



The Development of a Calibration Methodology for a Realistic Primary Settling Tank (PST) Model

by

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ABSTRACT

The comprehensive characterisation of influent waste to water and resource recovery facilities (WRRFs) is key to tracking the material elements through the entire WRRF system to ensure accurate prediction of system behaviour/performance or avoidance of system failure. Current models for activated sludge (AS) and anaerobic digestion (AD) unit processes of WRRF are well verified. However, previous models that replicated primary sedimentation units assumed that all the total settleable solids (TSS) components settled at the same velocities, which resulted in poor predictions of primary sludge characteristics and subsequently poor AD model predictions (with the PST underflow linked to AD in plant-wide settings).

In this investigation, the raw wastewater entering the WRRF via the primary settling tank (PST) is comprehensively characterised by categorising the TSS according to inorganic settleable solids (ISS), biodegradable particulate organics (BPO) and unbiodegradable particulate organics (UPO), each with five settling velocity distributions profiles. The BPO is further defined in terms of its elemental composition and hydrolysis rate kinetic constants to allow for accurate prediction of the AD system performance, when linked to the virtual PST. With the composition of raw wastewater and primary sludge (PS) known the settled wastewater that leads to the activated sludge (AS) system can be determined using the principles of material mass balance over the PST unit process.

This project introduces (i) the modification of the University of Cape Town Primary Sedimentation Unit (UCTPSU) physical process model of Polorigni (2020), by the inclusion of hydrolysis and acid fermentation bio-processes and (ii) calibration of the UCTPSU model through (a) the performance of a sensitivity analysis on the modified UCTPSU model and (b) utilisation of information generated from settleometer tests and augmented bio-methane potential (ABMP) tests to accurately predict the characteristics of PS to AD and settled wastewater to AS systems, hence allow for accurate tracking of elements along the entire WRRF, when using the model for design and optimised operation of WRRF systems. The settleometer, AD and ABMP tests showed that primary sewage sludge (or the total settleable solids) fractionated according to the particle size and density, and their corresponding wastewater characteristics were determined. The findings also showed that the unbiodegradable particulate organics formed the largest total settleable solid components removed from the PST underflow.

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ABBREVIATIONS

AAD	Anoxic-Aerobic Digestion	MBi	Mass balance across the device for the measured 'I' concentration
ABMP	Augmented Biological Methane Potential	MLISS	Mixed Liquor Inorganic Settleable Solids
AD	Anaerobic Digestion System/Reactor	MLVSS	Mixed Liquor Volatile Settleable Solids
AD_SS	Anaerobic Digestion Reactor at a Steady-State Condition	MLSS	Mixed Liquor Settleable Solids
AS	Activated Sludge	M_RWWi	Mass of influent raw wastewater (in mg) in the measured 'I' concentration
ASM2	Activated Sludge Model No. 2	M_SWWi	Mass of settled (overflow) wastewater (in mg) in the measured 'I' concentration
BMP	Biological Methane Potential	M_TSSi	Mass of Total Settleable Solids (in mg) in the measured 'I' concentration
BPO	Biodegradable Particulate Organics	ND	Nitrification-Denitrification
BPO_PS	Primary Sludge Biodegradable Particulate Organics	NDEBPR	Nitrification-Denitrification Enhanced Biological Phosphorus Removal
BSO	Biodegradable Soluble Organics	OHOs	Ordinary Heterotrophic Organisms
COD	Chemical Oxygen Demand	OP	Orthophosphate
CSTR	Continuously Stirred Tank Reactor	PDWWTW	Potsdam Wastewater Treatment Works
EDC	Electron Donating Capacity	PAOs	Phosphorus Accumulating Organisms
FAS	Ferrous Ammonium Sulphate	PE	Parameter Estimation
FBSO	Fermentable Biodegradable Soluble Organics	PHA	Poly-Hydroxy-alkanoate
FSA	Free and Saline Ammonia		
GT	Gravity Thickeners		
ID	Internal (PVC Column) diameter		
ISS	Inorganic Settleable Solids		

PP	Polyphosphate	USO	Unbiodegradable Soluble Organics
PS	Primary Sludge	VFA	Volatile Fatty Acid; same as SCFA
PST	Primary Settling Tank	VSS	Volatile Settleable Solids
PSVD	Primary Settling Velocity Distribution	WAS	Waste Activated Sludge
PVC	Poly-vinyl Chloride	WQL	Water Quality Laboratory
PWM_SA	Plant-wide Model of South Africa	WRG	Water Research Group
PWM_SA_AD	Anaerobic Digestion Unit of PWM_SA	WRRFs	Water Resource Recovery Facilities
PWM_SA_AD_BMP	Batch Test Adjusted PWM_SA_AD for ABMP Test Modelling	WWTPs	Wastewater Treatment Plants
SCFA	Short Chain Fatty Acid	WW	Wastewater
SRC	Standard Regression Coefficient		
SRT	Solids Retention Time		
SS	Steady-State		
TKN	Total Kjeldahl Nitrogen		
TP	Total Phosphorus		
TSS	Total Settleable Solids		
UCT	University of Cape Town		
UCTADM	University of Cape Town Anaerobic Digestion Model		
UCTSDM3P	Three-Phase University of Cape Town Sludge Digestion Model		
UCTPSU	University of Cape Town Primary Sedimentation Unit		
UPO	Unbiodegradable Particulate Organics		

NOMENCLATURE

S/N	Name	Description
1.	%	Percentage
2.	*gam_bp	EDC of the biodegradable particulate portion of biomass decay
3.	*gam_bps	EDC of the biodegradable particulate influent organics
4.	*gam_e	EDC of endogenous residue
5.	*gam_f	EDC of fermentable organics
6.	*gam_o	Electron donating capacity (EDC) of organism mass
7.	*gam_up	EDC of the unbiodegradable particulate organics
8.	*gam_us	EDC of the unbiodegradable soluble organics
9.	A _c	Baseline values containing unbiodegradable materials obtained at the end of control ABMP test.
10.	Alpha_B	1st group of BPO settling fraction
11.	Alpha_I	1st group of ISS settling fraction
12.	Alpha_U	1st group of UPO settling fraction
13.	A _T	Equivalent mass of unbiodegradable material (UPO) from seed added that remains till end of experiment
14.	b _{AC}	Decay rate constant for acetogens
15.	b _{AD}	Decay rate constant for acidogens
16.	b _{AM}	Decay rate constant for acetoclastic methanogens
17.	b _{HM}	Decay rate constant for hydrogenotrophic methanogens
18.	b _{OHO_AD}	Decay rate constant for OHOs in AD
19.	b _{PAO_AD}	Decay rate constant for PAOs in AD
20.	b _{AD}	Biomass death rate
21.	B _c	Mass of biodegradable organic material (BPO) in control ABMP reactor added
22.	Beta_B	2nd group of BPO settling fraction
23.	Beta_I	2nd group of ISS settling fraction
24.	Beta_U	2nd group of UPO settling fraction
25.	B _T	Equivalent mass of seed biodegradable material (BPO) with characteristics determined using data from the control ABMP reactor
26.	C1	Control test 1
27.	C2	Control test 2
28.	C ₄ H ₆ O ₂	Poly-hydroxy-alkanoates
29.	C ₆ H ₁₂ O ₆	Glucose
30.	Ca ²⁺	Calcium
31.	Ca ₃ (PO ₄) ₂	Calcium Phosphate
32.	CaCO ₃	Calcite
33.	C _{av}	Control tests average
34.	CH ₃ CH ₂ COO ⁻	Propionate
35.	CH ₃ COO ⁻	Acetate
36.	CH ₄	Methane
37.	CH _{Ybp} OZ _{bp} N _{Abp} P _{Bbp} S _{Cbp}	Biodegradable particulate organics
38.	CH _{Ybps} OZ _{bps} N _{Abps} P _{Bbps} S _{Cbps}	Primary sludge biodegradable particulate organics

39.	$\text{CH}_{\text{Ye}}\text{O}_{\text{Ze}}\text{N}_{\text{Ae}}\text{P}_{\text{Be}}\text{S}_{\text{Ce}}$	Endogenous residue
40.	$\text{CH}_{\text{Yf}}\text{O}_{\text{Zf}}\text{N}_{\text{Af}}\text{P}_{\text{Bf}}\text{S}_{\text{Cf}}$	Fermentable Biodegradable Soluble Organics
41.	$\text{CH}_{\text{Yo}}\text{O}_{\text{Zo}}\text{N}_{\text{Ao}}\text{P}_{\text{Bo}}\text{S}_{\text{Co}}$	Ordinary heterotrophic organisms
42.	$\text{CH}_{\text{Yo}}\text{O}_{\text{Zo}}\text{N}_{\text{Ao}}\text{P}_{\text{Bo}}\text{S}_{\text{Co}}$	Phosphate accumulating organisms
43.	$\text{CH}_{\text{Yo}}\text{O}_{\text{Zo}}\text{N}_{\text{Ao}}\text{P}_{\text{Bo}}\text{S}_{\text{Co}}$	Autotrophic nitrifying organisms
44.	$\text{CH}_{\text{Yo}}\text{O}_{\text{Zo}}\text{N}_{\text{Ao}}\text{P}_{\text{Bo}}\text{S}_{\text{Co}}$	Acidogens
45.	$\text{CH}_{\text{Yo}}\text{O}_{\text{Zo}}\text{N}_{\text{Ao}}\text{P}_{\text{Bo}}\text{S}_{\text{Co}}$	Acetogens
46.	$\text{CH}_{\text{Yo}}\text{O}_{\text{Zo}}\text{N}_{\text{Ao}}\text{P}_{\text{Bo}}\text{S}_{\text{Co}}$	Acetoclastic methanogens
47.	$\text{CH}_{\text{Yo}}\text{O}_{\text{Zo}}\text{N}_{\text{Ao}}\text{P}_{\text{Bo}}\text{S}_{\text{Co}}$	Hydrogenotrophic methanogens
48.	$\text{CH}_{\text{Yu}}\text{O}_{\text{Zu}}\text{N}_{\text{Au}}\text{P}_{\text{Bu}}\text{S}_{\text{Cu}}$	Unbiodegradable Soluble Organics
49.	$\text{CH}_{\text{Yup}}\text{O}_{\text{Zup}}\text{N}_{\text{Aup}}\text{P}_{\text{Bup}}\text{S}_{\text{Cup}}$	Unbiodegradable particulate organics
50.	Cl^-	Chloride
51.	CO_2	Carbon dioxide
52.	CO_3^{2-}	Carbonate
53.	$\text{COD_per_mol_}[\text{Comp_Index}]$	Array components providing the COD of each
54.	C_T	Mass of UPO in substrate added
55.	D_T	Mass of BPO in substrate added
56.	f_AC	Methanogenic acetogen fraction of live organisms
57.	f_AD	Acidogenic fraction of live organisms
58.	f_AM	Acetoclastic methanogen fraction of live organisms
59.	f_Biomass	Live organism fraction of biodegradable portion of dead biomass
60.	f_HM	Hydrogenotrophic methanogen fraction of live organisms
61.	f_iat	ISS/TSS ratio
62.	$f_\text{U_Inf}$	Fraction of Influent VSS_Inf that is unbiodegradable particulate organic substrate
63.	$f_\text{U_Org}$	Unbiodegradable endogenous residue fraction of inoculum seed sludge VSS
64.	$f_\text{XU_Bio_lysis}$	The unbiodegradable fraction of biomass that accumulates on lysis with death regeneration model
65.	f'_Sbp	Fraction of biodegradable particulate organics
66.	f'_Sup	Fraction of unbiodegradable particulate organics
67.	Gamma_B	3rd group of BPO settling fraction
68.	Gamma_I	3rd group of ISS settling fraction
69.	Gamma_U	3rd group of UPO settling fraction
70.	H^+	Hydrogen ion
71.	H_2	Dissolved hydrogen
72.	H_2O	Water
73.	$i_\text{Ca_PP_mol_perP}$	Molar fraction of Ca/P in polyphosphate
74.	$i_\text{H_Org_mol_perC}$	H/C: organisms

75.	i_H_SF_mol_perC	H/C: fermentable soluble
76.	i_H_SU_mol_perC	H/C: unbiodegradable soluble
77.	i_H_XBInf_mol_perC	H/C: PS biodegradable particulate
78.	i_H_XBOrg_mol_perC	H/C: biodegradable particulate
79.	i_H_XUInf_mol_perC	H/C: unbiodegradable particulate
80.	i_H_XUOrg_mol_perC	H/C: endogenous residue
81.	i_HF_mol_perC	H/C: fermentable soluble
82.	i_HU_mol_perC	H/C: unbiodegradable soluble
83.	i_K_PP_mol_perP	Molar fraction of K/P in polyphosphate
84.	i_Mg_PP_mol_perP	Molar fraction of Mg/P in polyphosphate
85.	i_N_Org_mol_perC	N/C: organisms
86.	i_N_SF_mol_perC	N/C: fermentable soluble
87.	i_N_SU_mol_perC	N/C: unbiodegradable soluble
88.	i_N_XBInf_mol_perC	N/C: PS biodegradable particulate
89.	i_N_XBOrg_mol_perC	N/C: biodegradable particulate
90.	i_N_XUInf_mol_perC	N/C: unbiodegradable particulate
91.	i_N_XUOrg_mol_perC	N/C: endogenous residue
92.	i_O_Org_mol_perC	O/C: organisms
93.	i_O_SF_mol_perC	O/C: fermentable soluble
94.	i_O_SU_mol_perC	O/C: unbiodegradable soluble
95.	i_O_XBInf_mol_perC	O/C: PS biodegradable particulate
96.	i_O_XBOrg_mol_perC	O/C: biodegradable particulate
97.	i_O_XUInf_mol_perC	O/C: unbiodegradable particulate
98.	i_O_XUOrg_mol_perC	O/C: endogenous residue
99.	i_P_Org_mol_perC	P/C : organisms
100.	i_P_SF_mol_perC	P/C: fermentable soluble
101.	i_P_SU_mol_perC	P/C: unbiodegradable soluble
102.	i_P_XBInf_mol_perC	P/C: PS biodegradable particulate
103.	i_P_XBOrg_mol_perC	P/C: biodegradable particulate
104.	i_P_XUInf_mol_perC	P/C: unbiodegradable particulate
105.	i_P_XUOrg_mol_perC	P/C: endogenous residue
106.	ISS_BM	ISS to biomass for X_{oh} and X_{pa}
107.	ISS_Under	Inorganic settleable solids in the PST underflow
108.	ISS _i	Influent inorganic settleable solids
109.	K_ALK	Saturation coefficient for alkalinity (HCO ₃ ⁻)
110.	K_CO2	Rate constant for CO ₂ exchange
111.	K_I_H_AM	H ⁺ inhibition for acetoclastic methanogens
112.	K_I_H_HM	H ⁺ inhibition for hydrogenotrophic methanogens
113.	K_I_H2	Inhibition coefficient for H ₂ in acidogenesis

