is a refractory polymer which remains after biodegradable matter has been digested. The hydrolysis rate is dependent on the production of enzymes, absorption and diffusion of enzymes, pH, and the particle size of the waste undergoing digestion (Ziemiński and Frąc, 2012, Logan, 2016).

2.1.1.2 Acidogenesis

Ziemiński and Frąc (2012) details that water-soluble substrates are produced by acidifying archaea, examples include hydrogen, carbon dioxide, aldehydes, alcohols, and some short-chain acids (SCFA) such as pentanoic, butyric, propionic, acetic and formic acid. Hydrogen sulphide and ammonia are two other products of acidogenesis that cause an intense, unpleasant smell (Ziemiński and Frąc, 2012, Logan, 2016)**.**

2.1.1.3 Acetogenesis

According to Logan (2016), acetate and hydrogen are produced from the acid phase products using acetogenic microorganisms. Hydrogen has an inhibitory effect on AD microorganisms hence the need to establish a symbiosis between acetogenic archaea and hydrogenotrophic archaea that use hydrogen in a process called syntrophy. The efficiency of an AD digester is dependent on acetogenesis because about 70% of methane is produced as a result of acetates production, because of this acetates are an important intermediate of methane production (Ziemiński and Frąc, 2012, Speece, 1983).

2.1.1.3 Methanogenesis

Methane is produced using acetic acid and hydrogen. It is produced in the preceding phases by methanogenic archaea (Logan, 2016). Even though only a limited number of archaea are capable of producing methane from acetic acid, most of the methane in AD is produced heterotrophic methane archaea that convert the acetic acid. Autotrophic methanogens consume H_2 creating ideal conditions for the growth of acid archaea which leads to the production of short-chain organic acids during the acidification stage (Ziemiński and Frąc, 2012, Speece, 1983).

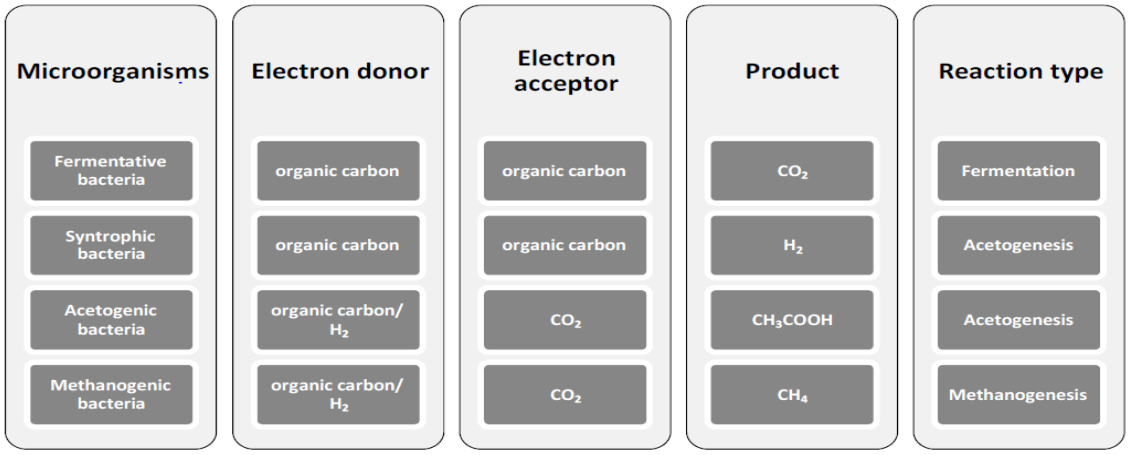


Figure 0-9: Cooperation of microorganism in degrading organic matter adapted from Ziemiński and Frąc (2012)

2.1.2 Physico-chemical process

These are gas-liquid transfer and association/dissociation processes that occur without biological mediation such as:

i. Liquid reactions (aqueous weak acid/base chemistry)
ii. Gas-liquid exchanges such as the bubbling out of CO_2 and CH_4
iii. Liquid-solid transformations such as solubilisation/precipitation processes (Batstone et al., 2002, Harding, 2009).

The processes mentioned above are essential when modelling AD because:

- Several biological inhibitors such as dissolved gas concentration, free acids and bases and pH can be expressed in the anaerobic model
- Important performance variables such as carbonate alkalinity and gas flow rely on an accurate approximation of physico-chemical changes (Batstone et al., 2002).

2.1.2.1 Liquid-liquid reactions (aqueous weak acid/base chemistry)

Harding (2009) notes that anaerobic digesters contain diverse weak acid/base systems comprising several chemical species at various molar concentrations. The various species concentrations arising from AD are dependent on the composition and concentration of the substrate that directly affects the aqueous concentration of the AD product. The pH in the AD is a function of the influent organics and inorganics composition (Harding, 2009, Logan, 2016).

2.1.2.2 Gas-liquid transfer

Gases that dissociate to form ions in an aqueous solution such as hydrogen sulphide, ammonia and carbon dioxide have complicated equilibrium relationships (Lizarralde et al., 2015). In a typical wastewater treatment plant carbon dioxide, ammonia, oxygen, nitrogen, methane, hydrogen and hydrogen sulphide are usually considered. The specific gases considered are

selected according to the AD system being investigated (Lizarralde et al., 2015, Harding, 2009).

The gas-liquid equilibrium kinetic rate relationship is determined by the difference between the dissolved gas saturation concentration and the contact area between the aqueous and gaseous phase. The gas saturation concentration in the liquid is equivalent to the multiple of the gas mass transfer coefficient (Kla) and the gas partial pressure. The gas mass transfer coefficient depends on the solubility of the gas under consideration moreover the solubility depends on mixing in the reactor. The gas-phase contact area is determined by the configuration of the reactor.

2.1.3 Inhibition levels

Inhibitors are compounds that prevent microorganisms from functioning (Tortora et al., 2004). There are several aspects that affect inhibition. Microorganisms may recover after perturbations, which may irreversibly change the microorganism such that it cannot recover from the effects of the inhibitor even though the inhibitory material will be absent. The system has to be restarted by the addition of new microorganisms. On the other hand, the microorganisms may merely be inhibited, and afterwards, they recover after some time has passed, this time is known as the lag period (Schnurer and Jarvis, 2010). During the lag period, the microorganisms do not grow due to inhibitory effects, it may also mean the system is growing organisms that can handle the inhibitory substance, the organisms may already be present but not in large numbers during the lag phase they increase their numbers. To avoid the total collapse of the system during the lag phase, there may be a need to increase retention time or reduce the organic load in a continuous system or else the organisms would be washed out (Schnurer and Jarvis, 2010).

2.1.4 Anaerobic digestion stability and control

According to Chen et al. (2008), in AD, methanogens and acid making archaea have very different sensitivity to digester conditions, growth kinetics, physiology, and nutritional needs. The inability to sustain the balance between the needs of the two archaea groups is the main reason for reactor failure. Process inhibitors are principal causative agents for AD instability because they exist in substantial quantities in wastewater and sludge. A substance is said to be inhibitory if its presence cases a hostile shift in microbial population or reticence of microbial growth. This shown by a reduction in steady-state CH_4 production and build-up of organic acids (Chen et al., 2008, Logan, 2016).

Perturbations such as ingress of inhibitors, a rapid drop in temperature, or a sharp increase OLR have the capacity of increasing SCFA (Sötemann et al., 2005a).

To avoid AD perturbations an appropriate system configuration and comprehensive control of operational parameters are essential to maintaining environmental variables stable and within optimum ranges. Hydrogen and propionate have a crucial role in methanogenesis, and because of this, they are vital intermediate products of AD, making them important system indicators. Furthermore, hydrogen propionate and acetate are more sensitive to system disturbances than pH, CH_4 composition and biogas production (Labatut and Gooch, 2012).

To optimize AD through technology, the fundamental process associated with the process, namely microbiology of AD has to be thoroughly understood. Knowing the ecology and role

of the microbial population is necessary for improving control of biochemical reactions as the process is ultimately reliant on active biomass for production efficiency (Tabatabaei et al., 2010). In AD, acidogens and methanogens differ widely in terms of growth kinetics, nutritional needs, physiology and sensitivity to ambient conditions. The inability to balance the requirements of acidogens and methanogens is the main cause of process instability (Chen et al., 2008).

2.1.4.1 Volatile fatty acids

Volatile fatty acids (VFA) concentration is perhaps the most sensitive process performance indictor (Remigi and Buckley, 2006). It can be an inhibitor and lead to system instability and collapse. VFAs includes a set of six compounds which are butyric acid/butyrate, caprioic acid/caproate, propionic/propionate, enanthic acid/enanthate evaleric acid/valerate and acetic/acetate of which acetate is principal. In a properly designed and run digester VFA total concentration is usually less than 500 mg/l in acetic acid form. An abrupt rise in VFA concentration shows possible digester instability, hence it is required that VFA be measured intermittently to identify problems timeously (Labatut and Gooch, 2012).

2.1.4.2 Molecular Hydrogen

In a manner similar to that of VFA, the concentration of molecular hydrogen is also sensitive to system disturbances and is suitable for early detection of process perturbations. Nevertheless, because it is present in minute quantities and requires complex equipment to measure it is not a suitable process monitoring parameter for the AD system (Labatut and Gooch, 2012).

2.1.4.3 pH

AD requires the maintenance of a neutral pH in the range of 6.5-6.7. Of the various microorganism populations required in AD, methanogens are the most vulnerable to deactivation because of a low pH (Labatut and Gooch, 2012, Ziemiński and Frąc, 2012). Altering digester operational parameters or ingress of toxic substances may cause system imbalance and accrual of VFAs if the system is not well buffered, the pH will decrease to less than optimum. Subject to the extent and period of the pH drop, biogas produced will be reduced and may stop completely (Labatut and Gooch, 2012).

2.1.4.4 Alkalinity

Alkalinity is a measurement of the concentration of alkaline/basic substances. Carbon dioxide, bicarbonate and carbonate are examples of compounds that add to the alkalinity in AD processes (Schnurer and Jarvis, 2010). The AD buffer capacity is dependent on the alkalinity in the digester. Bicarbonate (HCO_3^-) ions are the main basis of the AD buffer system, maintaining the pH at 6.5-7.6. (Labatut and Gooch, 2012). The amount of HCO_3^- present is dependent on the fraction of CO_2 gas, as shown by **equation 0-2** (Schnurer and Jarvis, 2010).

$$CO_2 + H_2O \leftrightarrow H_2CO_3 \leftrightarrow HCO_3^- + H^+ \leftrightarrow CO_3^{2-} + 2H^+ \quad \textbf{0-2}$$

There are two quantities that can be measured to when specifying AD alkalinity, namely bicarbonate alkalinity (BA) and total alkalinity (TA).

2.1.4.5 Ripley Ratio

According to Logan (2016), the importance of alkalinity and VFA in determining pH of AD processes, digester stability can be monitored and determined using the Ripley Ratio. The ratio of VFA to TA concentration is the Ripley Ratio. An increase of the Ripley Ratio indicates that digester stability has decreased due to the build-up of VFAs with no corresponding increase in the system's buffering capacity. If the Ripley Ratio exceeds 0.25 process failure is likely. Conversely, a decrease in the Ripley Ratio shows an increase in digester stability due to the increase in pH buffering capacity (Logan, 2016).

2.1.4.6 Temperature

Temperature is one of the most important parameters to consider in AD. With oxygen present, heat is evolved by the degradation of organic matter, in an anaerobic environment, very little heat is evolved, and most of it is used in the formation of CH_4. Thus for microorganisms to thrive an external heat source is required. In AD a process can either be mesophilic (37 to 39^oC) or thermophilic (40 to 55^oC). When a stable operating temperature has been reached temperature variations should be avoided, ± 0.5C^o variation gives the best performance although deviations of up to ± 2 to 3C^o are acceptable (Labatut and Gooch, 2012, Ziemiński and Frąc, 2012, Chen et al., 2008). Methanogens are more vulnerable to temperature variations than other organisms hence the need to maintain a stable temperature in the AD, and this is usually achieved through agitation, and insulation (Schnurer and Jarvis, 2010). Running the process outside the control temperature range results in less biogas being produced, reduced waste stabilization and in the long run, digester failure (Labatut and Gooch, 2012).

2.1.4.7 Biogas production

Biogas production is one of the key factors to monitor in AD. Biogas contains mainly CH_4 and CO_2, as well as small amounts of hydrogen sulphide, nitrogen, ammonia and other gases. The CH_4 methane is produced dependent on the volatile solids (VS) stabilized in the digester. CH_4 production must be steady with time, and any decline below the standard production rate shows possible digester upset (Labatut and Gooch, 2012).

2.1.4.8 Volatile Solids

Labatut and Gooch (2012) describe volatile solids (VS) as the quantity of organic material in waste, and it is used to calculate the digester OLR. The change in the VS composition of the influent and the effluent in the AD gives a measure of how much waste has been stabilized. The degree of organic material stabilization is principally dependent on the AD setup and the substrates' physicochemical parameters (Labatut and Gooch, 2012, Logan, 2016).

2.2 Co-digestion

The simultaneous anaerobic digestion of two or more waste streams where one is more biodegradable than the other to improve the biodegradability of the less biodegradable waste stream is called co-digestion (Remigi and Buckley, 2006). Co-digestion is known to considerably increase biogas yields while using the pre-existing treatment plant. The increased biogas yields are primarily caused by the higher OLR, synergy between substrates, and reduced inhibitory effects due to dilution also improve digestate stability (Jensen et al., 2014).

Co-digestion has several advantages, some of them are (Remigi and Buckley, 2006)

- It is more cost-effective than mono-digestion
- It can dilute inhibitors in concentrated effluents and increase nutrients
- It can increase co-metabolism for the detoxification of organic inhibitors.

The dilemma in choosing a co-substrate is usually between financial and technical constraints. Theoretically, a co-substrate should maintain the digester stability, maintain the Chemical Oxygen Demand (COD) removal levels and improve methane yields. But from a financial perspective the cost of moving and storing the co-substrate from the source to the digester, the cost of increased digestate and the cost of dewatering it, the cost of maintaining the pre-treatment facilities should be considered (Tormo et al., 2015).

The co-digestion needs to have a positive effect on the process of energy balance. The cost of establishing and running the co-digestion facility should not outweigh the savings reaped from co-digestion. The source of industrial effluent should be close to the AD plant site to reduce transport costs (Tormo et al., 2015).

The effluent should be easily obtainable with as little characteristic variation as possible. Harmony of the co-substrate with the main substrate is vital. The co-substrate should have characteristics that complement the main substrate. The water, organic, and nutrient content should stabilize that of the main substrate. The co-substrate must also dilute the inhibitory effects of the main substrate (Haak et al., 2015).

2.3 Case studies of mesophilic laboratory and full-scale sewage sludge co-digestion

There are various co-digestion examples; some of them are detailed below. Biogas production and sewage sludge stabilization are given for each case. Anaerobic digestion also results in sludge stabilization. Sludge is malodourous and also rots in the presence of pathogens. Anaerobic digestion stabilizes sludge by removing volatiles solids and solids (Peirce et al., 1998). In many of the studies, the co-substrate was a waste stream with an undefined composition.

2.3.1 Waste activated sludge, food waste and fruit/vegetable waste co-digestion

The study used a waste activated sludge fed with food waste, fruit and vegetable waste in a mass ratio of 1:2:1 on a 2 m^3 laboratory-scale continuously stirred reactor (CSTR) with an HRT of 15 d. The range of OLR used was 1.2 to 8 kg $m^{-3}d^{-1}$ of VS. The approximate waste stabilization was 62-70%. The process was steady approximate biogas produced at a range of 0.9-5.3 m^3 $m^{-3}d^{-1}$. The results also showed that as the

OLR was increased, there was a reduction the extent of waste stabilization, the CH_4 composition and the pH thereby reducing the process stability (Liu et al., 2012b).

2.3.2 Co-digestion of sewage sludge and waste glycerine

Two 1.3 m^3 laboratory-scale CSTR a solids residence time (SRT) of 20 d were used. Primary sludge and waste glycerine were the co-digestates. The first reactor was fed with primary sludge only while the second was fed with primary sludge and waste glycerine at a mass ratio of 77: 23 OLR of 1.04 $m^{-3}d^{-1}$of VS. The biogas production increased by 83% and the waste stabilization increased by 63%. Increasing the relative proportion of glycerine decreased process stability (Razaviarani et al., 2013b).

2.3.3 Co-digestion of sewage sludge and grease trap waste

Two 1.3 m^3 laboratory-scale CSTR digesters were used with an SRT of 20 d. The first was loaded with sewage sludge only while the second was loaded with primary sludge and grease trap waste at a mass ratio of 77: 23, and OLR of 1.58 $m^{-3}d^{-1}$of VS. The biogas production rate improved by 67% and the waste stabilization increased by 50%. The digester became unstable due to increased amounts of LCFA (Razaviarani et al., 2013a).

2.3.4 Co-digestion of sewage sludge, food waste and fruit/vegetable waste

A laboratory-scale CSTR with a 2 m^3 volume and an HRT of 20 d. Primary sludge: fruit waste: food waste in a mass ratio of 2: 1:1 with an OLR was 6 kg $m^{-3}d^{-1}$of VS. The biogas production rate was 4.25 m^3 $m^{-3}d^{-1,}$ and the waste stabilization was 65% (Liu et al., 2012a).

2.3.5 Co-digestion of sewage sludge and domestic organic waste

Studies on a full-scale digester were carried out in a 2000 m^3 CSTR with an HRT of 20 d. Two runs were conducted the first run was conducted with primary sludge and waste activated sludge only and the second was fed with a combination of primary sludge and waste activated sludge to organic waste mass ratio of 3:1 with an OLR of 1.01 kg $m^{-3}d^{-1}$of VS. The waste stabilization efficiency improved from 71% to 81%. The biogas production improved by 80% (Zupančič et al., 2008).

2.3.6 Co-digestion of sewage sludge and fruit waste

A full-scale CSTR reactor of 1 350 m^3 volume with a residence time of 40 days was used. Two experiments were conducted, the first used primary sludge and waste activated sludge only while the second experiment was fed with primary sludge and waste activated sludge: fruit waste ratio of 90:10. The specific methane yield of 0.446 m^3kg^{-1} of VS, from 0.317 m^3kg^{-1} VS in the first experiment showing a 40% increase (Koch et al., 2016).

2.3.7 Co-digestion of sewage sludge, glucose and glucose intermediates

Batch reactions were conducted in 525ml serum flasks, and the flasks were purged with argon. The main substrate was anaerobic sludge and the co-substrates were glucose-

acetate, ethanol butyrate and propionate. The reactors were dosed with 1-5 g/L of the co-substrate mixture to test how much they influence acetoclastic methanogenesis. All experiments were conducted at 35°C. Glucose, ethanol, VFA, methane hydrogen and carbon dioxide concentration were measured. The concentrations of the intermediate and by-products of the digestion of glucose were observed during the experiments indicating that glucose was digested in multiple stages. The concentration of the observed intermediate product was used to determine the stoichiometric values of the different stages of glucose digestion for use in the development of a kinetic model. The model developed had five stages for the degradation of glucose which were a) acidogenesis b) ethanol degrading- acetogenesis c) acetoclastic methanogenesis d) hydrogenotrophic methanogenesis. Other components of the process that were modelled the reactor pH, bacterial decay and inhibition of the degradation steps. The model showed that the two most important reactions are acidogenesis and acetoclastic methanogenesis (Kalyuzhnyi, 1997, Kalyuzhnyi and Davlyatshina, 1997).

2.4 History of Co-digestion at Amanzimtoti Wastewater Treatment Works

The development of the co-digestion was funded by the Water Research Commission under project number K5/2001 while the capital costs were covered by the eThekwini Municipality. The project title was "Co-digestion of high strength / toxic organic effluents in anaerobic digesters at wastewater treatment works". It was initiated in the year 2011, and its objectives were:

1. To investigate the possibility of co-digesting high strength organic and/ toxic effluents with municipality sewage sludge using the capacity of the available digester units at the wastewater treatment works.
2. To develop a protocol to test the effect of industrial effluent before dosing in the wastewater treatment works on the overall performance of the digesters.

The Pollution Research Group, which is under the Department of Chemical Engineering at the University of KwaZulu-Natal, provided scientific support to the eThekwini Municipality for the duration of the project.

2.4.1 Acquisition and identification of kinetic parameters

The Pollution Research Group developed and commissioned Anaerobic Sequencing Batch Reactors (AnSBR) to investigate the parameters needed a co-digestion model. AnSBR was selected because it was had a low-cost method and was easy to operate. The results of the parameter acquisition procedure were that when the AnSBR was dosed with ethanol while pH values and biogas flowrate were measured continuously, only five parameters could be identified. The parameters that are identifiable are carbon dioxide gas mass transfer coefficient, ethanol dosage and parameters associated with the degradation of ethanol (Osborne et al., 2012b).

2.4.2 Development of a model

A simulation of the co-digestion of concentrated industrial waste and sewage sludge from Amanzimtoti Wastewater Treatment Works was conducted by Osborne et al. (2012b) using a steady-state form of the UCT ADM2 model. The different types of UCT models are described in section 0. The focus was on the Ripley Ratio, hydraulic retention time and concentrated waste feed to primary sludge ratio (Osborne et al., 2012a).

2.4.3 Refurbishing Amanzimtoti Co-digestion Pilot digester

A digester at Amanzimtoti Wastewater Works was refurbished and fitted with a mixing pump. Mixing homogenises the sludge composition fulfilling the requirements for modelling the Amanzimtoti Co-digestion pilot digester reactor kinetics. As detailed in **section 2.1.2.2** mixing has an effect on the solubility of gasses, and carbon dioxide is an important gas in biogas production. Hence a better understanding of the impact of mixing on digester kinetics is important. Three 5 m^3 storage tanks were also erected. The mixing pump was a Rotamix system which provided a 432 m^3/h flowrate. The digester was also fitted with gas flowmeter, pH meter and sludge flow meter. The pump and instruments were controlled using an automated system. The storage tanks were also fitted with two pumps, one for receiving concentrated industrial effluent and another for pumping the concentrated effluent to the digester. Flow meters and level sensors were also installed on the storage tank system. The whole storage system was controlled automatically. A laboratory was built at the Amanzimtoti Wastewater Treatment Works next to the refurbished digester. The laboratory was used to screen potential candidate effluents for co-digestion. The laboratory was used to collect experimental data that was used for parameter acquisition. This was completed in 2011.

2.4.4 Development of reactor models

Two batch reactors were dosed by Logan (2016) with 0.065 L expired fruit juice and 9 g of glucose. The two doses had COD values of 1.54 g COD/L and 1.74 g COD /L, respectively. The reported expired fruit juice COD was 130 000 Mg/L O_2. The two experiments were used to test whether glucose can be used to represent fruit juice in a model. The goal was to use the glucose model to predict the performance of a digester dosed with fruit juice. The model was developed on the WEST platform using the UCT ADM 3P model. It was concluded that the model could adequately simulate the digestion of expired fruit juice. The information obtained using the batch reactors experiments and batch reactor model was used to develop a model of the Amanzimtoti Co-digestion Pilot digester (Logan, 2016).

All laboratory-scale digesters showed higher levels of methane production and waste stabilization. Generally, all the full-scale digesters reviewed had improved methane yield and waste stabilization except for Koch et al. (2016), where stabilization was not specified.

Koch et al. (2015) gives results that indicate that VS reduction of up to 35% of food waste can be achieved without destabilizing the process. The variety of substrates used in co-digestion improves nutritional equilibrium resulting in a more flexible process with a more robust microbial population (Mata-Alvarez et al., 2014).

It should be noted that reliable anaerobic co-digestion modelling is necessary to enable forecasting in a clear and measurable manner so that the potentially harmful impact of mixing multiple waste streams in AD is eliminated. Furthermore modelling may decrease the capital and time used in laboratory research in the development of co-substrate choices and loading rates (Mata-Alvarez et al., 2014). The above case studies did not involve any modelling which limits the amount of information that can be extracted from the investigation because there are no consistent experimental conditions.

2.5 Anaerobic Digestion Models

A mathematical model is a collection of equations that express the relationships between critical process parameters in AD such as OLR, biogas volumes, design parameters, and other pertinent parameters in a technically measurable way (Bozinis et al., 1996).

Models are classified as either dynamic or steady-state. Steady-state models are comparatively less complicated; they relate input and output variables of importance under steady-state conditions, permitting for various operational parameters. Models such as this are unable to capture temporal variations in microorganisms during shifts from one steady-state condition to another. However, steady-state models are used to forecast residual substrate concentration, biogas yield and optimal retention time for the breakdown of various wastewaters (Bozinis et al., 1996).

More complicated models are needed to capture the dynamic properties existing at start-up and during various operational perturbations in AD. A comprehensive chemical reaction path has to be used at all stages, employing differential equations, resulting in models that are difficult to solve mathematically; usually, iteration based algorithms are needed to solve them when implementing the model. Computers are used to simulate dynamic models for transient states, identifying potentially harmful operational conditions, where transitional digestion products such as LCFAs may cause substantial inhibition of digestion. Thus simulating a process reduces the need for costly experimental identification of toxic materials by constructing pilot digesters (Bozinis et al., 1996).

A compromise is made between complexity and accuracy of the model. Accuracy is dependent on how many parameters and state variables are involved. A decision has to be made between using a mechanistically derived model and a data-driven model. The selection and details of the model are also partly dependent on how much is already known about the process (Lauwers et al., 2013).

Modelling complicated biological processes includes many factors. A modeller may be unable to deduce some of the factors from experimental data through regression methods, these factors are said to be unidentifiable, and the rest of the factors are termed identifiable (Little et al., 2010).

If parameters are not identifiable, then the next step would be examining parameter sensitivity. This can be done using either global methods or local sensitivity; usually, the latter is used. In certain situations, parameters can be obtained from the literature if the parameters of the experiments are satisfactorily comparable (Lauwers et al., 2013).

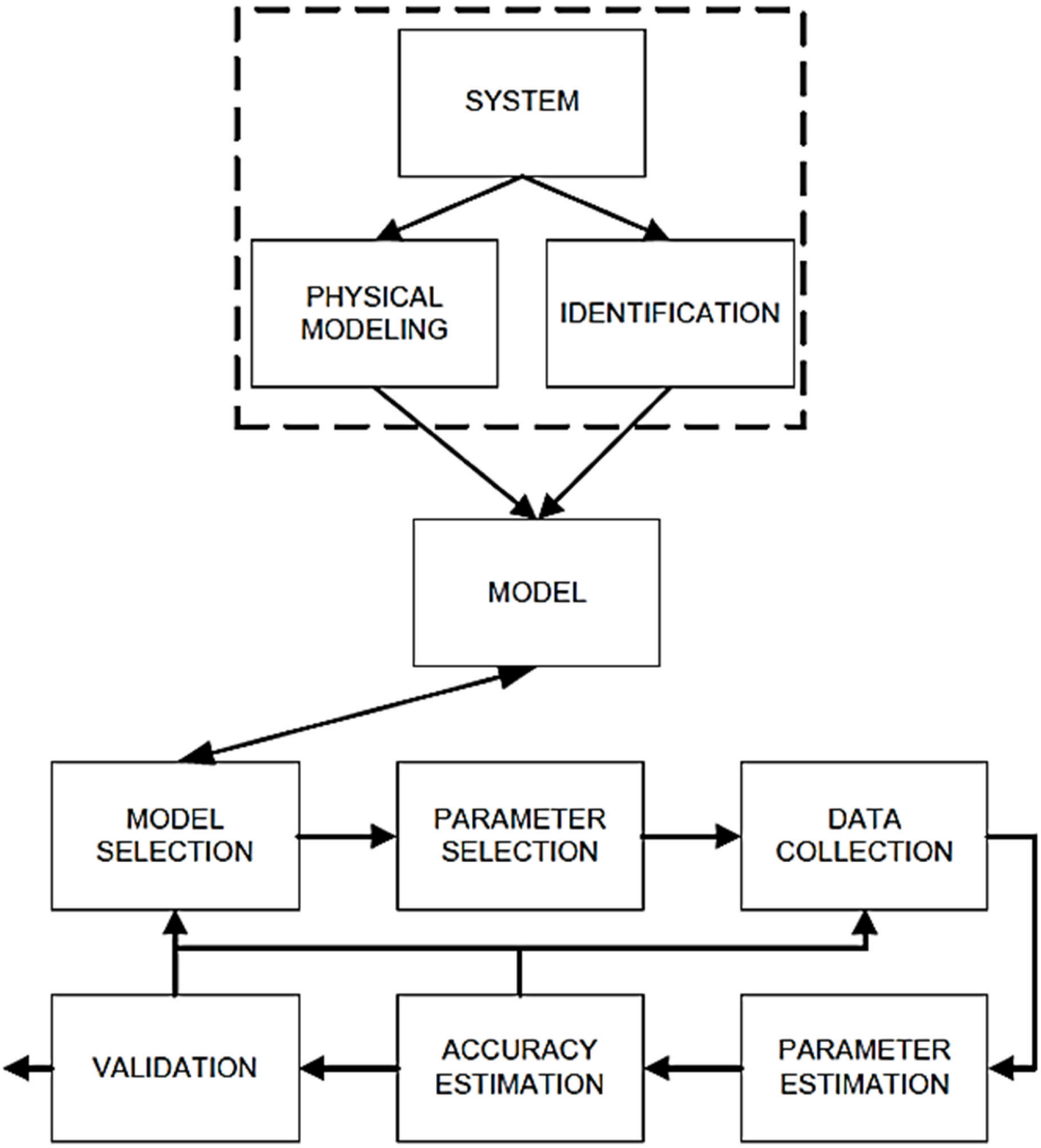


Figure 0-10: Dynamic model method (Lauwers et al., 2013)

In AD determining the available active biomass in the sludge is difficult. Nevertheless, this is usually achieved through (i) assuming that the microorganism concentration does not change (ii) fixing a percentage of the VS concentration to each microorganism population (iii) use of preliminary microorganism concentration estimated from initial digester simulation (iv) use of state-estimators calculated from known parameters (Lauwers et al., 2013).

According to Mahadevan (2009), various factors add to the uncertainty of a system model when it gives predictions. These factors include modelling errors, input variables, approximations

and assumptions, imprecise and sparse data and measurement errors. Lauwers et al. (2013) state that the determination of active biomass has its associated uncertainty which has to be estimated according to how the experiments are carried out. The measured parameters covariance matrix and the sensitivity analysis are used. The confidence interval for the approximated parameters may also be established. When the uncertainty is too high, more experiments should be done. The experimental set up should be developed to produce as much information on the estimated values as possible. In reality, one test with the proposed substrate will not give enough data to know all the values with enough reliability. The reason is that the speed of digestion is determined by the slowest stage in digestion in this instance, it is usually the hydrolysis or the methanogenesis depending on the characteristics of the substrate. In such situations altering the experimental configuration will enable the approximation of the non-limiting kinetics. Pre-existing literature may be used as a source for the unknown parameters (Lauwers et al., 2013).

The product model has to be validated. The quality is measured in terms of the coefficient of determination. The trends of how the data estimates compare with measured values are inspected. If the model predictions are not good enough, a new experimental configuration or a different model has to be used to improve the quality of the statistics (Lauwers et al., 2013).

2.5.1 Anaerobic co-digestion models

Many anaerobic co-digestion models have been produced and used in anaerobic co-digestion investigations. A key feature of recent anaerobic co-digestion models is their ability to ascertain the optimal OLR and ratio of co-substrates and substrates for maximum cost efficiency and energy hence avoiding organic overload. Most anaerobic co-digestion models are mechanistic, and they link important operation parameters (such as OLR and HRT) to digester performance (Xie et al., 2016).

Additionally, contemporary anaerobic co-digestion models are able to simulate process failure hence the enable advantageous working conditions during operation. Digester failure is a common problem in anaerobic co-digestion operation. It is signified by an irreversible drop in pH values and the death of active hydrogenotrophic and acetoclastic methanogens (Xie et al., 2016).

2.5.2 Anaerobic Digestion Model 1

The Anaerobic Digestion Model 1 (ADM1) is based on the assumption that the system is perfectly mixed in its description of AD reactions. ADM1 models physicochemical and biochemical reactions, as shown in **Figure 0-11**.

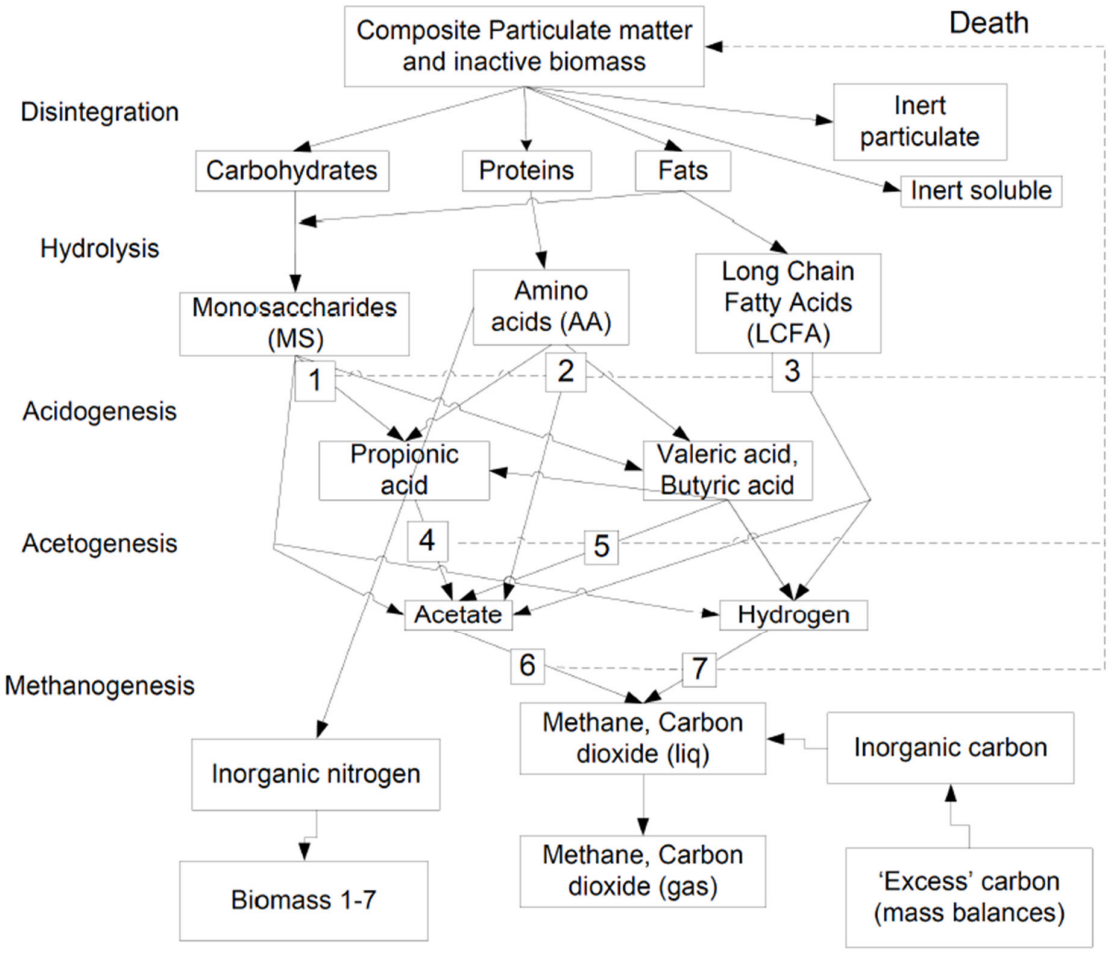


Figure 0-11: ADM1 reaction description (Lauwers et al., 2013)

The model assumes that the extracellular biochemical processes are 1st order as well as using Monod Kinetics for substrate absorption and microbial development. Dead biomass in the model is expressed in terms of 1st order kinetics and is measured as a combined particulate matter. Inhibition to biomass activity caused by pH is also contained in the model (Lauwers et al., 2013).

The ADM1 has algebraic algorithms derived from charge balance continuity, and weak acid/base chemistry. The algorithms are used to model biological processes in AD for the prediction of pH. The algorithms and calculations operate outside of the kinetic model of the ADM1. Weak acid/base water chemistry is not part of the AD kinetic model; hence the algebraic calculations for pH are also outside of the ADM1 model, which are also derived from charge balance. Calculating pH outside the kinetic model can not be easily applied to weak acid/base processes in gas/liquid/solid phases which include precipitation of various minerals (Sötemann et al., 2005b).

The ADM1 has demonstrated that it is a potent means of forecasting and controlling AD. Characterization of proteins, carbohydrates and lipids involves acquiring data that is not usually available for sewage sludge and this makes ADM1 too complicated for everyday use (Demitry, 2016).

2.5.3 Importance of temperature correction in modelling

The ADM1 model has been developed for mainly two temperature, which are 35°C and 55°C. ADM1 contains various gas-liquid transfer reactions, physio-chemical equilibriums, and biochemical reactions, all whose value depends on temperature. A better understanding of AD process parameter temperature dependence is necessary when using the ADM1 at temperatures other than 35°C (Bergland et al., 2015). The Van't Arrhenius equation is used to describe the AD kinetics dependence on temperature.

The Van't Hoff-Arrhenius equation for temperature coefficients is given in **equation 0-3**.

$$k_{T_{k2}} = k_{T_{k1}}\, \theta^{(T_k1 - T_k2)} \qquad \textbf{0-3}$$

Where:

$k_{T_{k2}}$ is the coefficient at the temperature T_k2

$k_{T_{k1}}$ is the coefficient at the temperature T_k1.

θ is the temperature-activity coefficient correction factor.

T_k1 and T_k2 are the reference and actual temperatures, respectively ((Bergland et al., 2015)Kelvin) (Metcalf et al., 2003, Bergland et al., 2015).

2.5.4 University Of Cape Town Anaerobic Digestion Model 1

Because of the difficulties of acquiring data on lipids, carbohydrates and proteins, the hydrolysis of these three components was combined to one step which involves a general species with a formula ($C_XH_YO_ZN_A$) which describes biodegradable substances in sewage sludge. This is a reasonable simplification considering that the final products of hydrolysis are similar, that is SCFAs (Sötemann et al., 2005b).

The composition of Carbon (C), Hydrogen (H), Oxygen (O), and Nitrogen (N) has to be measured to calculate the values of X, Y, Z, and A in the general formula. These calculations are done using direct measurements and modelling output data. Glucose was selected as the idealised end product of the anaerobic digestion of the proposed sewage sludge general formula $C_XH_YO_ZN_A$. It was selected because the action of microorganisms on it are well known, and acidogenesis using glucose will not be likely to be a rate-determining step, and its build-up will not happen even if an AD fails (Sötemann et al., 2005b).

The University Of Cape Town Anaerobic Digestion Model 1 (UCT ADM1) also had the partial pressure of hydrogen added in the model scheme to improve model when a digester fails.

Acidogenesis was separated into two stages under high and low hydrogen partial pressure. Under high hydrogen partial pressure propionic and acetic acids are produced along with H_2 and CO_2.but under low hydrogen partial pressure no propionic acid is produced while the rest of the products remain the same (Sötemann et al., 2005b).

2.5.5 UCT ADM 3P.

AD containing phosphorus (P) sludge requires the inclusion of the phosphates in the weak acid/base system as the discharge of microbial P or polyphosphates has an impact on alkalinity as well as encourages mineral precipitation. Consequently, for better forecasting of pH, the model needs the composition of N and P to be incorporated in the three-phase weak acid/base chemical and physical system (Brouckaert et al., 2010).

Extensions to include ionic components and reactions of the P containing sludge were added to the model. The mathematical representation of the processes was adjusted to handle the greater number of variables in the UCT ADM1. The ionic and biological reactions were represented by kinetic formulas, whereas initially, the biological reactions were expressed as equilibrium reactions (Brouckaert et al., 2010).

2.5.6 Wastewater treatment model simulators

There are various simulators available, namely ASIM, BioWin, EFOR, GPS-X, SIMBA, STOAT and WEST. This project was a continuation of work done by Logan (2016), which used the WEST modelling software; hence WEST was also used in the project.

2.5.6.1 WEST modelling platform

WEST is a platform with a block library that contains a list of components that can be used to create a virtual wastewater system by dragging and dropping the components. A typical example is shown in:

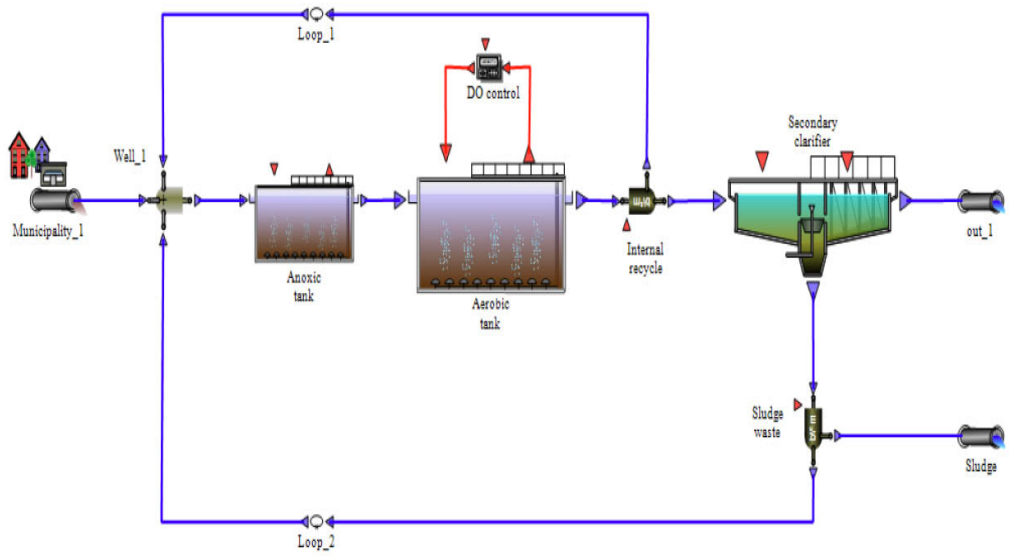


Figure 0-12: Typical block set up and connections as it appears on the WEST modelling platform

The dimension and sizes of the components can be adjusted to suit the needs of the user. The

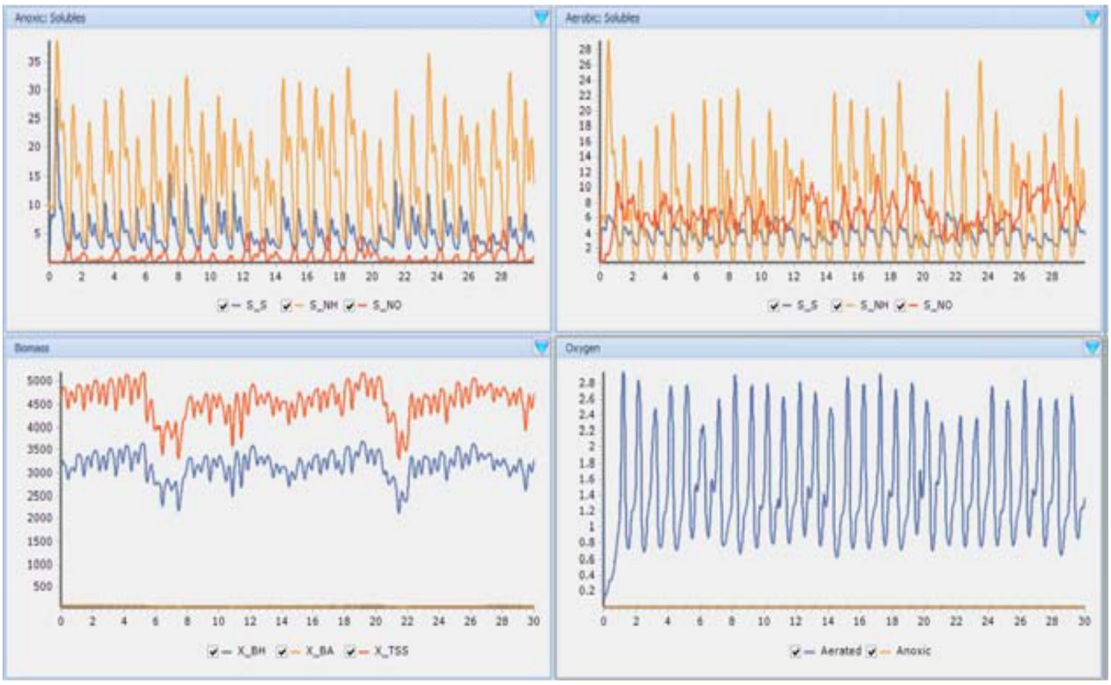


Figure 0-13: Results of a typical simulation on theWEST modelling patform.

system can be simulated at both steady-state and dynamic conditions.

WEST allows for the user to give different parameters weighting according to the priorities they want. A user can choose to give pH a higher weighting than biogas flowrate.

The platform is programmed to for overall species like acetoclastic methanogens, and the sub-species that fall under acetoclastic methanogens are all classified in one group. In reality, only a portion of the subspecies of the acetoclastic population may be active in a given sample of sewage sludge. All the biomass in the model is assumed to be active biomass. Active biomass is the component of biomass that grows through the degradation of nutrients in the sludge.

2.6 Parameter acquisition

Mathematical models are able to help control complicated and usually unstable AD systems; nevertheless, this is subject to the reliability of kinetic model parameters in the important reactions (Lübken et al., 2015).

The biggest problem with models is that they are complex; they are made up of various non-linear differential equations (NDE) with large sets of parameters that one has to adjust. Though a model may reliably approximate a system, the necessary adjustments will require numerous experiments and a lot of computing power to optimize the model. Moreover, the model is only as good as the input parameters fed to it; poor performance is to be expected if the parameters are not well adjusted (Martinez et al., 2012).

The main problem with AD modelling is that there were very few dependable, validated parameters and parameter acquisition techniques. Parameter estimates with realistic uncertainty are now more useful and practically applicable as a result of the use of iterations in parameter estimation techniques and the statistical techniques for estimating parameter uncertainty (Batstone et al., 2004). Some of the difficulties encountered in approximation in of parameters in AD processes are co-relationships between important parameters, inadequate identifiability, and difficult application of the appropriate dynamic test to the system (Batstone et al., 2004).

Bouallagui et al. (2010) used semi-continuous laboratory-scale reactors to simulate the full-scale digester in Tunisia. The results showed that the laboratory-scale experiments were able to approximate the performance of the full-scale digester. This is a possible parameter acquisition method for the Amanzimtoti Co-Digestion Pilot Project.

2.7 Sensitivity analysis

Sensitivity analysis is used to determine whether a chosen parameter or variable is sensitive to changes in model variables or parameters. A sensitivity analysis is conducted for each selected parameter. The parameters with the highest sensitivity are adjusted in an optimization procedure using WEST to improve the profile fitting between the measured data and the predicted values (Logan, 2016).

Osborne et al. (2012b) conducted a sensitivity analysis using a variation of the UCT ADM1 called the UCT ADM2 model. The UCT ADM2 model was used to describe the physico-chemical and biological system of an Anaerobic sequencing batch reactor. The reactor was dosed with ethanol. The parameters most sensitive to pH and biogas flow rate were those associated with the degradation of ethanol as well as the ethanol dosage.

Osborne et al. (2012b) recommended that the biomass concentration should be approximated while other parameters should be set at literature values.

2.7.1 Simplifying the UCT ADM 3P model

The UCT ADM 3P model has various parameters that had to be considered. Simplifying the model was done for easier collection of data and application in the model. Most models are high-dimensional and contain a high number of stoichiometric and kinetic parameters. Although the highly complex model is necessary to represent process dynamics over a wide range of operating conditions, this can cause substantial computational strain for analysis and simulation moreover it requires extensive experimental programs to establish the parameter values that are needed. Overall model validity is not always necessary for some applications, and in such cases, a simpler model with the limited operating scope is more beneficial (Anderson et al., 2000, Janssen et al., 2000).

The advantages of simplifying the model are:

1. Makes the project application more cost-effective
2. Operation of the model has fewer input requirements, and fewer types of data are needed in fewer numbers.
3. A simpler model is easier to combine and/or transfer to other models.
4. Interpreting a simplified model is easier. A model with fewer parameters is easier to understand than a model with additional parameters (Rexstad and Innis, 1985).
5. Controller tuning is easier and more efficient

2.7.2 Problem specification

Problem specification is a critical step in the modelling process which involves analysing the problem so that the modeller may determine clear objectives that the model should fulfil. The objectives guide how the model is developed (Olsson and Newell, 1999). During problem specification certain conditions need to be clarified, for example, the time scale of the solution, the environmental conditions, the system boundaries, the expected accuracy of the results and the degree of uncertainty (Dochain and Vanrolleghem, 2005).

Biomass action in anaerobic sludge is heavily affected by temperature (Van Lier et al., 1996, Donoso-Bravo et al., 2013). Nevertheless, it has hardly been considered explicitly for modelling anaerobic systems. Most industrial wastewater treatment plant are normally operated at constant temperature; hence temperature effects are also considered constant (Donoso-Bravo et al., 2013).

The current UCT ADM 3P uses default temperature coefficient derived from literature values and the work done by Logan (2016)was done at 35^{o}C only. The model was used on a laboratory batch reactor with the intention to transfer the batch reactor kinetic data to the ACP model. The ACP operates at ambient temperature, but the laboratory batch reactor was operated at 35^{o}C (Logan, 2016).

2.7.3 Data collection

Data needs to be collected to initialise, calibrate and validate a model. The data required includes design and operational data, hydrodynamic data, composition and concentration of microbial species populations and effluent streams composition (Mhlanga, 2008).

The elemental composition of sewage sludge inert soluble, particulate and organic fraction is different for each wastewater treatment plant. Even when the other data from wastewater treatment plants are similar, the fractionation of the sewage sludge is different. Thus a model is specific to a particular wastewater treatment plant. Plant specific data is needed in order to develop a model so as to ensure that the model reflects the performance of the plant. The data needed for calibration is typically sourced from (Donoso-Bravo et al., 2011):

- Literature
- Pilot-scale and laboratory-based experiments
- Grab samples
- Full-scale-plant data
- Full-scale plant mass balance
- Off-line and on-line plant data (Mhlanga, 2008).

2.7.4 Model implementation

The system of equations used to describe a plant in WEST is used for simulation. When a model is implemented during the simulation, the ordinary differential equations are numerically integrated, and the algebraic equations are solved simultaneously. The methods available for numerical integration in WEST are the

- Fixed step integrator
- The stiff solver (VODE)
- Adaptive step-size integrator (RK4ASC)(Mhlanga, 2008)

The fixed step-size integrator uses a constant step for each integration of the ordinary differential equations. There are various fixed-step integrators in WEST. The stiff solvers achieve high sensitivity in stiff systems. Stiff system have large differences in the time constraints in their processes. The VODE (rdrr.io, 2019) stiff solver is available in WEST. The adaptive solver varies the step size to optimize the speed and accuracy of the calculation.

2.7.5 Parameter estimation

Parameter estimation is usually based on minimisation or maximising a goodness-of-fit criterion such as Weighted Least Squares, Least Squares or Maximum Likelihood. The objective is to generate values for parameters within the model. There are various powerful estimation algorithms available for parameter estimation, no matter how powerful they are all dependent on the quality of the experimental data (Dochain and Vanrolleghem, 2005).

2.7.5.1 Parameter selection

The parameters with the greatest influence on the selected measured variables are selected using sensitivity analysis (Osborne et al., 2012b).(See **section 0**). The degradation of ethanol was studied with a focus on parameter identification for regression. The results showed that the identifiable parameters for which pH and biogas flowrate are sensitive are limited to those associated with acetoclastic methanogenesis and ethanol dosing (Osborne et al., 2012b).

2.7.5.2 Calibration

Calibration is when a model is adapted to fit information from the plant under study. The quantity and quality of the information used for calibration and the objective of the study determine how the model is calibrated (Mhlanga, 2008).

The information is obtained using well-controlled and specific experiments at bench and pilot scale under the assumption that known operating conditions are maintained. Values from small-scale plants are not always reliable because setting up the small-scale plant exactly the same way as the full-scale plant is difficult which changes the behaviour of the microbial population and the conditions that have an influence on parameters which are being determined. Moreover, the calculations and experiments are based on the assumption that the coefficients are constant while the nature of the wastewater may change in a matter of hours. Wastewater composition has a profound influence on model behaviour, and this amplifies the challenges of the calibration procedure (Jeppsson, 1996).

2.7.6 Validation

An assessment of the quality of the model prediction is used to validate the model. Thus the parameters from the calibration are also tested for accuracy. Validation confirms how confident a modeller is on the predictive capability of the model. Validation can be done either through cross-validation or direct validation (Donoso-Bravo et al., 2011).

Direct validation is when the model is evaluated in terms of how many experimental data fits the data generated by the model. Cross-validation is when model-generated data is compared to fresh, experimental data to confirm model predictions (Donoso-Bravo et al., 2011).

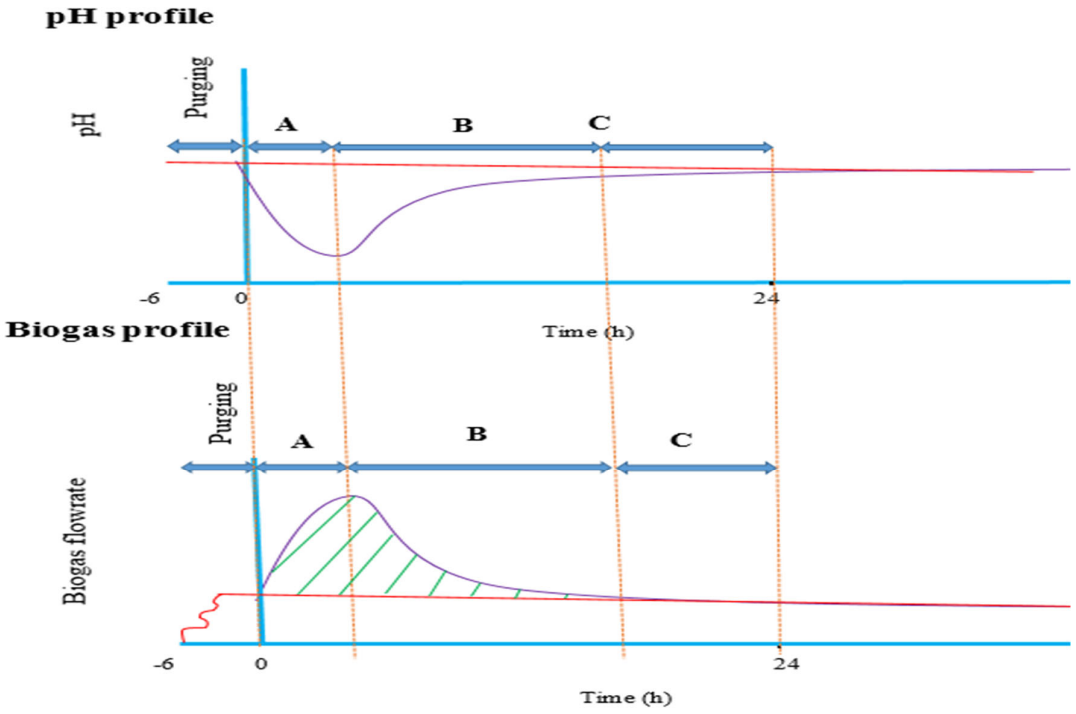


Figure 0-14: Typical characteristics of fruit juice digestion adapted from Kalyuzhnyi (1997), Osborne et al. (2012b) and Logan (2016),

The pH and biogas flowrate profile developed by Kalyuzhnyi (1997), Osborne et al. (2012b) and Logan (2016) is given in the diagram **Figure 0-14.** The experimental data used to validate the model must be reproducible for it to be useful in the validation procedure. Hence replicate experiments have to be conducted, and their consistency analysed before they are used for validation (Downing, 2004). The validation procedure confirms that the models that have been developed can be used to control the Amanzimtoti Co-digestion Pilot digester. **Figure 0-14** shows the typical characteristics of fruit juice digestion adapted from Kalyuzhnyi (1997), Osborne et al. (2012b) and Logan (2016) that can be used to validate the prediction quality of the UCT ADM 3P model. Logan (2016) conducted experiments where two experiments were conducted simultaneously using digester sludge from the ACP. In the first instance, expired fruit juice was dosed, and in the other nothing was dosed. The results of Logan (2016)'s experiments showed that the pH values and biogas flowrate of the first experiment converged to become similar to the experiment where nothing was dosed. The red line in both the pH and biogas profile represents endogenous anaerobic digestion when nothing is dosed in the digester. At - 6 h sludge is added to the digester and then during the period labelled **Purging** oxygen is displaced after sealing the digester by allowing an anaerobic environment to develop in the digester. After Purging expired fruit juice is dosed at time 0 h causing the pH value to decrease while the biogas flowrate increases at the same time. The green shaded area in the biogas profile represents the volume of biogas produced from the digestion of expired fruit juice.

According to the UCT ADM 3P, the period labelled **A** represents the production of VFA, which lowers the pH, the decrease has the potential to destabilise the digester. This will happen if the digester is overloaded with expired fruit juice. The VFA is consumed and causes a rise in biogas production until it reaches the highest value at the same time when the pH value is at its lowest. During period **B,** the rate of VFA production is less than the consumption for the production of biogas, hence the biogas production rate decreases. In period **C,** all the fruit juice has been consumed, and the pH and the biogas reach a steady state as the LCFA in the sludge are digested as endogenous digestion resumes it predominance. The recovery of the pH value after it decreases (within 24 h) indicates that a safe amount of expired of fruit juice has been dosed.

According to the UCT ADM 3P, the pH is also expected to recover to the initial pH as shown in **Figure 0-14** (Kalyuzhnyi, 1997, Kalyuzhnyi and Davlyatshina, 1997, Logan, 2016, Osborne et al., 2012b, a). As indicated in **section 2.1.4.3,** pH is one of the critical parameters for digester stability and control hence validating the pH model prediction is more important than validating the biogas production. In the pH profile period **A** and period **B** are the most important and a model's ability to model the decline and recovery of the pH are used to assess the quality of the validation.

According to Bond et al. (2011), the methane yield from co-digestion is additive, hence stoichiometrically determined methane yield can be used to do a material balance. The material balance is used to confirm how much more biogas can be collected by adding a co-substrate. The biogas produced from the laboratory screening experiments can be compared to the theoretical yield to determine if all the co-substrate has been digested. Trapezoidal Riemann sum (Anton et al., 2010) was used by Logan (2016) to calculate the biogas volume produced in each experiment. The area shaded in green on the pH profile represent the volume of biogas produced by digesting the expired fruit juice. The consistency of volume produced was used to confirm whether the amount of expired fruit juice dosed was the same in each experiment. This was based on the assumption that the dosing the same amount of fruit juice in each experiment

will result in the same amount of biogas produced. The dosed amount should produce a biogas flowrate that is within the limits of the equipment.

2.7.6.1 Criteria for validating the replicate experimental pH values and biogas flowrate from the laboratory screening experiments

The criteria used to validate the quality of the experimental data that is generated from laboratory screening batch reactors is summarised from **section 2.76**.

Table 0-2 shows that the criteria for validating the replicate pH values and biogas flowrate experimental data comparing the time taken to reach minimum pH for replicate experiments summarised from s**ection 0.**

Criteria	***Indicator***
1. Time taken to reach minimum pH after addition of expired fruit juice	*Maximum difference of 1 h allowable for the time taken to reach minimum pH after addition of expired fruit juice*
2. Safe ratio of fruit juice to sludge	*Recovery of pH in 24 hrs (within the safe operating range)*
3. Material balance	*Maximum difference of 50% allowable for the volume of biogas produced (area under biogas profile)*
4. Equipment limits	*Flowrate limits to between 20 mL - 50 mL*

2.7.6.2 Criteria for validating the pH values and biogas flowrate from the model predictions

The criteria used to validate the quality of the model after regressing the data from the laboratory screening batch reactors is summarised from **section 0**.

Table 0-3 shows the three criteria for validating the pH values and biogas flowrate predicted by the model summarised from **section 0**

Criteria	***Indicator***
1. Matching of initial experimental conditions the initial model conditions	*Maximum pH value difference of 0.1 between initial model pH and initial experiment pH*
2. Reaction rate	*Maximum difference of 1 h or less for the time taken to reach minimum pH*
3. Matching the buffering capacity	*Maximum difference of 0.1 or less in minimum pH value*
4. Matching the buffering capacity	*Difference in recovery of pH monitored by inspection*
5. Material balance	*Maximum difference of 50% allowable for the volume of biogas produced (area under biogas profile)*

2.8 Conclusions from the literature survey

Although AD offers several benefits, more research needs to be done to improve process control and stability. As a result of these challenges wastewater treatment plants are designed to compensate for lack of stability and ease control by incorporating excess capacity to reduce the risk of failure. Although the plants are designed with the excess capacity, they are still conservatively operated, which increases poor performance. To realise the full potential of the process, a better understanding of AD and effective process control and monitoring is required.

Co-digestion can improve biogas production while offering several advantages, as stated in **section 0,** but because of the variations of the composition of co-substrates, process stability and control are complicated. AD operates within a narrow range of pH values, and the introduction of co-substrates increases process perturbations. Effective process control is of paramount importance in co-digestion, and the most important parameter in process control is pH. In this project, a method was developed to control the co-digestion of the expired fruit juice process effectively.

2.8.1 Modelling pH

In this project, CO_2 partial pressure (p_{CO2}) had the greatest impact on pH. It was also assumed that during normal (pH 6.5-7.5) operations, other components such as VFAs have a limited impact on pH. Details of normal operating pH are given in **section 0**. When p_{CO2} increases, the pH is lowered if the alkalinity is constant. When p_{CO2} decreases pH rises if the alkalinity is

constant. As detailed in **section 2.1.4.4,** alkalinity gives a digester buffering capacity. From **equation 0-4** the removal of CO_2 does not affect alkalinity. It is also noteworthy that the removal of carbon dioxide is dependent on the Kla of carbon dioxide. pH is modelled by accounting for the ability of a system's to increase or decrease the dissolved carbon dioxide (Olsson and Newell, 1999).

$$CO_3^{2-}(aq) + 2H^+(aq) \rightarrow H_2CO_3 \rightarrow\uparrow CO_2(g) + H_2O(liq) \qquad \textbf{0-4}$$

The details of how the pH model was built are detailed in **Appendix A**. **Section 2.1.2.2** gives details of the importance of gas mass transfer coefficients as well as digester mixing in gas-liquid equilibrium. As detailed in **section 0** carbon dioxide is the most important gas in digester pH hence determining the Kla for carbon dioxide is necessary for pH modelling.

2.8.2 STAGE 1: Data acquisition from the laboratory batch reactor

Case studies show that co-digestion does have a positive impact on AD but only for a specific OLR. Exceeding the specific ORL results in digester instability. This reinforces the assertion that co-digestion requires process control to reduce the probability of digester failure. The feedback control loop in **Figure 0-7** was the method proposed to control the digester. The data acquisition STAGES are STAGE 1 and STAGE 4, which correspond to the experiments in which the pH values and biogas flowrate profiles were measured in the case studies described in **section 0**.

The Laboratory Batch Reactor will be seeded from the Amanzimtoti Co-digestion Pilot Project digester and dosed with a single dose of expired fruit juice, the pH values and biogas flow rates will be measured. The experiments will be run at 25°C and 35°C. As indicated in **section 0,**

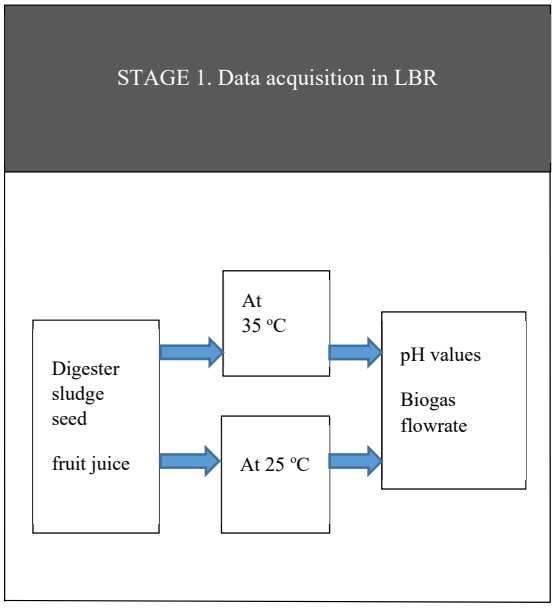


Figure 0-15: STAGE 1 of the feedback control loop shows that the Laboratory Batch Reactor will be seeded from the Amanzimtoti Co-digestion Pilot Project digester and dosed with a single dose of expired fruit juice, the pH values and biogas flowrates will be measured. The experiments will be run at 25°C and 35°C

the ADM1 model and model based on the ADM1 Model were designed for use for 35°C. Experiments conducted at temperatures other than 35°C require temperature correction. The data acquired from these experiments will be the pH profile and the biogas profile over 23 h. This data will be passed on to STAGE 2.

2.8.3 STAGE 2: Calibration and validation of laboratory batch reactor model

Modelling can be used to improve the understanding of AD as well as to improve process control. Modelling can also capture the effect of co-substrates in AD. This improves the understanding of AD while simultaneously improving process control.

The WEST modelling platform detailed in **section 2.5.6** will be used for all modelling activities in the feedback control loop. The biogas flowrate and pH data, which will be obtained in STAGE 1 and 4 will be used in the development of models as part of the second and fifth STAGEs of the feedback control loop.

The pH values and biogas values collected over 23 from STAGE 1 will be combined with literature values in the initial simulations to calibrate models of the LBR at 35°C and 25°C.

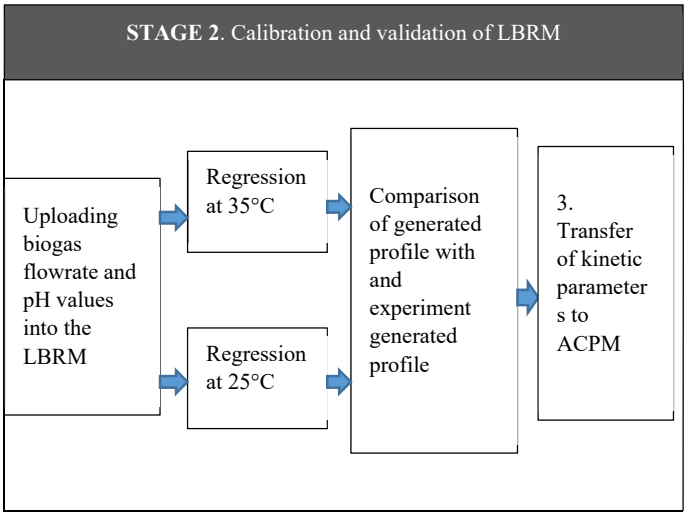


Figure 0-16: STAGE 2 of the feedback control loop shows that the pH values and biogas values from STAGE 1 will be combined with literature values in the initial simulations to calibrate models of the LBR at 35°C and 25°C.

To get the temperature correction coefficient indicated in **section 2.5.3,** regression is required. Hence **Figure 0-16** shows that regression will be done at the two temperature.

2.8.4 STAGE 3. Transfer of kinetic parameters to Amanzimtoti Co-digestion Pilot Project Model

STAGE 3 of the feedback control loop consists of mathematical operations which will be used to adjust results for transfer of extensive properties from the laboratory batch reactor (0.0065 m^3) to the Amanzimtoti Co-digestion Pilot Project (2 000 m^3) due to their differences in scale and methods of operation.

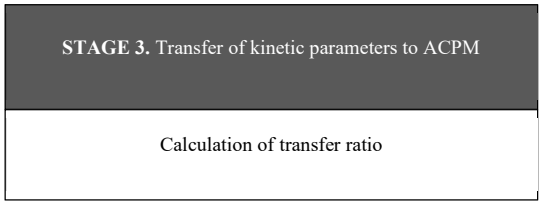


Figure 0-17: STAGE 3 of the feedback control loop where extensive properties of the laboratory batch reactor will be transferred to the Amanzimtoti Co-digestion Pilot Project digester

2.8.5 Stage 4.0: Estimation of the ACP carbon dioxide gas mass transfer coefficient (Kla)

The importance of the carbon dioxide mass transfer coefficient in the modelling the ACP pH is detailed in **section 0**. To estimate the Kla, two experiments will be conducted for 23 h each. They will be done by maintaining normal daily primary sludge dosage while varying the pump mixing duration.

40 m^3 of primary sludge will be dosed once per day in 2 h. During normal ACP operation, the mixing pump is turned on for three hours and off for three hours 24/7. The first set of experimental data will be collected over 23 while the mixing pump will be cycled on for two hours and off for four hours. The second set of experimental data will be collected over 23 h while the mixing pump will be turned on for four hours and off for two hours. Greater and lesser than normal mixing times will be selected to test their influence on the Kla value

The pH values and biogas flowrate experimental data over 23 h will be uploaded to the WEST modelling platform and regressed separately. The regression will be done using the ACPM model developed using the kinetic data transferred from STAGE 3 on the WEST modelling platform. Two values for Kla will be obtained, representing the upper and lower limit of Kla.

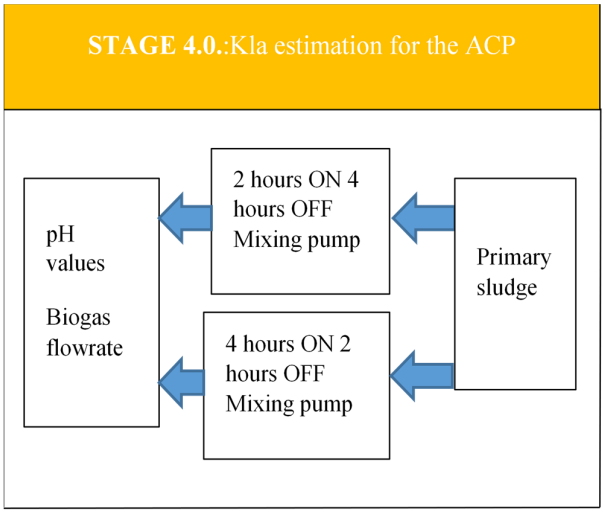


Figure 0-18 shows that two experiments will be conducted to approximate the Kla value. The first set of experimental data will be collected over 23 while the mixing pump will be cycled on for 2 h and off for 4 h. The second set of experimental data will be collected over 23 h while the mixing pump will be turned on for 4 h and off for 2 h

2.8.6 STAGE 4: Data acquisition from the Amanzimtoti Co-digestion Pilot Project

STAGE 4 will consist of a single experiment to determine the effect of fruit juice on the digestion process. A single experiment will be conducted. 40 m^3 of primary sludge (pumped in two hours) will be dosed first then five cubic meters of expired fruit juice (pumped over an

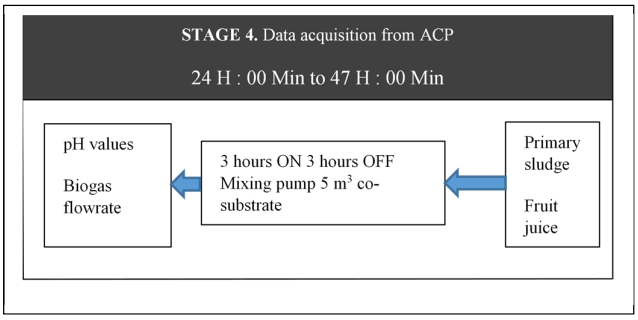


Figure 0-19 shows that a single experiment will be used to determine the effect of fruit juice on the digestion process. 40 m^3 of primary sludge (pumped in 2 h) will be dosed first then 5 m^3 of expired fruit juice (pumped over an hour) will be dosed while the mixing pump will be on for 3 h and off for 3 h for 23 h (normal operation).

hour) will be dosed while the mixing pump will be on for three hours and off for three hours for 23 h (normal operation).

2.8.7 STAGE 5: Calibration and validation of the Amanzimtoti Co-digestion Plant Model

pH and biogas flowrate values collected over 23 h from STAGE 4, and the average Kla value from STAGE 4.0 will be used to develop a model for the Amanzimtoti Co-digestion Pilot Project.

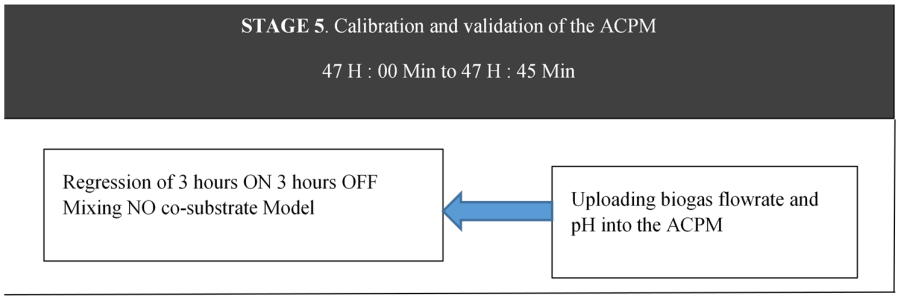


Figure 0-20 shows that pH values and biogas flowrate from STAGE 4 and the average Kla value from STAGE4.0 will be used to develop a model for the Amanzimtoti Co-digestion Pilot Project

The WEST modelling platform will be used for all the activities of STAGE 5. The pH values and biogas flowrate experimental data over 23 h from STAGE 4 as well as the Kla value estimated in **section 2.8.5** will be used for regression to calibrate the ACPM.

2.8.8 STAGE 6: Transfer of kinetic parameters in the feedback control loop

STAGE 6 of the feedback control loop is the same as STAGE 3 of the feedback control loop. The difference is that the inverse of the ratio used in STAGE 3. STAGE 6 consists of mathematical operations which will be used to adjust results for transfer of extensive properties

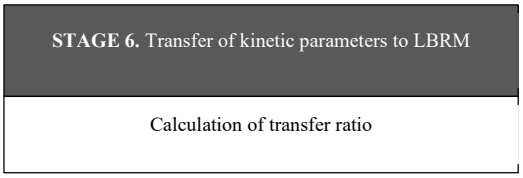


Figure 0-21: STAGE 6 of the feedback control loop consists of mathematical operations which will be used to adjust results for transfer of extensive properties from the Amanzimtoti Co-digestion Pilot Project (2 000 m^3) to the laboratory batch reactor.

from the Amanzimtoti Co-digestion Pilot Project (2 000 m^3) to the laboratory batch reactor (0.0065 m^3) due to their differences in scale and methods of operation.