114.	K ⁺	Potassium
115.	Kdis_cal	Dissolution of calcite
116.	Kdis_cap	Dissolution of calcium phosphate
117.	Kdis_mag	Dissolution of magnesite
118.	Kdis_mgkp	Dissolution of K-struvite
119.	Kdis_newb	Dissolution of newberyite
120.	Kdis_stru	Dissolution of struvite
121.	kH_F_AD_hyd	Hydrolysis rate constant for FBSO
122.	kH_PHA_AD_hyd	Hydrolysis rate constant for poly-hydroxy-alkanoates (PHA)
123.	kH_PP_AD_hyd	Hydrolysis rate constant for polyphosphate (PP)
124.	K _{kp} Mg _{mp} Ca _{cp} PO ₃	Polyphosphate
125.	kM_BInf_AD_hyd	Hydrolysis rate constant for BPO_PS
126.	kM_BInf_AD_hyd	Hydrolysis rate constant for X_B_Inf
127.	kM_BOrg_AD_hyd	Hydrolysis rate constant for BPO
128.	kM_BOrg_AD_hyd	Hydrolysis rate constant for X_B_org
129.	kM_fPP_PAO_PHAstor	Maximum rate for PP release with anaerobic PHA storage
130.	K _s	substrate and acidogenic biomass concentration ratio, at which the specific hydrolysis rate is half its upper limit (k _M) at saturation
131.	KS_AC	Half saturation coefficient for acetogens
132.	KS_AD	Half saturation coefficient for acidogens
133.	KS_AM	Half saturation coefficient for acetoclastic methanogens
134.	KS_BInf_AD_hyd	Half sat coefficient for BPO_PS (for sewage organics)
135.	KS_BInf_AD_hyd	Half saturation coefficient for X_B_Inf (Primary sludge)
136.	KS_BOrg_AD_hyd	Half sat coefficient for BPO (for organics from biomass death)
137.	KS_BOrg_AD_hyd	Half saturation coefficient for X_B_Org (organics from biomass death)
138.	KS_HM	Half saturation coefficient for hydrogenotrophic methanogens
139.	Lambda_B	4th group of BPO settling fraction
140.	Lambda_I	4th group of ISS settling fraction
141.	Lambda_U	4th group of UPO settling fraction
142.	Mg ²⁺	Magnesium
143.	MgCO ₃	Magnesite
144.	MgHPO ₄	Newberyite
145.	MgKPO ₄ .6H ₂ O	K-struvite
146.	MgNH ₄ PO ₄ .6H ₂ O	Struvite
147.	MM_C	Molar mass of carbon
148.	MM_H	Molar mass of hydrogen
149.	MM_N	Molar mass of nitrogen
150.	MM_O	Molar mass of oxygen
151.	MM_P	Molar mass of phosphorous

152.	MM_S	Molar mass of sulphur
153.	mu_AC	Max specific growth rate for acetogens
154.	mu_AD	Max specific growth rate for acidogens
155.	mu_AM	Max specific growth rate for acetoclastic methanogens
156.	mu_HM	Max specific growth rate for hydrogenotrophic methanogens
157.	MW_[Comp_Index]	Array components providing the molar mass of each
158.	n	Number (1,2,3....)
159.	Na ⁺	Sodium
160.	NH ₄ ⁺	Ammonium
161.	O ₂	Dissolved oxygen
162.	Out.X_ISS	Inorganic settleable solids in the PST overflow
163.	Out.X_U_Inf	Influent unbiodegradable particulate organics in the PST overflow
164.	Out.X_VSS	Volatile settleable solids in the PST overflow
165.	Out.X_B_Inf	Influent biodegradable particulate organics in the PST overflow
166.	PO ₄ ³⁻	Phosphate
167.	R	Sludge age
168.	r _h	Hydrolysis rate
169.	S _{bpi}	Influent particulate biodegradable COD
170.	S _{bsae}	Effluent volatile fatty acid COD
171.	S _{bsai}	Influent VFA COD
172.	S _{bsfi}	Influent fermentable biodegradable soluble COD
173.	S _{bsi}	Influent biodegradable soluble COD
174.	S _m	COD concentration in methane
175.	SO ₄ ²⁻	Sulphate
176.	S _{pe}	Effluent particulate COD
177.	S _{pi}	Total influent particulate COD
178.	S _{se}	Total effluent soluble COD
179.	S _{si}	Total influent soluble COD
180.	S _{ti}	Total influent COD
181.	Stoi_CO3_decay	Coefficient of CO ₃ ²⁻ in the decay process
182.	Stoi_ER_decay	Coefficient of X_U_Org in the decay process
183.	Stoi_H_decay	Coefficient of H ⁺ in the decay process
184.	Stoi_H2O_decay	Coefficient of water in the decay process
185.	Stoi_NH4_decay	Coefficient of NH ₄ ⁺ in the decay process
186.	Stoi_PO4_decay	Coefficient of PO ₄ ³⁻ in the decay process
187.	Stoi_SO4_decay	Coefficient of SO ₄ ²⁻ in the decay process
188.	S _{upi}	Influent particulate unbiodegradable COD
189.	S _{usi}	Influent unbiodegradable soluble COD
190.	T1a	Batch test of column 1
191.	T1Ave	Batch test of column 1 average

192.	T1b	Batch test of column 1 duplicate
193.	T2a	Batch test of column 2
194.	T2Ave	Batch test of column 2 average
195.	T2b	Batch test of column 2 duplicate
196.	T3a	Batch test of column 3
197.	T3Ave	Batch test of column 3 average
198.	T3b	Batch test of column 3 duplicate
199.	T4a	Batch test of column 4
200.	T4Ave	Batch test of column 4 average
201.	T4b	Batch test of column 4 duplicate
202.	T5a	Batch test of column 5
203.	T5Ave	Batch test of column 5 average
204.	T5b	Batch test of column 5 duplicate
205.	TempCoeff	Rate temperature coefficient
206.	Temperature	System temperature
207.	Tref	Reference Temperature
208.	TSS_Under_s	Sub-component total settleable solids in the PST underflow
209.	Under_X_B_Inf	Influent biodegradable particulate organics in the PST underflow
210.	Under_X_U_Inf	Influent unbiodegradable particulate organics in the PST underflow
211.	Under_X_VSS	Volatile settleable solids in the PST underflow
212.	V_gas	Volume of gas in the reactor
213.	V_liq	Volume of liquid in the reactor
214.	V _s	Settling velocities
215.	Vs_s_X_B_Inf1	Settling velocities for sub-component_X_B_Inf1
216.	Vs_s_X_B_Inf2	Settling velocities for sub-component_X_B_Inf2
217.	Vs_s_X_B_Inf3	Settling velocities for sub-component_X_B_Inf3
218.	Vs_s_X_B_Inf4	Settling velocities for sub-component_X_B_Inf4
219.	Vs_s_X_B_Inf5	Settling velocities for sub-component_X_B_Inf5
220.	Vs_s_X_ISS1	Settling velocities for sub-component_X_ISS1
221.	Vs_s_X_ISS2	Settling velocities for sub-component_X_ISS2
222.	Vs_s_X_ISS3	Settling velocities for sub-component_X_ISS3
223.	Vs_s_X_ISS4	Settling velocities for sub-component_X_ISS4
224.	Vs_s_X_ISS5	Settling velocities for sub-component_X_ISS5
225.	Vs_s_X_U_Inf1	Settling velocities for sub-component_X_U_Inf1
226.	Vs_s_X_U_Inf2	Settling velocities for sub-component_X_U_Inf2
227.	Vs_s_X_U_Inf3	Settling velocities for sub-component_X_U_Inf3
228.	Vs_s_X_U_Inf4	Settling velocities for sub-component_X_U_Inf4
229.	Vs_s_X_U_Inf5	Settling velocities for sub-component_X_U_Inf5
230.	VSS/TSS	VSS/TSS ratio
231.	VSS_Under_s	Sub-component volatile settleable solids in the PST underflow

232.	X_Lim	Minimal concentration in sludge blanket
233.	X_T	Threshold suspended solids concentration
234.	Y_AC	Acetogenesis biomass yield
235.	Y_AD	Lo H2 Acidogenesis biomass yield
236.	Y_AH	Hi H2 Acidogenesis biomass yield
237.	Y_AM	Acetoclastic Methanogenesis biomass yield
238.	Y_HM	Hydrogenotrophic Methanogenesis biomass yield
239.	Y _{AD}	Biomass yield
240.	Z _{AD}	Acidogenic biomass

CHAPTER 1.0: INTRODUCTION

This chapter gives an overview of the proposed project, the development of a calibration methodology for a realistic primary settling tank (PST) model. An elaborate problem statement that informs the need for the purposed project, study scope and objectives are detailed in this chapter.

1.1 THE PROPOSED PROJECT

This project proposes calibration of the modified University of Cape Town Primary Sedimentation Unit (UCTPSU) model that replicates the primary settling tank, within an integrated plant-wide model. The project will be conducted in the Water Research Group (WRG) in the Department of Civil Engineering at the University of Cape Town (UCT), supervised by Dr. David Ikumi and co-supervised by Professor George A. Ekama.

1.2 PROBLEM STATEMENT

The objective of wastewater treatment is to remove solid materials (at the primary treatment stage), biologically treat and digest supernatant and dissolved organic materials (in its secondary and tertiary stages). The wastewater treatment plant also removes inorganics and nutrients (mainly nitrogen (N) and phosphorus (P)) to ensure effluent quality that meets the required environmental criterion (Zhang *et al.*, 2011). However, with rapidly growing populations in developing countries, wastewater treatment plants (WWTPs) have been struggling to meet the strict effluent discharge regulations required to protect the regions' water resources. Moreover, the globally shifting paradigm (i.e. converting these WWTPs to water and resource recovery facilities (WRRFs) and transforming water-stressed cities to water-sensitive regions) have necessitated re-thinking the strategy behind waste treatment processes towards recovery of water, nutrients (N) and (P) and energy. To ensure that decision making processes are based on scientifically sound principles, tools (mathematical models) that provide expert information on the WRRFs can be used in strategy evaluation. A significant input to these mathematical models is the characteristics of the sewage waste entering the system. Once reaching the treatment plant, the raw sewage is usually taken

through a physical process of solid/liquid separation. The main unit operation in these physical processes is the primary sedimentation tank (PST).

The utilization of primary sedimentation tanks (PSTs) is a well-known strategy towards reducing the quantity of solids fed to the activated sludge (AS) systems, where the biological conversions of influent sewage occurs. The PST, removes settleable solids (once settled, are known as primary sludge; PS) from the influent and thereby reduces organic loads to the AS systems, hence lowering energy and volume requirements for water and resource recovery facilities (WRRFs) as a whole. Moreover, the biodegradable organics in primary sludge (PS; the PST underflow) are often channeled to anaerobic digestion (AD) systems, where their stabilization process results in the generation of biogas (that could be converted to energy savings). The major challenge in the treatment plant sedimentation has been the inability to accurately predict the recovered nutrient and energy corresponding to the elemental mass compositions (EMCs) of the digested primary sludge.

Most of the current models have been able to predict the PST output (i.e., PS) from the influent TSS with reasonable accuracy (Bachis *et al.*, 2015; Maruéjols *et al.*, 2015). From Ekama *et al.* (2011) compiled data set on anaerobic digestion of primary sludge (AD_PS), the EMCs of the biodegradable particulate organics (BPO) of , and the free and saline ammonia (FSA) from produced the volatile settleable solids (VSS) in the primary sludge were determined. It was also observed that Sötemann *et al.* (2005a) elemental analysis of PS from two full scale WWTPs closely correlated with Ekama *et al.* (2011) evaluation. However, characterizing that PS in terms of biodegradable and unbiodegradable particulate as well as inorganic suspended solids is not achievable through these models. In actual fact, the PS has experimentally revealed to settle in different proportions of 70-80% of the unbiodegradable particulate organics (UPO), 80-90% of the inorganic settleable solids (ISS) and 40-60 % of biodegradable particulate organics (BPO) (Wentzel *et al.*, 2006; Ikumi *et al.*, 2014). To obtain these proportions, it then follows that these components should settle at different velocities. In a parallel study (Polorigni *et al.*, 2020), an improved TSS-based primary settling tank model is developed that includes correct proportions of unbiodegradable particulate organic (UPO), biodegradable particulate organic (BPO, including the BPO characteristic empirical formula, i.e., x , y , z , a and b of $C_xH_yO_zN_aP_b$) and inorganic suspended solid (ISS) in correct proportions. This study therefore extends the UCTPSU model to include bioprocesses of hydrolysis and

fermentation and calibrates it by performance of a general sensitivity analysis and parameter determination, using experimentally generated data (from a settleometer connected to augmented bio-methane potential test).

1.3 SCOPE OF THE STUDY

The scope of the study will be strictly limited to the extension and calibration of the developed PST model using WEST® simulation platform (Vanhooren *et al.*, 2003). The model calibration will be achieved by employing the required analytical procedures on experimental data (obtained from settleometer, steady-state anaerobic digestion, and augmented biochemical methane potential tests).

1.4 STUDY OBJECTIVES

The main objective of the current study focusses on the development and calibration of a realistic PST model in terms of settling velocities, TSS fractionations and underflow sludge fermentation. These predictions will help maximize nutrient and energy recovery and predict real PS characteristics. The accurate characterization of PS and settled wastewater in application of plant-wide model is essential to simulate strategies for optimization of energy and nutrient recovery from the influent wastewater. To accomplish this overall goal, these sub-objectives were established:

- I. Acid generation characteristics of the UCTPSU model will be established including the hydrolysis and fermentation processes. This modification to the UCTSPU model may later on provide interesting control possibilities, since the VFAs produced could supply readily biodegradable carbon sources for growth of PAOs in plant and/or substrate for denitrification.
- II. Perform a sensitivity analysis on the modified UCTPSU model as part of the model calibration procedure.
- III. Utilize results experimentally generated, from (i) a settleometer that separates the settleable organics in municipal wastewater into different settling velocity groups together with (ii) augmented bio-methane potential tests performed on the solids collected by the settleometer, to calibrate the UCTPSU model.

CHAPTER 2.0: LITERATURE REVIEW

2.1 INTRODUCTION

This section reviews some of the relevant literature required for the development of the objectives of this project. Since this project focuses on calibration of the University of Cape Town Primary sedimentation Unit (UCTPSU) model, a brief background to the relative model viz, point settler, anaerobic digestion and bio-methane potential were discussed.

2.2 TOWARDS MODELLING PRIMARY SEDIMENTATION UNITS

Primary sedimentation refers to physical processes of solid-liquid separation in primary clarifiers or settlers, which are usually referred to as primary settling tanks (PSTs). It is usually the last stage of a series of different process of the primary treatment, which include pumping, screening, grit removal, flow distribution and balancing. A portion of the TSS referred to as settleable solids (SS) flocculate and get enmeshed to settle in the sedimentation basin to be disposed as primary sludge (PS). Hence, the remaining suspended solids, which are non-settleable, as well as the dissolved compounds constitute the supernatant (settled wastewater) that is conveyed to the biological reactors for secondary treatment and mediated by the organisms mediating wastewater processes. Since settleable particles naturally gravitate in the wastewater, it appears that settling is the common solid/ liquid separation technique (Piro *et al.*, 2011). In addition, the fundamental parameter controlling particle's settleability in primary sedimentation is the particle's settling velocity (Davis, 2011). Gravitational settling occurs in several ways as pointed out by Metcalf and Eddy (2003), such as discrete particle settling, flocculent particle settling and hindered or zone settling.

2.2.1 DISCRETE SETTLING

Discrete settling involves particles settling individually, at a constant settling velocity and without any significant interaction with others (Davis, 2011). Hence, particle sizes, shapes as well as densities are not altered and assimilated to spheres (Chebbo and Gromaire, 2009). This directly implies that that the terminal velocity is instantaneously reached and remains constant. As such, the wastewater is a suspension of a low solids concentration (Metcalf and Eddy, 2003). Sand and grit are usually removed under discrete settling.

Davis (2011) expresses the settling velocity from Stokes' law which under laminar flow conditions, states that:

$$v_s = \frac{g (\rho_s - \rho) d^2}{18 \mu} \quad (2.1)$$

Where: v_s is the particle settling velocity in m/s

d is the particle diameter in m

g is the acceleration due to gravity in m/s²

ρ_s is the density of particle in kg/m³

ρ is the density of fluid in kg/m³

μ is the dynamic viscosity in Pa.s

However, despite the actual non-discretization of particles in a PST, discrete modelling could still be used to provide a representation of primary sedimentation with particle settling velocities.

2.2.2 FLOCCULENT SETTLING

Flocculent settling is quite dominant in primary settling tanks, as well as in the upper layer of second clarifiers (Takacs *et al.*, 1991). In this type of sedimentation, particles coalesce and increase in mass to settle at a faster rate. The wastewater is usually a dilute suspension of particles and there's removal of a portion of the untreated water, as well as chemical flocs (Metcalf and Eddy, 2003). Described by Davis (2011) as Type II sedimentation, this settling phenomenon cannot be accurately modelled by Stokes' law since particles vary in size and shape through flocculation, as well the specific gravity variation due to the air entrapped into the flocs. As a result, settling column tests such as the ViCAs (Vitesse de Chute en Assainissement) can instead be used to model this behavior.

2.2.3 ZONE SETTLING

This settling type is a settling regime that is also referred to as hindering settling. Because of the high concentration of particles, the free area between them decreases and hence the inter-forces hamper the processes. As a result, particles settle as a mass of unit, in a "zone" or "blanket" fashion (Takacs *et al.*, 1991; Davis, 2011). Column tests are used to determine the settling characteristics associated with the solid flux theory (Metcalf and Eddy, 2003).

The role of primary sedimentation has been overlooked over years, due to the difficulties arising in describing the above-mentioned processes, from both optimization and modelling perspectives. Furthermore, the primary settler has been weakly replicated in the virtual plant-wide model setup, because it is mostly considered as an input to most of the main unit process models (i.e., activated sludge and anaerobic digestion systems), hence not directly influential in the modelling processes (Bachis *et al.*, 2015).

A wide range of models have been developed through various studies (Lessard and Beck, 1988; Otterpohl and Freund, 1992; Gernaey *et al.*, 2001; Maruejouis *et al.*, 2012; Bachis *et al.*, 2015). Each model developed has its advantages and disadvantages, as laid out in Table 2.1 below. Some models were quite simplistic by making use of retention time with a single variable (Otterpohl and Freund, 1992) or address scouring with the hydraulic behavior of the primary clarifier (Lessard and Beck, 1988), in an empirical fashion. Other models comprised of combined physical and biological processes that were it extremely complex to develop and calibrate (Lessard and Beck, 1988; Gernaey *et al.*, 2001). Hence, there is a need to redefine the development of primary settling tank models with the objective of a better WRRF processes description and a holistic plant-wide optimization. This led to a new generation of promising models using the particle settling velocity theory (Vallet, 2011; Maruéjouis *et al.*, 2012; Bachis *et al.*, 2015).

After evaluating these models, it appears that their predicted PST solids removals are TSS sensitive but do not characterize the removed TSS according to the relevant TSS components of ISS, UPO and BPO. This is because the data used to calibrate these models were measured in terms of TSS only, of which the composition was not included in these data collections. Therefore, the research gaps to be addressed in this project will include elaborating a more-detailed experimental campaign, to allow for the calibration of the PST model towards achievement of such detailed predictions. Furthermore, the composition of the TSS removed is usually incorrect with respect to the proportions of its components - the TSS in these models is assumed to be removed in equal proportions of its constituents (and subsequently at the same settling velocity). This was first noted by Sötemann *et al.* (2005b) and recently highlighted in the PST model implemented in the Benchmark Simulation Model No. 2 for Phosphorus (Batstone *et al.*, 2015). However, Wentzel *et al.* (2006) and Ikumi *et al.* (2014) have observed that BPO, UPO and ISS settle out in the PST in different proportions of 30-40%,

60-70% and 70-90% respectively. PST models that do not model the removal of the BPO, UPO and ISS material well, do not model the split of these materials between the primary sludge anaerobic digester (where energy is generated) and settled wastewater activated sludge system (where energy is consumed) well, with the result that the energy self-sufficiency of the wastewater treatment plant is not adequately predicted.

Table 2.1: Comparison of Reviewed Primary Sedimentation Unit Models (Polorigni, 2020)

Model	Description	Strengths	Gaps
Dynamic lumped-parameter model (Lessard and Beck, 1988) Aim: Settling characteristics of influent components and capacity of soluble removal	Use of continuously stirred tank reactors (CSTR) A distinction is made between the removable and non-removable compounds The soluble removal is included	The removable fraction is modelled into settleable and non-settleable fractions The model attempted to assign settling velocities to different types of sewage The soluble COD and ammonium removals are described	The sludge settling velocity is not adequately described The primary sludge is not characterized The solid profile distribution is not considered
Simple model of a primary clarifier (Otterpohl and Freund, 1992) Aim: Predict the PST buffering behavior and consider the change of inflow characteristics	Dilution of wastewater fractions per reactor volumes The removal of particulate fractions is based on hydraulic retention time	The regression analysis makes the model easy to be built A good COD particulate removal could be predicted	The biodegradability is not considered Only COD is modelled The solids distribution and flow patterns cannot be described
Dynamic model of a clarification-thickening (Takacs <i>et al.</i> , 1991) Aim: Propose an alternative settling velocity model to dynamically replicate the clarification and thickening functions of a clarifier	The solid flux theory and a material mass balance around each layer of a one-dimensional settler are used A special settling velocity equation for simulation of dilute and concentrated suspensions is developed	The model can simulate the solids profile in a column test under steady state and dynamic conditions, by means of the underflow and effluent suspended solids concentrations It can be applied to primary and secondary clarifiers	The settling velocity equation only holds for zone settling and fails to properly describe discrete and flocculent settlings The velocity profile distribution is not properly described as it makes use of a single concentration to determine the velocity.
Reactive clarifier model (Gernaey <i>et al.</i> , 1988) Aim: Model development of a primary clarifier to be used in WEST®	Based on Takacs <i>et al.</i> (1991) model Use of a settling velocity model for clarification and thickening	The influent COD is split into characteristics compatible with the activated sludge model No.1 (ASM1) Good prediction of effluent COD An extensive description of biological reactions (COD and ammonium removal through hydrolysis, ammonification) An attempt to link the model to the ASM1 is highlighted	Soluble COD is not well described by incorporating a particulate fraction Particles are assumed to have the same velocity Settling parameters not completely determined Primary sludge characterization is not addressed
Phenomenological retention tank model with the PSVD theory (Maruejouis <i>et al.</i> , 2011)	It is based on Lessard and Beck (1991) model	Successful full-scale data testing The solid distribution is addressed by a PSVD model using three particle classes	A validation with many other events is limited

Aim: Improve sedimentation model by incorporating the PSVD	Particle settling description under dynamic flows The ViCAs protocol is used for velocity characterization	with assigned time varying fractions of the influent TSS A good effluent TSS prediction	Organics and nutrient fractionation are not considered. The incorporation of WWTP state variables linking unit processes with the PST model has not been done
New dynamic water quality model for stormwater basins (Vallet <i>et al.</i> , 2014) Aim: Replicate the behavior of particulate pollutants in a basin	A distribution explains the particle settling velocities ViCAs experiments are used for velocity characterization Hydraulic and soluble models are also included, alongside to the particle's components	Three settling velocities are used to describe the distribution of particles associated with the pollutants The ViCAs results proved to be a good input into the model and virtual settling simulations were successful	In the context of a PST, this model needs to characterize the different particles with regards to their biodegradability The theoretical simulations are not sufficient to validate the model performance
New modelling approach with the PSDV theory (Bachis <i>et al.</i> , 2015) Aim: Sedimentation modelling with the PSVD and primary sludge characterization	PSVD model used for solids distribution ViCAs protocol is used for velocity characterization	PSVD model improved by using five particle classes with assigned time varying fractions of the influent TSS Good effluent TSS prediction Implementation on the CEPT strategy ASM1 fractionation from primary treatment	Biodegradability is partially addressed ST model is still to be properly link to the activated sludge model (ASM) Link to other unit processes (such as the anaerobic digester and the activated sludge system)

Hence a better model for the PST fractionation of the effluent primary sludge is required. It then follows that the PSVD theory (Bachis *et al.*, 2015) can serve as a good tool to model the removals of these components, under different settling velocities. In fact, this theory can account for solids distribution, based on the settling velocity of particles (Matko *et al.*, 1996). Furthermore, if the primary sludge is characterized, it will be possible to provide a much-detailed prediction in terms of primary effluent output.

Primary settling tanks are used for primary sedimentation of wastewater to generate primary sludge, which is then fed into the anaerobic digester for energy recovery purposes. Mathematical models have been developed to simulate the removal of particulates in the PST, by means of different solids settling principles. However, these models are all TSS-based and as such, it has been increasingly difficult to accurately predict the primary sludge (PS) composition, which is an input into downstream unit processes such as the anaerobic digestion (AD). The knowledge of the solids characteristic component compositions would be useful when applying plant-wide mathematical models in prediction of PS fed AD performance and also the performance of the activated sludge (AS) system that is fed the settled wastewater (the supernatant generated after primary sedimentation).

Primary clarifiers have not been modelled extensively because of the complexity in representing the sedimentation phenomena. Moreover, prior to the development of plant-wide models, the mathematical models focused on prediction of effluent quality from distinct unit processes such as activated sludge. Because the various WRRF unit processes are linked, their operations impact the performance of other downstream (and upstream, where recycling is involved) unit processes. Further, the tracking of energy (chemical oxygen demand - COD), nutrients (N and P) and water became essential with the utilization of plant-wide models to provide more holistic solutions to recovery of resources and generation of good effluent quality. Within this plant-wide model, the current PST unit process models have not been able to track the organic and inorganic materials removals appropriately; hence the compositions of primary sludge (to the AD unit process) as well as the settled wastewater (to the AS system) are not properly estimated. This project works towards development and verification of a model that realistically depicts the removal of solids materials (BPO, UPO and ISS) and caters for the determined primary sludge and settled wastewater compositions such that resource recovery can be optimized at a plant-wide level.

To propose a realistic model of the PST, two approaches could be used, depending on the settling process under consideration. Discrete settling assumes a constant velocity and no significant interaction with others (Davis, 2011) whereas flocculent settling considers particles that coalesce and increase in mass, to settle at a faster rate (Metcalf and Eddy, 2003). In that regard, a discrete particle settler was developed, and the insights drawn from this model were used to build a much more realistic PST dynamic model, under flocculent conditions. The Flocculent model is an extension of existing modelling approach of Bachis *et al.* (2015), which is described further below.

2.3 THE NEW MODELLING APPROACH OF BACHIS *ET AL.* (2015)

The model of Bachis *et al.* (2015) is based on a settling velocity distribution that is covered by five particle classes representing the TSS. The particle settling velocities are experimentally determined through the ViCAs protocol (Chebbo and Gromaire, 2009) and assigned to the different particle classes which are modelled as fractions of the influent TSS. The fractions are determined from observing the relationship between the particle settling velocity distribution (PSVD) curves extracted from the ViCAs experiments and the TSS concentrations. As a result,

a vertical gradient of the concentrations of each of these particles classes can be predicted by splitting the settler into several layers and performing a solids mass balance around each layer. The settling processes defined in this approach is based on the settling configuration described in the primary settling tank model of Takacs *et al.* (1991). Here, the settler (of area A and height H) is divided in 10 layers of equal thickness (V_L and H_L) and a solid flux analysis is applied, by considering the downwards solids flux that continuously flows through the layers. A minimum sludge blanket concentration (X_{MIN}) is defined as well as a maximum threshold concentration (X_{LIM}) which is established to regulate that downwards flux that can be sustained by the layer below the layer of interest.

The downwards flux is defined as the sum of the bulk liquid flux and the gravity settling flux. The bulk liquid flux (J_{UP}/J_{DN}) is due to the movement of the liquid in the settler and can either be upwards or downwards, depending on the position of the layer of interest with regards to the feed layer. It is therefore defined as the product of the solids concentration of the i^{th} layer (C_i) and the liquid bulk velocity (V_{UP}/V_{DN}), from the equations:

$$J_{UP} = C_i \times V_{UP} \quad (2.2)$$

$$J_{DN} = C_i \times V_{DN} \quad (2.3)$$

The gravity settling flux (J_G), which is due to the solids settling under the gravity force, is expressed as the product of the concentration of the solids in the i^{th} layer (C_i) and the settling velocity of the solids (V_s - these velocities extracted from the ViCAs experiments), from the equation:

$$J_G = C_i \times V_s \quad (2.4)$$

According to the solids flux analysis, the gravity settling flux can be expressed under the following constraints:

From the 1st to the 4th layer: If $C_i < X_{LIM}$, $J_G = C_i \times V_s$. But if $C_i > X_{LIM}$, $J_G = \min (J_{Gi}, J_{Gi-1})$

From the 5th layer (feed layer) to the 9th layer, $J_G = \min (J_{Gi}, J_{Gi-1})$

These conditions show that J_G depends on the solid concentration of the layer below the layer of interest.

As such, to perform solids mass balances around each layer, it is important to understand relationships established among layers as well as the input and outputs of solids to these layers. First, they are categorized into five groups, namely the top layer, the layers above the

feed layer, the layers below the feed layer and the bottom layer. Figure 2.1 below depicts a layered settler configuration.

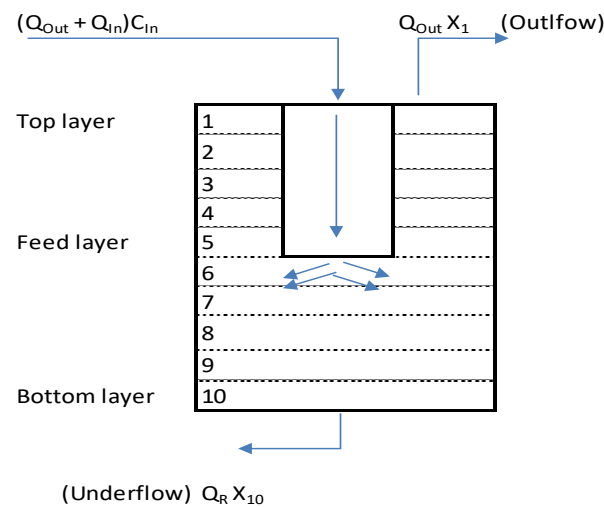


Figure 2.1: Layered settler model, adapted from Takacs *et al.*, (1991)

From this configuration, the primary settling tank receives the influent flow at the 5th layer and it is then distributed across all the other layers. Takacs *et al.* (1991) states two assumptions, which are as follow:

- 1) The incoming solid flux distribution is instantaneous and uniform across the whole cross-sectional area of the layers.
- 2) The vertical flow is the only flow considered.

Solids therefore move across layers in a dynamic fashion and these movements are summarized in Table 2..

Table 2.2: Solids movement summary across the layered model and adapted from Takacs <i>et al.</i> (1991)					
Layer	Before settling (Input)			After settling (Output)	
	Feed	Settling	Bulk liquid flux	Settling	Bulk liquid flux
Top layer	Not considered	Not considered	Upwards	Considered	Upwards
Layers above feed layer	Not considered	Considered	Upwards	Considered	Upwards
Feed layer	Considered	Considered	-	Considered	Upwards – downwards
Layers below feed layer	Not considered	Considered	Downwards	Considered	Downwards
Bottom layer	Not considered	Considered	Downwards	Not considered	Downwards

2.4 MASS BALANCES

Based on these definitions above as well as fluxes considered, solids mass balances are performed around each layer of the settler. It is important to note that mass balances are achieved when the solids concentration per layer is constant. Examples of solid mass balances mathematical modelling are depicted for the feed layer and 6th layer below.

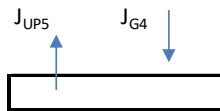


Figure 2.2: Input in layer 5

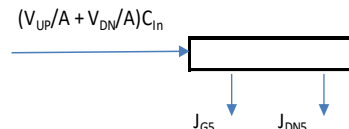


Figure 2.3: Output from layer 5

For the 5th layer

Inputs: $J_{UP5} - J_{G4}$

Output: $-J_{G5} - J_{DN5} + \left(\frac{V_{UP}}{A} + \frac{V_{DN}}{A}\right) * C_{In}$

Since the input must be equal to the output, it yields to:

$$-J_{G5} - J_{DN5} + \left(\frac{V_{UP}}{A} + \frac{V_{DN}}{A}\right) * C_{In} = J_{UP5} - J_{G4} \quad (2.5)$$

But

$$\left(\frac{V_{UP}}{A} + \frac{V_{DN}}{A}\right) * C_{In} = (Q_{out} + Q_R) * C_{In} = Q_{In} * C_{In} = F_{In} \quad (2.6)$$

Where: F_{in} is the influent flux of solids.

$$(-J_{G5} - J_{DN5} + F_{in} - J_{UP5} - J_{G4}) = 0 \quad (2.7)$$

Which leads to $dC_i/dt = 0$

And subsequently

$$(1/H_L) \times (-J_{G5} - J_{DN5}) + ((1/V_L) \times F_{in}) = 0 \quad (2.8)$$

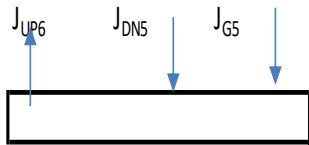


Figure 2.4: Input in layer 6

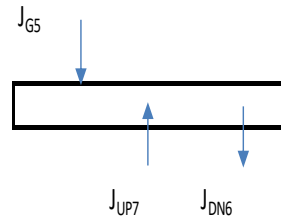


Figure 2.5: Output from layer 6

For the 6th layer

Inputs: $J_{UP6} - J_{DN5} - J_{G5}$

Output: $J_{UP7} - J_{G6} - J_{DN5}$ (2.9)

Since the input must be equal to the output, it yields to:

$$J_{UP6} - J_{G6} - J_{DN6} - J_{UP6} + J_{DN5} + J_{G5} = 0$$

Which leads to $dC_i/dt = 0$

$$\text{Subsequently, } (1/HL) \times (J_{UP7} - J_{G6} - J_{DN6} - J_{UP6} + J_{DN5} + J_{G5}) = 0 \quad (2.10)$$

A summary of the solid mass balances across the model is depicted in Figure 2. below.