2.9 Overall conclusion

The combination of STAGE 1, STAGE 2, STAGE 3STAGE, STAGE 4, STAGE 5, and STAGE 6 gives rise to **Figure 0-22**.

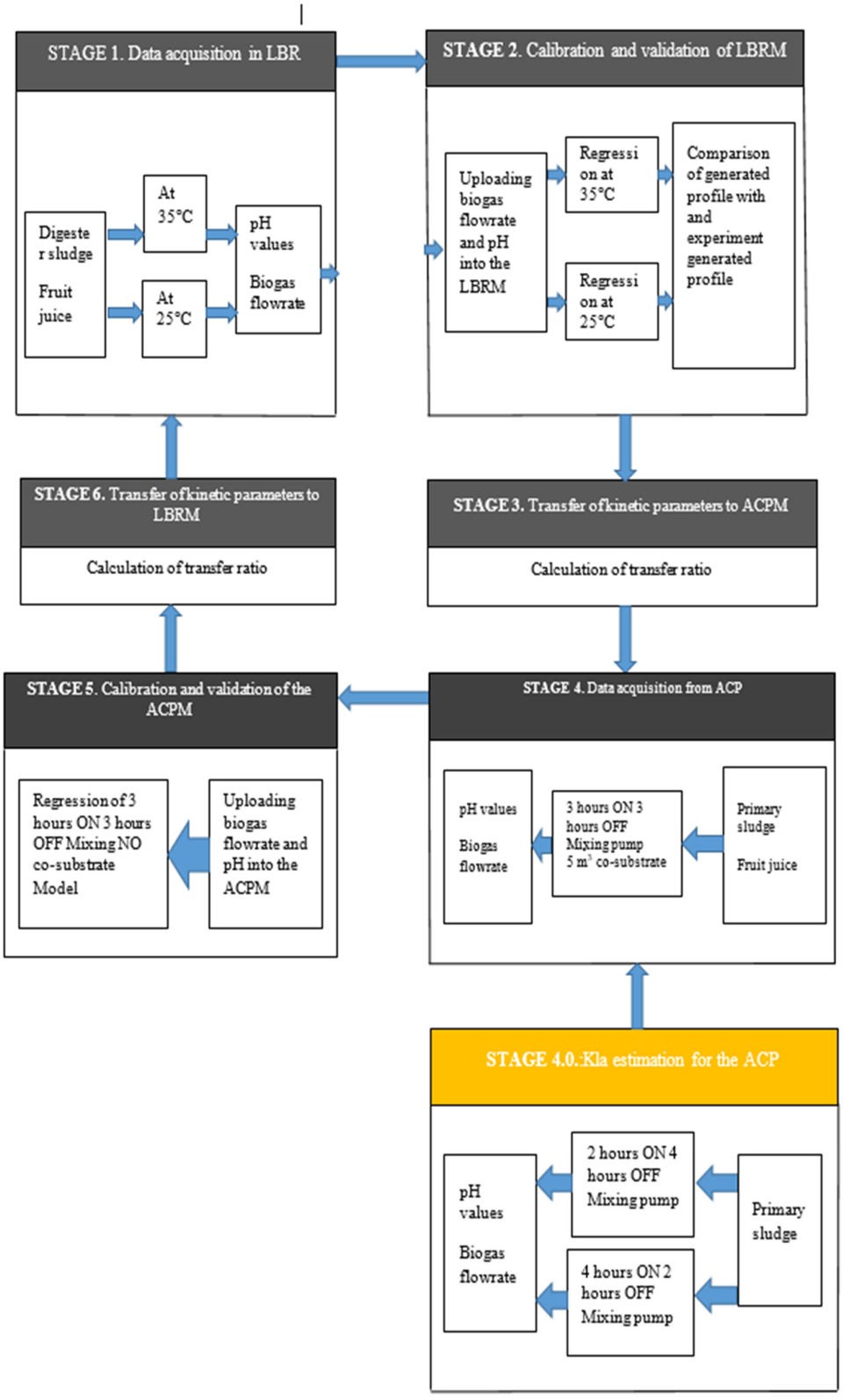


Figure 0-22 shows the details of the overall feedback control loop for each stage

2.10 The necessity of simplifying the model

The UCT ADM 3P model in WEST modelling platform is complex and can be used to model anaerobic digestion under a variety of conditions which require a large set of parameters to represent them. The objective was to predict the short term effect of dosing the digester with fruit juice co-substrate. The UCT ADM 3P model has approximately 600 parameters. Approximately 60 were relevant to the project. Instead of rewriting the model to remove the irrelevant parameters, it was set to values that had little or no impact on the model under the conditions that were being tested. The details of the parameters are listed in **Appendix B, Appendix C and Appendix D.**

This reduced set of parameters could be used in the calibration and validation procedure as indicated in **section 2.8.3** and **section 0**; however, the number of parameters (60) was still too high and would make the computation complex and time consuming for the experimental procedure. Adjusting all the parameters required to get the highest possible accuracy requires high computational and data cost; moreover, this can lead to poor parameter identifiability because of the non-linear nature of the model. Even when there is enough data available to identify every model parameter to produce a model that reproduces the experimental data accurately, calibration can show that model is overcalibrated. The overcalibrated model will not be able to predict digester performance under different conditions (Donoso-Bravo et al., 2011). Osborne et al. (2012b) confirmed that increasing the number of parameters used for regression reduces the accuracy of the model.

Because of the limitations of parameter identification, identifying all the parameters was not possible hence the key to modelling the influence of expired fruit juice in the digestion process was selecting only the parameters with the greatest influence from the available data and fixing the rest of the parameters to literature values.

The feedback control loop cycle was designed for short term prediction of the ACP's response to a dose of fruit juice. From the time the fruit juice is delivered to the storage tanks, to the time that the fruit juice is dosed less than 24 h. There is only enough time to go through the feedback control loop cycle once, and only a single set of conditions can be identified and tested in the procedure. There is no time to test more conditions. Considering that the target was short term prediction of the effects of fruit juice as long as the tested condition enables successful short term prediction any deficiencies in the model can be rectified through successive use of the feedback control loop. Long term prediction can be undertaken in parallel with short term prediction but it was not the objective of the study.

In the current project analysis of digester sludge before and after co-digestion was not considered. As indicated in the paragraph above analysing the digester sludge would the time needed for completing the feedback control loop. Moreover, the information gained from analysing the digester sludge may not necessarily improve the predictions of the model.

The combined knowledge of the co-substrate and sludge characteristics, together with a model sensitivity analysis enabled the most important model parameters to be identified and used in the hypothesis.

2.11 Parameter selection

According to Kalyuzhnyi and Davlyatshina (1997), the two most important reactions in glucose degradation are methanogenesis and acidogenesis. An investigation by Osborne et al. (2012b) into the co-digestion of sewage sludge and ethanol showed that biogas flowrate and pH are sensitive to carbon dioxide gas mass transfer coefficient, ethanol dosage and parameters associated with the degradation of ethanol (maximum specific growth rate, half-saturation constant and biomass concentration). In the current study the co-digestion of digester sludge and fruit juice, was assumed to be sensitive to the same parameters.

The degradation of glucose, as indicated in **section 0,** is described by the Monod equation. From the two reactions acidogenesis and acetoclastic methanogenesis, acetoclastic methanogenesis was selected as the focus of the sensitivity analysis because it is the main pathway for anaerobic digestion of sugars (Ziemiński and Frąc, 2012, Speece, 1983). From **section2.10,** the necessity of simplifying the model was explained; hence as long as the selection enabled the achievement of the project objectives, a single reaction would suffice.

To further simplify the regression procedure, the minimum number of parameters possible was selected from the various parameter associated with acetoclastic methanogenesis in **equation 0-5.**

$$R\_am = mu\_am[X\_am] \times \frac{[S\_Ac]}{k_{s\_am} + [S\_Ac]} \qquad \textbf{0-5}$$

Where:

R_am (g/day) is the acetoclastic methanogenesis reaction rate

mu_am (1/day) is the acetoclastic methanogens the maximum specific growth rate

k_{s_am} (g/m^3) is the acetoclastic methanogenesis half-saturation constant

$[X\_am]$ (g) is the acetoclastic methanogens biomass concentration

$[S\_Ac]$ (g/m^3) is the acetate substrate concentration

At low $[S\_Ac]$ concentration, the reaction rate R_am is sensitive to k_{s_am}. At high $[S\_Ac]$ concentration R_am is sensitive to the maximum specific mu_am. mu_am and k_{s_am} are potential parameters that can be identified for use in the regression procedure, but noise in biogas flowrate data at low substrate concentration reduces the practicality of identifying k_{s_am} for regression in the onsite laboratory facility. The reaction rate is directly proportional to the biomass concentration $[X\_am]$ (Logan, 2016, Osborne et al., 2012b). The objective of the current project was to control the process by determining the highest concentration of fruit juice that can be dosed without the reaction failing hence substrate concentration will be high when the digester fails, and k_{s_am} will not be a viable parameter for regression At high substrate concentration R_am is sensitive to mu_am hence it is a viable parameter for identification. But in the dosing of the Amanzimtoti Co-digestion Pilot digester, the substrate concentration will be limited to reduce the chances of digester failure; hence the mu_am value used for regression was obtained from the literature. The half-saturation constant (k_{s_am}) and the acetate substrate concentration $[S\_Ac]$ was set at literature values.

Equation 0-5 contains the product of *mu_am* and [*X_am*] indicating that they can be interchanged for regression. Logan (2016) used *mu_am* for his regression, but in the current project, *X_am* was selected.

From the list given by Osborne et al. (2012b) in **section 0,** some parameters were selected to be fixed at literature values, and some were used during the regression. Carbon dioxide mass transfer coefficient (Kla), Hydrogen ions, and Carbonate ions were selected for regression because they were key parameters in the modelling of pH. The details of how pH is modelled in the literature are given in **Appendix A**. Temperature is the parameter in the hypothesis proposed in **section 0;** therefore, it was selected for regression**.** Glucose concentration represents fruit juice in the model, and the feedback control loop was designed to control the dosing of fruit juice; hence glucose concentration was part of the regressed parameters.

Osborne et al. (2012b) note that when the yield coefficient is fixed, the biomass concentration becomes experiment-specific. Hence in this study, the biomass concentration was experiment-specific which would improve the model's ability to capture the acetoclastic methanogens' response to fruit juice dosing.

Table 0-4: Parameters used in regression and literature sourced parameters in the model

Parameters	
Determined by Regression	***Literature sourced values***
Carbon dioxide mass transfer coefficient (Kla)	*Half-saturation constants for* 1. *Acidogens,* 2. *Acetogens,* 3. *Acetoclastic methanogens* 4. *Hydrogenoclastic methanogens*
Temperature (Temp)	*Temperature coefficient*
Hydrogen ions	*Mass of organics* • *unbiodegradable* • *biodegradable*
Carbonate ions	*VFA*
Glucose concentration in co-digestate	*Calcium*
	Magnesium
	Chlorine
	Ammonium ions
	• *Mass of:* • *Acetogens* • *Acidogens* • *Hydrogenoclastic methanogens*
	Yield of • *Acidogens,* • *Acetogens,* • *Acetoclastic methanogens* • *Hydrogenoclastic methanogens* • *Acetoclastic methanogens*
	• *Mass of biodegradable influent* • *Mass of unbiodegradable influent*
	• *Mass of biodegradable organics* • *Mass of unbiodegradable organics*

Parameters that were manipulated in the model are in the ***Determined by Regression*** column, and those in the ***Literature sourced values*** column were set at literature values. The source of the literature values was Logan (2016).

2.12 Temperature hypothesis

The investigation by Logan (2016) and (Kalyuzhnyi and Davlyatshina, 1997) were undertaken at 35°C, which is the standard temperature for ADM1 based models, as indicated in **section 2.5.1**. The details of these two case studies are given in **section 0**. The reaction kinetics are faster at 35°C than at 25°C. Conducting data acquisition experiments at 35°C is faster, which improves the speed of the data acquisition. In this project, 35°, C experiments were conducted as well as additional runs at 25°C. As indicated in **section 11,** many parameters used

in the model were set at literature values; hence it was important for the literature source to have similar conditions to those being tested. Using 35°C in the current project would enable the literature values to improve the model's predictive capability. The Amanzimtoti Co-digestion Pilot Project operates at 25°C while data acquisition was made at 35°C; hence it was hypothesised that:

> ***"Kinetic data collected from the Laboratory Batch Reactor Model at 25°C and 35°C can be transferred to the Amanzimtoti Co-digestion Pilot Project Model."***

Figure 0-23 shows how the ***temperature hypothesis*** is tested. And **Figure 0-24** shows how the ***temperature hypothesis*** circled in green in fits in the overall activities of the project as a preparatory step.

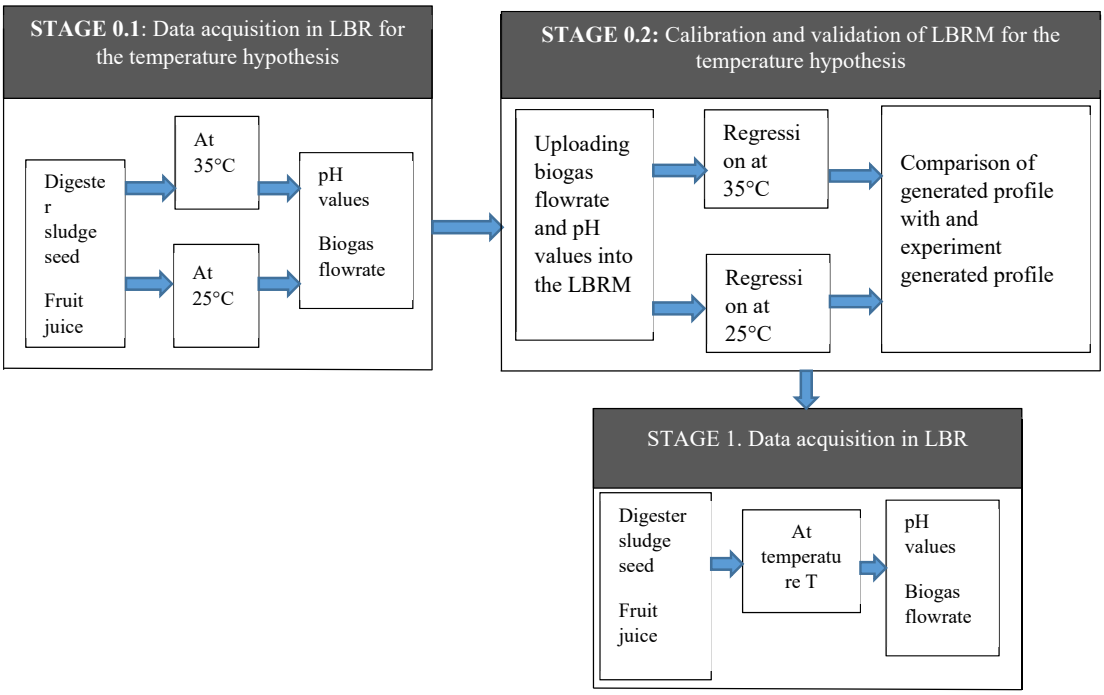


Figure 0-23: ***Temperature hypothesis*** test shows that the result of the hypothesis test (STAGE 0.1, STAGE 0.2) was used in STAGE 1 of the feedback control loop

2.13 Feedback control loop hypothesis

[X_am] represents a model construct for active biomass in the model. The difference between active biomass and biomass is that active biomass are the microorganisms that digest nutrients in the sludge, but biomass represents microscopic living organisms present in the sludge. Evaluating active biomass concentration through experiments is difficult and time-consuming; hence it can only be indirectly determined using the model construct. Most laboratory methods can determine biomass concentration but not active biomass concentration (Yücesoy et al., 2012). Determining active biomass concentration requires isolating the active biomass from the rest of the microbial population in the sludge. These challenges make it an ineffective

method for use in short term prediction for AD. Hence using the model to evaluate it indirectly was chosen for its simplicity and quick evaluation.

The project was designed to control the Amanzimtoti Co-digestion Pilot Project (ACP) by using data obtained from the LBR using a model. The control protocol based on the process model had to be sensitive, fast, and simple; hence it was hypothesised that:

> ***"Acetoclastic methanogen biomass concentration, biogas flowrate, and pH can be used to fit experimental data from the Laboratory Batch Reactor to the Laboratory Batch Reactor Model. Laboratory Batch Reactor Model data can be transferred to the Amanzimtoti Co-digestion Pilot Project Model. Amanzimtoti Co-digestion Pilot Project Model data can be transferred to the Laboratory Batch Reactor Model"***

The ***feedback control loop hypothesis*** will be tested using the feedback control loop shown in **Figure 0-24**.

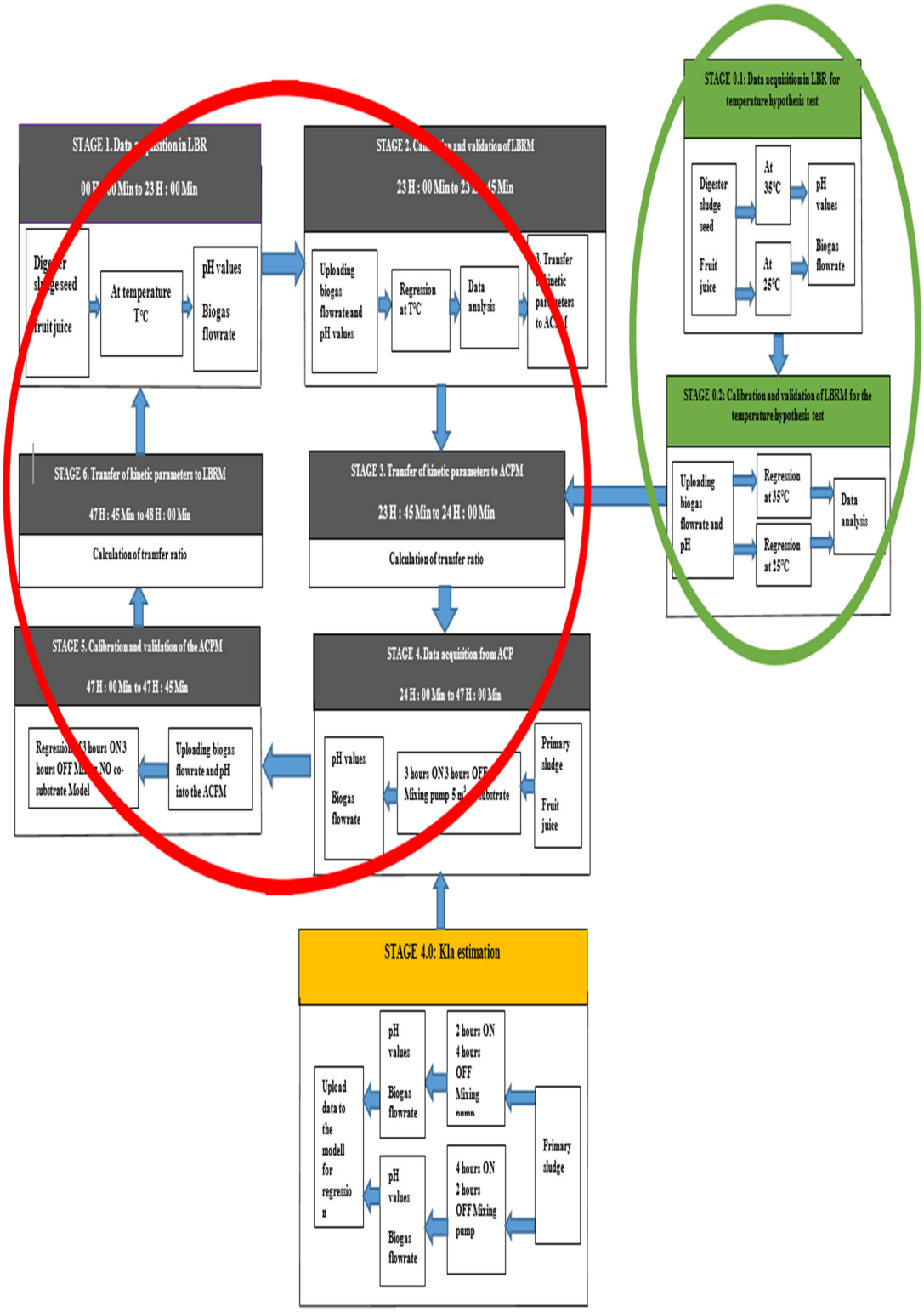


Figure 0-24: The diagram shows the preparatory steps which are STAGE 0.1 and STAGE 0.2 (green circle) for the ***temperature hypothesis*** as well as the ***feedback control loop hypothesis*** (red oval) STAGE 1, STAGE 2, STAGE 3, STAGE 4, STAGE 5 and STAGE 6.

2.14 Modelling approach

In this chapter, the information from the literature is used to guide the modelling procedures. The modelling approach that will be used is similar to the steps recommended by Lauwers et al. (2013) in **section 0 Figure 0-10**. The difference in the current project will be that it will be applied to digesters with different configurations at different temperatures to form a feedback control loop.

The ***temperature hypothesis*** will use the parameters selected in **section 11** for regression. And the result of the ***temperature hypothesis*** will be used for STAGE 1 of the ***feedback control loop hypothesis*** in **section 13**.

The pH value and biogas flow rate data obtained during experimental operations using the Laboratory Batch Reactor will be used in the model regression. The pH value will be given a higher weighting (priority) during regression as it is the more important indicator of digester stability (Labatut and Gooch, 2012, Chen et al., 2008). The details of digester stability and control are given in **section 0**.

The current project will use a similar WEST model in which expired fruit juice will be represented by glucose as done by Logan (2016) in **section 0**. Glucose will be used as an analogue of fruit juice in the model. The same laboratory screening batch reactor and the same source of digester sludge will also be used. In the current project, the control loop hypothesis will be tested by dosing the Amanzimtoti Co-digestion Pilot Project digester with co-substrate using the materials and methods described in **Chapter 0**.

2.15 Literature Review Summary

The biggest challenge of exploiting anaerobic digestion's potential is process control. .pH is critical for digester control. Co-digestion has been conducted as a viable method to improve biogas yields with limited success because of increased process control challenges.

The Water Research Commission, EThekwini Municipality and the Pollution Research Group, initiated a project to develop the Amanzimtoti Co-digestion Pilot digester, its model as well as a model-based control process for it. The model developed for the Amanzimtoti Pilot digester was called the UCT ADM 3P. The UCT ADM 3P model was developed based on the ADM 1 model.

The current project is a continuation of the work started by the Water Research Commission, EThekwini Municipality and the Pollution Research Group, to develop the Amanzimtoti Co-digestion Pilot digester control process. A feedback control loop was decided as the means to control the dosing of co-substrates. The screening experiments for co-substrates had to be conducted in 24 h, and the modelling activities conducted during the control procedure had to be simple and short.

Chapter 3: Materials and Methods

This chapter presents the steps taken to investigate hypothesises (***temperature hypothesis*** and ***feedback control loop hypothesis***) detailed in **section 0** and **section 0**. The materials used for data acquisition are detailed in **section 0**, the methods used to test the ***temperature hypothesis*** are detailed in **section 0** and the methods used to test the ***feedback control loop hypothesis*** are detailed in **section 0,** and the summary is given in **section 0**.

3.1 Materials

Laboratory screening experiments were conducted at the Amanzimtoti Wastewater Works laboratory site. The operating temperatures used were based on the ***temperature hypothesis*** in **section 0** at 25°C and 35°C using laboratory equipment described in **section 0**. The ACP was also dosed as part of the ***feedback control loop hypothesis*** (**section 0**) investigation. The materials used for the ACP data acquisition experiments are detailed in **section 0**.

3.1.1 Laboratory equipment

A laboratory located at Amanzimtoti Wastewater Treatment Works was used to conduct screening experiments. The equipment list is given in **Table 3-1**.

Table 0-5: shows the list of laboratory equipment used for screening experiments detailing the name and use of the main components

Equipment name	***Use***
DR890 Calorimeter	*COD and Ammonia measurement*
6.5 L PVC jacketed reactors	*Reaction vessels*
Water bath	*Temperature regulation*
Magnetic stirrer	*Mixing reactor contents*
0-20 ml/min flow meter	*Biogas flow measurement*
Thermometer	*Temperature measurement*
pH meter	*pH measurement*
Desktop computer	*Data logging*
LabView	*Data logging software.*
Display unit	*Conversion of signals from analogue to digital*

The reactors were set up according to **Figure 0-25**. The two reactors were connected to a water bath to regulate the temperature.

Figure 0-25: Laboratory screening batch reactor one and two, both with pH, temperature probes at the top and magnetic stirrers at the bottom. The reactors also have airtight transparent lids at the top.

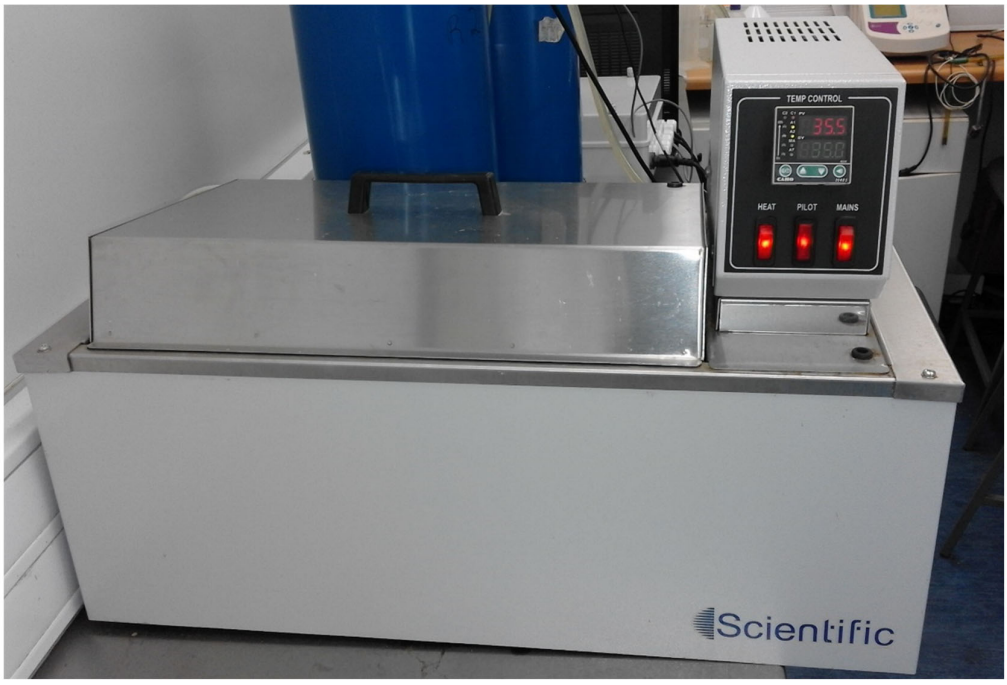


Figure 0-26: Water bath with thermostat for temperature control. The control panel and LCD temperature display are shown. The water bath has a pump inside for circulating the water in the reactors.

Figure 0-27: shows the display unit for gas flow, temperature, and pH. Inside the unit, there is an analogue to digital signal converter that converts physical readings to digital data

A pump inside the water bath was used to circulate the water in the reactor jackets. One reactor was connected to a water bath set at 35°C, and another was set at 25°C. A temperature probe and a pH probe was connected to each reactor. Pipes were also connected to each reactor and connected to gas flow meters for flow measurement.

The pH, temperature, and flow meter each had a separate display unit and were also connected to an analogue to digital converter. The analogue to digital converter changed signals from analogue to digital form so that it could be logged by the Labview data logging software.

3.1.2 Amanzimtoti Pilot Project

The ACP is located in Durban, South Africa. The plant capacity is given in **Table 0-6.**

Table 0-6: Amanzimtoti works plant daily hydraulic loading, total digestion capacity and digestion capacity in use (Logan, 2016)

Parameter description	***Quantity***
Hydraulic Loading Rate (ML/day)	*22*
Total digestion capacity (m^3)	*13 ,300*
Digestion capacity in use (m^3)	*9 ,350*

The ACP is made up of a refurbished digester with 2 000 m^3 capacity and is shown in **Figure 0-28**.

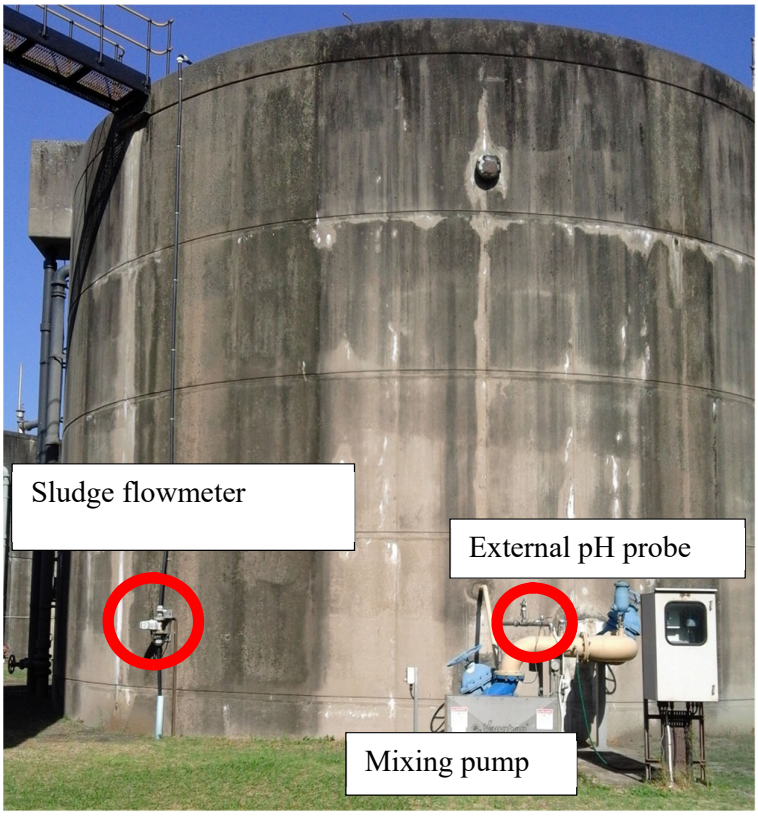


Figure 0-28: Digester number 1 at Amanzimtoti works with external pH probe. The digester also has a gas flowmeter and sludge flow meter.

There are also three JoJo tanks used for the storage of fruit juice, and they are shown in **Figure 0-29**.

The ACP consists of two parts, the three storage tanks, and the anaerobic digester. The storage tanks have a maximum capacity of 15 m^3. They have a transfer pump for receiving fruit juice from road tankers. The storage tank system also has a dosing pump that is used to dose the digester and also circulate the fruit juice within the tanks to keep solids in the fruit juice in suspension. The digester has a Vaughan jet mixer that is turned on three hours and off for three hours 24/7to circulate the digester sludge.

The digester has probes that measure temperature, pH, gas composition, biogas flow rate, sludge flowrate, and dosing flowrate online. The storage tank system has level sensors for volume measurement. The storage system is monitored and controlled automatically.

Although the ACP is a pilot digester for co-digestion, it is normally operated without dosing any expired fruit juice. It operates a semi-batch system where there is an average of 40 m^3 of primary sludge added daily while simultaneously offloading an equivalent amount of digester sludge from the top of the digester.

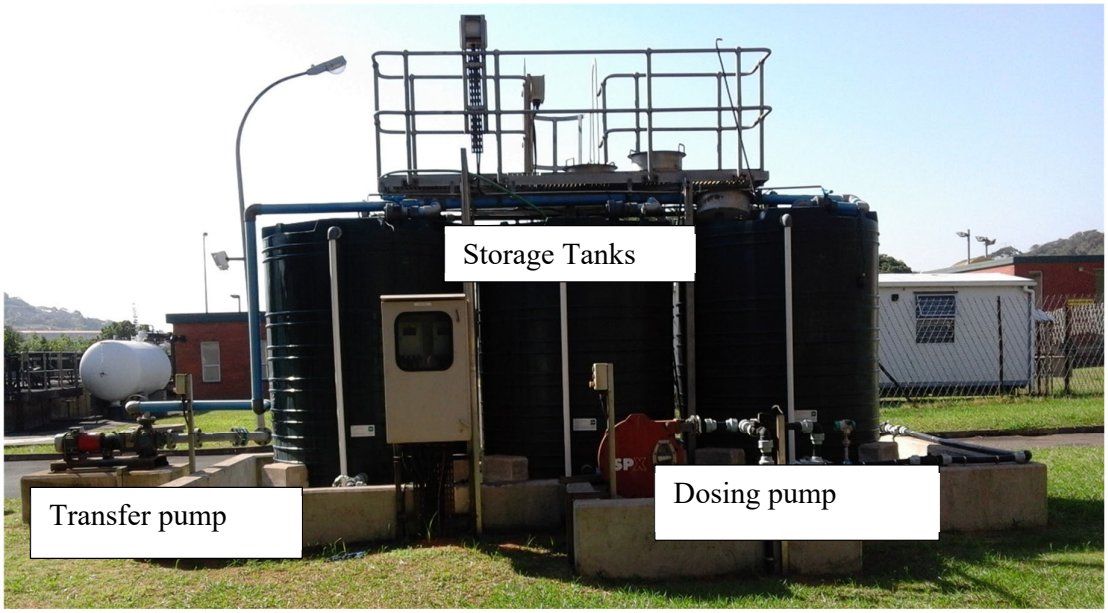
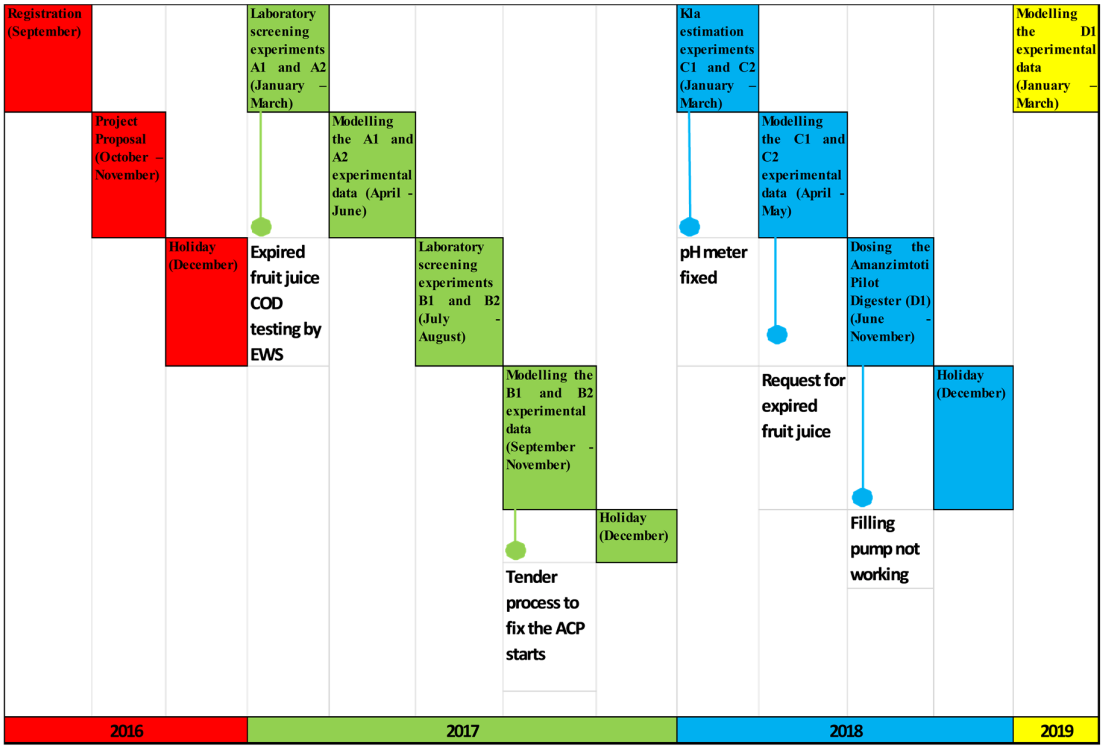


Figure 0-29: JoJo tanks with 5 m^3 capacity each used for the storage of fruit juice. The tanks are filled from road tankers using the transfer pump. The dosing pump is used to dose the ACP.

3.1.3 Timeline for the methodology

Table 0-7 shows the timeline used to implement the project methodology



The methodology was implemented according to **Table 0-7**. Two litres of expired fruit juice were delivered in May 2017 by the eThekwini municipality for use in the LBR screening experiments. Five cubic meters of expired fruit juice delivered to the storage tanks in **Figure 0-29** in September 2018 for use in ACP.