2.5 PRIMARY SLUDGE CHARACTERIZATION

To model PST removals in correct proportions, as well as accurately predicting the inputs into subsequent unit processes, the primary sludge needs to be comprehensively characterized. This characterization can be split into two experimental phases. The first phase consists of characterizing the primary sludge based on their settling velocities and settling mass fractions, and the second section determines the biodegradability of these different fractions.

2.5.1 SLUDGE SETTLEABILITY METHODS

Settleability characteristics of primary sludge (PS), generate particle velocity distributions that can adequately feed into a PSVD model. Owing to the density of particles, the PS can be characterized in different mass fractions. Methods such as the ViCAs protocol (Chebbo and

Gromaire, 2009) and the settleometer method (Poinapen *et al.*, 2009) can be used. See Figure 2.7 (below) for its experimental setup.

2.5.2 PARTICLE EFFLUENT VELOCITY (ViCAs) PROTOCOL

Chebbo and Gromaire (2009) have elaborated the well-known ViCAs operating protocol highlighted in some of the above-mentioned PST models (Maruejols *et al.*, 2012; Vallet *et al.*, 2014; Bachis *et al.*, 2015). It has been developed to measure settling velocities of suspended particles (carried by stormwater or combined sewage) and hence generate the distribution of these velocities. The protocol is based on the principle of homogeneous suspension to avoid pre-treatment and sample modification - this requires for the tests to be performed immediately after sampling.

The apparatus consists of a sedimentation column made of polyvinyl chloride (PVC), with an internal diameter of 70 mm and a height of 64 cm (see Figure 2.). The column is filled a homogeneous wastewater sample to about 60 cm and allowed to settle at defined time intervals. At every time interval, the sludge mass, which is later analyzed to determine its TSS content, is collected by a receptacle and replaced by another one for the next time interval. From these cumulated masses at different time intervals, it is possible to generate the distribution curves of settling velocities. Because particles do not settle over the same height, statistical tools are used to generate settling velocities distribution curves. Material mass balances verifications are performed to determine losses or gains throughout the experiment and evaluate the accuracy of the measurements.

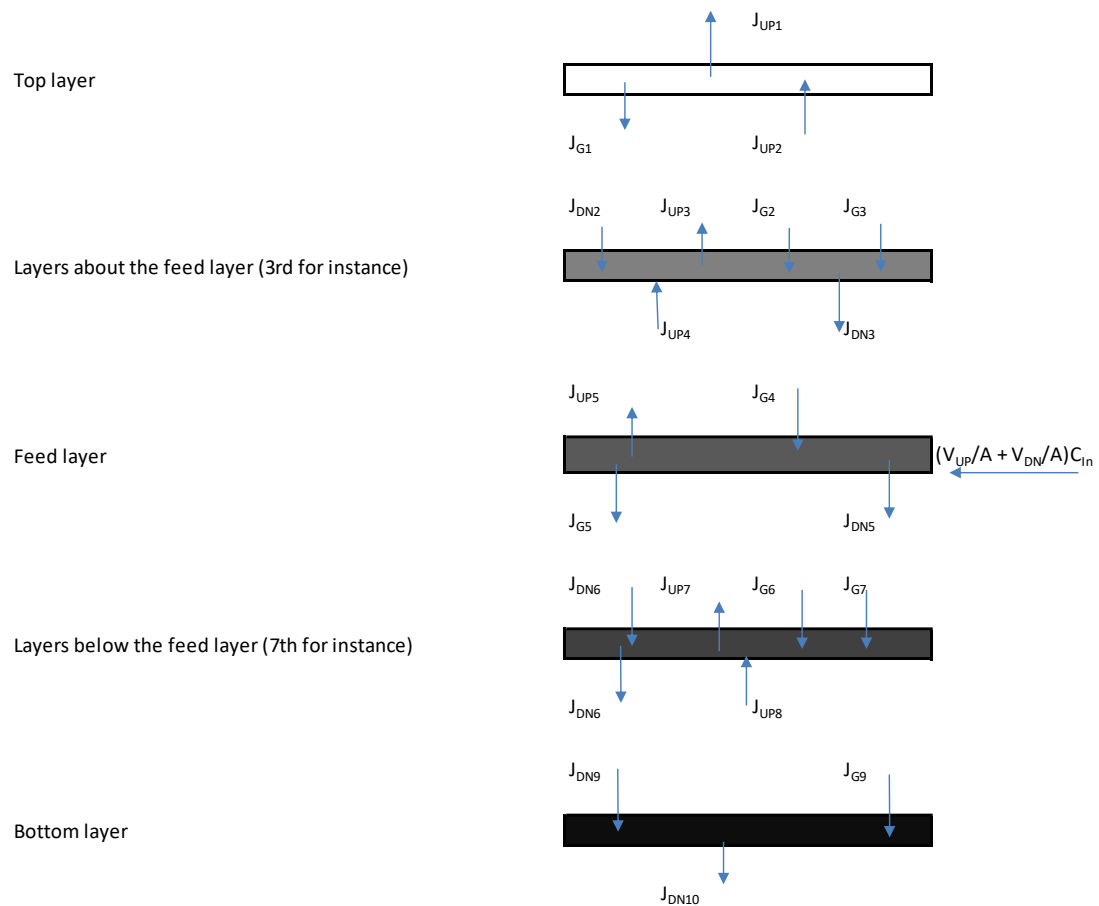


Figure 2.6: Solids balance throughout all the layers and adapted from Takacs *et al.* (1991)

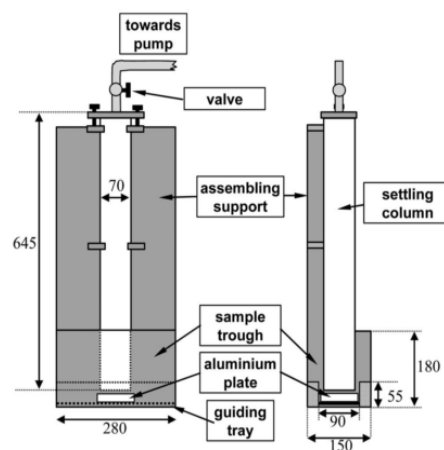


Figure 2.7: ViCAs protocol experimental set up (Chebbo and Gromaire, 2009)

2.6 FERMENTATION OF PRIMARY SLUDGE

Barker and Dold (1995) reported that achieving low effluent phosphorus (P) concentrations in enhanced biological phosphorus removal (EBPR) systems is difficult with low organic strength wastewaters, particularly where the influent COD:P ratio is low. This low COD:P ratio becomes more difficult in nitrifying systems with low influent COD:TKN ratios because denitrification of nitrate recycled to unaerated zones reduces the amount of readily biodegradable COD (RBCOD) available to promote biological P removal. Various means for addressing low influent COD:P (and COD:TKN) have been applied successfully; for example, addition of an external carbon source; addition of acid-fermented primary sludge supernatant to the anaerobic zone; and accumulating sludge in the primary settling tank (PST) to promote in situ fermentation, with elutriation of the sludge blanket to transfer VFAs and RBCOD to the primary effluent (Lilley *et al.*, 1990; Banister and Pretorius, 1998; Ahn and Speece, 2006; Wu *et al.*, 2010). All these approaches involve adding carbon (from the significant VFA and/or RBCOD content) that is generated external to the activated sludge EBPR system. However, one consequence is an increase in activated sludge production; also, the fermentation products will add to the nitrogen and phosphorus load to the EBPR system (Eastman and Ferguson, 1981; Zehnder and Gujer, 1983). Temperature, pH, solids retention time, return sludge flow rate, solids concentrations and dewatering are the major parameters that influence fermentation process in wastewater treatment plants (Eastman and Ferguson, 1981; Elefsiniotis, 1993; Gupta *et al.*, 1986; Lilley, 1990; Banister and Pretorius, (1998); Chanona *et al.*, (2006)).

2.7 ANAEROBIC DIGESTION

Anaerobic digestion (AD) is one of the biological treatment processes that has gained popularity for two important reasons: lower sludge production marked as chemical oxygen demand (COD) reduction (without the use of oxygen or nitrate) and production of useful head gases of high calorific value at the expense of the applied waste load (Ghosh & Pohland, 1974). This means AD converts sludge organic solids (and also decomposition of inorganic solids) into biogas such as methane (CH₄) used as renewable fuel for heating digesters, fuel vehicles and space heating; carbon dioxides (CO₂) and traces of other gases under anaerobic conditions. Apart from these two major advantages, Guerrero *et al.* (2009) defined three additional advantages as lower energy consumption, lower space requirements and lower overall costs.

This bioprocess is one of the ways to stabilize sludge during treatment process and stabilizing here means to lessen problems related to presence of pathogenic organisms, sludge odor and putrescence (Peirce & Vesilind, 1998). Moreover, the stabilized sludge can be used as soil conditioner or disposed if it contains large portion of unrequired substance like metals (hence, undesirable for soil) or properly disposed as an admixture on a sanitary landfill site (Ikumi, 2011). Several literature exists that asserts the stability-treatment process achieved through AD. Eastman and Ferguson (1981) reported that AD is used in treatment plants to stabilize large fraction of organic wastewater in the treatment plant. Wu (2015) also reported that sludge treatment process is used to completely digest primary sludge (PS) and waste activated sludge (WAS).

However, the operations of AD applies the same principles at all place by focussing on developing, and maintaining a large, stable, viable population of methane-forming bacteria. To achieve this, the following principles must be implemented: (i) Efficient contact time between nutrient resources in the substrate and bacteria (this means there must be uniform mixing); (ii) controlled anaerobic condition; and (iii) adequate retention time to allow the two-stage processes to be completed. Hence, in view of achieving optimal design and operation, microbiology and biochemistry of AD plants must be balanced (in between the acid- and hydrogen formation, to maintain favourable pH). If system imbalance occur after balancing microbiology and biochemistry, it means there is poor system design influenced by environmental and operational variables (Parkin & Owen, 2008).

2.7.1 VARIABLES OF ANAEROBIC DIGESTION SYSTEM

According to Ghosh and Pohland (1974), hydrolysis process is the rate-limiting step of the overall AD process since it enables sequestration of simple and small forms (liquefied form) of the degraded complex waste, as the liquefied form can pass through cell walls for use as energy or nutrient sources (Sötemann *et al.*, 2005). Literature focus more on methanogenic phase with little attention paid to the acidogenic phase. However, further study will improve knowledge on acidogenic phase at different operational and environmental situations. Acidogenesis increases the concentration of produced soluble organics (in primary settling tank) and suitable as energy feed for two-stage biological denitrification system. Although low pH (below normal range of 6.8 to 7.5 that favors methanogenic growth) and low temperature improves organic matter solubility and fermentation (hereby increasing the production of

soluble organics), and production is maximized when methane production is well reduced by reducing the retention time (Eastman and Ferguson, 1981). Since methanogens perform central role in the digestion process, acetates, propionate and hydrogen (that act as process indicators) are the intermediate products of AD required to be monitored in the system (as they determine the pH value and size of biogas produced). Moreover, anaerobic digestion is linked to the other unit treatment systems and there are cases where products of this process require recycling to upstream unit processes of the WWTP. However, the major disadvantage in AD process is that generation of methane gas contributes to global warming with potential of about 11 times greater than that of carbon dioxide. A 20% reduction in global warming may be achieved by utilization of organic wastes and residues for the production of bio-fuels and chemicals, both by preventing methane emission and by replacing fossil fuels (Ikumi, 2011). There are two types of AD processes in an AD treatment plant which are Mesophilic (characterized by high retention time of 15-30 *d* and temperature of 30-35 °C) and Thermophilic (defined to function at a higher temperature of 55 °C but shorter retention time like 12-14 days) digestions (Peirce & Vesilind, 1998). These digestion processes have more benefits than problems (like poor digester performance and system failure). Parkin and Owen (2008) explained that the performance of digestion system is determined by the reasonable proportion (in relative balance) of major types of anaerobic bacteria. These problems often happen due to poor process control and inadequate operation management ((Graef and Andrews (1974); Elefsiniotis (1993); Labatut and Gooch (2012)). Adequate control of operational parameters (like hydraulic retention time, HRT and solids retention time, SRT) and proper system configuration can be achieved to prevent digester upset and maintain steady environmental variables like influent characteristics, reactor configuration, pH, temperature and available trace minerals (Elefsiniotis and Oldham, 1994).

As established in the previous paragraphs that AD is multi-processed but classified into a two- stage process, the four organisms responsible for these processes are acidogens, acetogens, acetoclastic methanogens and hydrogentrophic methanogens. Zehnder and Gujer (1983) identified, as proposed by Kaspar in 1977, six different conversion processes that occur in the degradation of particulate organic materials to methane (which has potential for reuse). The particulate organics are hydrolyzed to organic monomers that can be used as substrates by fermentative organism (amino acids, sugars) or by anaerobic oxidizers (fatty

acids). Acetate and hydrogen (or intermediate compounds like volatile fatty acids) are the products of these degradation reactions and are the main components that determine the formation of microbial methane (as two systems further convert acetate and hydrogen to methane). The six processes include: (i) Hydrolysis of particulate organics such as lipids, proteins, and carbohydrates. This is the first activity that occurs described as when complex organics are broken down into simple organics (like monomers and dimers), small enough to be transported across cell membranes of acidogens (ii) Fermentation of amino acids and sugars (iii) Anaerobic oxidation of long chain fatty acids and alcohols (iv) Anaerobic oxidation of intermediary products such as volatile fatty acids with the exception of acetate (v) Conversion of acetate to methane, and (vi) Conversion of hydrogen to methane.

Labatut & Gooch, (2012) reported that at VFA concentrations over 1,500 – 2,000 mg/L, biogas production might be limited by inhibition. However, rather than a specific concentration, it is a sudden and steady increase of VFAs in the effluent that can be a sign of a digester upset (hence digester failure, if not monitored). In conventional applications, these six conversion processes that explain anaerobic digestion have been defined to be two-phase processes, acid-forming and methane forming (Demirel & Yenigün, 2002; Parkin & Owen, 2008) because ultimate sludge stabilization is based on the growth and metabolism of two groups of microorganisms, which are very different from each other in terms of physiology, nutritional requirements, growth kinetic capabilities, and sensitivity to environmental stresses. Other factors that can influence the performance level of an AD system are retention time, pH and system temperature, feeding rate and mixing condition and presence of toxins (McCarthy, 1974; Parkin and Owen, (2008); Guerrero *et al.*, (2009)).

2.7.2 ANAEROBIC DIGESTION (AD) SYSTEM STEADY STATE MODELS

Steady state models are based on the slowest process kinetic rate (i.e. hydrolysis) that governs the overall behavior of the system. Therefore, steady state models allow the system design and operating parameters, such as reactor volume and recycle ratios, to be estimated reasonably simply and quickly from system performance criteria specified for the design, such as effluent quality. Once approximate design and operating parameters are known, these can serve as input to the more complex simulation models to investigate dynamic behavior of the system and refine the design and operating parameters. A steady state AD model is therefore useful to:

- estimate retention time, reactor volume, gas production and composition for a required system performance like COD (or VSS) removal,
- investigate the sensitivity of the system performance to the design and operation parameters,
- provide a basis for cross-checking simulation model results, and
- estimate product stream concentrations for design of down- (or up-) stream unit operations of the wastewater treatment plant (Sötemann *et al.*, 2005; Brouckaert *et al.*, 2010; and Ikumi *et al.*, 2014).