3.2 Temperature hypothesis

The ***temperature hypothesis (*****section 2.12*****)*** states that:

> ***"Kinetic data collected from the Laboratory Batch Reactor Model at 25^{o}C and 35^{o}C can be transferred to the Amanzimtoti Co-digestion Pilot Project Model."***

The ***temperature hypothesis*** is composed of STAGE 0.1 and STAGE 0.2, which are preparatory stages for the ***feedback control loop hypothesis***. Before operating the feedback control loop STAGE 0.1 and STAGE 0.2 need to be conducted once, and then the main stages of the feedback control loop which are STAGE 1, STAGE 2, STAGE 3, STAGE 4, STAGE 5 and STAGE 6 can be conducted. After going through all the six stages of the feedback control loop, there is no need to go through STAGE 0.1 and STAGE 0.2 again. Operating the feedback control loop will start at STAGE 1 instead of STAGE 0.1.

Figure 0-30 shows how the ***temperature hypothesis*** is tested. STAGE 0.1 consists of laboratory screening experiments conducted at 35°C and 25°C. As indicated in **section 0** the experimental data that will be used in the modelling procedure has to be validated to confirm

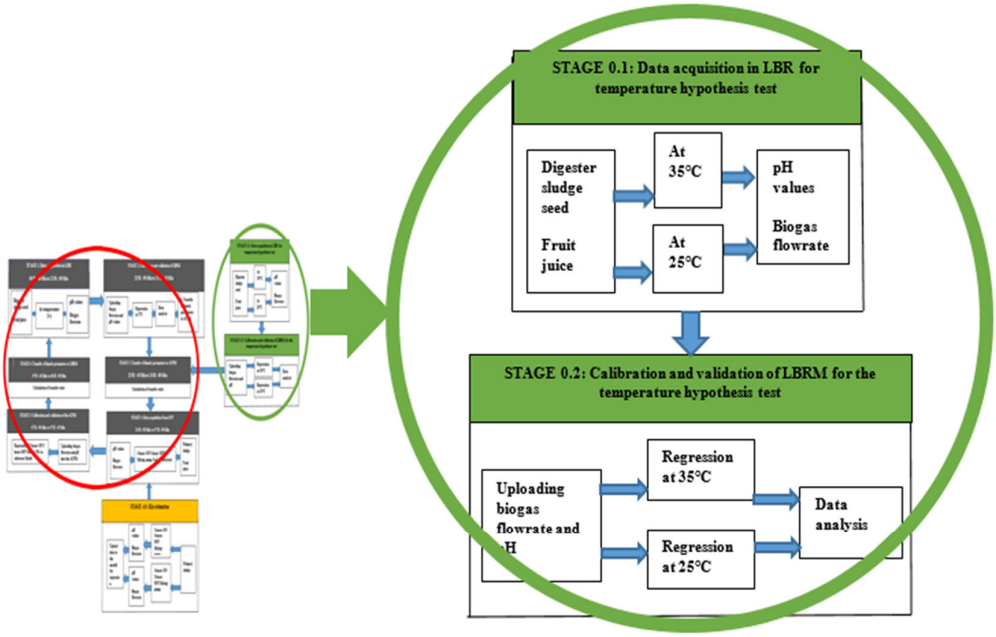


Figure 0-30: Shows a minimised version of **Figure 0-24** in section 0 on the left with only the portion relevant to the *temperature hypothesis* magnified and shown on the right side. The result of the hypothesis test (STAGE 0.1 and, STAGE 0.2) was used in STAGE 1 of the feedback control loop

its reproducibility hence, two replicate experiments were conducted simultaneously at each temperature; A1 and A2 at 35°C and B1 and B2 at 25°C. The pH values and biogas flowrate data collected from the experiments were used for regression in the model (STAGE 0.2).

The details of the materials used for the screening experiments are given in **section 0**. The details of the method used for STAGE 0.1 are given in **section 0** and the details of how the regression was conducted in **section 3.2.2.**

3.2.1 Method for STAGE 0.1

In this section, the method for data acquisition for the batch reactors described in **section 0**. The method was applied in STAGE 0.1. There were three steps in the data acquisition process; which are the feeding phase, the reaction phase, and the decanting phase.

The equipment described in **section 0** was arranged, as shown in **Figure 0-31**. The temperature probes, pH probes, and gas flowmeters were all calibrated according to methods described in

Figure 0-31: Laboratory screening equipment showing two batch reactors connected to a water bath, pH probes, temperature probes, gas flow meters and a desktop for data logging

Error! Reference source not found. before they were used for the duplicate experiments (A1, A2, B1 and B2). **Figure 0-33** shows an overview of the operating procedure used for the equipment described in **Figure 0-31**. The details of the operational procedure are given in **section 3.2.1.1**, **section 0, section 0, section 3.2.1.5,** and **section 3.2.1.5.**

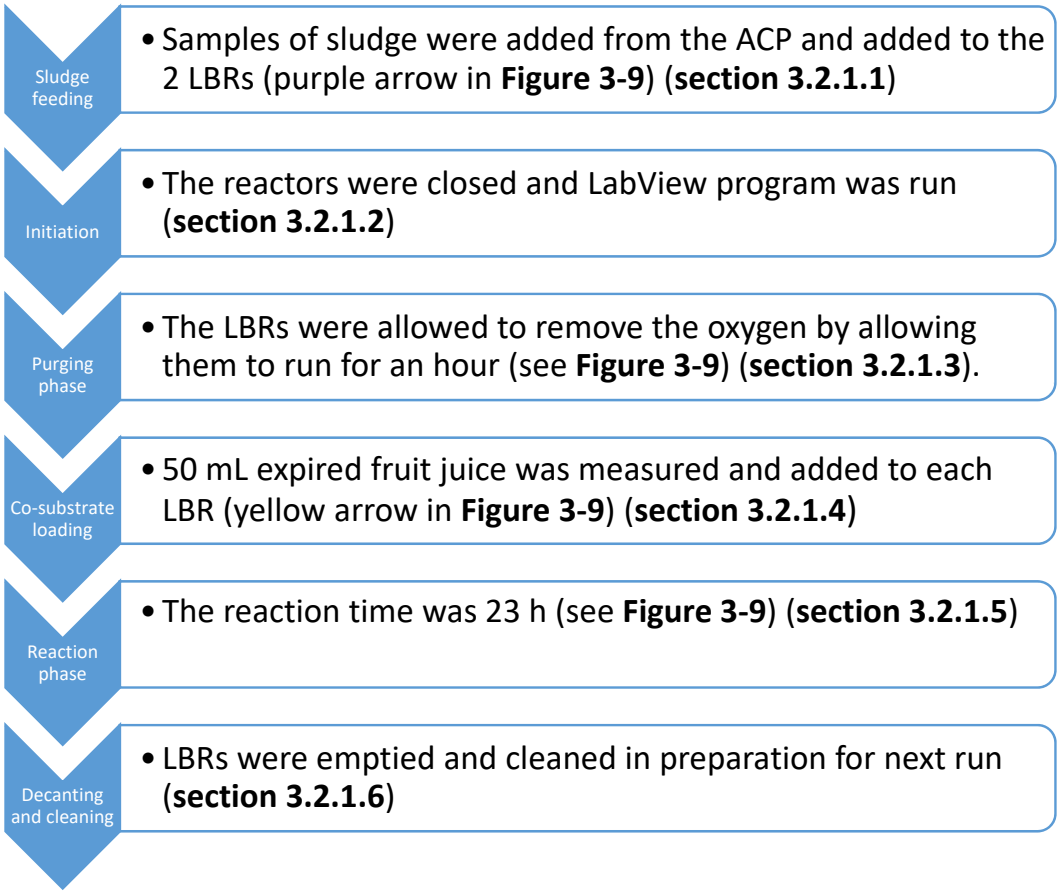


Figure 0-33: Standard operating procedure for the laboratory screening reactions showing the different activities conducted for data acquisition

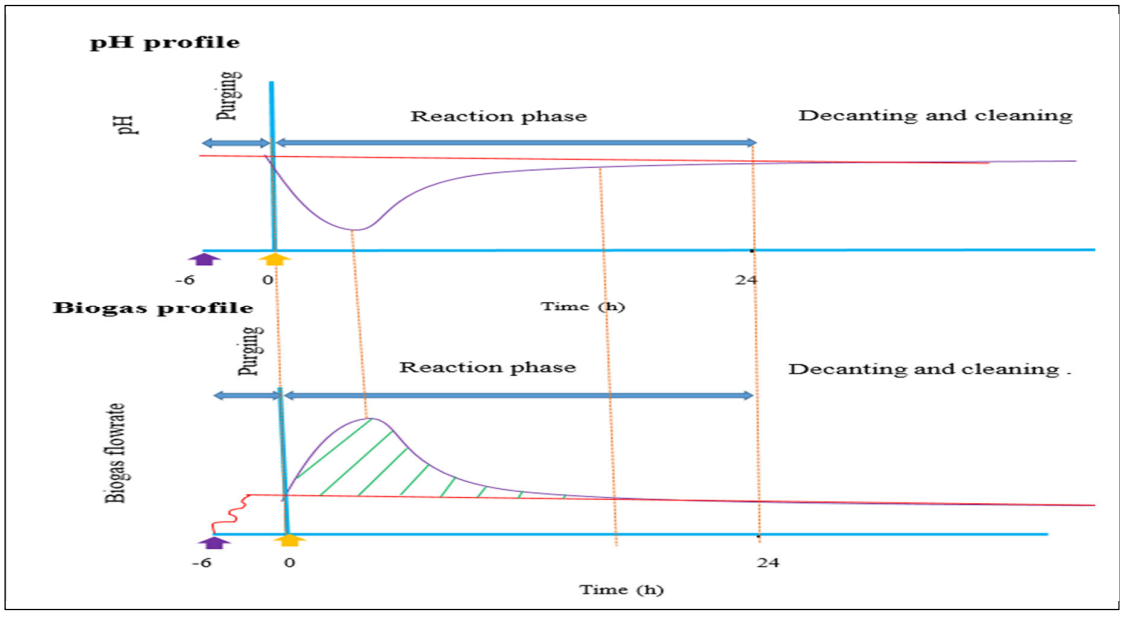


Figure 0-32 shows the relationship between the standard operating procedure for the laboratory screening reactions pH and biogas profile

3.2.1.1 Sludge loading

Prior to collection, the ACP mixing pump was run for at least an hour to ensure that the sludge was well mixed. During collection, the sampling valve was opened for at least 10 minutes to avoid collecting sludge that was stagnant in the pipes as well as to ensure that the samples collected were representative of the sludge in the ACP. As can be seen in **Figure 0-28**, the sampling point is located next to the pH probe on the pipe shown in the diagram. To collect a sample representative of the digester, the sludge in the pipe had to be expelled by running the mixing pump.

The sludge used in the LBR was collected from the ACP and loaded into the LBR immediately after collection. 4 L of digester sludge was used in each reactor. A 5 L beaker with an accuracy of plus/minus 200 mL. The magnetic stirrers were turned on immediately after loading, and the glass lids were monitored to ensure that the digester sludge was actually circulating. The digester sludge used was from the same digester whose sludge was characterised by Logan (2016) in (**section 0**) preparation for the modelling procedure in **section 3.2.2**. As indicated in **section 0,** the digester sludge will not be analysed before or after the co-digestion process, and the reasons were given.

3.2.1.2 Initiation

The reactor lids were closed tightly closed, and all valves except the gas outlet were closed. The gas flow meters were monitored closely, and if reactors are gas-tight, the displays show a gradual rise in gas flow. A gas-tight environment to ensure anaerobic conditions are maintained during the reaction by preventing ingress of air, hence any errors that occur during sealing can distort the results. Since the LBR operated at different temperatures, each reactor was connected to a separate water bath. One water bath temperature was set to 35°C and the other water bath was set to 25°C. The inbuilt pumping system in each water bath ensured that the temperature of the water bath was the same as that of the LBR jackets. The magnetic stirrers kept the sludge in the LBRs well mixed.

3.2.1.3 Purging phase

As indicated in **section 2.11,** carbonate ion concentration is important in the pH value of the sludge. The purging of air allows for the CO_2 to accumulate in the reactor and reach equilibrium while at the same time removing the dissolved oxygen in the digester sludge and oxygen in the headspace. This allows the pH of the reactor to stabilize. The purging time also allows for the temperature of the sludge to adjust and match the water bath temperatures.

3.2.1.4 Co-substrate loading

After the one hour of purging elapsed a 50 mL of fruit juice was added to both reactors. The fruit juice dosed was stored in a 2 L container in a cold room. After dosing the digesters, the biogas flowrate is monitored using LabView.

3.2.1.5 Reaction phase

The reaction was allowed to run for 23 h. By monitoring the profile generated by the LabView software during the digestion process, the complete consumption of the co-substrate can be observed, and the experiment terminated when the biogas flowrate is similar to flowrate at start-up.

3.2.1.6 Decanting and cleaning

The sludge was removed, and the vessels were disinfected with 90% ethanol to prevent cross-contamination by microbial species from the first experiment.

3.2.2 Methods for STAGE 0.2

The methods used for STAGE 0.2 are detailed in this section. The WEST modelling platform was used for all the activities of STAGE 0.2. The first step in STAGE 0.2 is to upload the biogas and pH values collected over 23 h for each experiment on the platform for validation. The validation is done by inspection using the features described in **section 0.**

As indicated in **section 2.7.6** the consistency of the time taken to reach the minimum pH and the consistency of the time taken for the profile to recover are the main parameters used to validate the duplicate pH profile. The second step is to upload the data into the WEST modelling platform and use it for regression. As indicated in **section 2.7.6** the ability to accurately model the time taken to reach the minimum pH and the time taken for the profile to recover are the main parameters used to validate the duplicate experiments' pH model. The third step is to use a mathematical tool to calculate the amount of biogas produced to confirm that the COD of gas produced is similar to that of the expired fruit juice.

The data from the laboratory screening experiments were validated by inspecting whether it conformed to expected phenomena associated with expired fruit juice digestion.

The data of Logan (2016) was used for reference. The features that are taken note of are the peak, bottom, and recovery rate of the biogas flowrate and pH identified in **Figure 0-14**.

3.2.2.1 Procedure for Regression of 25°C and 35°C data

pH is a key parameter for process control, as indicated in **section 2.8.1** hence during the regression was given a higher weighting. During the regression, the model initiates mathematical computations that are done using the regression parameters discussed in **section 11** to generate profiles similar to the uploaded data. Details about the weighting system in the WEST modelling platform are given in **section 2.5.6.1**. In the WEST modelling platform, the first step when modelling the pH is to adjust the pH of the model so that it matches the initial pH of the experimental data. This is done by adjusting the carbonate ion (CO_3^{2-}) and the hydrogen ion (H^+) in the model settings. If the initial model carbonate ion and the hydrogen ion is accurate, the model will prediction will maintain the same initial pH value. If it is not the initial pH prediction will shift to another value.

Logan (2016) used the model developed by (Osborne et al., 2012b, a). The model used literature sources temperature coefficient correction. The details of the importance of temperature coefficient correction in modelling are given in **section 2.5.3**. The literature-based

temperature coefficient in the model was replaced with the Van't Hoff-Arrhenius equation for temperature coefficients from Metcalf et al. (2003). The Van't Hoff-Arrhenius equation for temperature coefficients is given in **section 2.5.3**. The model code for temperature correction coefficient was edited to include the Van't Hoff-Arrhenius equation. The data obtained from the 35°C experiment was regressed first, and its corresponding temperature coefficient was used in the model for the 25°C temperature correction factor.

The ***temperature hypothesis*** was tested in the model using the temperature coefficient correction factor. This was done by inspecting whether the generated profile features that fit the experimental data from STAGE 0.2.

Trapezoidal Riemann sum detailed in **section 2.7.6** was used to calculate the biogas volume produced in each experiment. The consistency of volume produced was used to confirm whether the amount of fruit juice dosed was the same in each experiment. This was based on the assumption that dosing the same amount of fruit juice in each experiment will result in the same amount of biogas produced (Anton et al., 2010).

3.3 Feedback control loop hypothesis

The ***feedback control loop hypothesis*** states that:

> ***"Acetoclastic methanogen biomass concentration, biogas flowrate, and pH can be used to fit experimental data from the Laboratory Batch Reactor to the Laboratory Batch Reactor Model. Laboratory Batch Reactor Model data can be transferred to the Amanzimtoti Co-digestion Pilot Project Model. Amanzimtoti Co-digestion Pilot Project Model data can be transferred to the Laboratory Batch Reactor Model"***

Experimental data from the Laboratory Batch Reactor is collected in STAGE 1 and is used in the WEST modelling platform for regression to develop the Laboratory Batch Reactor Model in STAGE 2. Laboratory Batch Reactor Model data can be transferred to the Amanzimtoti Co-digestion Pilot Project Model in STAGE 3. Amanzimtoti Co-digestion Pilot digester data is collected in STAGE 4 and is used on the WEST modelling platform for regression in STAGE 5. Amanzimtoti Pilot Project digester Model data can be transferred to the Laboratory Batch Reactor Model in STAGE 6.

3.3.1 STAGE 1 of the feedback control loop: Data acquisition in the Laboratory Batch Reactor

STAGE 1 consisted of the laboratory screening experiments in the LBRs. Once the parameter selection and laboratory screening experiment operating temperature (25°C/35°C) has been confirmed from STAGES 0.1 and STAGE 0.2, the feedback control loop procedure can begin. The details of how STAGE 1 screening experiments were conducted are given in **section 3.3.1.1.**

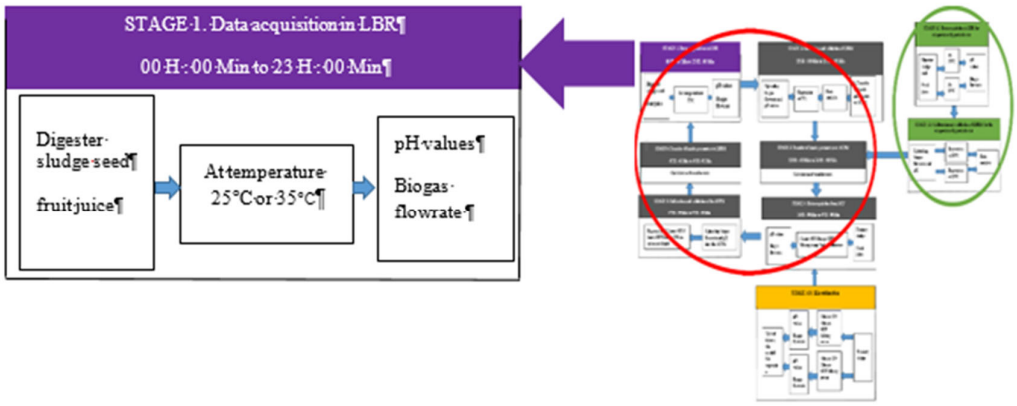


Figure 0-34 shows a minimised version of **Figure 0-24** in **section 2.13** on the right with only the portion relevant to STAGE 1 magnified and shown on the left side. STAGE 1 activities were conducted in 23 h. The temperature determined in the ***temperature hypothesis*** (25°C/35°C) is used as the operating temperature for STAGE 1.

3.3.1.1 Method for STAGE 1

The laboratory screening method for STAGE 1 is the same as that of STAGE 0.2. The same steps (feeding phase, the reaction phase, and the decanting phase) were also used. The details of STAGE 0.2 are given in **section 3.2.2**. The same equipment, described in **section 0,** is also used. The difference is that at STAGE 1, the experiments are done only at the temperature determined by the ***temperature hypothesis*** (25°C/35°C).

3.3.2 STAGE 2 of the feedback control loop: Calibration and validation of the laboratory batch reactor model

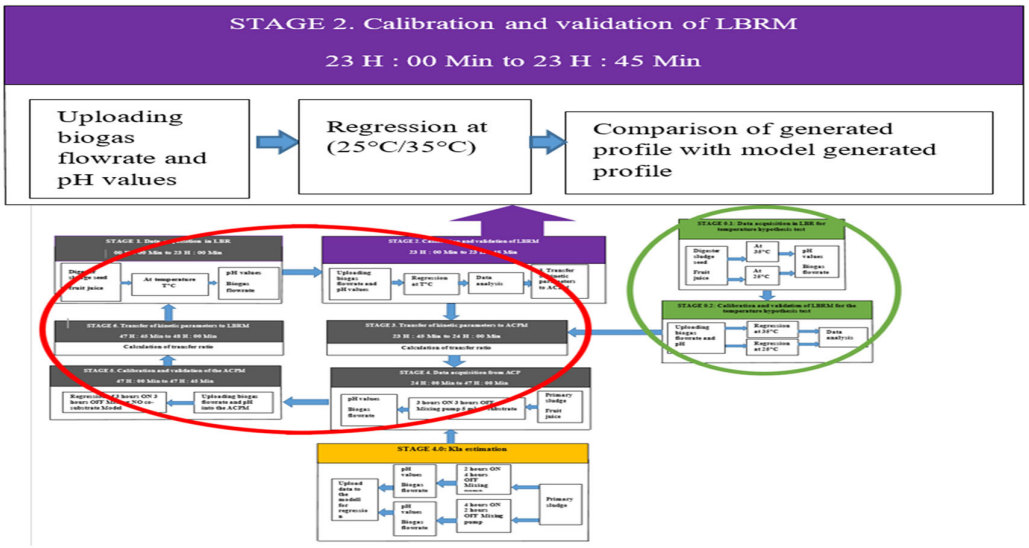


Figure 0-35 shows a minimised version of **Figure 0-24** in **section 2.13** at the bottom with only the portion relevant to STAGE 2 magnified and shown at the top. STAGE 2 operation takes 1 h and operations were done on the WEST modelling platform. The temperature (25°C/35°C) is determined by the ***temperature hypothesis***.

3.3.2.1 Methods for STAGE 2

The methods for STAGE 2 of the feedback control loop are the same as those of STAGE 0.2. Once the temperature has been determined in STAGE 0.2, it will be used for STAGE 1 and STAGE 2. In this instance, the data from the selected temperature (25°C/35°C) was used in STAGE 1 and STAGE 2 instead of redoing it. The conclusions of the data analysis and regression conducted in **section 3.3.2.1** will be the same as those of STAGE 0.2.

3.3.3 STAGE 3 of the feedback control loop: Transfer of kinetic parameters from Laboratory Batch Reactor Model to the Amanzimtoti Co-digestion Pilot Project

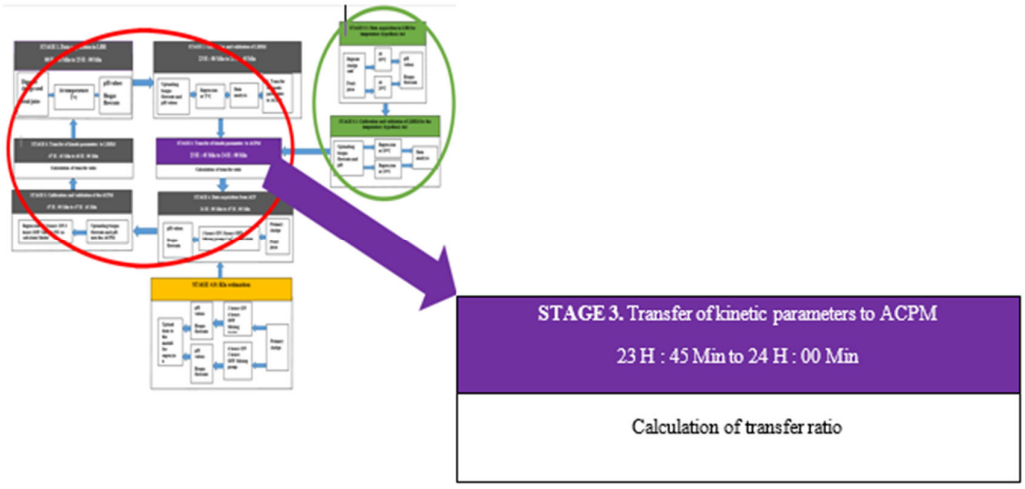


Figure 0-36 shows a minimised version of **Figure 0-24** in **section 2.13** on the left with only the portion relevant to STAGE 3 magnified and shown on the right side. STAGE 3 of feedback control loop takes five minutes and is conducted on the WEST modelling platform. The transfer ratio is calculated using the volume of the ACP and the LBR

The WEST modelling platform was used for all the activities of STAGE 3.

3.3.3.1 Method for STAGE 3

The ratio of the ACP digester sludge volume (2 000 m^3) to LBR sludge volume (0.004 m^3) was used as the basis for the transfer of extensive properties. The WEST modelling platform has an inbuilt function that enables the transfer of kinetic parameters which only require the input of the transfer ratio; hence the process takes 5 minutes to complete.

3.3.4 Stage 4.0 Carbon dioxide gas mass transfer coefficient (Kla) estimation

Before dosing the ACP in STAGE 4 is was necessary to estimate the carbon dioxide Kla value of the digester. The importance of the Kla value as detailed in **section 2.1.2.2** and **section 0**. To estimate the Kla, two experiments were conducted for 23 h each. They were done by maintaining normal daily primary sludge dosage while varying the pump mixing duration.

The materials used for estimating Kla are detailed in **section 0.** The primary sludge comes from the secondary settlers at Amanzimtoti Wastewater Treatment Works. 40 m^3 of primary sludge was dosed in two hours once per day. The experiments were conducted according to **Figure 0-37**.

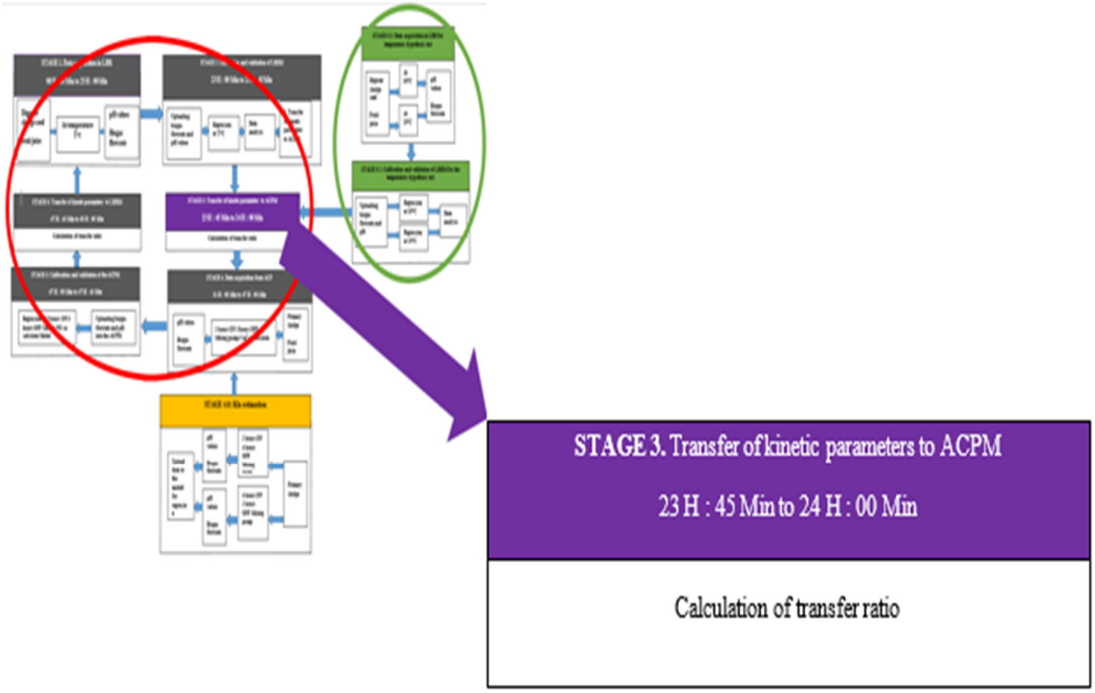


Figure 0-37 shows a minimised version of **Figure 0-24** in **section 2.13** on the left with only the portion relevant to the estimation of Kla magnified and shown on the right side. The experiments were conducted to estimate the Kla value of the ACP.

3.3.4.1 Method for estimating the carbon dioxide gas mass transfer coefficient (Kla)

The operation of the mixing pump is automated. During normal ACP operation, the mixing pump is turned on for three hours and off for two hours 24/7. The first set of experimental data was collected every five minutes for 23 while the mixing pump was cycled on for two hours and off for four h. The second set of experimental data was collected over 23 h while the mixing pump was turned on for four hours and off for two hours. Greater and lesser than normal mixing times were selected to test their influence on the Kla value

The pH values and biogas flowrate experimental data over 23 h were uploaded to the WEST modelling platform and regressed separately. The regression was done using the ACPM model developed using the kinetic data transferred from STAGE 3 on the WEST modelling platform. Two values for Kla were obtained representing the upper and lower limit of Kla. Experimental data for pH and biogas were used to calibrate the model using the objective function and parameters selected in **section2.11, section 2.12,** and **section 2.13**. The average Kla was used in the model.

3.3.5 STAGE 4 of the feedback control loop: data acquisition from the Amanzimtoti co-digestion Pilot Project sludge data

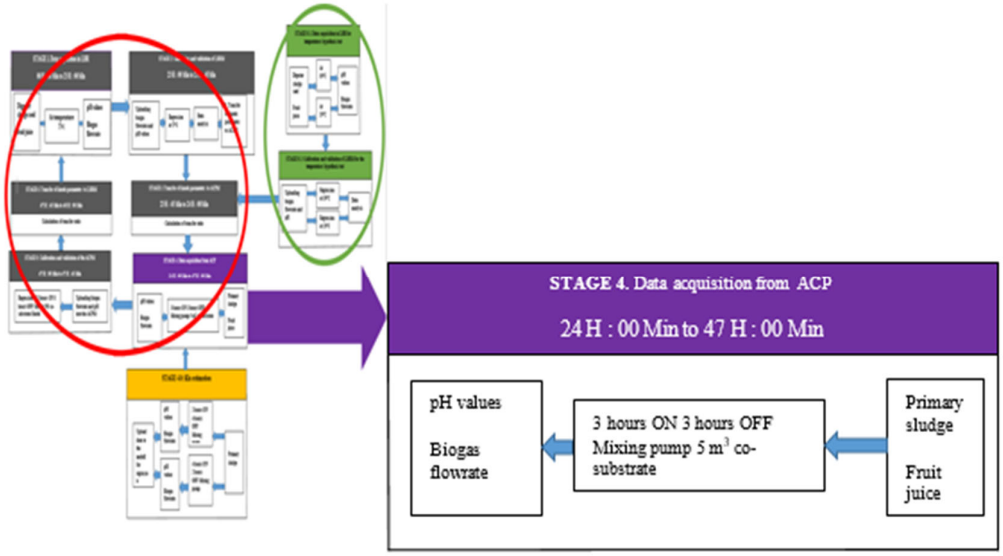


Figure 0-38 shows a minimised version of **Figure 0-24** in **section 2.13** on the left with only the portion relevant to STAGE 4 magnified and shown on the right side. One experiment was conducted to test the effect of dosing the fruit juice in the ACP.

STAGE 4 consisted of a single experiment to determine the effect of fruit juice on the digestion process. The materials used for the experiment are detailed in **section 0.**

3.3.5.1 Method for STAGE 4

The expired fruit juice was delivered to the storage tanks described in **section 0** by a tanker truck. The dosing pump, which is part of the storage tank system, was used to dose the expired fruit juice into the ACP. A flow meter on the piping system is used to measure the volume of expired fruit juice dosed.

The experiment was conducted according to **Figure 0-38**. 40 m^3 of primary sludge was dosed in two hours, and 5 m^3 of expired fruit juice was dosed in one hour while the mixing pump was on for three hours and off for three hours for 23 h (normal operation).

3.3.6 STAGE 5 of feedback control loop: calibration and validation of the Amanzimtoti Co-digestion Pilot Project model

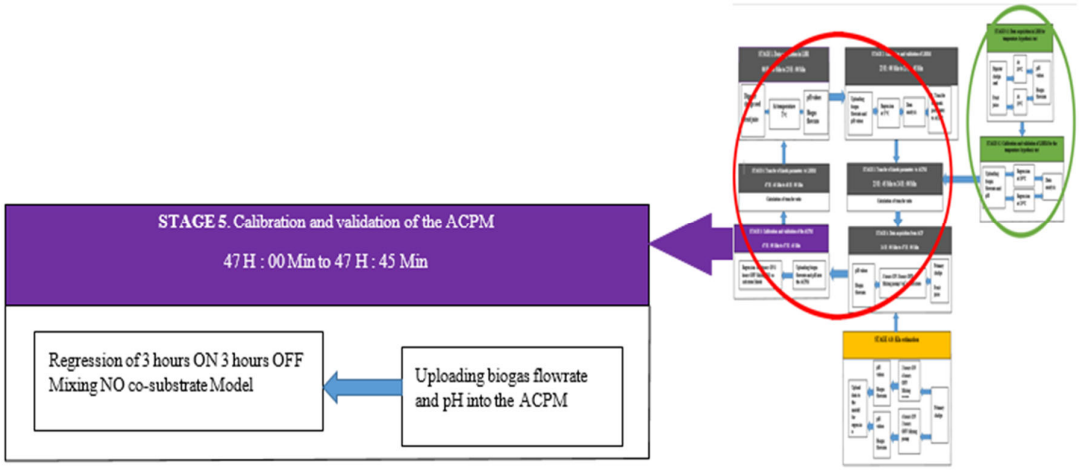


Figure 0-39 shows a minimised version of **Figure 0-24** in **section 2.13** on the right with only the portion relevant to STAGE 5 magnified and shown on the left side.

Figure 0-39 show STAGE 5 was conducted. The details are given in **section 0**.

3.3.6.1 Methods for STAGE 5

The WEST modelling platform was used for all the activities of STAGE 5. The pH values and biogas flowrate experimental data over 23 h from STAGE 4 as well as the Kla value estimated in **section 0,** were used for regression to calibrate the ACPM.

3.3.6.2 Procedure for Testing digester dosing limit

After the model fitting, the ACPM was used as a representative of the ACP. This was in fulfilment of the original objective in **section 1.6** of ascertaining the limit of how much fruit juice could be dosed before the digester failed. Model simulations with higher expired fruit juice analogue (glucose) dosages were conducted. This enabled the use of the ACPM to test the limits of dosing by increasing the expired fruit juice analogue (glucose) dosage in the model. The model output was the maximum safe dosage of the expired fruit juice analogue (glucose).

3.3.7 STAGE 6 of the feedback control loop: Transfer of kinetic parameters to Laboratory Batch Reactor Model

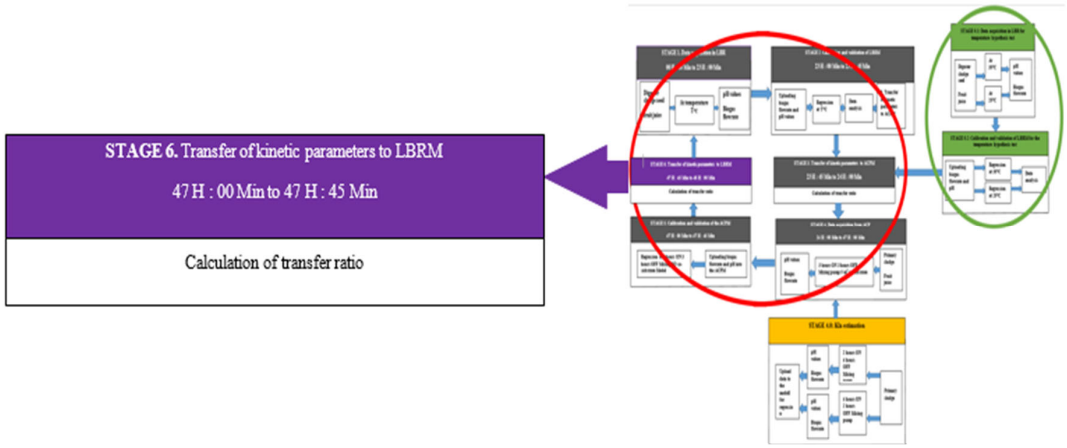


Figure 0-40 shows a minimised version of **Figure 0-24** in **section 2.13** on the right with only the portion relevant to STAGE 6 magnified and shown on the left side. The data from the ACPM is transferred to the LBRM

The WEST modelling platform was used for all the activities of STAGE 6.

3.3.6.1 Method for STAGE 6

The inverse of the ratio used to transfer kinetic data from the LBRM to the ACPM is used in the model to reverse the process done in STAGE 3. The ratio of the LBR sludge volume (0.004 m^3) to the ACP digester sludge volume (2 000 m^3) was used as the basis for the transfer of extensive properties.

3.4 Materials and Methods Summary

Two Laboratory Batch Reactors were used to conduct laboratory screening experiments. The Amanzimtoti Co-digestion Pilot Digester was used to test the influence of expired fruit juice anaerobic digestion.

The method used to test the ***Temperature hypothesis*** and the ***Feedback control loop hypothesis*** was based on the six stages of the feedback control loop. Experimental data from the Laboratory Batch Reactor was collected in STAGE 1 and is used in the WEST modelling platform for regression to develop the Laboratory Batch Reactor Model in STAGE 2. The Laboratory Batch Reactor Model data can be transferred to the Amanzimtoti Co-digestion Pilot Project Model in STAGE 3. The Amanzimtoti Co-digestion Pilot digester data was collected in STAGE 4 and was used on the WEST modelling platform for regression in STAGE 5. The Amanzimtoti Pilot Project digester Model data was transferred to the Laboratory Batch Reactor Model in STAGE 6.

Chapter 4: Results and Discussion

In this chapter, the results of the test conducted to test the ***Temperature hypothesis*** in **section 4.1** and the ***Feedback control loop hypothesis*** results are given in **section 4.2** while **section 0** details the conclusion to the temperature hypothesis and **section 0** gives the conclusion to the results and discussion.

4.1 Temperature hypothesis 35°C results

STAGE 0.1 and STAGE 0.2 tested the ***Temperature hypothesis.*** Two experiments were conducted at each temperature according to **Table 0-8**. The COD of the expired fruit juice was used to calculate the organic loading rate of the LBRs. The expired fruit juice COD chemical

Table 0-8: ***Temperature hypothesis*** conditions for STAGE 0.1 and STAGE 0.2. Two experiments were conducted at each temperature A1 and A2 at 35°C, B1 and B2 at 25°C

Run	***Units***	***A1***	***A2***	***B1***	***B2***
Temperature	***(°C)***	*35*	*35*	*25*	*25*
Total reactor volume	***(L)***	*6.5*	*6.5*	*6.5*	*6.5*
PS added Volume	***(L)***				
Digester sludge volume	***(L)***	*4*	*4*	*4*	*4*
Fruit Juice added	***(L)***	*0.05*	*0.05*	*0.05*	*0.05*

analysis average result was 130 000 mg COD/L with an error of ± 10 000 mg COD/L.

As indicated in **section 0,** the project was conducted over three years. The main reason for this was the challenges with fixing equipment on the ACP. Most of the problems on the digester were either mechanical of sensors. The process of fixing them required a long process which involved off-site personnel. At one point in time, a tender process was conducted to fix the ACP. The length of time taken to conduct the project raised concerns for the stability of the digester.

The pH meter, the biogas flow meter and the gas analyser were not working consistently from September 2016 to May 2018 hence it was not possible to pH value and biogas production to monitor the state of the ACP. Nevertheless, the records of how the ACP was dosed with primary sludge were available onsite. These records indicated that from 2012 to 2018, 40 m^3 were dosed in the ACP consistently. The consistent dosing of primary sludge was the only indication that the operation of the ACP was steady; hence it was concluded that the condition of the digester sludge was stable.

4.1.1 Results for the data acquisition experiments in the Laboratory batch Reactor for the *Temperature hypothesis* (STAGE 0.1)

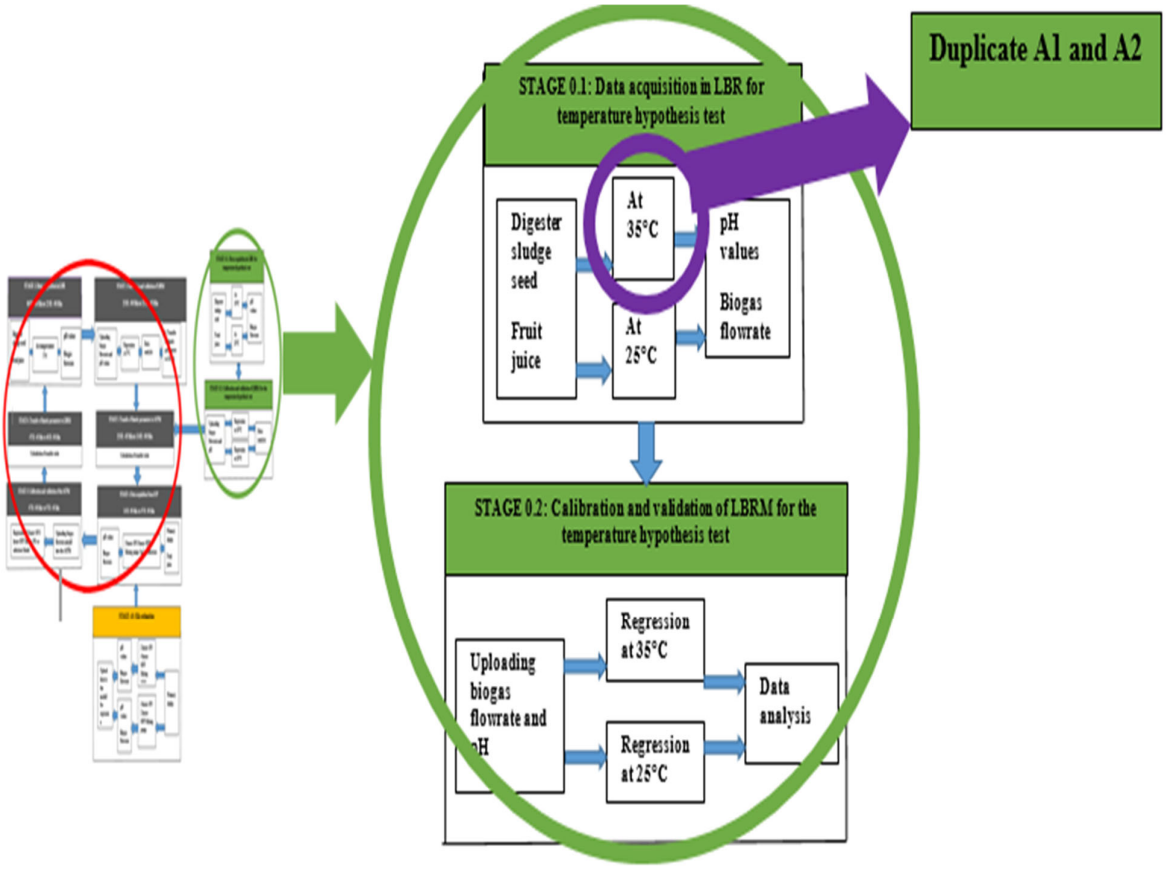


Figure 0-41 shows that A1 and A2 are duplicate experiments for testing the *Temperature hypothesis*

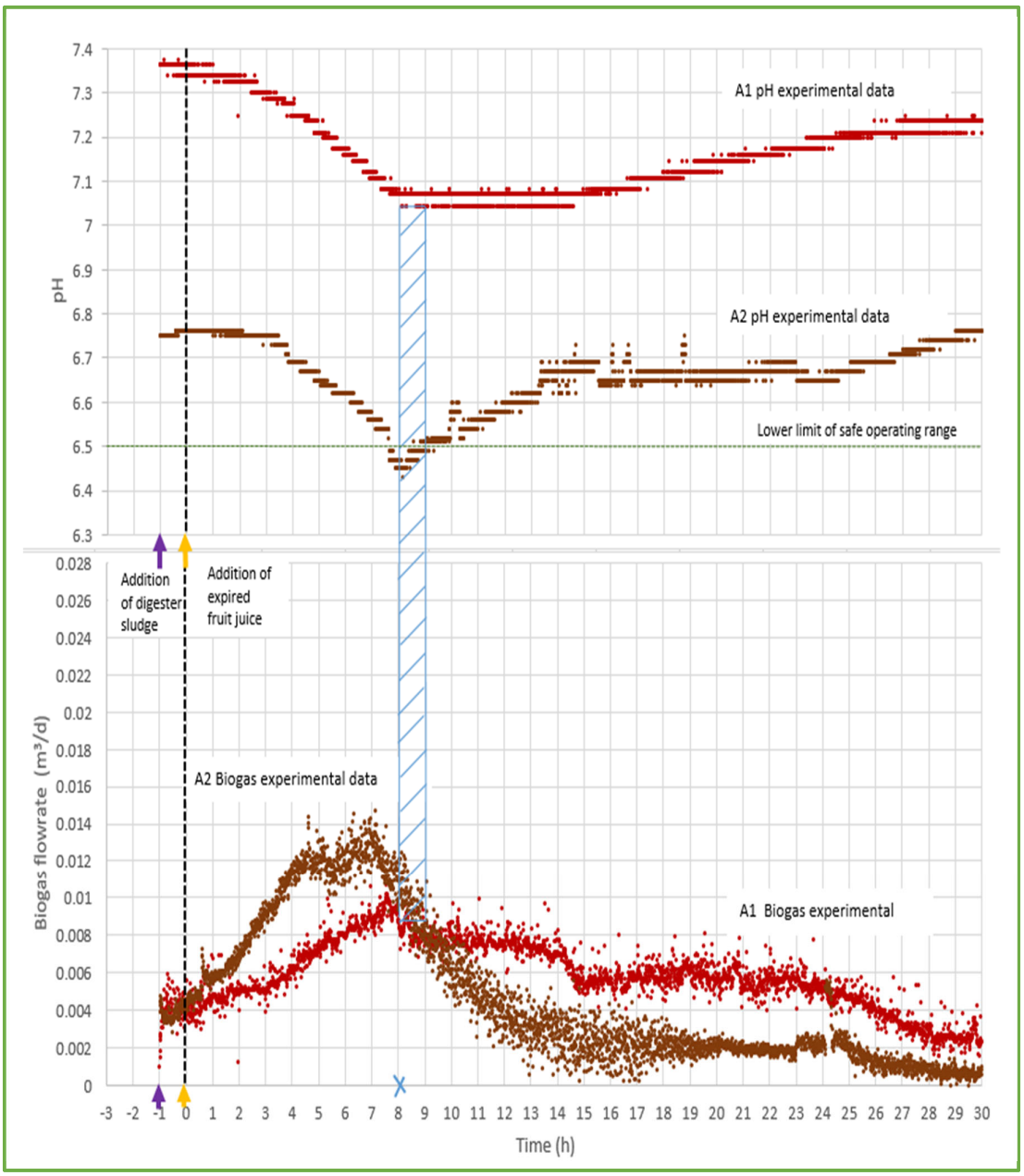


Figure 0-42 shows the pH and biogas profiles for the duplicate experiments A1 and A2 where 4 L of digester sludge, 50 mL of expired fruit juice was added to the LBRs and the experiment was conducted at 35°C. The time when the sludge, and the expired fruit juice was added are indicated by the purple arrow and the yellow arrow. The blue column shows that the lowest pH value of A1 and A2 occurs at approximately the same time.

The pH and biogas profile of the duplicate experiments A1 and A2 are shown in **Figure 0-42**. Digester sludge from the ACP was loaded into the LBRs at time -1 h (purple arrow). The LBRs were sealed and purged for one hour according to the methodology in **section 0**.

The pH value of A1 and A2 at time 0 h was 7.37 and 6.76, respectively. The pH values of A1 and A2 gradually decreased until they reached the minimum values simultaneously at time 8 h. The minimum pH values of A1 and A2 were 7.05 and 6.43, respectively. Although the minimum pH value for A2 is below the safe range (6.5-7.5), the pH subsequently increased to values within the safe operating range and maintained its pH within the safe operating range. Hence the results for A2 are acceptable. The pH values of both A1 and A2 after 24 h recover to values above the lower safe operating limit hence according to the second criteria in **section 2.7.6.1** the dosage used in both duplicates was validated as safe.

According to the first validation criteria described in **section 2.7.6.1,** the difference in the time taken to reach the minimum pH for the duplicate experiments fall within the acceptable range (1 h) and are therefore valid.

The volume of biogas produced by both A1 and A2 was calculated according to the method described **in section 3.2.2.1**. The volume of biogas produced by A1 and A2 was 0.0095 m^3 and 0.0080 m^3, respectively.

The volume of gas produced is by A1 and A2 has a difference of less than 50% hence according to the third criteria given in **section 2.7.6.1** the biogas data is valid.

4.1.2 Results for calibrating and validating the Laboratory Batch Reactor Model (STAGE 0.2)

The WEST modelling platform was used for all the activities of STAGE 0.2, as indicated in **section 3.2.2**.

4.1.3 Results for modelling the first duplicate experiment at 35°C (A1)

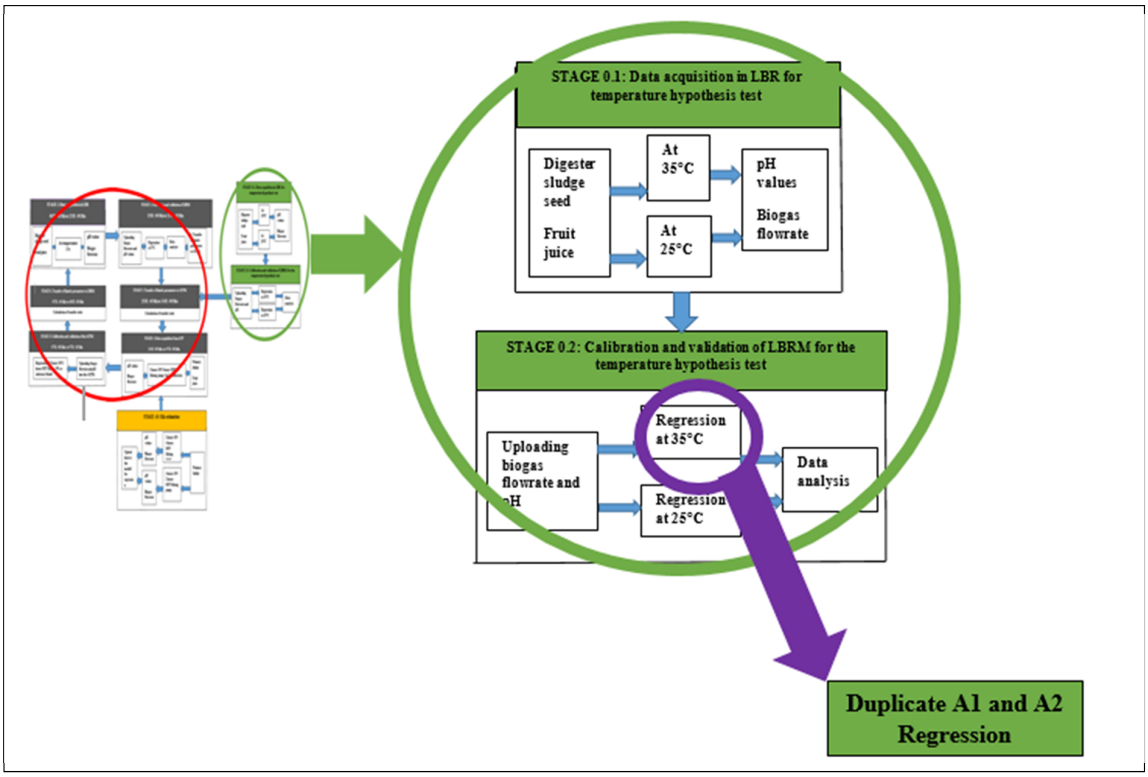


Figure 0-43 shows that duplicate experiments A1 and A2 were used for regression in STAGE 0.2 of the ***Temperature hypothesis***

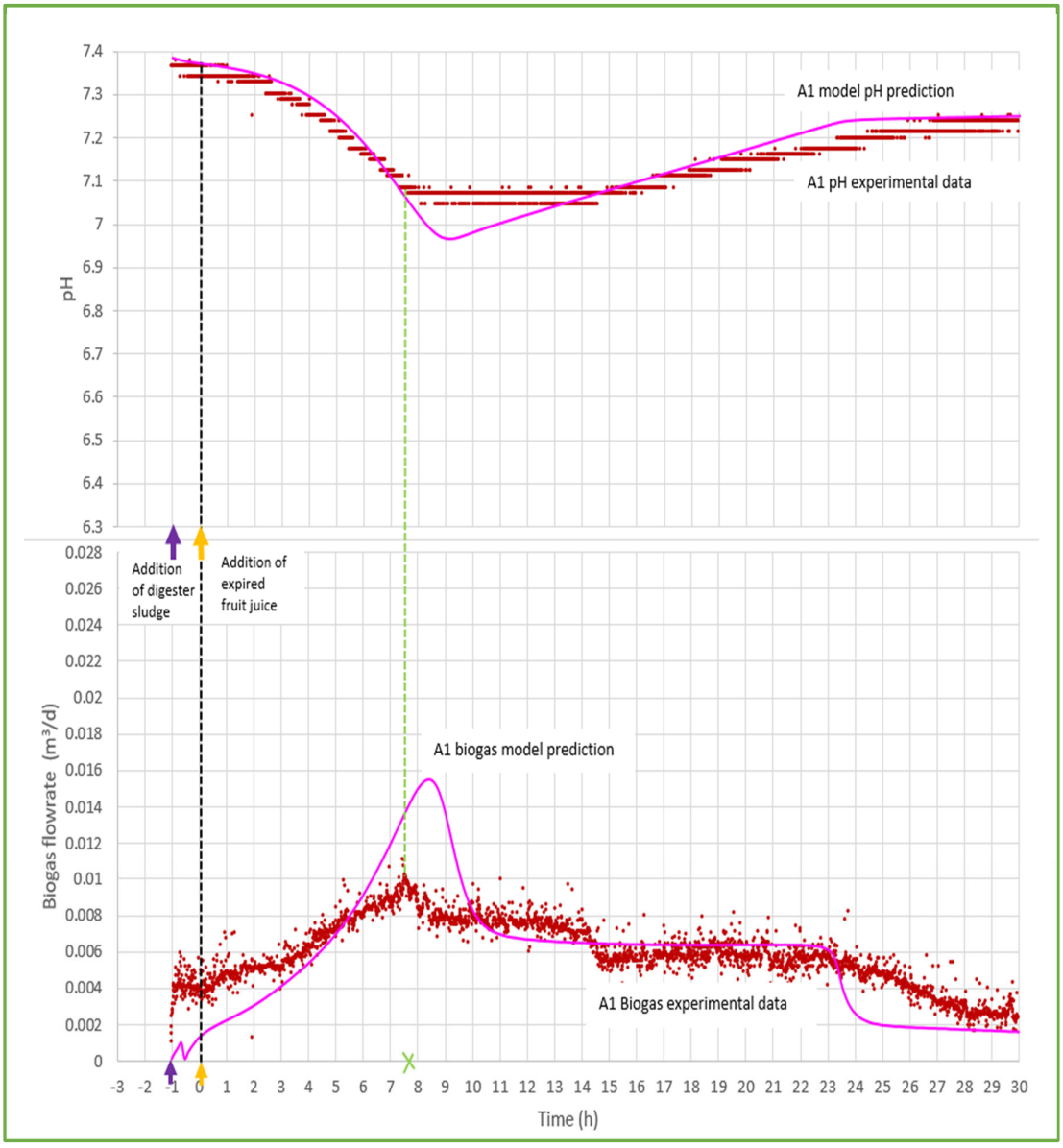


Figure 0-44 shows the pH and biogas profile of the duplicate experiment A1 and its corresponding model prediction. The duplicate experiment was conducted at 35°C with a dose of 50 mL expired fruit juice. The model prediction produced after a regression was conducted at 35°C with a dose of 7 g expired fruit juice analogue (glucose).

The duplicate experiment was conducted at 35°C with a dose of 50 mL expired fruit juice. The model prediction was produced after a regression was conducted at 35°C with a dose of 7 g expired fruit juice analogue (glucose) on the WEST modelling platform. As indicated in **section 2.7.6** the ability to accurately model the time taken to reach the minimum pH and the time taken for the profile to recover are the main parameters used to validate the duplicate experiments' pH model.

Figure 0-44 shows the pH value predicted by the model at time 0 h is 7.37, which was the same as the experimental data. Hence according to the first criteria described in **section 2.7.6.2**

meets the first requirement for validation. The minimum model pH value was also predicted to occur at 9 h while the experimental data showed a minimum value at time 8 h. The difference in time taken to reach the minimum pH value was 1 h, which, according to the second criteria in **section 2.7.6.2** meets the second requirement for validation. Moreover, the model predicted a minimum value of 6.97, while the experimental data showed a minimum of 7.05. The difference in minimum pH value is less than 0.1, which, according to the third criteria in **section 0** meets the second requirement for validation. The model predicted pH after 24 h was 7.24 while the experimental data showed a value of 7.20. The model accurately predicts the increase of the pH value after the minimum value is reached, which, according to the fourth criteria in **section 2.7.6.2** meets the requirement for validation. Overall the model was able to meet all the requirements to validate the pH profile prediction.

When 50 mL of expired fruit juice was dosed, the biogas flowrate started to increase. The volume of biogas predicted by the model and the volume produced by duplicate experiment A1 was calculated according to the method described in **section 3.2.2.1**. The volume of biogas predicted by the model was 0085 m^3while the duplicate experiment A1 produced was 0.0095 m^3. The difference in biogas volume is less than 50 %, which, validates the expired fruit juice dosage and its corresponding fruit juice analogue (glucose) according to the fifth criteria in **section 2.7.6.2**. The parameter values that were used in the model before the regression as well as the parameter values obtained after the regression are given in **Table 0-9**.

Table 0-9: shows the values of the kinetic parameters (Carbonate ion, Hydrogen ion, Mass of acetoclastic methanogens) that were selected during the parameter selection (**section 2.11**). The values before the regression and after the regression of the A2 experimental data are detailed.

Parameter	*Unit*	*Value Before Calibration*	*Value After Calibration*	*Change in Value*
Carbonate ion	-	*22.55*	*22.33*	-
Hydrogen ion	-	*0.422*	*0.455*	+
Mass of acetoclastic methanogen	-	*1.2257*	*1.2467*	+

4.1.4 Results for modelling the second duplicate experiment at 35°C (A2)

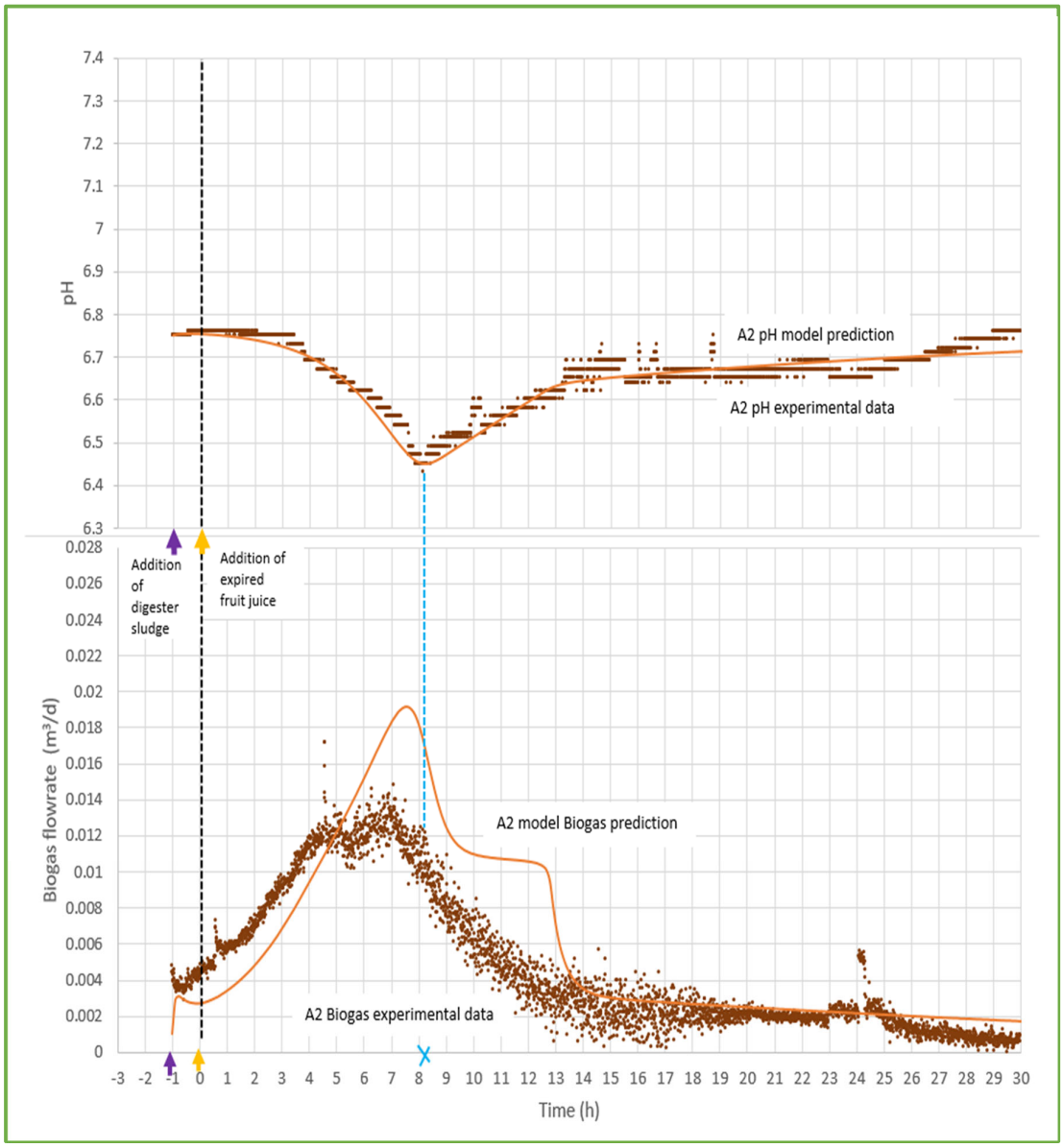


Figure 0-45 shows the pH and biogas profile of the duplicate experiment A2 and its corresponding model prediction. The duplicate experiment was conducted at 35°C with a dose of 50 mL expired fruit juice. The model prediction produced after a regression was conducted at 35°C with a dose of 7 g expired fruit juice analogue (glucose).

The duplicate experiment was conducted at 35°C with a dose of 50 mL expired fruit juice. The model prediction was produced after a regression was conducted at 25°C with a dose of 7 g expired fruit juice analogue (glucose) on the WEST modelling platform. As indicated in **section 0** the ability to accurately model the time taken to reach the minimum pH and the time taken for the profile to recover are the main parameters used to validate the duplicate experiments' pH model.

Figure 0-45 shows the pH value predicted by the model at time 0 h is 6.67, which was the same as the experimental data; according to the first criteria described in **section 0** meets the first requirement for validation. The minimum model pH value was also predicted to occur at 8 h, which was the same as the experimental data according to the second criteria in **section 0** meets the second requirement for validation. Moreover, the model predicted a minimum value of 6.43, which was the same as the experimental data according to the third criteria in **section 0** meets the second requirement for validation. The model also predicted the pH value after 24 h as 6.70, which was the same as the experimental data. The model accurately predicts the increase of the pH value after the minimum value is reached, which, according to the fourth criteria in **section 0** meets the requirement for validation. Overall the model was able to meet all the requirements to validate the pH profile prediction.

When 50 mL of expired fruit juice was dosed, the biogas flowrate started to increase. The volume of biogas predicted by the model and the volume produced by duplicate experiment A2 was calculated according to the method described **in section 3.2.2.1**. The volume of biogas predicted by the model was 0085 m^3while the duplicate experiment A2 produced was 0.0080 m^3. The difference in biogas volume is less than 50 %, which, according to the fifth criteria in **section 0** meets the second requirement for validation. The parameter values that were used in the model before the regression as well as the parameter values obtained after the regression are given in **Table 0-10**.

Table 0-10: shows the values of the kinetic parameters (Carbonate ion, Hydrogen ion, Mass of acetoclastic methanogens) that were selected during the parameter selection (**section 2.11**). The values before the regression and after the regression of the A2 experimental data are detailed.

Parameter	***Unit***	***Value Before Calibration***	***Value After Calibration***	***Change in Value***
Carbonate	-	*24*	*25.3*	+
Hydrogen ion	-	*0.61*	*0.63*	+
Mass of acetoclastic methanogen	-	*1.9286*	*2.1255*	+

4.1.5 Results of the transfer of kinetic parameters from Laboratory Batch Reactor Model to the Amanzimtoti Co-digestion Pilot Project in the *Feedback control loop hypothesis* (STAGE 3)

The ratio of the ACP digester sludge volume (2 000 m^3) to LBR sludge volume (0.004 m^3) was used as the basis for the transfer of extensive properties. The ratio used was 500 000.

4.1.6 Results of the carbon dioxide gas mass transfer coefficient (Kla) estimation (STAGE 4.0)

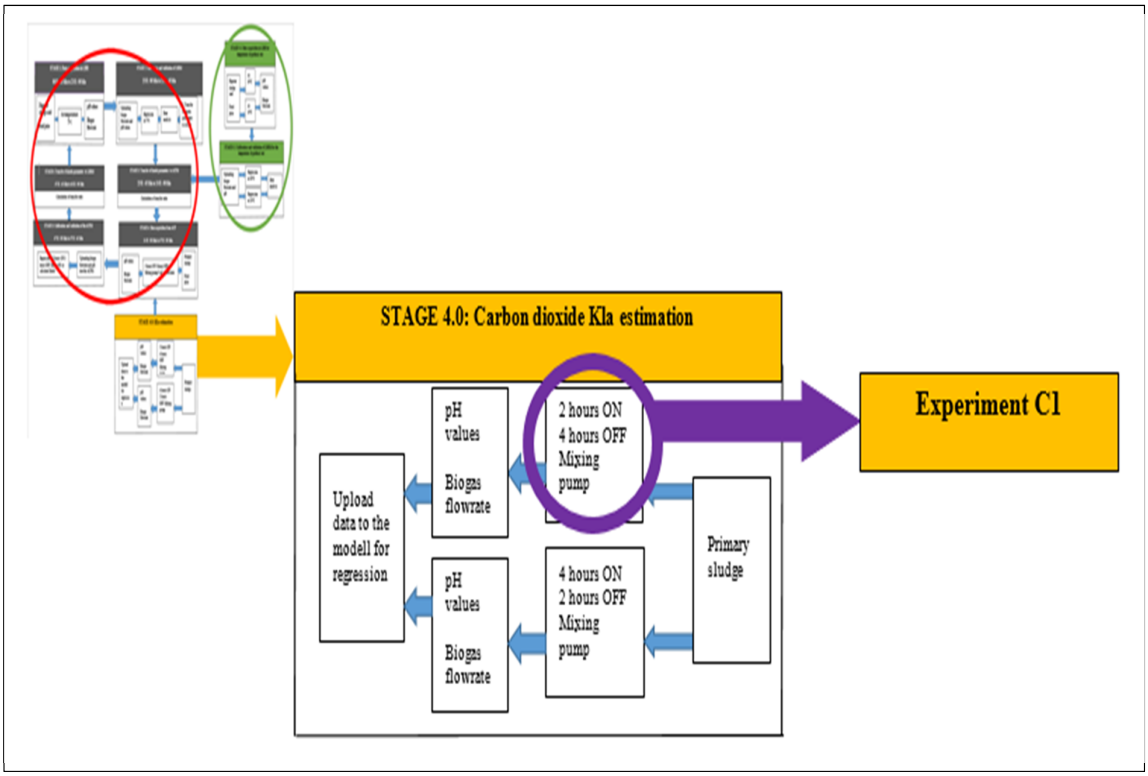


Figure 0-46 shows experiment C1 where 40 m^3 of primary sludge was dosed to estimate the Kla value of the Amanzimtoti Co-digestion Pilot plant.

Two experiments were (C1 and C2) conducted according to the methodology in **section 0**. The mixing pump was turned ON for two hours and then turned OFF for four hours as indicated in **Figure 0-46**.

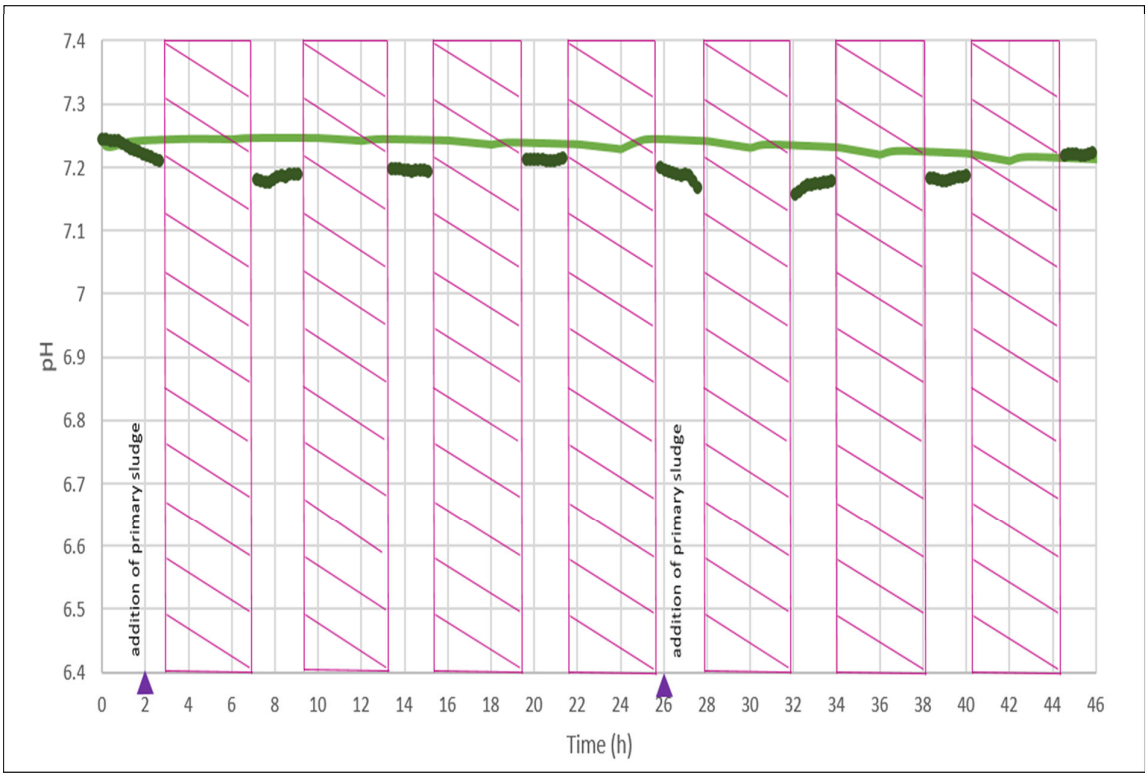


Figure 0-47 shows the results of the pH values during the experiments to determine carbon dioxide gas mass transfer coefficient (Kla) estimation (STAGE 4.0) experiments conducted on the ACP, and its corresponding model prediction. The mixing pump was turned ON for 2 h and OFF for 4 h (grey box), while 40 m^3 primary sludge was dosed (purple arrow) once every day in both the ACP and the ACP model.

The results of the carbon dioxide gas mass transfer coefficient (Kla) estimation (C1) experiments conducted on the ACP and its corresponding model prediction are shown in **Figure 0-47**. The pH value at time 0 h for the model as well as the experimental data was 7.24, according to the first criteria described in **section 0** meets the first requirement for validation. The pH value of the experimental data was maintained at approximately 7.2 throughout the experiment while the model predicted an average of 7.23, according to the third criteria in

Table 0-11: shows the values of the kinetic parameters (Carbonate ion, Hydrogen ion, Mass of acetoclastic methanogens) that were selected during the parameter selection (**section 2.11**). The values before the regression and after the regression of the C1 (ON 2 h and OFF for 4 h) experimental data are detailed.

Parameter	***Unit***	***Value Before Calibration***	***Value After Calibration***	***Change in Value***
Carbonate	-	*9 350 000*	*9 250 064*	-
Hydrogen ion	-	*177 500*	*178 976*	+
Mass of acetoclastic methanogen	-	*900 000*	*825 287*	-
Kla	d^{-1}	*5.3590*	*5.4532*	+

section 0 validates the buffering capacity predicted by the model. The parameter values that were used in the model before the regression as well as the parameter values obtained after the regression are given in **Table 0-11**.

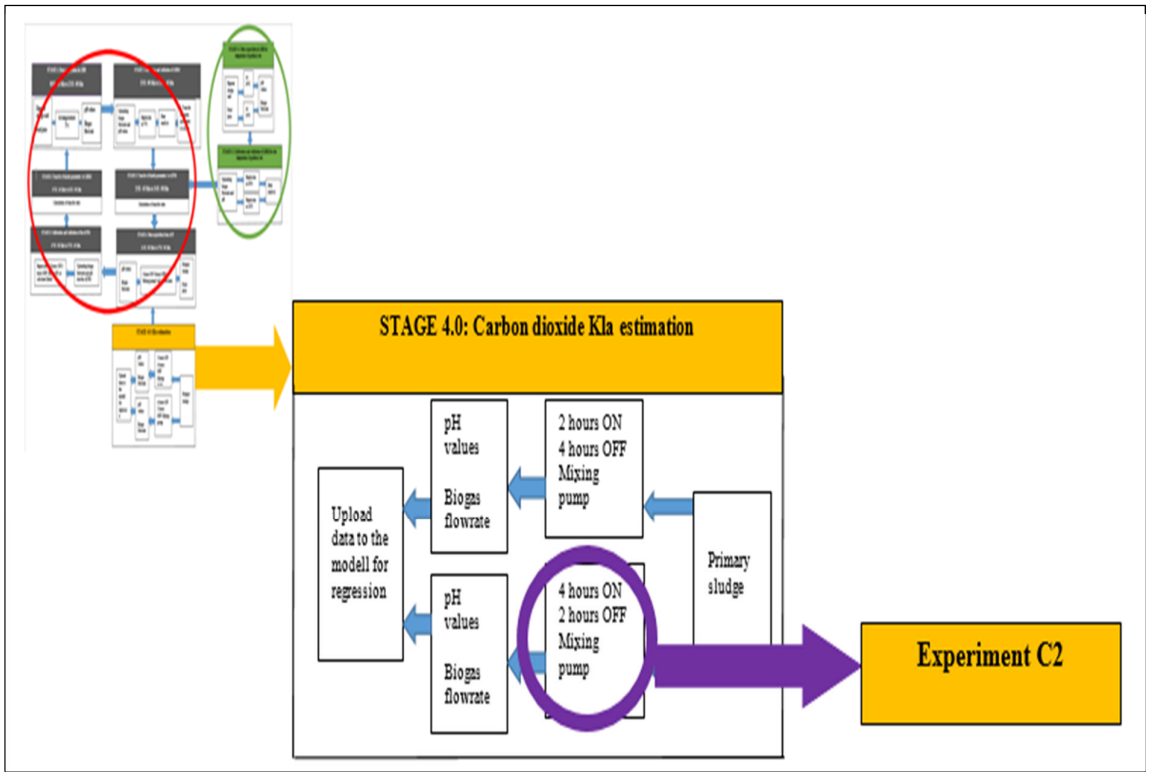


Figure 0-48 shows experiment C2 where 40 m^3 of primary sludge was dosed to estimate the Kla value of the Amanzimtoti Co-digestion Pilot plant.