2.8 BIOCHEMICAL METHANE POTENTIAL (BMP) TEST

The BMP test measures the biodegradability (biodegradable fraction of organics) of a substrate by comparing the methane production of a control sample (only containing anaerobic digestion seed inoculum) to that of a test sample (containing organic waste and anaerobic digestion seed inoculum). The difference in biogas produced between the test and control samples is an indication of the potential methane that can be produced through the anaerobic digestion of the organic waste (Moody *et al.*, 2009). The limitations experienced by this system, despite its simplicity, comes from its result inconsistency which can be influenced by many factors like headspace volumes and pressure, environmental conditions and even system's configuration (Botha, 2015). This therefore calls for a more reliable means of determining biodegradability of tested organics (or sample). In this current study, an augmented BMP will be used to measure organics biodegradation and test for its consistency by measuring the organic-bound compositions that are generated (like the free and saline ammonia, ortho-phosphate, and biogas).

2.9 CONCLUSION

In the literature review, the need for a refined knowledge of settled wastewater fractionations as described by Bachis *et al.* (2015) and Polorigni (2020) will undermine the assumed percentage set for each settleable components (ISS, UPO and BPO) and establish more realistic fractionations that is system-derived, by using calibration and experimental methods. The ABMP test will assist in determining the elemental mass composition. This finding will help monitor and predict the possible amount of nutrient that can be produced

and the energy that can be generated through biogas (CH_4 and CO_2) production. The next chapter is establishing practical and important procedures that will be followed to estimate the proportionate total settleable solids (TSS) that settles based on their inherent settling properties, unbiodegradable particulate organics of the primary sewage sludge (PSS), elemental mass compositions of the bio-organics, and the parameters that significantly affect PSS.

University of Cape Town

CHAPTER 3.0: METHODOLOGY

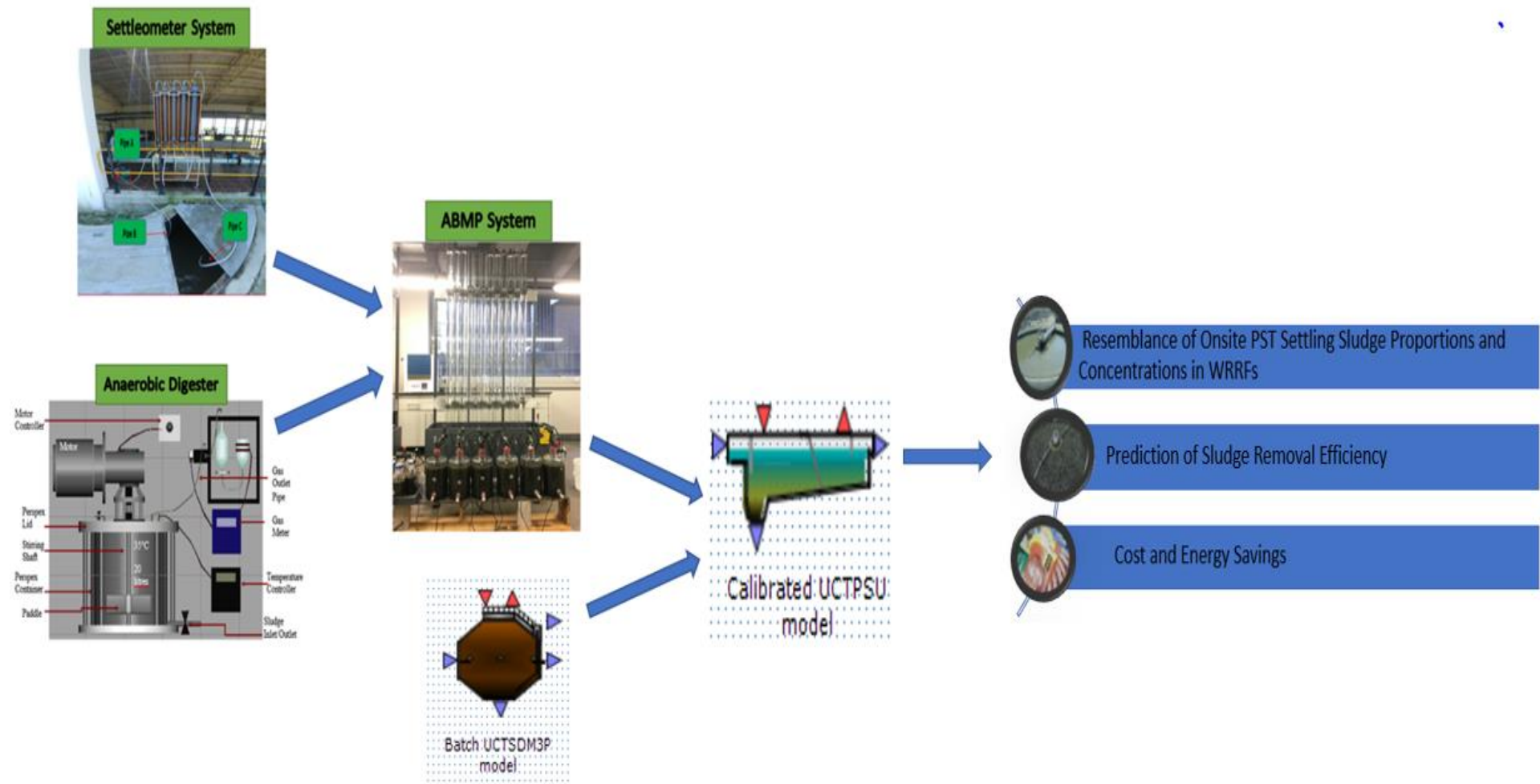


Figure 3.1: Pictorial Description of the Study Objectives (calibrating modified UCTPSU model)

3.1. INTRODUCTION

This chapter provides a comprehensive description of experimental and analytical procedures applied to achieve the study objectives. The three integrated experiments conducted are (I) settleometer running and testing, (II) running anaerobic digestion reactor at a steady-state conditions (AD_SS), and (III) augmented bio-methane potential (ABMP) test. Each of the experiments are described and explained from sections 3.2 – 3.4. The chapter also gave an appropriate overview for the plant-wide model of South Africa (PWM_SA) in terms of its components, species and speciation routine, variables, and parameters. The model descriptions focused on the University of Cape Town Sludge Digestion Model (UCTSDM3P) and the University of Cape Town Primary Sedimentation Unit (UCTPSU) model as these two models (coupled with the proposed experimental procedures) formed the basis of the proposed calibration methodology.

3.2 SETTLEOMETER EXPERIMENT

3.2.1 EQUIPMENT DESIGN CRITERIA

A settleometer (Figures 3.2 and 3.3) is an instrument developed (by the University of Cape Town (UCT) Engineering workshop) to separate influent raw wastewater and suspended particles based on innate settling velocities (V_s) and hence generate the distribution of their settling velocities. The design principle for the settleometer was established by Moosbrugger *et al.* (1995). The apparatus consists of five vertical transparent interconnected plastic tubes made of polyvinyl chloride (PVC) with equal height (1 m tall) and increasing internal diameters (45.2 mm to 134.4 mm), operating at a constant flow rate. The fastest settling particles settle and remain in the first column which has the smallest diameter and where the settling velocity (V_s) is highest and the slowest settling particles settle in the last column where the diameter is the largest and the lowest V_s . As the V_s decreases between the successive columns, sludge samples generated from the settling within the columns are divided according to particle size and density (Poinapen *et al.*, 2009). Once the percentage sludge mass retained and the sludge concentrations are found in each column, they can be plotted against their up-flow velocities. The resulting graph will depict the settling profile of the sludge at different up-flow velocities (Poinapen *et al.*, 2009).

Before testing the settleometer, it needed to be serviced by first pumping clean water through it to test for any leakages. Once all problem areas were located, they were serviced and repaired. This step was repeated to ensure that the settleometer was fully functional. Following this, the upflow velocity for each cylinder was calculated by sucking fresh water through the system at flow rates ranging from 0.6 l/min to 1.2 l/min using Equation 3.1.

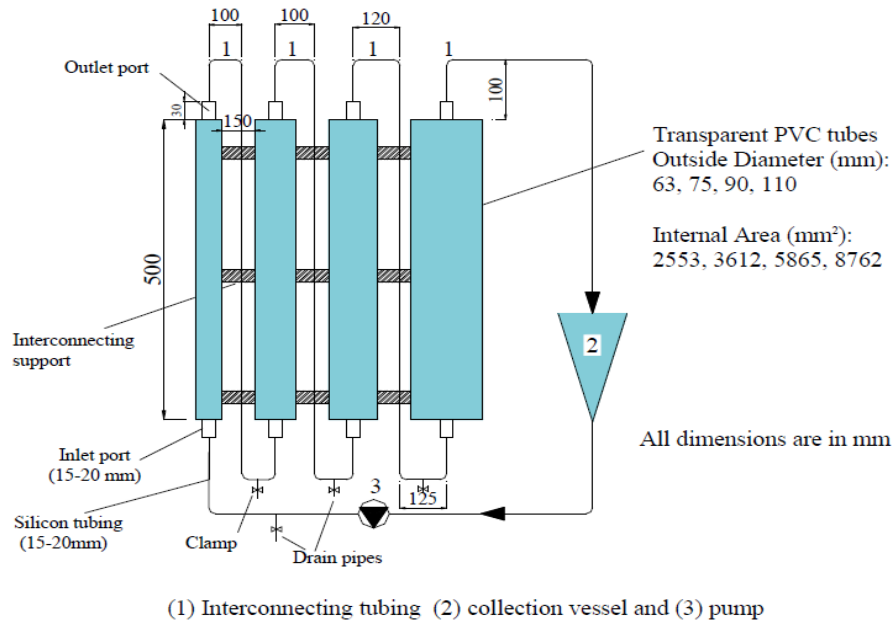


Figure 3. 2: Schematic Diagram of Settleometer

$$V_{up} = \frac{Q}{A_{in}} \quad (3.1)$$

Where Q is the input flow rate,

A_{in} is the internal cross-sectional area of the cylinder, and

V_{up} is the calculated up-flow velocity inside the cylinder.

To ensure that no solids are broken down before moving through the settleometer, it was decided that the water would be required to be sucked through the system instead of being pumped through it. Once the pump was primed with water in the system, the system was reversed. To check for possible leakage, water was now being sucked through the settleometer from the smallest cylinder and exiting out the largest cylinder. Once the settleometer was proved to be fully functional, it was ready to run raw wastewater through the system. The raw wastewater fed into the settleometer is taken from the inlet works of the Potsdam wastewater treatment works (PDWWTW; in Cape Town, South Africa).

3.2.2 SETTLEOMETER ON-SITE TESTING AND RUNNING

Due to the pump noise and lack of space to accommodate its size, the settleometer trial run was performed on-site (PDWWTW) using tap water. Two settleometer runs were conducted as trial runs to observe all possible human operation errors and observe the functionality of the equipment. The functionality was tested under the influence of water for round 1 and primary sewage sludge flowing through the inlet works for round 2 (Figure 3.3 below).

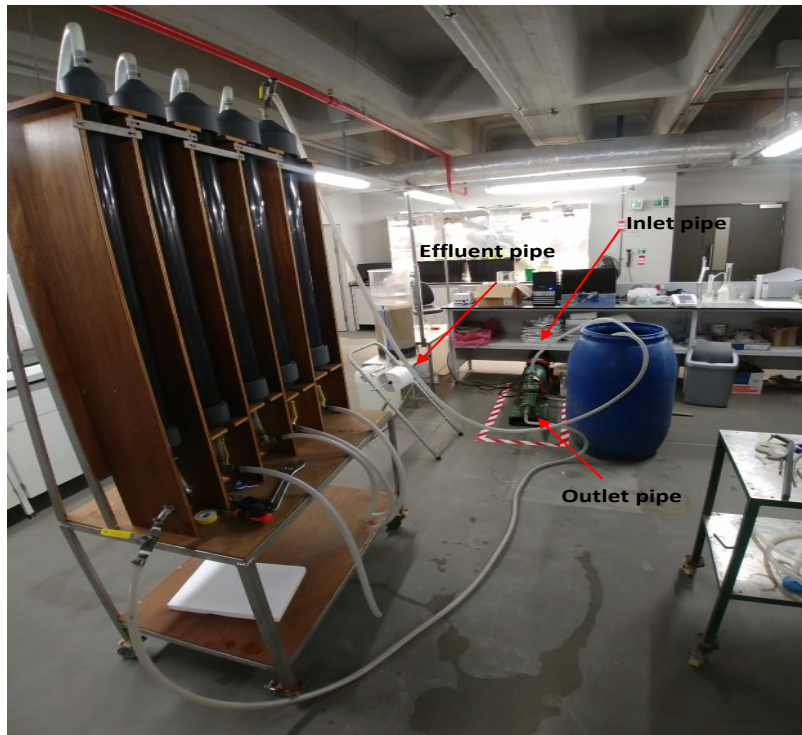


Figure 3. 3: UCT Settleometer Trial Run in Water Quality Laboratory (WQL)

Although the flow rate would reduce due to the increasing pressure loss in each PVC column, a simplified illustration was considered by applying the principle of mass conservation i.e. it was assumed that the effluent flow rate equals the influent flow rate. The principle of mass conservation was applied to determine flow rate of the settleometer by constantly measuring the effluent discharge at specific time intervals of 25 mins. This measured effluent flow rate is assumed to be the actual influent flow rate since flow is conserved in the system. Hence, the consistently measured effluent flow rate was estimated to be the conserved flow and that was 1.13 l/min. Similarly, a second trial test was performed but at a flow rate of 0.86 l/min, to determine the optimum flow rate that would allow for maximum settling.

In Figure 3.4 (below), Pipe A (representing the inlet pipe) is the connecting pipe between the pump and the settleometer (flowing from the smallest inner diameter to the largest inner

diameter). Pipe B is the outlet pipe that serves as the link between the flowing raw wastewater in the inlet works and the suction pump that transport the wastewater to the settleometer. Pipe C represents the overflow (or effluent) flowing out of the settleometer. Following the success of the on-site trial runs at PDWWTW, two succeeding settleometer tests were carefully conducted, to improve on human operation errors that must have occurred in the previous runs. To initiate the tests, the pump is set at the desired but allowable pumping flow rate (0.845 l/min), until a steady flow is achieved without any disturbances to the pump.

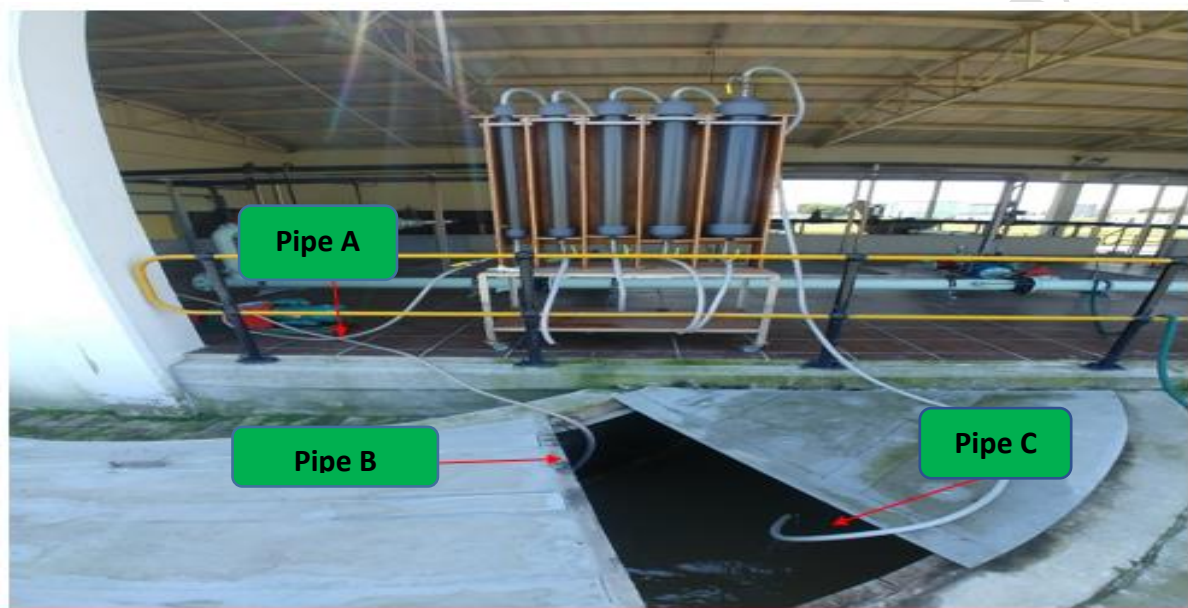


Figure 3. 4 depicts the positioning of the Settleometer device at PDWWTW Inlet Works (Cape Town).