The second experiment (C2) conducted to estimate the carbon dioxide Kla was done according to **section 0**.

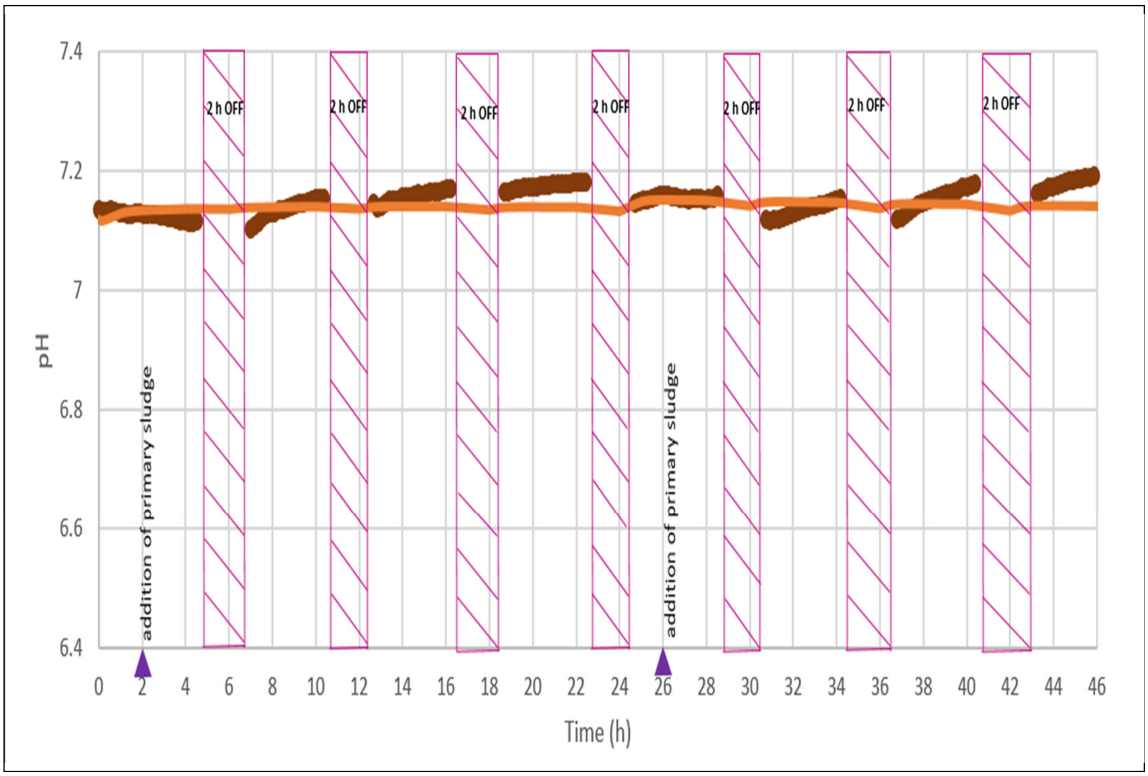


Figure 0-49 shows the results of the pH values during the experiments to determine carbon dioxide gas mass transfer coefficient (Kla) estimation (STAGE 4.0) experiments conducted on the Amanzimtoti Co-digestion Pilot Digester (ACP), and its corresponding model prediction. The mixing pump was turned ON for 4 h and OFF for 2 h (grey box), while 40 m^3 primary sludge was dosed (purple arrow) once every day in both the ACP and the ACP model.

The results of the carbon dioxide gas mass transfer coefficient (Kla) estimation (C2) experiments conducted on the ACP and its corresponding model prediction are shown in **Figure 0-49**. The pH value at time 0 h for the model was 7.13 while the pH value for the experimental data was 7.13, according to the first criteria described in **section 0** meets the first requirement for validation. The pH value of the experimental data was maintained at approximately 7.13 throughout the experiment while the model predicted an average of 7.14, according to the third criteria in **section 0** validates the buffering capacity predicted by the model. The parameter values that were used in the model before the regression as well as the parameter values obtained after the regression are given in **Table 0-12**.

Table 0-12: shows the kinetic parameters values (Carbonate ion, Hydrogen ion, Mass of acetoclastic methanogens) that were selected during the parameter selection (**section 2.11**). The values before the regression and after the regression of the C2 (ON 4 h and OFF for 2 h) experimental data are detailed.

Parameter	***Unit***	***Value Before Calibration***	***Value After Calibration***	***Change in Value***
Carbonate	-	*9350000*	*9064056*	-
Hydrogen ion	-	*181788*	*176528*	-
Mass of acetoclastic methanogen	-	*900000*	*825264*	-
Kla	d^{-1}	*15.3168*	*15.5687*	+

The estimated Kla value was the average of 5.4532 and 15.5687 from **Table 0-11** and **Table 0-12**, respectively. The resultant Kla value used was 10.

4.1.7 Results of the data acquisition experiments (STAGE 4) and the calibration and validation of the Amanzimtoti Co-digestion Pilot digester model (STAGE 5)

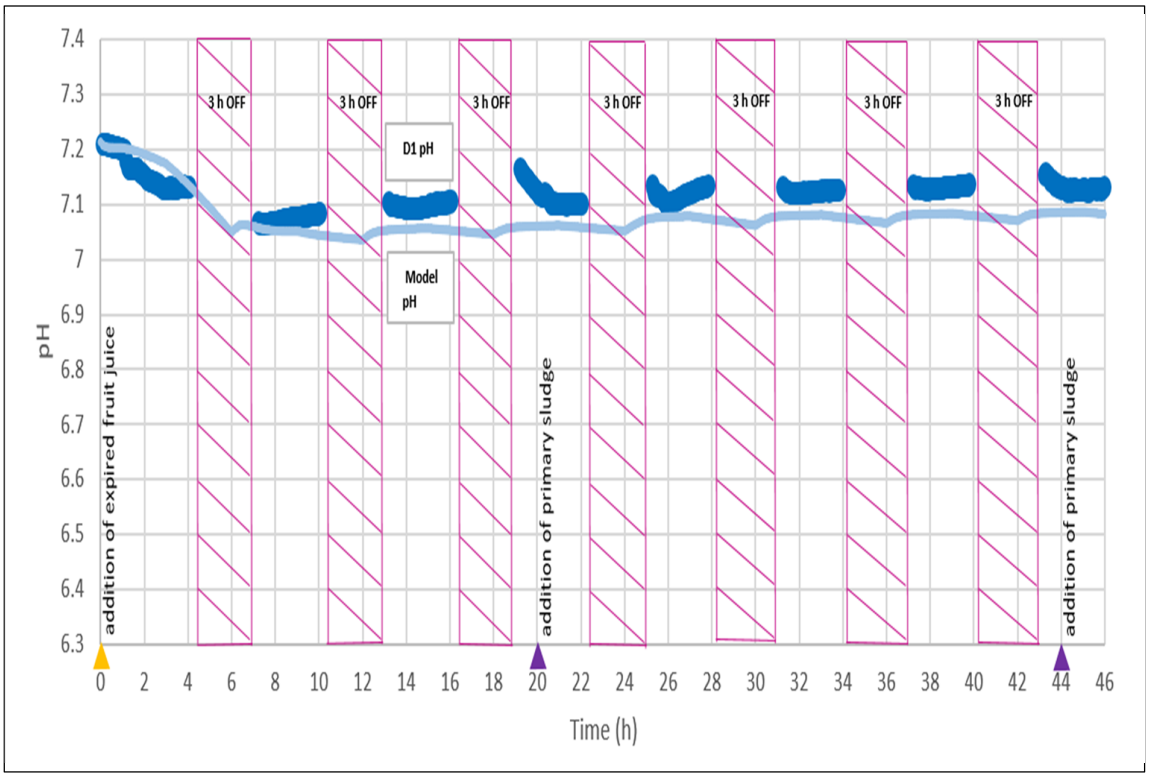


Figure 0-50 shows the results of the data acquisition experiment (D1) conducted on the Amanzimtoti co-digestion Pilot Digester (ACP)), and its corresponding model prediction, where the mixing pump was turned ON for 3 h and OFF for 3 h (grey box), while 5 m^3 of expired fruit juice (yellow arrow) and 40 m^3 primary sludge was dosed (purple arrow).

The results of the data acquisition experiments conducted on the Amanzimtoti co-digestion Pilot Digester (ACP) and its corresponding model prediction are shown in **Figure 0-50**. The pH value at time 0 h for the model as well as the experimental data was 7.13, according to the first criteria described in **section 0** meets the first requirement for validation. The pH value of the experimental data was maintained at approximately 7.13 throughout the experiment while the model predicted an average of 7.07, according to the third criteria in **section 0** validates the buffering capacity predicted by the model. The parameter values that were used in the model before the regression as well as the parameter values obtained after the regression are given in **Table 0-13**.

Table 0-13: shows the values of the kinetic parameters (Carbonate ion, Hydrogen ion, Mass of acetoclastic methanogens) that were selected during the parameter selection (**section 2.11**). The values before the regression and after the regression of the D1 experimental data are detailed.

Parameter	*Unit*	*Value Before Calibration*	*Value After Calibration*	*Change in Value*
Carbonate	*-*	*9350000*	*9397428*	+
Hydrogen ion	*-*	*178400.*	*183340*	+
Mass of acetoclastic methanogen	*-*	*900000*	*869919*	+

4.1.8 Results of the transfer of the kinetic parameters from the Amanzimtoti Coo-digestion Pilot Digester Model to the Laboratory Batch Reactor Model (STAGE 6)

The inverse of the ratio used in STAGE 3 (**section 4.1.5)** was used as the basis for the transfer of extensive properties. The ratio used was 2×10^{-4}.

4.2 Conclusion to 35°C *Feedback control loop hypothesis*

The ***feedback control loop hypothesis*** states that:

> ***"Acetoclastic methanogen biomass concentration, biogas flowrate, and pH can be used to fit experimental data from the Laboratory Batch Reactor to the Laboratory Batch Reactor Model. Laboratory Batch Reactor Model data can be transferred to the Amanzimtoti Co-digestion Pilot Project Model. Amanzimtoti Co-digestion Pilot Project Model data can be transferred to the Laboratory Batch Reactor Model"***

The Laboratory Batch Reactor (LBR) duplicate experiments (STAGE 0.1) A1 and A2 were validated according to the criteria stated in **section 0.** Moreover, the Laboratory Batch Reactor Models (LBRM) calibrated using experimental data (STAGE 0.2) from A1 and A2 by using Acetoclastic methanogen biomass concentration, biogas flowrate, and pH as parameters for regression. The models that were developed were validated according to the criteria stated in **section 0**. The kinetic parameters were from the LBRM were transferred to the ACPM (STAGE 3), and the ACPM model was calibrated (STAGE 4 and STAGE 5) using the experimental data (D1). The calibrated ACPM model was validated using the criteria in **section 0**. The ACPM kinetic was finally transferred to the LBRM. Hence the feedback control loop was successfully completed using LBR screening experiments conducted at 35°C. Therefore the ***feedback control loop hypothesis*** was proved.

4.2.1 Results for data acquisition in the LBR for the *Temperature hypothesis* (STAGE 0.1)

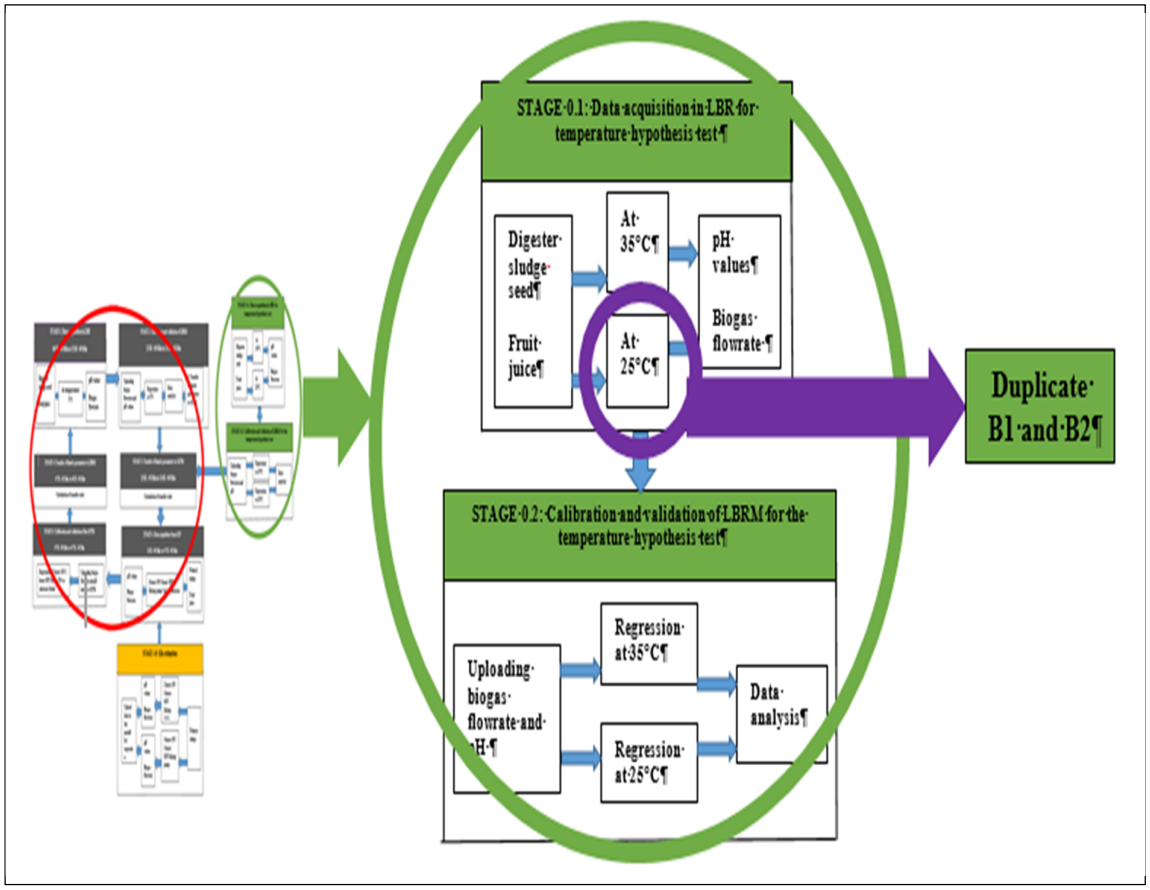


Figure 0-51 shows that B1 and B2 are duplicate experiments for testing the *Temperature hypothesis*

This section details the results of the data acquisition conducted in STAGE 0.1 at 25°C as shown in **Figure 0-51**.

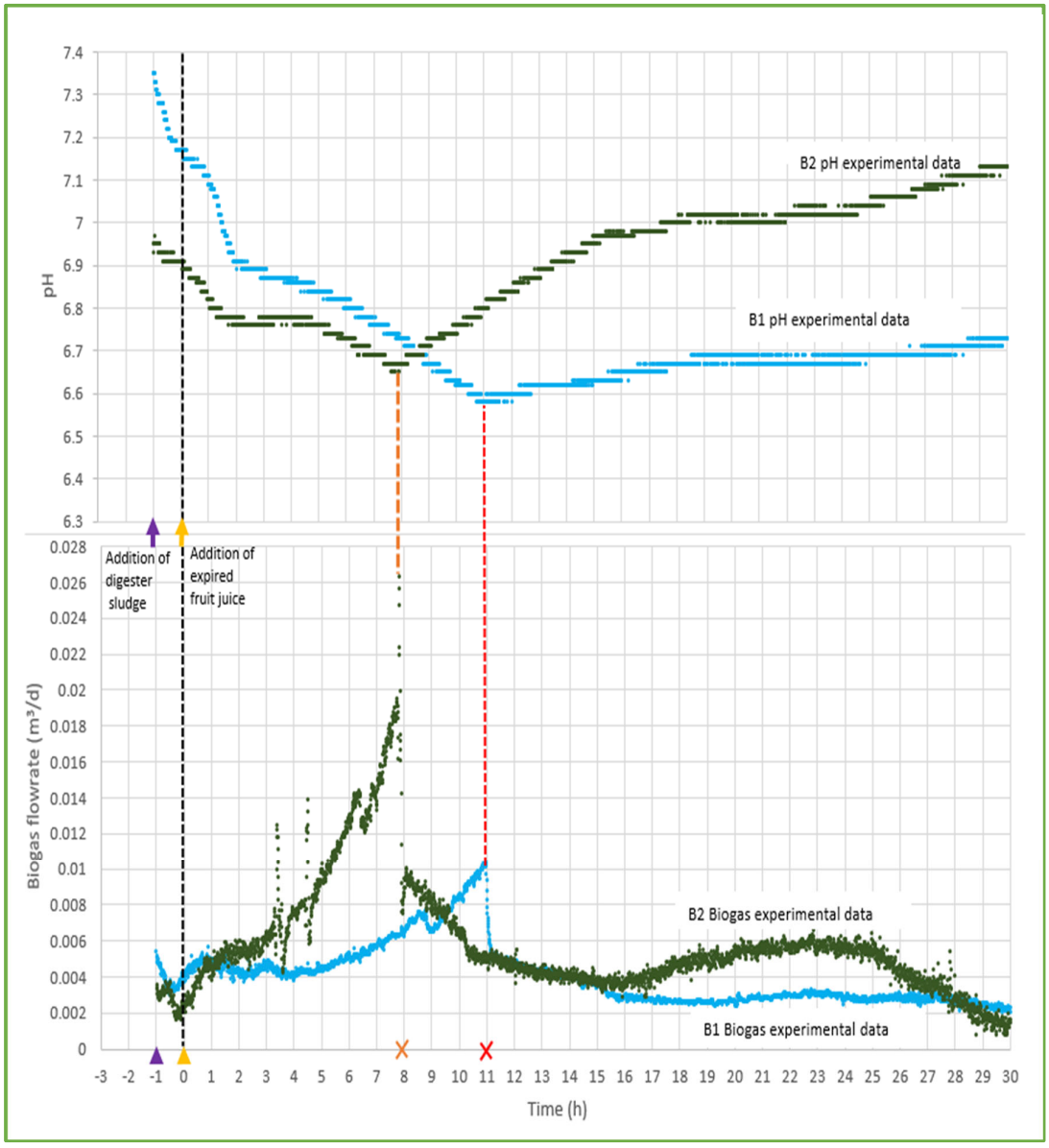


Figure 0-52 shows the pH and biogas profiles for the duplicate experiments B1 and B2 where 4 L of digester sludge, 50 mL of expired fruit juice was added to the LBRs and the experiment was conducted at 25°C. The brown and red dotted lines show that the lowest pH value coincides with the highest biogas flowrate. The time when the sludge and the expired fruit juice was added are indicated by the purple arrow and the yellow arrow.

The pH and biogas profile shown in **Figure 0-52** is of duplicate experiments B1 and B2. Digester sludge from the ACP was loaded into the LBRs at time -1 h indicated by a purple arrow. The LBRs were sealed and purged for one hour according to the methodology in **section 0**. At time 0 h, 50 mL of expired fruit juice was dosed, as shown by the yellow arrow line in **Figure 0-52**.

The pH value of B1 and B2 at time 0 h (purple arrow) was 7.17 and 6.91, respectively. The pH values of B1 and B2 gradually declined until they reached the minimum values at time 11 h (red X) and 8 h (brown X), respectively. The minimum pH values of B1 and B2 were 6.58 and 6.65, respectively. The pH value for B1 was gradually increased from 11 h, and after 24 h it reached a value of 6.67, which was lower than its pH value at time 0 h. The pH value for B2 gradually increased, and after 2 h the pH reached a value of 7.02, which was higher than its pH value at time 0 h.

According to the first validation criteria described in **section 0,** the difference in the time taken to reach the minimum pH for the duplicate experiments fall outside of the acceptable range (1 h) and are therefore invalid.

The volume of biogas produced by both B1 and B2 was calculated according to the method described **in section 3.2.2.1**. The volume of biogas produced by B1 and B2 was 0.00583 m^3 and 0.0088 m^3, respectively.

The volume of gas produced is by B1 and B2 has a difference of less than 50% hence according to the third criteria given in **section 0** the biogas data is valid

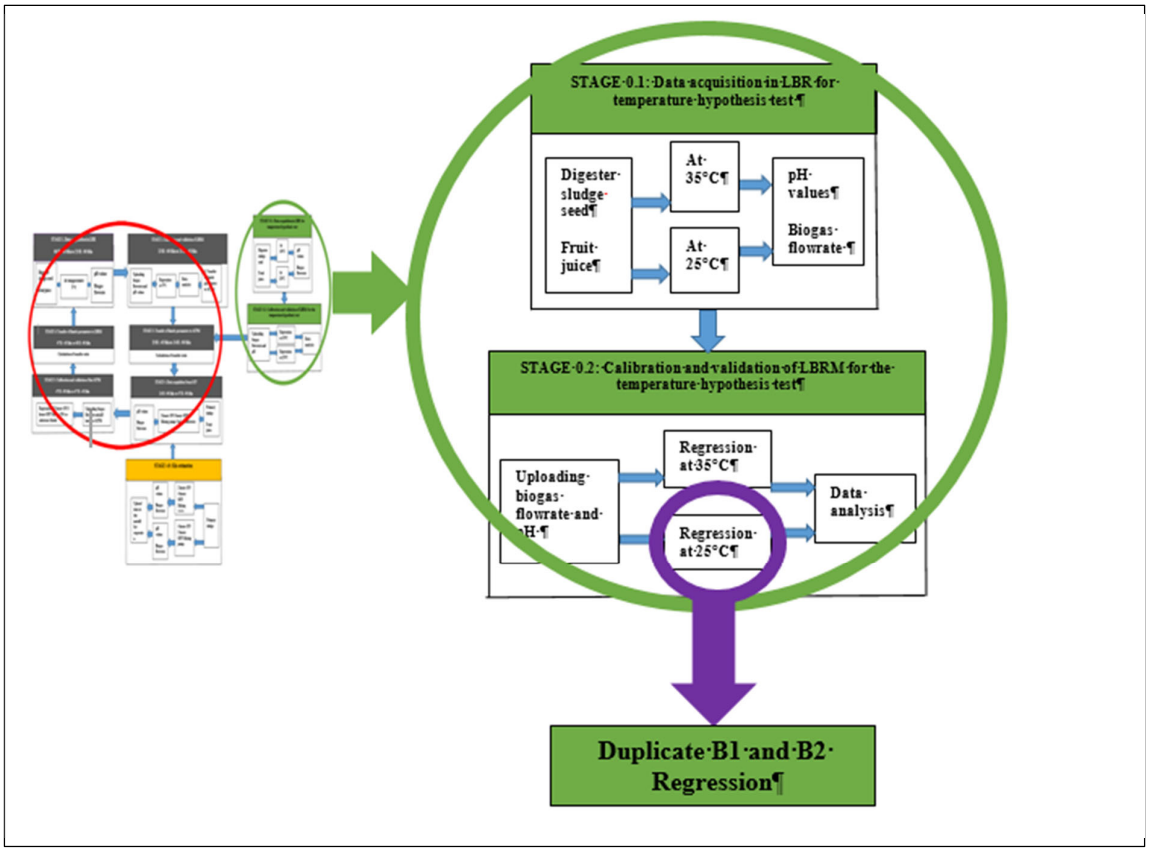


Figure 0-53 shows that duplicate experiments B1 and B2 were used for regression in STAGE 0.2 of the ***Temperature hypothesis***

4.2.2 Results for the data acquisition experiments in the Laboratory batch Reactor for the Temperature hypothesis (STAGE 0.1)

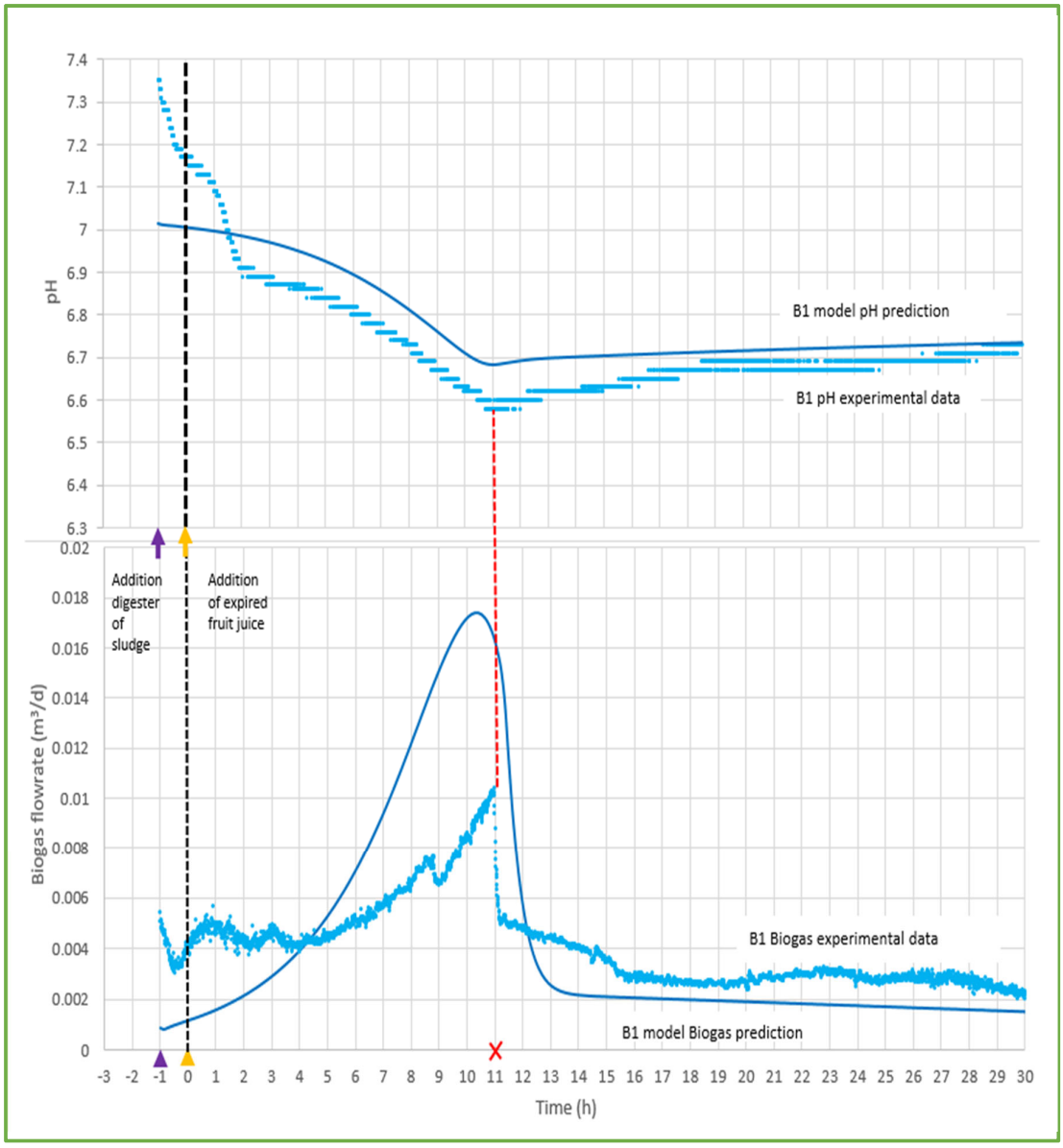


Figure 0-54 shows the pH and biogas profile of the duplicate experiment B1 and its corresponding model prediction. The duplicate experiment was conducted at 25°C with a dose of 50 mL expired fruit juice. The model prediction produced after a regression was conducted at 25°C with a dose of 7 g expired fruit juice analogue (glucose).

The duplicate experiment was conducted at 25°C with a dose of 50 mL expired fruit juice. The model prediction was produced after a regression was conducted at 25°C with a dose of 7 g expired fruit juice analogue (glucose) on the WEST modelling platform. As indicated in **section 0** the ability to accurately model the time taken to reach the minimum pH and the

time taken for the profile to recover are the main parameters used to validate the duplicate experiments' pH model.

Figure 0-54 shows the pH value predicted by the model at time 0 h is 7.01, while the experimental data showed a value of 7.17, which was different from the experimental data. The initial rapid drop in pH value was not captured by the model. The model only captures the second phase of the pH value decrease. Hence according to the first criteria described in **section 0,** the model does not meet the first requirement for validation. The minimum model pH value is predicted to occur at 11 h, which was the same as the experimental data. The difference in time taken to reach the minimum pH value was less than 1 h, which, according to the second criteria in **section 0** meets the second requirement for validation. Nevertheless, the model predicts a minimum value of 6.68, while the experimental data shows a minimum value of 6.58. The difference in minimum pH value is equal to 0.1, which, according to the third criteria in **section 0** meets the second requirement for validation. The model predicted pH after 24 h was 6.72 while the experimental data showed a value of 6.67 after 24 h. which, according to the fourth criteria in **section 0** meets the requirement for validation.Overall the model was unable to meet all the requirements to validate the pH profile prediction.

The area under the biogas flowrate profile is equal to the volume of the biogas produced during the co-digestion process, as indicated in **section 0**. The volume of biogas predicted by the model as calculated using the method described in **section 3.2.2.1** was 0.0073 m^3 while the duplicate experiment volume was 0.0058. The difference in biogas volume is less than 50 %, which, validates the expired fruit juice dosage and its corresponding fruit juice analogue (glucose) according to the fifth criteria in **section 0**. The parameter values that were used in the model before the regression as well as the parameter values obtained after the regression are given in **Table 0-15.**

Table 0-14: shows the values of the kinetic parameters (Carbonate ion, Hydrogen ion, Mass of acetoclastic methanogens) that were selected during the parameter selection (**section 0**). The values before the regression and after the regression of the D1 experimental data are detailed.

Parameter	***Unit***	***Value Before Calibration***	***Value After Calibration***	***Change in Value***
Carbonate	-	*22.55*	*22.33*	-
Hydrogen ion	-	*0.422*	*0.455*	+
Mass of acetoclastic methanogen	-	*1.2975*	*1.26146*	-

4.2.3 Results for modelling the second duplicate experiment at 25°C B2

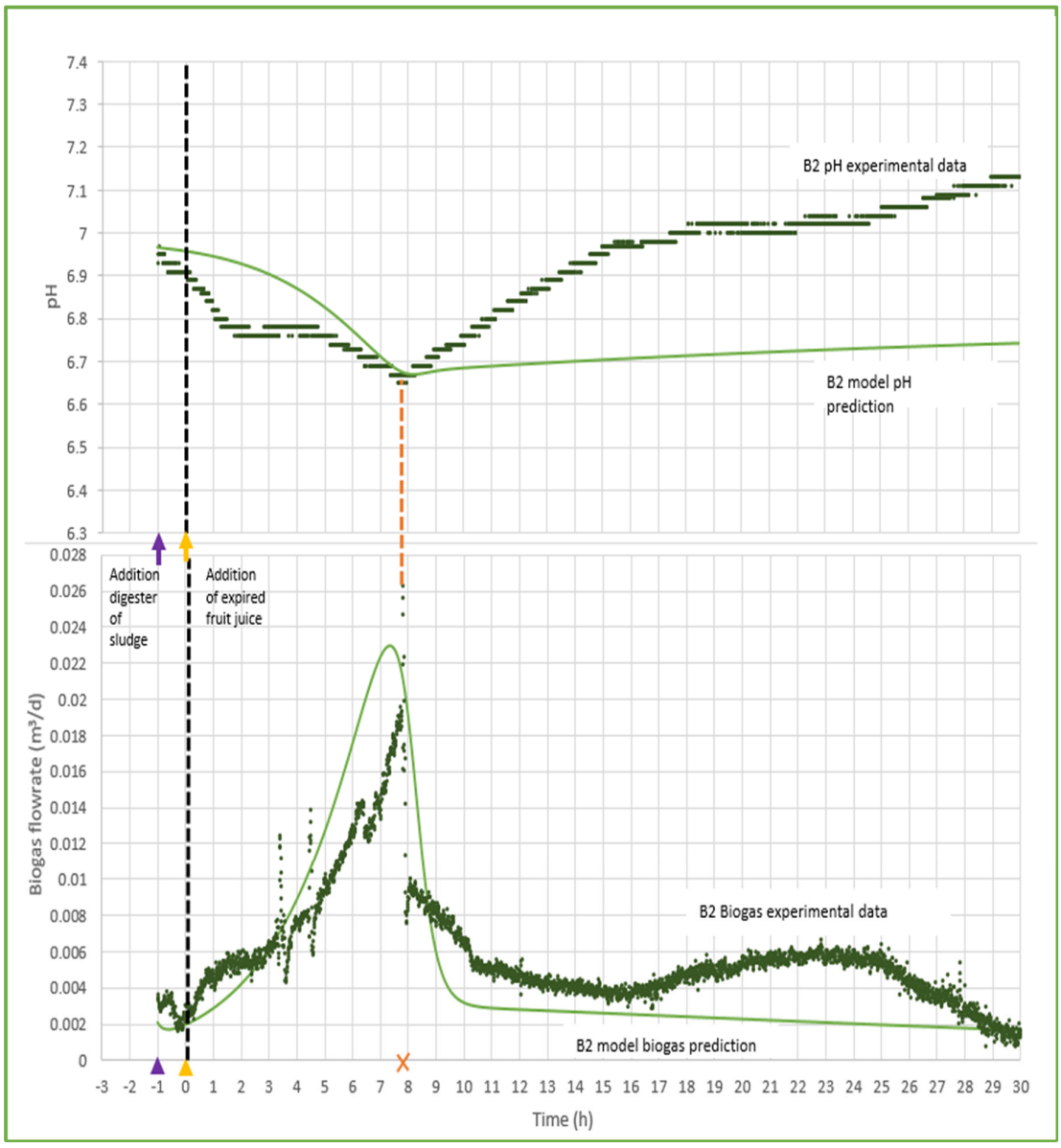


Figure 0-55 shows the pH and biogas profile of the duplicate experiment B2 and its corresponding model prediction. The duplicate experiment was conducted at 25°C with a dose of 50 mL expired fruit juice. The model prediction produced after a regression was conducted at 25°C with a dose of 7 g expired fruit juice analogue (glucose).

The duplicate experiment was conducted at 25°C with a dose of 50 mL expired fruit juice. The model prediction was produced after a regression was conducted at 25°C with a dose of 7 g expired fruit juice analogue (glucose) on the WEST modelling platform. As indicated in **section 0** the ability to accurately model the time taken to reach the minimum pH and the time

taken for the profile to recover are the main parameters used to validate the duplicate experiments' pH model.

Figure 0-55 shows the pH value predicted by the model at time 0 h is 6.96 while the experimental data showed a similar value of 6.91, which was the same as the experimental data. Hence according to the first criteria described in **section 0** meets the first requirement for validation. The minimum model pH value was also predicted to occur at 8 h, which was the same as the experimental data. There is no difference in time taken to reach the minimum pH value, which, according to the second criteria in **section 0** meets the second requirement for validation. Moreover, the model predicted a minimum value of 6.65, which was the same as the experimental data. The difference in minimum pH value is less than 0.1, which, according to the third criteria in **section 0** meets the second requirement for validation. The model predicted pH after 24 h was 6.73 while the experimental data showed a value of 7.02 after 24 h. The model was unable to predict the increase of the pH value after the minimum value is reached, which, according to the fourth criteria in **section 0** does not meet the requirement for validation. Overall the model was unable to meet all the requirements to validate the pH profile prediction.

The area under the biogas flowrate profile is equal to the volume of the biogas produced during the co-digestion process, as indicated in **section 0**. The volume of biogas predicted by the model as calculated using the method described in **section 3.2.2.1** was 0.0083 m^3 while the duplicate experiment volume was 0.0088. The difference in biogas volume is less than 50 %, which, validates the expired fruit juice dosage and its corresponding fruit juice analogue (glucose) according to the fifth criteria in **section 0**. The parameter values that were used in the model before the regression as well as the parameter values obtained after the regression are given in **Table 0-17.**

Table 0-16: shows the values of the kinetic parameters (Carbonate ion, Hydrogen ion, Mass of acetoclastic methanogens) that were selected during the parameter selection (**section 2.11**). The values before the regression and after the regression of the B2 experimental data are detailed.

Parameter	***Unit***	***Value Before Calibration***	***Value After Calibration***	***Change in Value***
Carbonate	-	*22*	*24.33*	+
Hydrogen ion	-	*0.45*	*0.53*	+
Mass of acetoclastic methanogen	-	*10.8612*	*9.7831*	-

4.3 Conclusion to *Temperature hypothesis*

The ***temperature hypothesis (*****section 0*****)*** states that:

> ***"Kinetic data collected from the Laboratory Batch Reactor Model at 25°C and 35°C can be transferred to the Amanzimtoti Co-digestion Pilot Project Model."***

The kinetic data collected from the Laboratory Batch Reactor Model at 35°C was successfully transferred to the Amanzimtoti Co-digestion Pilot Project Model. The success was determined by the ACPM's prediction of the ACP's response to the dosing of 5 m^3 expired fruit juice (D1) in **section** Error! Reference source not found.. Therefore the result of the ***Temperature hypothesis*** with regard to the 35°C Laboratory Batch Reactor Model kinetic data was a success.

The LBR duplicate experiments (STAGE 0.1) B1 and B2 were analysed according to the criteria stated in **section 0** and found invalid. Moreover, the LBRM models calibrated using experimental data (STAGE 0.2) from B1 and B2 were found invalid according to the criteria stated in **section 0**.

The key difference between 25°C and 35°C was that the time taken to reach the minimum pH value was inconsistent for the. Duplicate experiments A1 and A2 both took 8 h while B1 and B2 took 11 h and 8 h respectively. B1 and B2 were expected to take longer than A1 and A2 but only B1 took longer by three hours while B2 took the same time as A1 and A2. In **section 1.4** and **section 2.10** the key requirement for the project was to maintain a time of 24 h for the LBR screening experiments. Using the 25°C is feasible but it has a longer rate of reaction which can potentially increase the time taken to complete the feedback control loop. Therefore the ***Temperature hypothesis*** was not proved.

4.4 Results and Discussion Summary

The temperature hypothesis was not proved. Only the 35°C experimental data was successfully used in the Amanzimtoti co-digestion plant model. The 25°C did not meet the validation criteria. Moreover, the 25°C data had a longer reaction time than the 35°C data. More investigation is required to compare the reaction rate of the 35°C experiments to the 25°C experiments.

The feedback control loop hypothesis was proved. The feedback control loop can be used as a tool to control how much expired fruit juice can be dosed in the Amanzimtoti Co-digestion Pilot Digester. Although the feedback control loop was successful, the experimental procedure was plagued by instances where various components (temperature sensors, gas analysis sensor and gas flow meter) of the ACP were not functional. Moreover, there were serious delays when expired fruit juice deliveries were required, which resulted in only a single dose of five cubic meters of expired fruit juice being delivered.

Chapter 5: Conclusions

- The expired fruit juice Laboratory screening tests were successfully conducted in 24 h.
- Dosing a co-substrate daily in the ACP and updating parameters of the ACPM after each screening experiment to improve short term prediction removes the need for long term prediction of the ACPM.
- Temperature hypothesis was invalid.
- The 25°C laboratory screening experiments reaction time is too long for the requirements of the project.
- Feedback control loop hypothesis was proved
- The transfer of kinetic parameters from the LBRM obtained at 35°C to the ACPM was effective in the development of the ACPM.
- The simplified UCT ADM 3P model is effective characterizing the effect dosing fruit juice in both the ACP and the LBR.
- The LBR is effective in capturing the kinetic parameters of the ACP digester sludge at 35^{o}C
- Runs at 25°C were not effective in characterizing the effect of dosing fruit juice in the LBR after considering the time required to process the data. There were too many differences between the model prediction and the 25°C data. In contrast, the 35°C data was well predicted by the model, hence the 25°C path was discarded.
- Varying the mixing intensity in the ACP and modelling the pH data only was effective in estimating the Kla value of the ACP. The Kla estimate was good enough for use to predict ACP performance.
- Digester sludge only was effective, no need to dose PS in the LBR for characterizing the effect of fruit juice on digester sludge. The ACP is dosed with 40m^3 of PS per day. During the LBR experiments, only digester sludge was used, and the resultant data was good enough for use in calibrating the LBRM and the subsequent transfer of kinetic parameters to the ACPM,
- Glucose was an effective fruit juice analogue in the model for the ACPM and LBR.

Chapter 6: Recommendations

The feedback control loop technique can be used as a dosing guide for a daily dosage of low volumes of expired fruit juice.

Future research

The current model has glucose as a generic representative of the co-substrates in the model. The simplicity of glucose was good enough to be used in place of expired fruit juice in the model. There is a need to extend the model for materials more complex than fruit juice by developing other generic components in place of glucose. This would improve the utility and flexibility of the model. The current model can be used as a foundation on which these waste streams can be modelled.

ACP scientific recommendations

- Conduct more runs to confirm the limits of dosing as determined by the model. The model is effective in determining the limit of fruit juice that could be dosed in the ACP
- Methane flowrate and composition measurement should be done in preparation of using the biogas for power generation

ACP engineering recommendations

- Training municipality personnel to use WEST modelling software in preparation for officially handover to the municipality.
- Develop a better industrial waste collection system. There were persistent delays in getting fruit juice tankers on site. More has to be done by the municipality to allow regular collection of waste to enable regular dosing of the ACP.

LBR scientific recommendations

- Experimental methodology should be improved by analysing different co-substrates. Characterizing the effect of other co-substrates would enable a wider range of industrial effluent to be screened for the ACP.

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Appendix

1.1. Appendix A

Importance of pH modelling

pH was a key indicator of digester stability. Hydrogen ions, carbonate ions, phosphate ions, and VFAs were the main determinants of pH in the model. VFA and phosphate content was set according to sludge composition data from Logan (2016). During the regression, carbonate and hydrogen ion content was used to match the initial pH of sludge during experiments and the buffering capacity of the sludge. The buffering capacity was indicated by how much the sludge was able to counteract the drop in pH to match the experimental data

Brouckaert et al. (2010) note that due to the accumulation of CO_2 from the methanogenesis reactions the reactor headspace develops a partial pressure of the gas, some of the organics are broken down and remain in solution as carbonate (HCO_3^-). The combination of CO_2 and HCO_3^- establishes the digester pH. The modelling of AD pH, therefore, requires the integration of bioprocesses and mixed weak/acid-base chemistry in aqueous-gas phases (Brouckaert et al., 2010). The ACP has low P content; hence a two-phase acetate ammonium and inorganic carbon mixed weak acid/base chemistry are adequate.

During normal operation of AD VFAs are produced, causing the pH to drop. The pH also drops due to the presence of CO_2 from biogas production. The CO_2 dissolves in water to form an equilibrium system, as shown below (Demitry, 2016).

$$CO_2(g) \leftrightharpoons CO_2(aq) \qquad \textbf{0-6}$$

Carbonic acid is produced as follows (Snoeyink and Jenkins, 1980):

$$CO_2(aq) + H_2O \leftrightharpoons H_2CO_3 \qquad \textbf{0-7}$$

Acid dissociation of carbonic acid is shown below (Snoeyink and Jenkins, 1980):

$$H_2CO_3 \leftrightharpoons HCO_3 + H^+ \qquad \textbf{0-8}$$

$$HCO_3^- \leftrightharpoons CO_3^{-2} + H^+ \qquad \textbf{0-9}$$

In situations where there is inadequate buffering capacity, an abrupt drop in pH is experienced in the reactor. The buffering system (alkalinity) of the digester prevents rapid drops in pH.

Hydroxide ions (OH^-), carbonate (CO_3^{-2}) and bicarbonate (HCO_3^-) are the sources of buffering capacity in AD (Demitry, 2016). The equations are shown below (Snoeyink and Jenkins, 1980):

$$OH^- + H^+ \leftrightharpoons H_2O \quad \textbf{0-10}$$

$$CO_3^{2-} + H^+ \leftrightharpoons HCO_3^- \quad \textbf{0-11}$$

$$HCO_3^- + H^+ \leftrightharpoons H_2CO_3 \quad \textbf{0-12}$$

According to Sötemann et al. (2005a) pH is calculated based on three components of the model, namely a kinetic portion, a stoichiometric portion and a carbonate system of weak acid-base chemistry. The kinetic part is used to calculate how much methane is produced during a specified retention time as well as the percentage COD removed in the same span of time. The stoichiometric part determines the amount of ammonia, carbon dioxide and alkalinity based on the percentage COD removed. Digester pH is calculated from the carbonate system of weak acid and base, the carbon dioxide partial pressure and the alkalinity generated (Sötemann et al., 2005a).

Other variables such as Ca, Mg and NH_3 that had the potential of affecting pH were left at the same as the original model used by Logan (2016). From work done by Logan (2016), the Ca and Mg composition in the sludge was low enough that it did not cause precipitation; hence it was not used as a variable in the regression. NH_3 content was also set at an arbitrary value because NH_3 has a significant effect on the pH at a pH higher than 8 (Capri and Marais, 1975) which was outside of the operating (pH 6-7) conditions for this study.

If the initial conditions and other equations that were used represent the different processes in AD in the model are close to the experimental conditions the parameter estimation procedure would result in the model converging to match the objective function. The model's predictive capability is dependent on the objective functions.

Constructing the pH model

Components of the model

Components are a set of model units that are used to outline the complete material composition of the system. They served as mathematical constructs for material balances and stoichiometry.

Species of the model were the entities that are used to describe the actual molecules physically present in the system.

Components in pH modelling

Since the model was simplified, it was decided to focus on components associated with CO_2 since it had the greatest influence on digester pH. The chosen components were H^+, Ac^-, Pr^-, CO_3^+, and H_2O.

The species in the model were

H^+ - Hydrogen ion

Ac^- - Acetate ion

Pr^- -Propionate ions

HAc – Acetic acid

HPr – Propionic acid

HCO_3^- - Hydrogen carbonate ion

OH^- - Hydroxide ion

H_2CO_3 – Hydrogen carbonate acid

CO_3^- - Carbonate ion

Speciation equations for all species are identified, and the corresponding, equilibrium constants and stoichiometry for the formation of the species from the components are known and part of the system database.

pH can not be directly measured. It is indirectly calculated using equations developed for the proton condition or TOTH. TOTH is the total of all the excess H^+ after subtracting the H^+ deficiencies (Benjamin, 2014). To get the TOTH, there three equations that need to be solved simultaneously.

For example, the evolution of CO_2:

$$CO_3^{2-}(aq) + H^+(aq) \rightarrow HCO_3^- \quad \textbf{0-13}$$

$$HCO_3^- + H^+ \rightarrow H_2CO_3 \quad \textbf{0-14}$$

$$H_2CO_3 \rightarrow\uparrow CO_2(g) + H_2O(liq) \quad \textbf{0-15}$$

The equilibrium constant equations are the first set of equations which are:

$$K_{a1} = \frac{\{HCO_3^-\}}{\{CO_3^{2-}\}\{H^+\}} \quad \textbf{0-16}$$

$$K_{a2} = \frac{\{H_2CO_3\}}{\{HCO_3^-\}\{H^+\}} \quad \textbf{0-17}$$

$$K_{a3} = \frac{\{H_2O\}\{CO_2\}}{\{H_2CO_3\}} \quad \textbf{0-18}$$

K_{a1}, K_{a2}, and K_{a3} can be found in the system database. {} indicates the activity of a species.

The balance equations would be the second set of equations which are:

$$[H^+]_T \rightarrow [H^+] + [HCO_3^-] + 2[H_2CO_3] \quad \textbf{0-19}$$

$$[CO_3^{2-}]_T \rightarrow [CO_3^{2-}] + [HCO_3^-] + 2[H_2CO_3] \quad \textbf{0-20}$$

[] indicates the concentration of the species in brackets. The subscript T denotes the total concentration of a particular component which is found by adding all the species which contain the component.

The third set of equations that need to be solved are related to the activity coefficients for the evolution of CO_2.

$$\{HCO_3^-\} = \gamma_{HCO_3^-}[HCO_3^-] \quad \textbf{0-21}$$

$$\{CO_3^{2-}\} = \gamma_{CO_3^{2-}}[CO_3^{2-}] \quad \textbf{0-22}$$

$$\{H^+\} \rightarrow \gamma_{H^+}[H^+] \quad \textbf{0-23}$$

γ is the activity coefficient. The three sets of equations have to be solved numerically to get $\{H^+\}$, and the pH is found using the equation below.

$$pH = -log\{H^+\} \quad \textbf{0-24}$$

This is done by the equilibrium software for every component simultaneously(Benjamin, 2014).

2.1. Appendix B

Amanzimtoti co-digestion plant model digester variables

Table 0-18 Amanzimtoti co-digestion plant model digester variables

Name	*Value*	*Initial Value*	*Unit*
Category: Algebraic Variables			
Group: Concentration			
C(H2O)	*0*	*0*	*m3/d*
C(S_H)	*0*	*0*	*g/m3*
C(S_Na)	*0*	*0*	*g/m3*
C(S_K)	*0*	*0*	*g/m3*
C(S_Ca)	*0*	*0*	*g/m3*
C(S_Mg)	*0*	*0*	*g/m3*
C(S_NH)	*0*	*0*	*g/m3*
C(S_Cl)	*0*	*0*	*g/m3*
C(S_VFA)	*0*	*0*	*g/m3*
C(S_Pr)	*0*	*0*	*g/m3*
C(S_CO3)	*0*	*0*	*g/m3*
C(S_SO4)	*0*	*0*	*g/m3*
C(S_PO4)	*0*	*0*	*g/m3*
C(S_HS)	*0*	*0*	*g/m3*
C(S_NO2)	*0*	*0*	*g/m3*
C(S_NO3)	*0*	*0*	*g/m3*
C(S_Fer)	*0*	*0*	*g/m3*
C(S_Feo)	*0*	*0*	*g/m3*
C(S_Al)	*0*	*0*	*g/m3*
C(S_H2)	*0*	*0*	*g/m3*
C(S_CH4)	*0*	*0*	*g/m3*
C(S_U)	*0*	*0*	*g/m3*
C(S_F)	*0*	*0*	*g/m3*
C(S_Glu)	*0*	*0*	*g/m3*
C(S_O)	*0*	*0*	*g/m3*
C(X_U_Inf)	*0*	*0*	*g/m3*
C(X_B_Org)	*0*	*0*	*g/m3*
C(X_PAO_PP)	*0*	*0*	*g/m3*
C(X_PAO_Stor)	*0*	*0*	*g/m3*
C(X_Str_NH4)	*0*	*0*	*g/m3*
C(X_ACP)	*0*	*0*	*g/m3*
C(X_Str_K)	*0*	*0*	*g/m3*
C(X_Cal)	*0*	*0*	*g/m3*
C(X_Mag)	*0*	*0*	*g/m3*
C(X_Newb)	*0*	*0*	*g/m3*
C(X_OHO)	*0*	*0*	*g/m3*
C(X_PAO)	*0*	*0*	*g/m3*
C(X_AD)	*0*	*0*	*g/m3*
C(X_AC)	*0*	*0*	*g/m3*
C(X_AM)	*0*	*0*	*g/m3*
C(X_HM)	*0*	*0*	*g/m3*

C(X_U_Org)	*0*	*0*	*g/m3*
C(X_B_Inf)	*0*	*0*	*g/m3*
C(X_ANO)	*0*	*0*	*g/m3*
C(X_ISS)	*0*	*0*	*g/m3*
C(G_CH4)	*0*	*0*	*g/m3*
C(G_CO2)	*0*	*0*	*g/m3*
C(G_N2)	*0*	*0*	*g/m3*
COD(H2O)	*0*	*0*	*m3/d*
COD(S_H)	*0*	*0*	*g/m3*
COD(S_Na)	*0*	*0*	*g/m3*
COD(S_K)	*0*	*0*	*g/m3*
COD(S_Ca)	*0*	*0*	*g/m3*
COD(S_Mg)	*0*	*0*	*g/m3*
COD(S_NH)	*0*	*0*	*g/m3*
COD(S_Cl)	*0*	*0*	*g/m3*
COD(S_VFA)	*0*	*0*	*g/m3*
COD(S_Pr)	*0*	*0*	*g/m3*
COD(S_CO3)	*0*	*0*	*g/m3*
COD(S_SO4)	*0*	*0*	*g/m3*
COD(S_PO4)	*0*	*0*	*g/m3*
COD(S_HS)	*0*	*0*	*g/m3*
COD(S_NO2)	*0*	*0*	*g/m3*
COD(S_NO3)	*0*	*0*	*g/m3*
COD(S_Fer)	*0*	*0*	*g/m3*
COD(S_Feo)	*0*	*0*	*g/m3*
COD(S_Al)	*0*	*0*	*g/m3*
COD(S_H2)	*0*	*0*	*g/m3*
COD(S_CH4)	*0*	*0*	*g/m3*
COD(S_U)	*0*	*0*	*g/m3*
COD(S_F)	*0*	*0*	*g/m3*
COD(S_Glu)	*0*	*0*	*g/m3*
COD(S_O)	*0*	*0*	*g/m3*
COD(X_U_Inf)	*0*	*0*	*g/m3*
COD(X_B_Org)	*0*	*0*	*g/m3*
COD(X_PAO_PP)	*0*	*0*	*g/m3*
COD(X_PAO_Stor)	*0*	*0*	*g/m3*
COD(X_Str_NH4)	*0*	*0*	*g/m3*
COD(X_ACP)	*0*	*0*	*g/m3*
COD(X_Str_K)	*0*	*0*	*g/m3*
COD(X_Cal)	*0*	*0*	*g/m3*
COD(X_Mag)	*0*	*0*	*g/m3*
COD(X_Newb)	*0*	*0*	*g/m3*
COD(X_OHO)	*0*	*0*	*g/m3*
COD(X_PAO)	*0*	*0*	*g/m3*
COD(X_AD)	*0*	*0*	*g/m3*

COD(X_AC)	*0*	*0*	*g/m3*
COD(X_AM)	*0*	*0*	*g/m3*
COD(X_HM)	*0*	*0*	*g/m3*
COD(X_U_Org)	*0*	*0*	*g/m3*
COD(X_B_Inf)	*0*	*0*	*g/m3*
COD(X_ANO)	*0*	*0*	*g/m3*
COD(X_ISS)	*0*	*0*	*g/m3*
COD(G_CH4)	*0*	*0*	*g/m3*
COD(G_CO2)	*0*	*0*	*g/m3*
COD(G_N2)	*0*	*0*	*g/m3*
COD_HAc	*0*	*0*	*g/m3*
COD_HPr	*0*	*0*	*g/m3*
molality(H)	*0*	*0*	*mol*
molality(Na)	*0*	*0*	*mol*
molality(K)	*0*	*0*	*mol*
molality(Ca)	*0*	*0*	*mol*
molality(Mg)	*0*	*0*	*mol*
molality(NH4)	*0*	*0*	*mol*
molality(Cl)	*0*	*0*	*mol*
molality(Ac)	*0*	*0*	*mol*
molality(Pr)	*0*	*0*	*mol*
molality(HCO3)	*0*	*0*	*mol*
molality(SO4)	*0*	*0*	*mol*
molality(HPO4)	*0*	*0*	*mol*
molality(HS)	*0*	*0*	*mol*
molality(NO2)	*0*	*0*	*mol*
molality(NO3)	*0*	*0*	*mol*
molality(Fer)	*0*	*0*	*mol*
molality(Fe_OH_2)	*0*	*0*	*mol*
molality(Al_OH_4)	*0*	*0*	*mol*
molality(OH)	*0*	*0*	*mol*
molality(H2CO3)	*0*	*0*	*mol*
molality(CaCO3)	*0*	*0*	*mol*
molality(MgCO3)	*0*	*0*	*mol*
molality(CaHCO3)	*0*	*0*	*mol*
molality(MgHCO3)	*0*	*0*	*mol*
molality(CO3)	*0*	*0*	*mol*
molality(H2PO4)	*0*	*0*	*mol*
molality(MgPO4)	*0*	*0*	*mol*
molality(CaPO4)	*0*	*0*	*mol*
molality(MgHPO4)	*0*	*0*	*mol*
molality(CaHPO4)	*0*	*0*	*mol*
molality(PO4)	*0*	*0*	*mol*
molality(HAc)	*0*	*0*	*mol*
molality(HPr)	*0*	*0*	*mol*

molality(NH3)	*0*	*0*	*mol*
molality(CaSO4)	*0*	*0*	*mol*
molality(MgSO4)	*0*	*0*	*mol*
molality(CaOH)	*0*	*0*	*mol*
molality(NH4SO4)	*0*	*0*	*mol*
molality(NaHPO4)	*0*	*0*	*mol*
molality(NaHCO3)	*0*	*0*	*mol*
molality(MgH2PO4)	*0*	*0*	*mol*
molality(CaAc)	*0*	*0*	*mol*
molality(NaAc)	*0*	*0*	*mol*
molality(MgAc)	*0*	*0*	*mol*
molality(MgPr)	*0*	*0*	*mol*
molality(NaSO4)	*0*	*0*	*mol*
molality(MgOH)	*0*	*0*	*mol*
molality(H2S)	*0*	*0*	*mol*
molality(KSO4)	*0*	*0*	*mol*
molality(CaH2PO4)	*0*	*0*	*mol*
molality(KHPO4)	*0*	*0*	*mol*
molality(Feo)	*0*	*0*	*mol*
molality(Al)	*0*	*0*	*mol*
molality(Fer_HS_2)	*0*	*0*	*mol*
molality(Fer_HS_3)	*0*	*0*	*mol*
molality(FerHCO3)	*0*	*0*	*mol*
molality(FerSO4)	*0*	*0*	*mol*
molality(FerHPO4)	*0*	*0*	*mol*
molality(FerH2PO4)	*0*	*0*	*mol*
molality(Feo_OH_3)	*0*	*0*	*mol*
molality(Feo_OH_4)	*0*	*0*	*mol*
molality(FeoHPO4)	*0*	*0*	*mol*
molality(Al_OH_)	*0*	*0*	*mol*
molality(Al_OH_2)	*0*	*0*	*mol*
molality(Al_OH_3)	*0*	*0*	*mol*
molality(AlSO4)	*0*	*0*	*mol*
Group: Equilibrium			
TK	*0*	*0*	*K*
Group: Headspace			
CH4_molrate	*0*	*0*	
CO2_molrate	*0*	*0*	
HeadGas	*1*	*0*	*mol*
Henry_CH4	*0*	*0*	*atm.m3.Mol-1*
Henry_CO2	*0*	*0*	*atm.m3.Mol-1*
Henry_H2	*0*	*0*	*atm.m3.Mol-1*
Henry_NH3	*0*	*0*	*atm.m3.Mol-1*
PCH4_eq	*0*	*0*	*Pa*
PCO2_eq	*0*	*0*	*Pa*

PH2_eq	*0*	*0*	*Pa*
PNH3_eq	*0*	*0*	*Pa*
P_H2O	*100*	*0*	*Pa*
Q_Gas_Mol	*0*	*0*	*mol.d-1*
Group: kinetics			
Kd_ac	*0*	*0*	*1/d*
Kd_ad	*0*	*0*	*1/d*
Kd_am	*0*	*0*	*1/d*
Kd_hm	*0*	*0*	*1/d*
Kd_oh	*0*	*0*	*1/d*
Kd_pa	*0*	*0*	*1/d*
Kh_bp	*0*	*0*	*1/d*
Kh_bps	*0*	*0*	*1/d*
Kh_fs	*0*	*0*	*1/d*
Kh_polyp	*0*	*0*	*1/d*
Mu_ac	*0*	*0*	*1/d*
Mu_ad	*0*	*0*	*1/d*
Mu_am	*0*	*0*	*1/d*
Mu_hm	*0*	*0*	*1/d*
S_ALK_MonodTerm	*0*	*0*	*-*
S_A_MonodTerm	*0*	*0*	*-*
S_NH_MonodTerm	*0*	*0*	*-*
S_PO_MonodTerm	*0*	*0*	*-*
Tcorr	*0*	*0*	*dUnit/dUnit*
Group: Operational			
Kla_Actual	*0*	*0*	*1/d*
Q_Out	*0*	*0*	*m3/d*
Q_Over	*0*	*0*	*m3/d*
Temp_liq	*0*	*0*	*degC*
V	*0*	*0*	*L*
Group: Particulates			
TSS_factor	*0*	*0*	*dUnit/dUnit*
Group: Precipitation			
Driver_Str	*0*	*0*	
Driver_cal	*0*	*0*	
Driver_cap	*0*	*0*	
Driver_mag	*0*	*0*	
Driver_mgkp	*0*	*0*	
Driver_newb	*0*	*0*	
K_cal	*0*	*0*	
K_cap	*0*	*0*	
K_mag	*0*	*0*	
K_mgkp	*0*	*0*	
K_newb	*0*	*0*	
K_stru	*0*	*0*	

KspCorr	*0*	*0*	*dUnit/dUnit*
Ksp_cal	*0*	*0*	*dUnit/dUnit*
Ksp_cap	*0*	*0*	*dUnit/dUnit*
Ksp_mag	*0*	*0*	*dUnit/dUnit*
Ksp_mgkp	*0*	*0*	*dUnit/dUnit*
Ksp_newb	*0*	*0*	*dUnit/dUnit*
Ksp_stru	*0*	*0*	*dUnit/dUnit*
Ppt_cal	*0*	*0*	*mol*
Ppt_cap	*0*	*0*	*mol*
Ppt_mag	*0*	*0*	*mol*
Ppt_mgkp	*0*	*0*	*mol/kg*
Ppt_newb	*0*	*0*	*mol*
saturation_cal	*0*	*0*	*dUnit/dUnit*
saturation_cap	*0*	*0*	*dUnit/dUnit*
saturation_mag	*0*	*0*	*dUnit/dUnit*
saturation_mgkp	*0*	*0*	*dUnit/dUnit*
saturation_newb	*0*	*0*	*dUnit/dUnit*
saturation_stru	*0*	*0*	*dUnit/dUnit*
Group: P-release			
Kh_pha	*0*	*0*	*1/d*
Kh_pp	*0*	*0*	*1/d*
Group: Speciation			
IonicStrength	*0*	*0*	*mol/kg*
SpeciationError	*0*	*0*	
Totalmolality(H_)	*0*	*0*	*mol/L*
Totalmolality(Na_)	*0*	*0*	*mol/L*
Totalmolality(K_)	*0*	*0*	*mol/L*
Totalmolality(Ca_)	*0*	*0*	*mol/L*
Totalmolality(Mg_)	*0*	*0*	*mol/L*
Totalmolality(NH4_)	*0*	*0*	*mol/L*
Totalmolality(Cl_)	*0*	*0*	*mol/L*
Totalmolality(Ac_)	*0*	*0*	*mol/L*
Totalmolality(Pr_)	*0*	*0*	*mol/L*
Totalmolality(CO3_)	*0*	*0*	*mol/L*
Totalmolality(SO4_)	*0*	*0*	*mol/L*
Totalmolality(PO4_)	*0*	*0*	*mol/L*
Totalmolality(HS_)	*0*	*0*	*mol/L*
Totalmolality(NO2_)	*0*	*0*	*mol/L*
Totalmolality(NO3_)	*0*	*0*	*mol/L*
Totalmolality(Fer_)	*0*	*0*	*mol/L*
Totalmolality(Feo_)	*0*	*0*	*mol/L*
Totalmolality(Al_)	*0*	*0*	*mol/L*
actwater	*0*	*0*	*dUnit/dUnit*
gam1	*0*	*0*	*dUnit/dUnit*
p_H	*0*	*0*	

spectest1	*0*	*0*
spectest2	*0*	*0*
Category: Derived Variables		
Group:		
M(H2O)	*1000000000*	*2850000000*
M(S_H)	*77320.71*	*178400.5005*
M(S_Na)	*106204.99*	*1198625.85*
M(S_K)	*55254.96*	*500*
M(S_Ca)	*6016.87*	*500*
M(S_Mg)	*2406.74*	*500*
M(S_NH)	*793650.94*	*1198625.85*
M(S_Cl)	*26155.68*	*500*
M(S_VFA)	*15.2*	*384.1698*
M(S_Pr)	*90.81*	*0*
M(S_CO3)	*3225485*	*9350000*
M(S_SO4)	*9626.99*	*499.9670423*
M(S_PO4)	*595290.67*	*595746.9*
M(S_HS)	*0*	*0*
M(S_NO2)	*0*	*0*
M(S_NO3)	*0*	*0*
M(S_Fer)	*0*	*0*
M(S_Feo)	*0*	*0*
M(S_Al)	*0*	*0*
M(S_H2)	*0.34274*	*0.000628523*
M(S_CH4)	*0.34274*	*46677.18286*
M(S_U)	*10028.62*	*290621.2173*
M(S_F)	*9.065*	*0*
M(S_Glu)	*643.34*	*1206.272554*
M(S_O)	*0.01*	*0*
M(X_U_Inf)	*0.01*	*16498912.39*
M(X_B_Org)	*10462302.56*	*46508.825*
M(X_PAO_PP)	*14772.92*	*0*
M(X_PAO_Stor)	*0.01*	*0*
M(X_Str_NH4)	*0.01*	*0*
M(X_ACP)	*3.2714E-06*	*0*
M(X_Str_K)	*8.1785E-07*	*0*
M(X_Cal)	*8.178E-07*	*0*
M(X_Mag)	*8.178E-07*	*0*
M(X_Newb)	*8.178E-07*	*0*
M(X_OHO)	*8.178E-07*	*0*
M(X_PAO)	*99.06*	*0*
M(X_AD)	*0.01*	*10500*
M(X_AC)	*796324.32*	*44720.59432*
M(X_AM)	*354.04*	*900000*

M(X_HM)	*73165.14*	*768093.4338*	
M(X_U_Org)	*15043.68*	*412389.87*	
M(X_B_Inf)	*235234.96*	*226073.7702*	
M(X_ANO)	*61044.94*	*0*	
M(X_ISS)	*0.0005487*	*36672507.56*	
M(G_CH4)	*4339036.66*	*110000*	
M(G_CO2)	*2165*	*190000*	
M(G_N2)	*3322.58*	*0*	
Group: Gas			
CumulativeGas	*0*	*0*	*m3*
Group: Headspace			
P_CH4	*500*	*53202.25832*	*Pa*
P_CO2	*500*	*42513.26431*	*Pa*
Category: Input Variables			
Group: Influent			
Inflow(H2O)	*0*	*0*	*g/d*
Inflow(S_H)	*0*	*0*	*g/d*
Inflow(S_Na)	*0*	*0*	*g/d*
Inflow(S_K)	*0*	*0*	*g/d*
Inflow(S_Ca)	*0*	*0*	*g/d*
Inflow(S_Mg)	*0*	*0*	*g/d*
Inflow(S_NH)	*0*	*0*	*g/d*
Inflow(S_Cl)	*0*	*0*	*g/d*
Inflow(S_VFA)	*0*	*0*	*g/d*
Inflow(S_Pr)	*0*	*0*	*g/d*
Inflow(S_CO3)	*0*	*0*	*g/d*
Inflow(S_SO4)	*0*	*0*	*g/d*
Inflow(S_PO4)	*0*	*0*	*g/d*
Inflow(S_HS)	*0*	*0*	*g/d*
Inflow(S_NO2)	*0*	*0*	*g/d*
Inflow(S_NO3)	*0*	*0*	*g/d*
Inflow(S_Fer)	*0*	*0*	*g/d*
Inflow(S_Feo)	*0*	*0*	*g/d*
Inflow(S_Al)	*0*	*0*	*g/d*
Inflow(S_H2)	*0*	*0*	*g/d*
Inflow(S_CH4)	*0*	*0*	*g/d*
Inflow(S_U)	*0*	*0*	*g/d*
Inflow(S_F)	*0*	*0*	*g/d*
Inflow(S_Glu)	*0*	*0*	*g/d*
Inflow(S_O)	*0*	*0*	*g/d*
Inflow(X_U_Inf)	*0*	*0*	*g/d*
Inflow(X_B_Org)	*0*	*0*	*g/d*
Inflow(X_PAO_PP)	*0*	*0*	*g/d*
Inflow(X_PAO_Stor)	*0*	*0*	*g/d*

Inflow(X_Str_NH4)	*0*	*0*	*g/d*
Inflow(X_ACP)	*0*	*0*	*g/d*
Inflow(X_Str_K)	*0*	*0*	*g/d*
Inflow(X_Cal)	*0*	*0*	*g/d*
Inflow(X_Mag)	*0*	*0*	*g/d*
Inflow(X_Newb)	*0*	*0*	*g/d*
Inflow(X_OHO)	*0*	*0*	*g/d*
Inflow(X_PAO)	*0*	*0*	*g/d*
Inflow(X_AD)	*0*	*0*	*g/d*
Inflow(X_AC)	*0*	*0*	*g/d*
Inflow(X_AM)	*0*	*0*	*g/d*
Inflow(X_HM)	*0*	*0*	*g/d*
Inflow(X_U_Org)	*0*	*0*	*g/d*
Inflow(X_B_Inf)	*0*	*0*	*g/d*
Inflow(X_ANO)	*0*	*0*	*g/d*
Inflow(X_ISS)	*0*	*0*	*g/d*
Inflow(G_CH4)	*0*	*0*	*g/d*
Inflow(G_CO2)	*0*	*0*	*g/d*
Inflow(G_N2)	*0*	*0*	*g/d*
Category: Output Variables			
Group: Biogas			
Q_Biogas	*0*	*0*	*m3/d*
Q_CH4	*0*	*0*	*m3/d*
Q_CO2	*0*	*0*	*m3/d*
Q_N2	*0*	*0*	*m3/d*
Group: Concentrate			
Outflow(H2O)	*0*	*0*	*g/d*
Outflow(S_H)	*0*	*0*	*g/d*
Outflow(S_Na)	*0*	*0*	*g/d*
Outflow(S_K)	*0*	*0*	*g/d*
Outflow(S_Ca)	*0*	*0*	*g/d*
Outflow(S_Mg)	*0*	*0*	*g/d*
Outflow(S_NH)	*0*	*0*	*g/d*
Outflow(S_Cl)	*0*	*0*	*g/d*
Outflow(S_VFA)	*0*	*0*	*g/d*
Outflow(S_Pr)	*0*	*0*	*g/d*
Outflow(S_CO3)	*0*	*0*	*g/d*
Outflow(S_SO4)	*0*	*0*	*g/d*
Outflow(S_PO4)	*0*	*0*	*g/d*
Outflow(S_HS)	*0*	*0*	*g/d*
Outflow(S_NO2)	*0*	*0*	*g/d*
Outflow(S_NO3)	*0*	*0*	*g/d*
Outflow(S_Fer)	*0*	*0*	*g/d*
Outflow(S_Feo)	*0*	*0*	*g/d*

Outflow(S_Al)	*0*	*0*	*g/d*
Outflow(S_H2)	*0*	*0*	*g/d*
Outflow(S_CH4)	*0*	*0*	*g/d*
Outflow(S_U)	*0*	*0*	*g/d*
Outflow(S_F)	*0*	*0*	*g/d*
Outflow(S_Glu)	*0*	*0*	*g/d*
Outflow(S_O)	*0*	*0*	*g/d*
Outflow(X_U_Inf)	*0*	*0*	*g/d*
Outflow(X_B_Org)	*0*	*0*	*g/d*
Outflow(X_PAO_PP)	*0*	*0*	*g/d*
Outflow(X_PAO_Stor)	*0*	*0*	*g/d*
Outflow(X_Str_NH4)	*0*	*0*	*g/d*
Outflow(X_ACP)	*0*	*0*	*g/d*
Outflow(X_Str_K)	*0*	*0*	*g/d*
Outflow(X_Cal)	*0*	*0*	*g/d*
Outflow(X_Mag)	*0*	*0*	*g/d*
Outflow(X_Newb)	*0*	*0*	*g/d*
Outflow(X_OHO)	*0*	*0*	*g/d*
Outflow(X_PAO)	*0*	*0*	*g/d*
Outflow(X_AD)	*0*	*0*	*g/d*
Outflow(X_AC)	*0*	*0*	*g/d*
Outflow(X_AM)	*0*	*0*	*g/d*
Outflow(X_HM)	*0*	*0*	*g/d*
Outflow(X_U_Org)	*0*	*0*	*g/d*
Outflow(X_B_Inf)	*0*	*0*	*g/d*
Outflow(X_ANO)	*0*	*0*	*g/d*
Outflow(X_ISS)	*0*	*0*	*g/d*
Outflow(G_CH4)	*0*	*0*	*g/d*
Outflow(G_CO2)	*0*	*0*	*g/d*
Outflow(G_N2)	*0*	*0*	*g/d*
Group: Gas			
Gasflow(H2O)	*0*	*0*	*g/d*
Gasflow(S_H)	*0*	*0*	*g/d*
Gasflow(S_Na)	*0*	*0*	*g/d*
Gasflow(S_K)	*0*	*0*	*g/d*
Gasflow(S_Ca)	*0*	*0*	*g/d*
Gasflow(S_Mg)	*0*	*0*	*g/d*
Gasflow(S_NH)	*0*	*0*	*g/d*
Gasflow(S_Cl)	*0*	*0*	*g/d*
Gasflow(S_VFA)	*0*	*0*	*g/d*
Gasflow(S_Pr)	*0*	*0*	*g/d*
Gasflow(S_CO3)	*0*	*0*	*g/d*
Gasflow(S_SO4)	*0*	*0*	*g/d*
Gasflow(S_PO4)	*0*	*0*	*g/d*
Gasflow(S_HS)	*0*	*0*	*g/d*