Once a steady flow rate was achieved, the pump is stopped, and the system is flushed with tap water from the WWTW to rid the settleometer from all settled solids. Table 3.1 (below) gives the detailed summary of how each of the settleometer runs were conducted.

3.2.3 COLLECTION AND STORAGE

During each of the 4 settleometer runs, influent samples were fetched at an interval of 20 mins from time zero (0) till the last minute of each run. The collected influent samples for each run procedure were thoroughly mixed and a 5 l sample fetched.

Table 3. 1: 3rd Run for Settleometer Readings with 135 minutes Run Time (September 17, 2019)										
Test Categories	Units	PVC 1	PVC 2	PVC 3	PVC 4	PVC 5	M _{TSi}	M _{RWWi}	M _{SWWi}	MB _i
Measured Flow	<i>l/min</i>	-	-	-	-	-	-	1.13	1.13	MB
Volume	<i>l</i>	1.8	4.3	6.2	9.5	14.5	PVC ₋	-	-	MB
COD (unfilt.)	<i>mg/l</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
COD (filt.)	<i>mg/l</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
TKN	<i>mg/l</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
FSA	<i>mg/l</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
TP	<i>mg/l</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
OP	<i>mg/l</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
MLSS	<i>mg/l</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
MLVSS	<i>mg/l</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
MLISS	<i>mg/l</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
Alk.	<i>mg/l as CaCO₃</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
direct pH	<i>no unit</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
VFA	<i>mg/l</i>	Mea.	Mea.	Mea.	Mea.	Mea.	Calc.	Calc.	Calc.	MB
ID	<i>mm</i>	45.2	67.6	86.4	105.6	134.4	-	-	-	-
V_s	<i>m²</i>	Calc.	Calc.	Calc.	Calc.	Calc.	-	-	-	-
	<i>m³/min</i>	Calc.	Calc.	Calc.	Calc.	Calc.	-	-	-	-
	<i>m³/hr</i>	Calc.	Calc.	Calc.	Calc.	Calc.	-	-	-	-
	<i>m/hr</i>	Calc.	Calc.	Calc.	Calc.	Calc.	-	-	-	-
	<i>m/min</i>	Calc.	Calc.	Calc.	Calc.	Calc.	-	-	-	-
Abbreviations										
Filt and Unf	Filtered through Schleicher & Schull ME 25/21 0.45 micrometer membrane filters and Unfiltered samples respectively									
Mea. And Calc.	Measured as indicated in Table 3.2 (more details are given in result chapter) and calc. for direct calculation (using eq 3.1)									
M _{TSi}	Mass of total settleable solids (in mg) in the measured 'I' concentration									
M _{RWWi}	Mass of influent raw wastewater (in mg) in the measured 'I' concentration									
M _{SWWi}	Mass of settled (overflow) wastewater (in mg) in the measured 'I' concentration									
MB _i	Mass balance across the device for the measured 'I' concentration									
ID and V _{UP}	Internal column diameter (mm) and Up-flow velocity (in m/hr)									

While the setup was running, 1 l samples of the raw wastewater were taken at approximately 20 mins intervals till each run was completed (2 h). The effluent wastewater was discharged into a 200 l collection drum and the discharge started just after the influent raw wastewater had flowed through the interconnected 5 PVC columns. The effluent flow rate was estimated by recording the time it took a 3000 ml volumetric flask to fill up.

A 3000 ml volumetric flask was used in place of the 200 l collection drum in order to get more accurate timing of the flow rate and was justified by repeating the flow rate measurement about 3 times. The first run was completed after running the settleometer for 135 mins and its settled solids (together with its supernatants) in each column was emptied into separate 25 l containers.

The columns were emptied from the largest to the smallest cylinder to prevent supernatant overflow and sludge influx from a larger column to smaller column.

The pipe clamp at the top of the columns was loosened when emptying the columns to enhance the discharge of retained wastewater (supernatant and settled sludge) down the column. Each of 5-PVC-column samples in their receiving containers were thoroughly mixed before being collected into their respective 5 l containers. To ensure that all solids are flushed out of the system, clean water is pumped through the settleometer until all columns are completely saturated with water. The samples collected from the base of each PVC columns during the settleometer rounds were sampled for various tests (see Table 3.2 below). Altogether, 28 samples from the 4 settleometer runs were transported to WQL at UCT and were stored in the walk-in refrigerator (cold room) maintained at 4°C. Upon arrival, various analytical tests (listed in Table 3.2) were performed on all the collected samples (influent, 5 PVC columns and effluents). The full test result and result analysis for settleometer runs are well detailed in Appendix A.

3.3 REACTORS DESCRIPTION AND FEED PREPARATION

3.3.1 STEADY STATE MESOPHILIC ANAEROBIC DIGESTION OPERATION

The anaerobic digester (AD) is a continuously stirred tank reactor (CSTR) as depicted in Figure 3.5 (below). The reactor tank was manufactured from Perspex and cylindrical stainless-steel rods for structural support, to ensure a gas-tight seal. A stirrer driven by a single-phase motor was mounted on the top lid of the unit. The stirring shaft passed through the lid via a sealed

bearing to ensure the reactor is gas-tight under low positive gas pressures ($< 50 \text{ mm}$ water). A valve was also fitted at the base of the reactor to allow for feeding of influent sludge and removal of waste sludge in sampling and/or maintaining the AD sludge age. A gas outlet is also shown to be provided in the top lid. The gas-outlet pipe is connected to a wall-mounted gas counter. The anaerobic digester is operated at a temperature of approximately 35°C , optimal for mesophilic organisms. This temperature is controlled by means of heating rods dipped inside the AD reactor and connected to a temperature controller with a temperature probe in the reactor mixed liquor.

The AD is completely sealed, except for the provision of the gas outlet pipe and the access port, which was closed with a rubber bung. The access port is opened only once daily to measure the pH. The sludge inlet/ outlet pipe at the base of the AD, controlled by a valve, is only opened during the feeding process when waste sludge is drawn, and new feed sludge added. To monitor the AD system the general Tests (see Table 3.2) are done at least twice a week, while the pH, VFAs and alkalinity are monitored every second day. The total volume of the AD reactor tank is 25 l . However, the operating volume of AD is set at 20 l . The access point is opened once (or twice) daily for the ADs: to measure the in-situ pH, then to withdraw the required volume of waste sludge withdrawn via the stop-cock at the AD base and finally to restore the AD operating volume by adding the required volume of feed sludge (same as wasted volume, i.e. added batch-wise), thereby maintaining the prescribed 20 d sludge age.

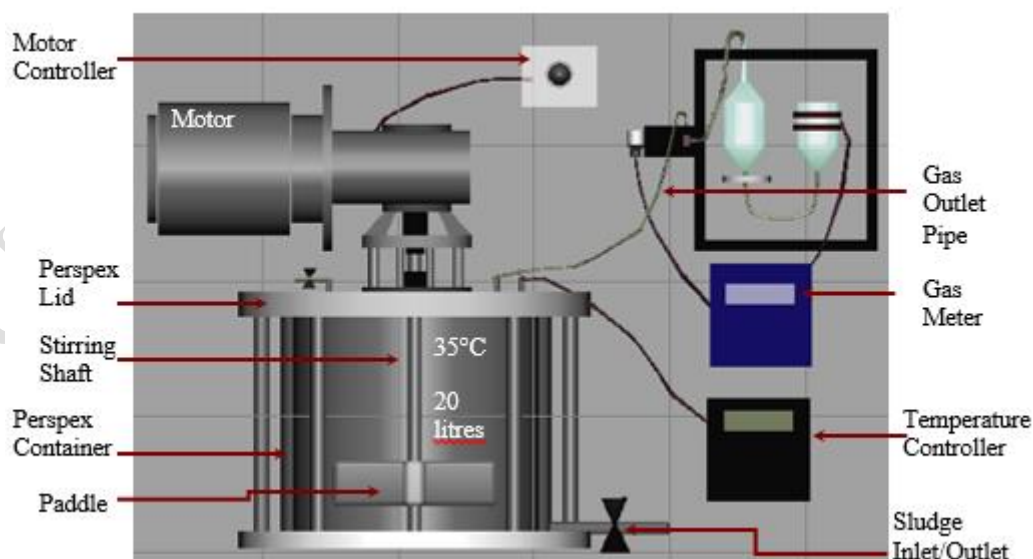


Figure 3. 5: Anaerobic digester used in research project

The anaerobic digestion (AD) system is fed primary sludge (PS) obtained from the underflow of the primary settling tank (PST) at the Potsdam wastewater treatment works (PDWWTW). This PS is collected in about 50 / batches and stored in the 4°C cold room of the UCT WQL. It is possible for the PS to undergo considerable anaerobic fermentation, causing increased short-chain fatty acid (SCFA) concentrations, even at low temperatures of 4°C. To limit the prospect of such characteristic alterations, PS storage is limited to a maximum of three months. Before the PS was fed to the AD, it is macerated to reduce its particle size - hence preventing blockages in the experimental systems and heated to above 35 °C to avoid causing a temperature shock to the temperature-sensitive methanogenic biomass. Figure 3.6 (below) shows the image of gas flow meter connected to the AD reactor to measure the produced biogas.

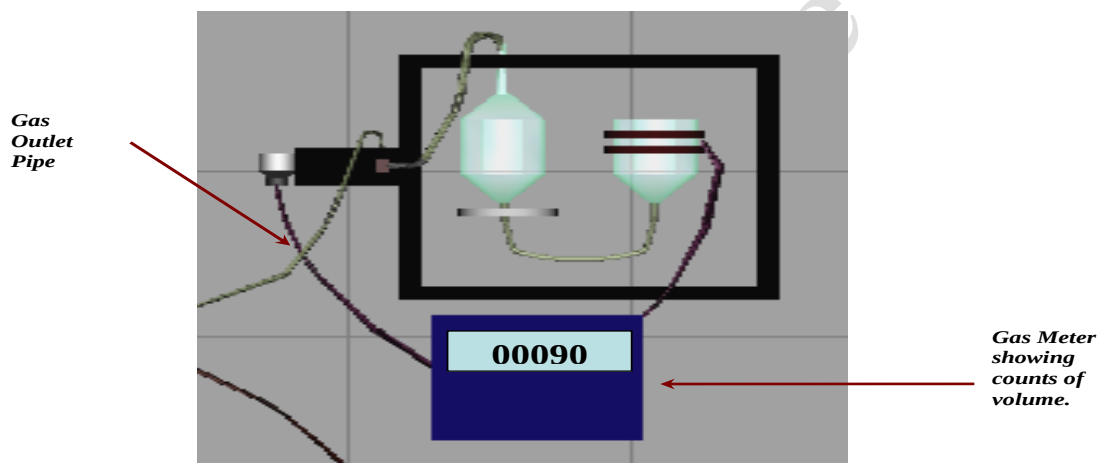


Figure 3. 6: Gas flow meter that measures the counts of produced biogas produced from the AD reactor.

3.3.2 AUGMENTED BIO-METHANE POTENTIAL TEST

The Bio-methane Potential (BMP) test is used to measure the potential yield of biogas (mainly methane and carbon dioxide) from the digestion of organic material in anaerobic batch conditions. The Augmented Bio-methane Potential (ABMP) test is run the same way as the BMP test, but also including few basic measurements of the chemical oxygen demand (COD; filtered and unfiltered), total, volatile and inorganic suspended solids (TSS, VSS and ISS) and the aqueous phase volatile fatty acids (VFA), H_2CO_3 alkalinity, free and saline ammonia (FSA) and orthophosphate (OP) concentrations and the pH (Botha, 2015). This shall be in the attempt to characterize the settled raw wastewater particles, which has been divided into various settling velocity groups.

The ABMP test uses a transparent glass bottle with a sample placed inside and the produced gas (methane gas, CH₄) escapes through tubing connected at the top of each bottle and is bubbled through a barrier solution into a measuring cylinder. Before the start of the test, water is sucked into the measuring cylinder using a vacuum pump. The gas produced displaces the water volume; therefore, by measuring the change in water level, the volume of gas produced over time by the sample can be determined. Various methods are being explored to measure the water level in the column continuously, however, on-line measurement using ultrasound and pressure sensors was the method applied in this project. This method will allow gas production rate versus time to be determined. Figure 3.7 (below) shows the ABMP test setup.



Figure 3. 7 ABMP Test Setup in WQL at UCT

This biomass is added to the ABMP reactor by a process known as seeding, in which a measured sample was drawn from the steady-state methanogenic reactor and placed into the ABMP reactor vessel at the start of the experiment (see section 3.3.1 above). The test samples collected from the 5-PVC columns shall be utilized by the seed inoculum present inside the ABMP reactor. The control (containing AD biomass seed supplied from the steady state AD effluent) and test (containing both the biomass seed and substrate) ABMP reactors were subjected to a long sludge age (> 40 d) in the ABMP reactors. The control and test samples were subjected to long sludge age to ensure in-situ biodegradables were completely

stabilized, hereby leaving unbiodegradable particulate organics (UPO) and inorganic settleable solids (ISS) as the remaining organics in the ABMP reactors. The initial starting concentrations of the ABMP reactor contents (inoculum and substrate) are sampled and measured. Also, sample is drawn from each reactor every 24 h for the first 12 d, after which a sample is taken every second day. This is done to ensure that enough mass remained inside the reactor until the end of the test. Reaction endpoint (no further biodegradation to occur) will be observed the moment gas production stops.

The composition of the biomass can be identified by using the bioprocess stoichiometry for methanogenic AD. The control test contains only the sludge seed, therefore, the carbon (C), nitrogen (N) and phosphorus (P) in the biomass endogenously respired becomes part of both the gaseous and aqueous products. Therefore, by measuring the difference in the various concentrations before the start of the test and at the end of the test, the COD, VSS, C, N and P of the biomass endogenously respired can be calculated.

Therefore, the biomass composition can be calculated provided accurate measurements are taken for the above-mentioned mass ratio parameters. The same procedure is then repeated for the batch test which contains biomass and a known concentration of organics. The results obtained indicate the concentrations of the various elements transferred to the gas and aqueous phases for both the biomass and the biodegradable organics.

$$C_{start} - C_{end} \quad (3.2)$$

$$[(T_{start} - T_{end}) - (C_{start} - C_{end})] \quad (3.3)$$

Where T and C respectively represent the test and control batches.

The change in concentration during this testing period is due to the breakdown of the residual biodegradable material inside the steady-state (SS) AD system effluent as well as a small (negligible) amount from endogenous respiration (as shown in Equation 3.2). The various concentrations of the organics can be measured by taking the difference between the start and end of the test, the COD, VSS, C, N and P of the biomass digested can be calculated (using Equation 3.3, above). As mentioned by Ekama and Brink (2008), the composition of the organic material can be identified using the elemental mass ratios, which in this case is applied to the biomass.

- I. The carbon (fc) content of the biomass: Using mixed weak acid/base chemistry and 5-point titration, the H_2CO_3 alkalinity can be accurately identified. Therefore, the C can

be tracked through the system by considering the change in concentration of CO_2 , CH_4 and H_2CO_3 alkalinity before and after the test.

- II. The nitrogen (fn) and phosphorus (fp) content of the biomass: The N and P content of the biomass in the control are calculated using a similar approach, which measures the change in concentration of FSA and OP before and after the test.
- III. The COD (fcv): The COD of the biomass lost is given by the difference between the methane COD before and after the test.
- IV. The VSS: The VSS of the biomass lost is the different between the VSS concentration before and after the test.

Therefore, the composition of the biomass can be calculated provided accurate measurements are taken for the above-mentioned mass ratio parameters.

3.4 SAMPLING AND TESTING

3.4.1 ANAEROBIC DIGESTION

Samples for analysis are collected from the AD influent and effluent. In order to check the stability of the AD on a routine basis, a five-point titration is conducted on a filtered effluent sample at least every second day. The in-situ pH and five-point titration method (Moosbrugger *et al.*, 1993) gives the H_2CO_3 alkalinity and VFA concentration. For optimal operation, the in-situ pH should be above 6.5 but preferably within the range of 7 and 8 (McCarty, 1974) and the H_2CO_3 alkalinity to VFA ratio should be maintained at more than 3:1 (Ripley *et al.*, 1986). During the intensive measuring periods, once the AD reach steady state (i.e., after the three sluge age periods, $20 \times 3 = 60 \text{ d}$), the influent and effluent, unfiltered and membrane filtered VFA, COD, TKN and FSA, TP and OP tests are performed to determine the extent of digestion and the COD, N and P mass balances over these digesters (See Table 3.2 below). The daily gas flow is measured by means of the wet tipping gas meter and gas samples are collected in 5 l impermeable Tedlar gasbags connected to the AD gas outlet pipes. The gas is analyzed to determine the CO_2 and CH_4 content as a requirement to establish a COD and carbon balance over the digesters.

In order to conduct the ABMP tests accurately, each test reactor required inoculation with methanogenic bacteria. This necessitated the operation of a methanogenic AD system onsite (in the WQL) to generate the required seed inoculum for the proposed ABMP test. This AD

system is run at SS to allow for the stability of the seed inoculum generated and for calculation of AD biomass concentrations using the mass balanced AD model, simulated at steady state. The AD is tested to have achieved SS (i.e., after the three sludge ages) when the mixed liquor concentrations (i.e., COD, TSS, VSS, etc.) are consistent and a mass balance is achievable over the reactor. This can be observed in the test results compiled in Appendix B.

All material that is fed into the reactor has 20 d to be broken down by the anaerobic bioprocesses. However, this is not always the case with SS AD systems due to the way in which they are fed. The SS AD system is mixed mechanically to try and achieve a homogenous distribution of products and reactants within the system. Yet, when effluent is drawn from the bulk liquid, it may still contain a portion of biodegradable organic material. This portion of biodegradable material would not be broken down in the reactor and may skew the total concentration of biodegradable material available in the PS (substrate).

During operation of the AD, half of this sludge was fed in the mornings and the other half in the evenings to avoid shock loading, which would result in digester failure. The pH level and alkalinity concentration of the feed and AD system were regularly monitored. In instances where the AD showed signs of failure, the loading rate on the digester is reduced to half the sludge mass per day and hydrogen carbonate added to the influent feed. Key factors to look out for in AD reactor are the pH range (6.7 – 8.0), biogas production (which could either inform on failing state of the reactor or complete degradation of the organics), Ripley ratio effect or the combination of these factors.

3.4.2 AUGMENTED BIOMETHANE POTENTIAL

This missing component of biodegradable material in AD can be accounted for by looking at the control ABMP reactor (using Equation 3.2). Preceding the ABMP test, the control batch reactors were diluted with a dilution factor of 2, because 1-part seed sludge was added to 1-part water, diluting the respective SS AD system effluent concentrations by half. This dilution factor is included during the test analysis to adjust the seed characteristics. Table 3.2 (above) highlights the analysis conducted on control and test batches of the ABMP.

Table 3.2 Summarises the test analysis that conducted on the three inter-connected experiments.						
Unit Process		Settleometer			AD	Batch AD
Abbr.	Meaning	Influent	Settled sludge in PVC columns	Effluent	Influent & Effluent	Influent & Effluent
COD	Chemical oxygen demand (<i>mgCOD/l</i> ; Open flux method)	Unf. & Filt.	Unf.	Unf.	Unf. & Filt.	Unf. & Filt.
TKN	Total Kjeldahl Nitrogen (<i>mgN/l</i> ; micro-Kjeldahl method)	Unf. & Filt.	Occ.	Unf.	Unf. & Filt.	Unf. & Filt.
FSA	Free and saline ammonia (<i>mgN/l</i> ; titrimetric method)	Filt.	Filt.	Filt.	Filt.	Filt.
NO ₃	Nitrates (<i>mgNO₃-N/l</i> ; Hydrazine reduction)	Occ.	-	-	-	-
Flow	Flumes, etc.	dir.	dir.	dir.	dir.	dir.
OP	Orthophosphate (<i>mgP/l</i> ; Vanado-Molybdatevanate color dev.)	Filt.	-	-	Filt.	Filt.
TP	Total phosphorous (<i>mgP/l</i> ; Sulfuric acid/Persulfatedigestion followed by OP test)	Unf & Filt	Occ.	Unf.	Unf. & Filt.	Unf. & Filt.
TSS	Total suspended solids (<i>mg/l</i> ; solids dried at 103-105 °C)	Unf.	Unf.	Unf.	Unf.	Unf.
ISS	Inorganic suspended solids (<i>mgN/l</i> ; solids ignited at 600 °C)	Unf.	Unf.	Unf.	Unf.	Unf.
OUR	Oxygen Utilization Rate (<i>mgO/l</i> ; (Randall <i>et al.</i> , 1991)	-	-	-	-	-
pH	Hydrogen power (using pH meter)	dir.	dir.	dir.	dir.	dir.
VFA	Volatile Fatty Acid content (as <i>mgHAc/l</i> ; 5 point titration (Moosbrugger <i>et al.</i> , 1992)	Filt.	Filt.	Filt.	Filt.	Filt.
H ₂ CO ₃ * Alk.	Hydrogen bicarbonate alkalinity (as <i>mgCaCO₃/l</i> ; 5-point titration)	Filt.	Filt.	Filt.	Filt.	Filt.
Cond.	Conductivity (<i>mS/m</i> ; using conductivity meter)	Filt.	Filt.	Filt.	Filt.	Filt.
Mg	Magnesium	-	-	-	Occ.	Occ.
K	Potassium	-	-	-	Occ.	Occ.
Ca	Calcium	-	-	-	Occ.	Occ.
Biogas	CO ₂ and CH ₄ produced	-	-	-		dir.
Filt. & Un	Filtered through Schleicher & Schull ME 25/21 0.45 micrometer membrane filters and unfiltered sample respectively					
dir. & Occ.	Direct measurement taken and occasional					

3.4.3 DESCRIPTION OF EXPERIMENTAL TEST METHODS USED

Water and wastewater treatment plants are described with the treated sewage and sludge materials, involving different categories of treatment phases or processes. The level of treatment applied could depend on the organic nature of waste or complexity of the treatment plant or both. Such descriptions can be inclined to be the physical and chemical characteristics of the treated wastewater. The decision to run classical laboratory tests (as against instrumental wet chemistry) on these samples to determine wastewater properties is premised on its simplicity, accessibility, its reduced cost of operation and efficiency to identify elemental mass compositions of the wastewater sample. The choice of the parameters to be tested is appropriate as it provides qualitative and quantitative data on the organic strength and nutrients present in the wastewater sample. Hence, the need to analyze the properties of wastewater by conducting laboratory tests to understand and interpret the actual components of wastewaters, irrespective of its source.

In this study, the PS characteristics will be determined by lab-testing the settleometer samples, biomass fetched from the SS AD system and the ABMP experiment (to further determine the actual EMCs of the test samples and also determine their hydrolysis rate). These analysis were performed on the seven samples collected from each settleometer rounds, influent and effluent AD, and control and test batches of the ABMP reactors include the following: Chemical Oxygen Demand (COD) tests; Total Kjeldahl Nitrogen (TKN) test and Free and Saline Ammonia (FSA) test; Total Phosphate (TP) and Ortho-Phosphate (OP) concentration test; Volatile Fatty Acids (VFA), H_2CO_3 alkalinity and pH measurements; Mixed Liquor Total and Volatile Settleable Solids (MLSS, MLVSS); gas composition analysis and flow rate measurement. The tests performed on the samples from the settleometer, ABMP and AD systems are briefly described below.

3.4.3.1 CHEMICAL OXYGEN DEMAND (COD)

The COD is measured using the dichromate and sulfuric acid open flux method, followed by a titration with ferrous ammonium sulfate (FAS) (Standard Methods, 1985). The COD test involves the reflux of a 10 ml sample in strongly acidic solution (5 ml sulfuric acid) with a known excess ($\sim 5 \text{ ml}$ at 0.25 N, where N means normality) of potassium dichromate ($\text{K}_2\text{Cr}_2\text{O}_7$). In principle, the organic matter is oxidized by the boiling dichromate. After boiling, the quantity of potassium di-chromate reduced is determined by titration, which gives the

electron donating capacity of the oxidized organic matter in terms of oxygen equivalent (Sawyer *et al.*, 1994).

3.4.3.2 TOTAL KJELDAHL NITROGEN (TKN) AND FREE AND SALINE AMMONIA (FSA)

The TKN and FSA concentration is measured using a micro-distillation method (Standard Methods, 1985, Semi-micro Kjeldahl method, 420B). The TKN is the combination of organic nitrogen (OrgN) and FSA. In the TKN test, the sample is digested with a sulfuric acid solution containing potassium sulfate (K_2SO_4) while using Mercuric sulfate as a catalyst. The digestion converts all organic nitrogen compounds such as proteins and peptides to ammonia. The sample is then steam distilled using a micro-distillation apparatus with sodium hydroxide and sodium thio-sulfate. On being stripped from sample as a gas, the ammonia generated from the OrgN and any ammonia originally present in the sample is condensed and dissolved in a boric acid solution turning it from purple to green. A sample is then titrated with standard sulfuric acid solution of normality 0.001 until it regains its purple color and the volume of acid titrated is deemed proportional to the TKN concentration. For the FSA concentration only, the sample is not digested but only steam distilled. The difference between the TKN and FSA is the organically bound N (OrgN).

3.4.3.3 TOTAL PHOSPHATES (TP) AND ORTHO-PHOSPHATES (OP)

The TP and OP are measured using the persulfate digestion method (Standard Methods, 1985, Method 424CIII) and the molybdate-vanadate colorimetric method (Standard Methods, 1985, Vanado-molybdo-phosphoric acid colorimetric method). In principle, ortho-phosphates react with molybdate, in the presence of vanadate, to form a yellow phospho-vando-molybdate solution. The intensity of the yellow color is proportional to the concentration of ortho-phosphate present and is measured by absorbance using a spectrophotometer. A Unicam 8625 UV/VIS spectrophotometer, set at a wavelength of $470\text{ }\mu\text{m}$, was used for this color intensity measurement and is valid up to a concentration of 300 mgP/l . Measurement of total phosphates requires conversion of organic and polyphosphates to ortho-phosphate through boiling the sample with sulfuric acid and potassium persulfate.

3.4.3.4 VOLATILE FATTY ACIDS (VFAS), $H_2CO_3^*$ ALKALINITY AND pH

The pH, volatile fatty acid (VFA in mgAc/l) and $H_2CO_3^*$ alkalinity (measured as mgCaCO_3/l) are measured using the 5-point titration method (Moosbrugger *et al.*, 1992). In this test, a sample of digester supernatant is titrated to five predetermined pH points with dilute hydrochloric

acid. The acid added to the 4 predetermined pH points and the in-situ pH are keyed into a computer program (Titra 5) which calculates the required H_2CO_3^* alkalinity (as mgCaCO_3/l) and VFA (as mgHAc/l) concentrations. A Metrohm Dosimat (715) and Metrohm pH meter (744) combo was used in the 5-point titration method.

3.4.3.5 MIXED LIQUOR SETTLEABLE SOLIDS (MLSS)

The MLSS concentration (measured in mg/l) is measured using the Total Settleable Solids (TSS) and Inorganic Settleable Solids (ISS) tests (Standard Methods, 1985). The TSS is obtained by first centrifuging a known volume (usually $2 \times 50 \text{ ml}$) of mixed liquor, decanting all the (usually) clear supernatant, transferring the collected solids to a clean and dry crucible of known mass and drying the solids at 105°C for 24 h. The ISS, performed subsequently, is obtained by incinerating the sample in a furnace at about 600°C for over 20 mins. The difference between the TSS and ISS gives the VSS.

3.4.3.6 GAS PRODUCTION AND COMPOSITION

The biogas volume produced is measured using gas meters connected to the AD system's gas outlet pipe, shown in Figure 3.5. Once the biogas production was known for a given AD steady state period, 5 l impermeable Tedlar gas bags are connected to the gas outlet pipes for the collection of gas samples. Thereafter, these samples are sent to a laboratory at the University of Stellenbosch (Department of Food Sciences) for analysis, using a gas chromatograph to give the percentage composition of methane, carbon dioxide and nitrogen of the total gas sample.

3.5 MODEL DESCRIPTION

A three phase plant-wide model of South Africa (PWM_SA; Brouckaert *et al.*, 2012) has been developed for simulating the biological processes of wastewater treatment, to track and predict the output of materials (COD, carbon (C), hydrogen (H), oxygen (O), nitrogen (N), phosphorus (P), magnesium (Mg), potassium (K) and calcium (Ca)) along the unit processes of a Water Resource Recovery Facility (WRRF). The PWM_SA model combines biological N and P removal activated sludge (AS), anaerobic digestion (AD) of primary sludge (PS) and AD or anoxic-aerobic digestion (AAD) of waste activated sludge (WAS) with interlinking non-reactive thickening physical unit operations. This is done through mapping of the various unit processes on an elemental component base. The PWM_SA model of Ikumi *et al.* (2015) originally comprised three sub-models, integrated for simulation of the entire WRRF under

various configurations (e.g. nitrification-denitrification (ND) excess biological P removal (EBPR) AS, NDEBPR AS system linked to an AD or an AAD for WAS stabilization). These sub-models include:

- I. The ionic speciation model (Brouckaert *et al.*, 2012). This model includes pairing of ionic components (the set of model ionic species is given in Table 3.4) and inter-phase transfers of component species. Table 3.5 gives an example of a set of equilibrium and mass balance equations used in the ionic speciation subroutine.
- II. The ASM2-3P model: This is the Activated Sludge Model No. 2 (ASM2, Henze *et al.*, 1995), modified to include the ionic speciation model (Brouckaert *et al.*, 2012), the Inorganic Settleable Solids (ISS) model of Ekama and Wentzel (2004) and including multiple mineral precipitation according to Musvoto *et al.*, (2000, 2003).
- III. The UCTSDM3P Model: This is the University of Cape Town Anaerobic Digestion Model (UCTADM; Sötemann *et al.*, 2005), modified to include the hydrolysis of multiple organic sludge types (PS, ND WAS, NDEBPR WAS and PS-WAS blends), the Ekama and Wentzel (2004) ISS model, multiple mineral precipitation processes according to Musvoto *et al.*, (2000, 2003) and the Brouckaert *et al.* (2012) aqueous speciation model which facilitates ionic speciation (Ikumi *et al.*, 2015).

To include WRRF strategies that involves primary sedimentation or raw sewage, the PWM_SA model has recently been extended to include the University of Cape Town Primary Sedimentation Unit (UCTPSU) physical process model (Polorigni *et al.*, 2020) that virtually replicates a primary settling tank, which is linkable to the AS system (PST overflow, being the settled wastewater, can be connected to the AS system), and the AD system (the PST underflow, being primary sludge (PS), can be connected downstream to the AD system). Hence UCTPSU (as the fourth sub-model of PWM_SA) is integrated with the 3 initial sub-models of PWM_SA to allow for simulation of primary sedimentation within a plant-wide setting.

For their compatibility, the ASM2-3P, UCTSDM3P and UCTPSU models have the same comprehensive set of model components as performed according to the supermodel approach (Jones and Takacs, 2004; Volcke *et al.*, 2006). The model components are given in Table 3.3 (below) and applied stoichiometric processes are listed in Table 3.6), including parameterized stoichiometry for the bioprocesses, and sharing the same ionic speciation

subroutine model. All the model components and parameters were defined and named according to the standard notational framework proposed by Corominas *et al.* (2010).

The models of interest for this study is based on PWM_SA, therefore, this chapter will begin with the description of the applied mathematical model terminologies, processes that define the reactions occurring in the applied model, and model progressions. The discussion will end by introducing the extensions and modifications made, in this project, to the PWM_SA model. Part of the basis of this study includes (i) extension of the UCTPSU of Poliorigni (2020) by inclusion of certain stoichiometric bioprocesses (see Section 3.8.2) and (ii) presentation of the methodology used for calibration of the UCTPSU model parameters (explained in Sections 5.5.2, 4.4 and 4.5).