Gasflow(S_NO2)	*0*	*0*	*g/d*
Gasflow(S_NO3)	*0*	*0*	*g/d*
Gasflow(S_Fer)	*0*	*0*	*g/d*
Gasflow(S_Feo)	*0*	*0*	*g/d*
Gasflow(S_Al)	*0*	*0*	*g/d*
Gasflow(S_H2)	*0*	*0*	*g/d*
Gasflow(S_CH4)	*0*	*0*	*g/d*
Gasflow(S_U)	*0*	*0*	*g/d*
Gasflow(S_F)	*0*	*0*	*g/d*
Gasflow(S_Glu)	*0*	*0*	*g/d*
Gasflow(S_O)	*0*	*0*	*g/d*
Gasflow(X_U_Inf)	*0*	*0*	*g/d*
Gasflow(X_B_Org)	*0*	*0*	*g/d*
Gasflow(X_PAO_PP)	*0*	*0*	*g/d*
Gasflow(X_PAO_Stor)	*0*	*0*	*g/d*
Gasflow(X_Str_NH4)	*0*	*0*	*g/d*
Gasflow(X_ACP)	*0*	*0*	*g/d*
Gasflow(X_Str_K)	*0*	*0*	*g/d*
Gasflow(X_Cal)	*0*	*0*	*g/d*
Gasflow(X_Mag)	*0*	*0*	*g/d*
Gasflow(X_Newb)	*0*	*0*	*g/d*
Gasflow(X_OHO)	*0*	*0*	*g/d*
Gasflow(X_PAO)	*0*	*0*	*g/d*
Gasflow(X_AD)	*0*	*0*	*g/d*
Gasflow(X_AC)	*0*	*0*	*g/d*
Gasflow(X_AM)	*0*	*0*	*g/d*
Gasflow(X_HM)	*0*	*0*	*g/d*
Gasflow(X_U_Org)	*0*	*0*	*g/d*
Gasflow(X_B_Inf)	*0*	*0*	*g/d*
Gasflow(X_ANO)	*0*	*0*	*g/d*
Gasflow(X_ISS)	*0*	*0*	*g/d*
Gasflow(G_CH4)	*0*	*0*	*g/d*
Gasflow(G_CO2)	*0*	*0*	*g/d*
Gasflow(G_N2)	*0*	*0*	*g/d*
Group: Headspace			
P_N2	*0*	*0*	*Pa*
f_CH4	*0*	*0*	*-*
f_CO2	*0*	*0*	*-*
f_H2O	*0*	*0*	*-*
f_N2	*0*	*0*	*-*
Group: Measured Data			
V_tot	*0*	*0*	*m3*
Group: Measurements			
CO3Alkalinity	*1180*	*0*	*g/m3*
CO3Alkalinity1	*1180*	*0*	*g/m3*

COD_s	*1000*	*0*	*g/m3*
Ca_Tot	*33*	*0*	*g/m3*
FSA	*45*	*0*	*g/m3*
ISSm	*13000*	*0*	*g/m3*
K_Tot	*5*	*0*	*g/m3*
Mg_Tot	*15*	*0*	*g/m3*
NH3Alkalinity	*20*	*0*	*g/m3*
OrthoP	*15*	*0*	*g/m3*
PO4Alkalinity	*20*	*0*	*g/m3*
TKN	*222*	*0*	*g/m3*
TP	*111*	*0*	*g/m3*
TSS	*11111*	*0*	*g/m3*
T_oper	*308.15*	*0*	*°K*
TotalAlkalinity	*1250*	*0*	*g/m3*
VFA	*33*	*0*	*g/m3*
VFAAlkalinity	*20*	*0*	*g/m3*
VSS	*15000*	*0*	*g/m3*
V_liquid	*1000*	*0*	*m3*
p_H_s	*7*	*0*	*g/m3*
Group: Underflow			
Underflow(H2O)	*0*	*0*	*g/d*
Underflow(S_H)	*0*	*0*	*g/d*
Underflow(S_Na)	*0*	*0*	*g/d*
Underflow(S_K)	*0*	*0*	*g/d*
Underflow(S_Ca)	*0*	*0*	*g/d*
Underflow(S_Mg)	*0*	*0*	*g/d*
Underflow(S_NH)	*0*	*0*	*g/d*
Underflow(S_Cl)	*0*	*0*	*g/d*
Underflow(S_VFA)	*0*	*0*	*g/d*
Underflow(S_Pr)	*0*	*0*	*g/d*
Underflow(S_CO3)	*0*	*0*	*g/d*
Underflow(S_SO4)	*0*	*0*	*g/d*
Underflow(S_PO4)	*0*	*0*	*g/d*
Underflow(S_HS)	*0*	*0*	*g/d*
Underflow(S_NO2)	*0*	*0*	*g/d*
Underflow(S_NO3)	*0*	*0*	*g/d*
Underflow(S_Fer)	*0*	*0*	*g/d*
Underflow(S_Feo)	*0*	*0*	*g/d*
Underflow(S_Al)	*0*	*0*	*g/d*
Underflow(S_H2)	*0*	*0*	*g/d*
Underflow(S_CH4)	*0*	*0*	*g/d*
Underflow(S_U)	*0*	*0*	*g/d*
Underflow(S_F)	*0*	*0*	*g/d*
Underflow(S_Glu)	*0*	*0*	*g/d*
Underflow(S_O)	*0*	*0*	*g/d*

Underflow(X_U_Inf)	*0*	*0*	*g/d*
Underflow(X_B_Org)	*0*	*0*	*g/d*
Underflow(X_PAO_PP)	*0*	*0*	*g/d*
Underflow(X_PAO_Stor)	*0*	*0*	*g/d*
Underflow(X_Str_NH4)	*0*	*0*	*g/d*
Underflow(X_ACP)	*0*	*0*	*g/d*
Underflow(X_Str_K)	*0*	*0*	*g/d*
Underflow(X_Cal)	*0*	*0*	*g/d*
Underflow(X_Mag)	*0*	*0*	*g/d*
Underflow(X_Newb)	*0*	*0*	*g/d*
Underflow(X_OHO)	*0*	*0*	*g/d*
Underflow(X_PAO)	*0*	*0*	*g/d*
Underflow(X_AD)	*0*	*0*	*g/d*
Underflow(X_AC)	*0*	*0*	*g/d*
Underflow(X_AM)	*0*	*0*	*g/d*
Underflow(X_HM)	*0*	*0*	*g/d*
Underflow(X_U_Org)	*0*	*0*	*g/d*
Underflow(X_B_Inf)	*0*	*0*	*g/d*
Underflow(X_ANO)	*0*	*0*	*g/d*
Underflow(X_ISS)	*0*	*0*	*g/d*
Underflow(G_CH4)	*0*	*0*	*g/d*
Underflow(G_CO2)	*0*	*0*	*g/d*
Underflow(G_N2)	*0*	*0*	*g/d*

3.1. Appendix C

Amanzimtoti co-digestion plant model digester dosing variable

Name	*Value*	*Initial Value*	*Unit*
Category: Algebraic Variables			
Group: Concentration			
C(H2O)	*0*	*0*	*m3/d*
C(S_H)	*0*	*0*	*g/m3*
C(S_Na)	*0*	*0*	*g/m3*
C(S_K)	*0*	*0*	*g/m3*
C(S_Ca)	*0*	*0*	*g/m3*
C(S_Mg)	*0*	*0*	*g/m3*
C(S_NH)	*0*	*0*	*g/m3*
C(S_Cl)	*0*	*0*	*g/m3*
C(S_VFA)	*0*	*0*	*g/m3*
C(S_Pr)	*0*	*0*	*g/m3*
C(S_CO3)	*0*	*0*	*g/m3*
C(S_SO4)	*0*	*0*	*g/m3*
C(S_PO4)	*0*	*0*	*g/m3*
C(S_HS)	*0*	*0*	*g/m3*
C(S_NO2)	*0*	*0*	*g/m3*
C(S_NO3)	*0*	*0*	*g/m3*
C(S_Fer)	*0*	*0*	*g/m3*
C(S_Feo)	*0*	*0*	*g/m3*
C(S_Al)	*0*	*0*	*g/m3*
C(S_H2)	*0*	*0*	*g/m3*
C(S_CH4)	*0*	*0*	*g/m3*
C(S_U)	*0*	*0*	*g/m3*
C(S_F)	*0*	*0*	*g/m3*
C(S_Glu)	*0*	*0*	*g/m3*
C(S_O)	*0*	*0*	*g/m3*
C(X_U_Inf)	*0*	*0*	*g/m3*
C(X_B_Org)	*0*	*0*	*g/m3*
C(X_PAO_PP)	*0*	*0*	*g/m3*
C(X_PAO_Stor)	*0*	*0*	*g/m3*
C(X_Str_NH4)	*0*	*0*	*g/m3*
C(X_ACP)	*0*	*0*	*g/m3*
C(X_Str_K)	*0*	*0*	*g/m3*
C(X_Cal)	*0*	*0*	*g/m3*
C(X_Mag)	*0*	*0*	*g/m3*
C(X_Newb)	*0*	*0*	*g/m3*
C(X_OHO)	*0*	*0*	*g/m3*
C(X_PAO)	*0*	*0*	*g/m3*
C(X_AD)	*0*	*0*	*g/m3*
C(X_AC)	*0*	*0*	*g/m3*
C(X_AM)	*0*	*0*	*g/m3*
C(X_HM)	*0*	*0*	*g/m3*

C(X_U_Org)	*0*	*0*	*g/m3*
C(X_B_Inf)	*0*	*0*	*g/m3*
C(X_ANO)	*0*	*0*	*g/m3*
C(X_ISS)	*0*	*0*	*g/m3*
C(G_CH4)	*0*	*0*	*g/m3*
C(G_CO2)	*0*	*0*	*g/m3*
C(G_N2)	*0*	*0*	*g/m3*
Group: Dimension			
V	*0*	*0*	*m3*
Group: Operational			
Q_In	*0*	*0*	*m3/d*
Q_Out	*0*	*0*	*m3/d*
Category: Derived Variables			
Group:			
M(H2O)	*1000000000*	*4000000000*	
M(S_H)	*1*	*20681*	
M(S_Na)	*1*	*1707781*	
M(S_K)	*1*	*10*	
M(S_Ca)	*1*	*10*	
M(S_Mg)	*1*	*10*	
M(S_NH)	*1*	*863568*	
M(S_Cl)	*1*	*4*	
M(S_VFA)	*1*	*6000000*	
M(S_Pr)	*1*	*10*	
M(S_CO3)	*1*	*1000000*	
M(S_SO4)	*1*	*10*	
M(S_PO4)	*1*	*463982*	
M(S_HS)	*0*	*0*	
M(S_NO2)	*0*	*0*	
M(S_NO3)	*0*	*0*	
M(S_Fer)	*0*	*0*	
M(S_Feo)	*0*	*0*	
M(S_Al)	*0*	*0*	
M(S_H2)	*1*	*10*	
M(S_CH4)	*1*	*10*	
M(S_U)	*1*	*413722*	
M(S_F)	*1*	*579824*	
M(S_Glu)	*0.1*	*1*	
M(S_O)	*0.1*	*1*	
M(X_U_Inf)	*0.1*	*23715190*	
M(X_B_Org)	*10*	*100*	
M(X_PAO_PP)	*10*	*0*	
M(X_PAO_Stor)	*10*	*0*	
M(X_Str_NH4)	*10*	*0*	

M(X_ACP)	*0.1*	*0*	
M(X_Str_K)	*0.1*	*0*	
M(X_Cal)	*0.1*	*1E+12*	
M(X_Mag)	*0.1*	*0*	
M(X_Newb)	*0.1*	*0*	
M(X_OHO)	*0.1*	*1*	
M(X_PAO)	*10*	*0*	
M(X_AD)	*10*	*100*	
M(X_AC)	*1*	*10*	
M(X_AM)	*1*	*10*	
M(X_HM)	*1*	*10*	
M(X_U_Org)	*1*	*10*	
M(X_B_Inf)	*10*	*50318540*	
M(X_ANO)	*10*	*100*	
M(X_ISS)	*10*	*52975560*	
M(G_CH4)	*0*	*0*	
M(G_CO2)	*0*	*0*	
M(G_N2)	*0*	*0*	
Category: Input Variables			
Group: Influent			
Inflow(H2O)	*0*	*0*	*g/d*
Inflow(S_H)	*0*	*0*	*g/d*
Inflow(S_Na)	*0*	*0*	*g/d*
Inflow(S_K)	*0*	*0*	*g/d*
Inflow(S_Ca)	*0*	*0*	*g/d*
Inflow(S_Mg)	*0*	*0*	*g/d*
Inflow(S_NH)	*0*	*0*	*g/d*
Inflow(S_Cl)	*0*	*0*	*g/d*
Inflow(S_VFA)	*0*	*0*	*g/d*
Inflow(S_Pr)	*0*	*0*	*g/d*
Inflow(S_CO3)	*0*	*0*	*g/d*
Inflow(S_SO4)	*0*	*0*	*g/d*
Inflow(S_PO4)	*0*	*0*	*g/d*
Inflow(S_HS)	*0*	*0*	*g/d*
Inflow(S_NO2)	*0*	*0*	*g/d*
Inflow(S_NO3)	*0*	*0*	*g/d*
Inflow(S_Fer)	*0*	*0*	*g/d*
Inflow(S_Feo)	*0*	*0*	*g/d*
Inflow(S_Al)	*0*	*0*	*g/d*
Inflow(S_H2)	*0*	*0*	*g/d*
Inflow(S_CH4)	*0*	*0*	*g/d*
Inflow(S_U)	*0*	*0*	*g/d*
Inflow(S_F)	*0*	*0*	*g/d*
Inflow(S_Glu)	*0*	*0*	*g/d*

Inflow(S_O)	*0*	*0*	*g/d*
Inflow(X_U_Inf)	*0*	*0*	*g/d*
Inflow(X_B_Org)	*0*	*0*	*g/d*
Inflow(X_PAO_PP)	*0*	*0*	*g/d*
Inflow(X_PAO_Stor)	*0*	*0*	*g/d*
Inflow(X_Str_NH4)	*0*	*0*	*g/d*
Inflow(X_ACP)	*0*	*0*	*g/d*
Inflow(X_Str_K)	*0*	*0*	*g/d*
Inflow(X_Cal)	*0*	*0*	*g/d*
Inflow(X_Mag)	*0*	*0*	*g/d*
Inflow(X_Newb)	*0*	*0*	*g/d*
Inflow(X_OHO)	*0*	*0*	*g/d*
Inflow(X_PAO)	*0*	*0*	*g/d*
Inflow(X_AD)	*0*	*0*	*g/d*
Inflow(X_AC)	*0*	*0*	*g/d*
Inflow(X_AM)	*0*	*0*	*g/d*
Inflow(X_HM)	*0*	*0*	*g/d*
Inflow(X_U_Org)	*0*	*0*	*g/d*
Inflow(X_B_Inf)	*0*	*0*	*g/d*
Inflow(X_ANO)	*0*	*0*	*g/d*
Inflow(X_ISS)	*0*	*0*	*g/d*
Inflow(G_CH4)	*0*	*0*	*g/d*
Inflow(G_CO2)	*0*	*0*	*g/d*
Inflow(G_N2)	*0*	*0*	*g/d*
Category: Output Variables			
Group: Effluent			
Outflow(H2O)	*0*	*0*	*g/d*
Outflow(S_H)	*0*	*0*	*g/d*
Outflow(S_Na)	*0*	*0*	*g/d*
Outflow(S_K)	*0*	*0*	*g/d*
Outflow(S_Ca)	*0*	*0*	*g/d*
Outflow(S_Mg)	*0*	*0*	*g/d*
Outflow(S_NH)	*0*	*0*	*g/d*
Outflow(S_Cl)	*0*	*0*	*g/d*
Outflow(S_VFA)	*0*	*0*	*g/d*
Outflow(S_Pr)	*0*	*0*	*g/d*
Outflow(S_CO3)	*0*	*0*	*g/d*
Outflow(S_SO4)	*0*	*0*	*g/d*
Outflow(S_PO4)	*0*	*0*	*g/d*
Outflow(S_HS)	*0*	*0*	*g/d*
Outflow(S_NO2)	*0*	*0*	*g/d*
Outflow(S_NO3)	*0*	*0*	*g/d*
Outflow(S_Fer)	*0*	*0*	*g/d*
Outflow(S_Feo)	*0*	*0*	*g/d*

Outflow(S_Al)	*0*	*0*	*g/d*
Outflow(S_H2)	*0*	*0*	*g/d*
Outflow(S_CH4)	*0*	*0*	*g/d*
Outflow(S_U)	*0*	*0*	*g/d*
Outflow(S_F)	*0*	*0*	*g/d*
Outflow(S_Glu)	*0*	*0*	*g/d*
Outflow(S_O)	*0*	*0*	*g/d*
Outflow(X_U_Inf)	*0*	*0*	*g/d*
Outflow(X_B_Org)	*0*	*0*	*g/d*
Outflow(X_PAO_PP)	*0*	*0*	*g/d*
Outflow(X_PAO_Stor)	*0*	*0*	*g/d*
Outflow(X_Str_NH4)	*0*	*0*	*g/d*
Outflow(X_ACP)	*0*	*0*	*g/d*
Outflow(X_Str_K)	*0*	*0*	*g/d*
Outflow(X_Cal)	*0*	*0*	*g/d*
Outflow(X_Mag)	*0*	*0*	*g/d*
Outflow(X_Newb)	*0*	*0*	*g/d*
Outflow(X_OHO)	*0*	*0*	*g/d*
Outflow(X_PAO)	*0*	*0*	*g/d*
Outflow(X_AD)	*0*	*0*	*g/d*
Outflow(X_AC)	*0*	*0*	*g/d*
Outflow(X_AM)	*0*	*0*	*g/d*
Outflow(X_HM)	*0*	*0*	*g/d*
Outflow(X_U_Org)	*0*	*0*	*g/d*
Outflow(X_B_Inf)	*0*	*0*	*g/d*
Outflow(X_ANO)	*0*	*0*	*g/d*
Outflow(X_ISS)	*0*	*0*	*g/d*
Outflow(G_CH4)	*0*	*0*	*g/d*
Outflow(G_CO2)	*0*	*0*	*g/d*
Outflow(G_N2)	*0*	*0*	*g/d*
Group: Energy			
MixingEnergy	*0*	*0*	*kWh*
PumpingEnergy	*0*	*0*	*kWh*
Group: Measurement data			
V_Buffer	*0*	*0*	*m3*

4.1. Appendix D

Amanzimtoti co-digestion plant model fruit juice storage tank

Name	*Value*	*Initial Value*	*Unit*
Category: Algebraic Variables			
Group: Concentration			
C(H2O)	*0*	*0*	*m3/d*
C(S_H)	*0*	*0*	*g/m3*
C(S_Na)	*0*	*0*	*g/m3*
C(S_K)	*0*	*0*	*g/m3*
C(S_Ca)	*0*	*0*	*g/m3*
C(S_Mg)	*0*	*0*	*g/m3*
C(S_NH)	*0*	*0*	*g/m3*
C(S_Cl)	*0*	*0*	*g/m3*
C(S_VFA)	*0*	*0*	*g/m3*
C(S_Pr)	*0*	*0*	*g/m3*
C(S_CO3)	*0*	*0*	*g/m3*
C(S_SO4)	*0*	*0*	*g/m3*
C(S_PO4)	*0*	*0*	*g/m3*
C(S_HS)	*0*	*0*	*g/m3*
C(S_NO2)	*0*	*0*	*g/m3*
C(S_NO3)	*0*	*0*	*g/m3*
C(S_Fer)	*0*	*0*	*g/m3*
C(S_Feo)	*0*	*0*	*g/m3*
C(S_Al)	*0*	*0*	*g/m3*
C(S_H2)	*0*	*0*	*g/m3*
C(S_CH4)	*0*	*0*	*g/m3*
C(S_U)	*0*	*0*	*g/m3*
C(S_F)	*0*	*0*	*g/m3*
C(S_Glu)	*0*	*0*	*g/m3*
C(S_O)	*0*	*0*	*g/m3*
C(X_U_Inf)	*0*	*0*	*g/m3*
C(X_B_Org)	*0*	*0*	*g/m3*
C(X_PAO_PP)	*0*	*0*	*g/m3*
C(X_PAO_Stor)	*0*	*0*	*g/m3*
C(X_Str_NH4)	*0*	*0*	*g/m3*
C(X_ACP)	*0*	*0*	*g/m3*
C(X_Str_K)	*0*	*0*	*g/m3*
C(X_Cal)	*0*	*0*	*g/m3*
C(X_Mag)	*0*	*0*	*g/m3*
C(X_Newb)	*0*	*0*	*g/m3*
C(X_OHO)	*0*	*0*	*g/m3*
C(X_PAO)	*0*	*0*	*g/m3*
C(X_AD)	*0*	*0*	*g/m3*
C(X_AC)	*0*	*0*	*g/m3*
C(X_AM)	*0*	*0*	*g/m3*
C(X_HM)	*0*	*0*	*g/m3*

C(X_U_Org)	*0*	*0*	*g/m3*
C(X_B_Inf)	*0*	*0*	*g/m3*
C(X_ANO)	*0*	*0*	*g/m3*
C(X_ISS)	*0*	*0*	*g/m3*
C(G_CH4)	*0*	*0*	*g/m3*
C(G_CO2)	*0*	*0*	*g/m3*
C(G_N2)	*0*	*0*	*g/m3*
Group: Dimension			
V	*0*	*0*	*m3*
Group: Operational			
Q_In	*0*	*0*	*m3/d*
Q_Out	*0*	*0*	*m3/d*
Category: Derived Variables			
Group:			
M(H2O)	*1000000000*	*10000000000*	
M(S_H)	*1*	*0*	
M(S_Na)	*1*	*0*	
M(S_K)	*1*	*0*	
M(S_Ca)	*1*	*0*	
M(S_Mg)	*1*	*0*	
M(S_NH)	*1*	*0*	
M(S_Cl)	*1*	*0*	
M(S_VFA)	*1*	*0*	
M(S_Pr)	*1*	*0*	
M(S_CO3)	*1*	*0*	
M(S_SO4)	*1*	*0*	
M(S_PO4)	*1*	*0*	
M(S_HS)	*0*	*0*	
M(S_NO2)	*0*	*0*	
M(S_NO3)	*0*	*0*	
M(S_Fer)	*0*	*0*	
M(S_Feo)	*0*	*0*	
M(S_Al)	*0*	*0*	
M(S_H2)	*1*	*0*	
M(S_CH4)	*1*	*0*	
M(S_U)	*1*	*0*	
M(S_F)	*1*	*0*	
M(S_Glu)	*0.1*	*1500000000*	
M(S_O)	*0.1*	*0*	
M(X_U_Inf)	*0.1*	*0*	
M(X_B_Org)	*10*	*0*	
M(X_PAO_PP)	*10*	*0*	
M(X_PAO_Stor)	*10*	*0*	
M(X_Str_NH4)	*10*	*0*	

M(X_ACP)	*0.1*	*0*	
M(X_Str_K)	*0.1*	*0*	
M(X_Cal)	*0.1*	*0*	
M(X_Mag)	*0.1*	*0*	
M(X_Newb)	*0.1*	*0*	
M(X_OHO)	*0.1*	*0*	
M(X_PAO)	*10*	*0*	
M(X_AD)	*10*	*0*	
M(X_AC)	*1*	*0*	
M(X_AM)	*1*	*0*	
M(X_HM)	*1*	*0*	
M(X_U_Org)	*1*	*0*	
M(X_B_Inf)	*10*	*0*	
M(X_ANO)	*10*	*0*	
M(X_ISS)	*10*	*0*	
M(G_CH4)	*0*	*0*	
M(G_CO2)	*0*	*0*	
M(G_N2)	*0*	*0*	
Category: Input Variables			
Group: Influent			
Inflow(H2O)	*0*	*0*	*g/d*
Inflow(S_H)	*0*	*0*	*g/d*
Inflow(S_Na)	*0*	*0*	*g/d*
Inflow(S_K)	*0*	*0*	*g/d*
Inflow(S_Ca)	*0*	*0*	*g/d*
Inflow(S_Mg)	*0*	*0*	*g/d*
Inflow(S_NH)	*0*	*0*	*g/d*
Inflow(S_Cl)	*0*	*0*	*g/d*
Inflow(S_VFA)	*0*	*0*	*g/d*
Inflow(S_Pr)	*0*	*0*	*g/d*
Inflow(S_CO3)	*0*	*0*	*g/d*
Inflow(S_SO4)	*0*	*0*	*g/d*
Inflow(S_PO4)	*0*	*0*	*g/d*
Inflow(S_HS)	*0*	*0*	*g/d*
Inflow(S_NO2)	*0*	*0*	*g/d*
Inflow(S_NO3)	*0*	*0*	*g/d*
Inflow(S_Fer)	*0*	*0*	*g/d*
Inflow(S_Feo)	*0*	*0*	*g/d*
Inflow(S_Al)	*0*	*0*	*g/d*
Inflow(S_H2)	*0*	*0*	*g/d*
Inflow(S_CH4)	*0*	*0*	*g/d*
Inflow(S_U)	*0*	*0*	*g/d*
Inflow(S_F)	*0*	*0*	*g/d*
Inflow(S_Glu)	*0*	*0*	*g/d*

Inflow(S_O)	*0*	*0*	*g/d*
Inflow(X_U_Inf)	*0*	*0*	*g/d*
Inflow(X_B_Org)	*0*	*0*	*g/d*
Inflow(X_PAO_PP)	*0*	*0*	*g/d*
Inflow(X_PAO_Stor)	*0*	*0*	*g/d*
Inflow(X_Str_NH4)	*0*	*0*	*g/d*
Inflow(X_ACP)	*0*	*0*	*g/d*
Inflow(X_Str_K)	*0*	*0*	*g/d*
Inflow(X_Cal)	*0*	*0*	*g/d*
Inflow(X_Mag)	*0*	*0*	*g/d*
Inflow(X_Newb)	*0*	*0*	*g/d*
Inflow(X_OHO)	*0*	*0*	*g/d*
Inflow(X_PAO)	*0*	*0*	*g/d*
Inflow(X_AD)	*0*	*0*	*g/d*
Inflow(X_AC)	*0*	*0*	*g/d*
Inflow(X_AM)	*0*	*0*	*g/d*
Inflow(X_HM)	*0*	*0*	*g/d*
Inflow(X_U_Org)	*0*	*0*	*g/d*
Inflow(X_B_Inf)	*0*	*0*	*g/d*
Inflow(X_ANO)	*0*	*0*	*g/d*
Inflow(X_ISS)	*0*	*0*	*g/d*
Inflow(G_CH4)	*0*	*0*	*g/d*
Inflow(G_CO2)	*0*	*0*	*g/d*
Inflow(G_N2)	*0*	*0*	*g/d*
Category: Output Variables			
Group: Effluent			
Outflow(H2O)	*0*	*0*	*g/d*
Outflow(S_H)	*0*	*0*	*g/d*
Outflow(S_Na)	*0*	*0*	*g/d*
Outflow(S_K)	*0*	*0*	*g/d*
Outflow(S_Ca)	*0*	*0*	*g/d*
Outflow(S_Mg)	*0*	*0*	*g/d*
Outflow(S_NH)	*0*	*0*	*g/d*
Outflow(S_Cl)	*0*	*0*	*g/d*
Outflow(S_VFA)	*0*	*0*	*g/d*
Outflow(S_Pr)	*0*	*0*	*g/d*
Outflow(S_CO3)	*0*	*0*	*g/d*
Outflow(S_SO4)	*0*	*0*	*g/d*
Outflow(S_PO4)	*0*	*0*	*g/d*
Outflow(S_HS)	*0*	*0*	*g/d*
Outflow(S_NO2)	*0*	*0*	*g/d*
Outflow(S_NO3)	*0*	*0*	*g/d*
Outflow(S_Fer)	*0*	*0*	*g/d*
Outflow(S_Feo)	*0*	*0*	*g/d*

Outflow(S_Al)	*0*	*0*	*g/d*
Outflow(S_H2)	*0*	*0*	*g/d*
Outflow(S_CH4)	*0*	*0*	*g/d*
Outflow(S_U)	*0*	*0*	*g/d*
Outflow(S_F)	*0*	*0*	*g/d*
Outflow(S_Glu)	*0*	*0*	*g/d*
Outflow(S_O)	*0*	*0*	*g/d*
Outflow(X_U_Inf)	*0*	*0*	*g/d*
Outflow(X_B_Org)	*0*	*0*	*g/d*
Outflow(X_PAO_PP)	*0*	*0*	*g/d*
Outflow(X_PAO_Stor)	*0*	*0*	*g/d*
Outflow(X_Str_NH4)	*0*	*0*	*g/d*
Outflow(X_ACP)	*0*	*0*	*g/d*
Outflow(X_Str_K)	*0*	*0*	*g/d*
Outflow(X_Cal)	*0*	*0*	*g/d*
Outflow(X_Mag)	*0*	*0*	*g/d*
Outflow(X_Newb)	*0*	*0*	*g/d*
Outflow(X_OHO)	*0*	*0*	*g/d*
Outflow(X_PAO)	*0*	*0*	*g/d*
Outflow(X_AD)	*0*	*0*	*g/d*
Outflow(X_AC)	*0*	*0*	*g/d*
Outflow(X_AM)	*0*	*0*	*g/d*
Outflow(X_HM)	*0*	*0*	*g/d*
Outflow(X_U_Org)	*0*	*0*	*g/d*
Outflow(X_B_Inf)	*0*	*0*	*g/d*
Outflow(X_ANO)	*0*	*0*	*g/d*
Outflow(X_ISS)	*0*	*0*	*g/d*
Outflow(G_CH4)	*0*	*0*	*g/d*
Outflow(G_CO2)	*0*	*0*	*g/d*
Outflow(G_N2)	*0*	*0*	*g/d*
Group: Energy			
MixingEnergy	*0*	*0*	*kWh*
PumpingEnergy	*0*	*0*	*kWh*
Group: Measurement data			
V_Buffer	*0*	*0*	*m3*

5.1. Appendix E

Theoretical COD Calculation

$$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 5H_2O$$

1 mole of $C_6H_{12}O_6$ (Mr = 180 g) requires 6 moles of O_2(Mr = 32 g))

This is equivalent to 1.067 g of Oxygen per gram of Glucose

6.1. Appendix F

Temperature coefficient model code editing

wwtp.VolumeUCTADConversionModel.kinetics.msl

```
/*****************************************************************************
 *
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 *
 * $Revision: 1$
 * $Date: 17. oktober 2013 14:30:45$
 *
 *****************************************************************************/

#ifdef PWM_SA

//state.V = parameters.V_liq ;
state.Tcorr = exp(parameters.TempCoeff * (state.Temp_liq - parameters.Tref));
state.Kh_fs =
    IF (parameters.KH_F_AD_hyd * state.Tcorr > 20.0 )
    THEN (20.0)
    ELSE (parameters.KH_F_AD_hyd * state.Tcorr);
state.Kh_bp =
    IF ((parameters.KM_BOrg_AD_hyd * state.Tcorr * (state.COD[X_B_Org] / state.COD[X_AD]) / (parameters.KS_BOrg_AD_hyd + (state.COD[X_B_Org] / state.COD[X_AD]))) > 20.0 )
    THEN (20.0)
    ELSE (parameters.KM_BInf_AD_hyd * state.Tcorr * (state.COD[X_B_Inf] / state.COD[X_AD]) / (parameters.KS_BInf_AD_hyd + (state.COD[X_B_Inf] / state.COD[X_AD])));

state.Kd_oh = parameters.b_OHO_AD * state.Tcorr;
state.Kd_pa = parameters.b_PAO_AD * state.Tcorr;
state.Kd_ad = parameters.b_AD * state.Tcorr / parameters.COD_per_mol[X_AD];
state.Kd_ac = parameters.b_AC * state.Tcorr / parameters.COD_per_mol[X_AC];
state.Kd_am = parameters.b_AM * state.Tcorr / parameters.COD_per_mol[X_AM];
state.Kd_hm = parameters.b_HM * state.Tcorr / parameters.COD_per_mol[X_HM];
state.Kh_pp = parameters.KH_PP_AD_hyd * state.Tcorr / parameters.MW_[X_PAO_PP];
state.Kh_pha = parameters.KH_PHA_AD_hyd * state.Tcorr / parameters.COD_per_mol[S_Glu];
state.Tk = state.Temp_liq + 273.15;
state.Mu_ad = parameters.mu_AD * state.Tcorr;
state.Mu_ac = parameters.mu_AC * state.Tcorr;
state.Mu_am = parameters.mu_AM * state.Tcorr;
state.Mu_hm = parameters.mu_HM * state.Tcorr;
/*
state.YAD = parameters.Y_AD * ((parameters.COD_per_mol[X_AD] / parameters.MW_[X_AD])/ (parameters.COD_per_mol[S_Glu] / parameters.MW_[S_Glu]));
state.YAH = parameters.Y_AH * ((parameters.COD_per_mol[X_AD] / parameters.MW_[X_AD])/ (parameters.COD_per_mol[S_Glu] / parameters.MW_[S_Glu]));
state.YAC = parameters.Y_AC * ((parameters.COD_per_mol[X_AC] / parameters.MW_[X_AC])/ (parameters.COD_per_mol[S_Pr] / parameters.MW_[S_Pr]));
state.YAN = parameters.Y_AM * ((parameters.COD_per_mol[X_AM] / parameters.MW_[X_AM])/ (parameters.COD_per_mol[S_VFA] / parameters.MW_[S_VFA]));
state.YHN = parameters.Y_HM * ((parameters.COD_per_mol[X_HM] / parameters.MW_[X_HM])/ (parameters.COD_per_mol[S_H2] / parameters.MW_[S_H2]));
```

7.1 Appendix G

Experimental Temperature fro runs A1, A2, B1 and B2

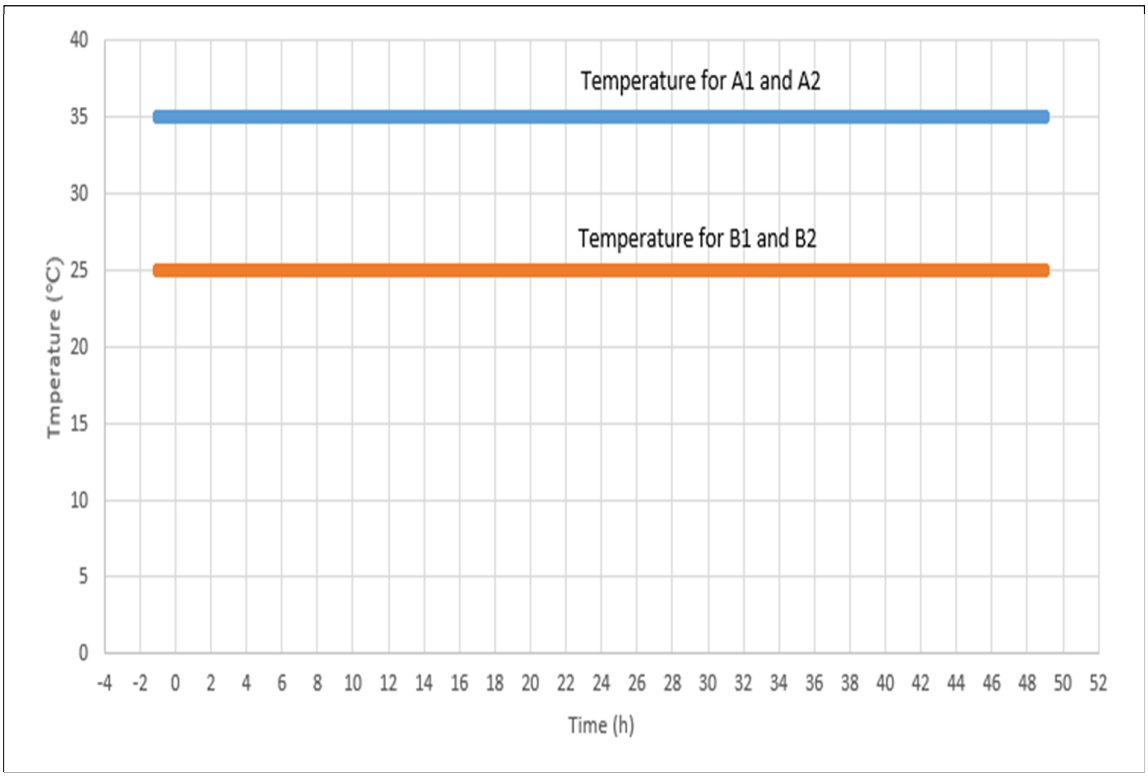

Figure 0-56 shows that duplicate experiments A1, A2, B1 and B2were were conducted at 35°C and 25°C , respectively without ant fluctuation.