3.6 MODEL TERMINOLOGY

3.6.1 MODEL COMPONENTS

The selection of the components for PWM_SA (as listed in Table 3.3) was made to universally represent all unit operations across the Water Resource Recovery Facilities (WRRFs). Each component is parameterised based on its COD and Molar concentrations (molality). Most of the model components are well known and clearly defined elemental compositions (e.g., ammonia is well known as NH_4^+). However, the organics of municipal wastewater are usually broken down to components of biodegradable and unbiodegradable particulate and soluble organics, i.e.: (i) BPO (biodegradable particulate organics, denoted as X_{Binf}), (ii) UPO (unbiodegradable particulate organics, denoted as X_{Uinf}), (iii) FBSO (Fermentable biodegradable soluble organics, denoted as S_{F}), (iv) USO (unbiodegradable soluble organics, denoted as S_{U}). Because of their varying composition, these organic components, together with the various biomass that mediate the biological treatment processes have been allocated parameterized elemental formulations (i.e., the X, Y, Z, A and B of $\text{C}_x\text{H}_y\text{O}_z\text{N}_a\text{P}_b$ are included as model parameters). The composition of organics and biomass was recently extended (Ghoor, 2020) to include S (sulfur) if required (hence the generic elemental formulation for organics is now $\text{CH}_y\text{O}_z\text{N}_a\text{P}_b\text{S}_c$).

The composition of these components is then specified by assigning the correct values to the parameters used to define their elemental composition (these values may be specific to the waste source and could vary from one treatment system to another). Therefore Table 3.3

indicates the composition of these editable components such as $\text{CH}_Y\text{O}_Z\text{N}_A\text{P}_B\text{S}_C$. Based on the notation of Corominas *et al.* (2010), Y, which is the subscript of the H (hydrogen) element is $i_H_X_{\text{Binf_mol_perC}}$ (see Table 3.6 for the list of all parameters including those used to define the elemental composition of organics) which now becomes easy to understand because the name is self-explanatory (Ghoor, 2020).

In Table 3.3, it is shown that the set of components representing micro-organism groups all have the same stoichiometric composition, they are grouped in Figure 4.2 based on the biological reactions they mediate - having the same stoichiometric composition does not render these biomass groups independent from the mass balance (stoichiometry) but they are kinetically independent and so are treated as model components, rather than as species. Figure 3.8 illustrates how model components in their masses are defined with initial values in WEST simulation platform.

3.6.2 SPECIES AND SPECIATION ROUTINE

Lizarralde *et al.*, (2015) defined species as chemical entities taken to be physically present in the system, and components are selected so that all species can be expressed as linear combination of these components. The concentrations of ionic species belonging to various weak acid/base sub-systems that are simultaneously present in solution, and govern pH, are governed by sets of aqueous phase equilibrium dissociation and mass balance equations. Since total concentrations are the appropriate quantities to use in material balance calculations, Brouckaert *et al.* (2012) included 13 total species components to represent the total concentrations of the various weak acid/base systems concerned, e.g. CO_3 represents CO_3^{2-} plus HCO_3^- plus H_2CO_3 plus various other aqueous ion pair (not precipitates) carbonate complexes present in the solution, such as MgCO_3 and CaHCO_3^+ .

The ion pairs that can be formed are listed in Table 3.4. The PWM_SA model has 47 ionic species and complexes participating in the ionic speciation subroutine. The concentrations of the 47 ionic species are related to the total concentrations of the 13 components by a set of 13 stoichiometric balances, together with a set of 30 equilibrium relationships (Ghoor, 2020).

Table 3.3: Model components used in PWM_SA (Ikumi et al., 2015; Ghoor, 2020)			
Component Name		Empirical formula	Notation
Solvent	Water	H ₂ O	H ₂ O
Total Dissolved Ionic Concentrations	Hydrogen ion	H ⁺	S_H
	Sodium	Na ⁺	S_Na
	Potassium	K ⁺	S_K
	Calcium	Ca ²⁺	S_Ca
	Magnesium	Mg ²⁺	S_Mg
	Ammonium	NH ₄ ⁺	S_NHx
	Chloride	Cl ⁻	S_Cl
	Acetate	CH ₃ COO ⁻	S_VFA
	Propionate	CH ₃ CH ₂ COO ⁻	S_Pr
	Carbonate	CO ₃ ²⁻	S_CO3
	Sulphate	SO ₄ ²⁻	SO ₄
	Phosphate	PO ₄ ³⁻	S_PO4
Soluble Organics	Dissolved hydrogen	H ₂	S_H2
	Dissolved oxygen	O ₂	S_O2
	Unbiodegradable Soluble Organics	CH _{YU} O _{ZU} N _{AU} P _{Bu} S _{Cu}	S_U
	Fermentable Biodegradable Soluble Organics	CH _{YF} O _{ZF} N _{AF} P _{Bf} S _{Cf}	S_F
	Glucose	C ₆ H ₁₂ O ₆	S_Glu
Particulates	Unbiodegradable particulate organics	CH _{Yup} O _{Zup} N _{Aup} P _{Bup} S _{Cup}	X_U_inf
	Biodegradable particulate organics	CH _{Ybp} O _{Zbp} N _{Abp} P _{Bbp} S _{Cbp}	X_B_Org
	Primary sludge biodegradable particulate organics	CH _{Ybps} O _{Zbps} N _{Abps} P _{Bbps} S _{Cbps}	X_B_Inf
	Polyphosphate	K _{Kp} Mg _{mp} Ca _{cp} PO ₃	X_PAO_PP
	Poly-hydroxy-alkanoate	C ₄ H ₆ O ₂	X_PAO_Stor
	Struvite	MgNH ₄ PO ₄ ·6H ₂ O	Xtr_NH4
	Calcium Phosphate	Ca ₃ (PO ₄) ₂	X_ACP
	K-struvite	MgKPO ₄ ·6H ₂ O	Xtr_K
	Calcite	CaCO ₃	X_Cal
	Magnesite	MgCO ₃	X_Mag
	Newberyite	MgHPO ₄	X_Newb
	Influent inorganic settleable solids		X_ISS
Microorganism Biomass	Ordinary heterotrophic organisms	CH _{Y0} O _{Z0} N _{A0} P _{B0} S _{C0}	X_OHO
	Phosphate accumulating organisms	CH _{Y0} O _{Z0} N _{A0} P _{B0} S _{C0}	X_PAO
	Autotrophic nitrifying organisms	CH _{Y0} O _{Z0} N _{A0} P _{B0} S _{C0}	X_ANO
	Acidogens	CH _{Y0} O _{Z0} N _{A0} P _{B0} S _{C0}	X_AD
	Acetogens	CH _{Y0} O _{Z0} N _{A0} P _{B0} S _{C0}	X_AC
	Acetoclastic methanogens	CH _{Y0} O _{Z0} N _{A0} P _{B0} S _{C0}	X_AM
	Hydrogenotrophic methanogens	CH _{Y0} O _{Z0} N _{A0} P _{B0} S _{C0}	X_HM
	Endogenous residue	CH _{Ye} O _{Ze} N _{Ae} P _{Be} S _{Ce}	X_U_Org
Gases	Carbon dioxide	CO ₂	G_CO2
	Methane	CH ₄	G_CH4

The equilibrium relationships formulated (in terms of species activities) are related to their concentrations by activity coefficients. Chemical reactions examined (with the defined components) are subject to pH values ranging between 5.0 and 9.0 (Lizarralde *et al.*, 2015). The species that were selected to be components in the bioprocess stoichiometry was based on those species adopted in well-known physicochemical models (PHREEQC and MINTEQA2) for ease of cross-referencing and model checking (Allison *et al.*, 1991). The ionic speciation model forms an important part of the PWM_SA model. The inclusion of this ionic speciation model required coding the ionic speciation routine (containing the aqueous phase equilibrium and mass balance reactions) in a separate C++ file, which is then linked to the WEST® simulation platform library. This separate coding was done to alleviate the numerical handling of these ‘instantaneous’ equilibrium reactions (Lizarralde *et al.*, 2015).

To account for possible occurrence of stiffness (resulting from reaction dynamics), time-step simulation (numerical resolution) is applied (differential algebraic equations or ordinary differential equation). These equations comprise the stoichiometry and kinetics of the slow physical (gas exchange and precipitation) and bioprocesses are solved resulting in the component values at the next time step. The new component values are then speciated into the species concentrations with an algebraic equation speciation routine. The speciation equations are not time-based because the endpoint of these extremely fast aqueous phase equilibrium processes is defined by the thermodynamics of the dissociation processes. This approach keeps separate the very fast aqueous equilibrium processes and slow physical and bioprocesses for fast runtimes and mathematically stable solver calculations. This approach may initially seem confusing because some species are also components (e.g. CO_3^{2-} and PO_4^{3-}) but the context makes clear what the variables are— in the differential equations they are components and in the speciation routine they are species (Ghoor, 2020).

3.6.3 MODEL VARIABLES

Within the simulation platform (in this project the selected platform was WEST®; Vanhooren *et al.*, 2003), model variables are divided into Algebraic, Derived, Input, and Output variable categories (Ghoor, 2020). Derived variables include the initial digester conditions and component masses which need to be specified within a reasonable range of the final simulation values prior to simulation. These initial masses allow the initial component and species concentrations to be calculated which are then fed into the kinetic expressions to

determine the kinetic rates of the bioprocesses at the initial and subsequent time steps (see Figure 3.8 for an example).

Table 3.4: Ionic Components, Species and Complex Ion Pairs

Dissolved Component	Ionic Component	Empirical Formula of Component	Ionic Species and Complexes
S_H	H ⁺		H ⁺ , OH ⁻ , HCO ₃ ⁻ , H ₂ CO ₃ , NH ₃ , HPO ₄ ²⁻ , H ₂ PO ₄ ⁻ , H ₃ PO ₄ , HAc, HPr, CaOH ⁺ , MgOH ⁺ , NaHCO ₃ , NaHPO ₄ ⁻ , CaHCO ₃ ⁺ , CaHPO ₄ , MgHCO ₃ ⁺ , MgHPO ₄ , MgH ₂ PO ₄ ⁺
S_Na	Na ⁺		Na ⁺ , NaHPO ₄ ⁻ , NaCO ₃ ⁻ , NaHCO ₃ , NaAc, NaSO ₄ ⁻
S_K	K ⁺		K ⁺
S_Ca	Ca ²⁺		Ca ²⁺ , CaCO ₃ , CaHCO ₃ ⁺ , CaPO ₄ ⁻ , CaHPO ₄ , CaSO ₄ , CaOH ⁺ , CaAc ⁺ , CaPr ⁺
S_Mg	Mg ²⁺		Mg ²⁺ , MgCO ₃ , MgHCO ₃ ⁺ , MgPO ₄ ⁻ , MgHPO ₄ , MgH ₂ PO ₄ ⁺ , MgSO ₄ , MgOH ⁺ , MgAc ⁺ , MgPr ⁺
S_NH	NH ₄ ⁺		NH ₄ ⁺ , NH ₃ , NH ₄ SO ₄ ⁻
S_Cl	Cl ⁻		Cl ⁻
S_VFA	CH ₃ COO ⁻		Ac ⁻ , HAc, CaAc ⁺ , NaAc, MgAc ⁺
S_Pr	CH ₃ CH ₂ COO ⁻		Pr ⁻ , HPr, CaPr ⁺ , MgPr ⁺
S_CO ₃	CO ₃ ²⁻		CO ₃ ²⁻ , HCO ₃ ⁻ , H ₂ CO ₃ , CaCO ₃ , MgCO ₃ , CaHCO ₃ ⁺ , MgHCO ₃ ⁺ , NaCO ₃ ⁻ , NaHCO ₃
SO ₄	SO ₄ ²⁻		SO ₄ ²⁻ , CaSO ₄ , MgSO ₄ , NH ₄ SO ₄ ⁻ , NaSO ₄ ⁻
S_PO ₄	PO ₄ ³⁻		PO ₄ ³⁻ , HPO ₄ ²⁻ , H ₂ PO ₄ ⁻ , H ₃ PO ₄ , MgPO ₄ ⁻ , CaPO ₄ ⁻ , MgHPO ₄ , CaHPO ₄ , NaHPO ₄ ⁻ , MgH ₂ PO ₄ ⁺

3.6.4 MODEL PARAMETERS

The parameters are the model constants which can be obtained from (i) measurement in an experimental system, (ii) calibration with a model or (iii) from literature. Examples of parameters include the kinetic rate constants, reference temperature, and maximum specific growth rate constants. The parameters may be changed between simulation runs if required through the user-interface, but they are held constant during a simulation.

Block Details : .AD_1				
Parameters Variables Description				
Name	Value	Unit	Initial Value	Default Value
Category: Derived Variables				
Group:				
M(H ₂ O)	7800		5000	7800
M(S_H)	0.306		0.1035	0.306
M(S_Na)	7.8E-06		1.25E-06	7.8E-06
M(S_K)	7.8E-06		4.895	7.8E-06
M(S_Ca)	7.8E-06		1.25E-06	7.8E-06
M(S_Mg)	7.8E-06		0.0397	7.8E-06
M(S_NH)	0.06		0.9948	0.06
M(S_Cl)	7.8E-06		0.49859423	7.8E-06
M(S_VFA)	7.8E-06		0.08	7.8E-06
M(S_Pr)	7.8E-06		1.25E-06	7.8E-06
M(S_CO ₃)	3.215		6.0105	3.215
M(S_SO ₄)	7.8E-06		1.2510032E-06	7.8E-06
M(S_PO ₄)	7.8E-06		0.046	7.8E-06
M(S_HS)	7.8E-06		1.25E-06	7.8E-06
M(S_H ₂)	7.8E-06		1.25E-06	7.8E-06
M(S_U)	7.8E-06		0.2197	7.8E-06

Figure 3.8: Illustration of defined initial values of components and masses in WEST simulation

Parameters can also be coded in as equations which are calculated at the beginning of the simulation. An example of this would be the electron donating capacity of the organisms (X_o – gam_o) which is determined from the biomass composition values. Because its value does not change during a simulation, it is considered a parameter rather than a variable. This is the main difference between parameters and variables. Table 3.6 provides a list of the parameters.

The electron donating capacity (EDC) of the different organism groups is calculated with the same Equation 3.4 but the terms in the equation change to those relevant to the specific component. So, the EDC of the organisms (X_o) is shown in Equation 3.5 where the terms inserted into Equation 3.4 are all related to organisms (Org). When calculating X (EDC) of fermentable soluble organics (S_F), gam_o becomes gam_f and “Org” in the parameters becomes “SF” e.g $i_{H_Org_mol_perC}$ becomes $i_{HF_mol_perC}$.

$$Y = 4k + l - 2m - 3n + 5p + 6s \quad (3.4)$$

Where: Biomass is represented by $C_kH_lO_mN_nP_pS_s$ and

k is assigned a value of 1.

$$gam_o = 4 + i_{H_Org_mol_perC} - 2 \times i_{O_Org_mol_perC} - 3 \times i_{N_Org_mol_perC} + 5 \times i_{P_Org_mol_perC} + 6 \times i_{S_Org_mol_perC} \quad (3.5)$$

Table 3.5: Example for Equilibrium and mass Balance for Ionic Speciation			
Weak Acid Sub-System	*Aqueous Phase Equilibrium Equations	Mass Balance Equation	
Ammonia	$[NH_3] = \frac{K_{NH_4} * [NH_3]}{(H^+)}$ $[NH_4SO_4^-] = \frac{SO_4^{2-} * [NH_4^+]}{(k_{NH_4SO_4})}$	$[N_T] = [NH_4^+] + [NH_3] + [NH_4SO_4^-]$	
*Where (H+) is the hydrogen ion activity, [X] the molar concentrations of species X and KX' is the thermodynamic equilibrium constant for species X, adjusted for Debye Hückel effects to account for the activity of ions in low salinity water (Stumm and Morgan, 1996).			

Table 3.6: List of Parameters of PWM_SA_AD				
Parameters		Descriptions	Values	Units
System Parameters	V_liq	Volume of liquid in the reactor	System specific	m ³
	V_gas	Volume of gas in the reactor		m ³
	Temperature	System temperature		°C
	Tref	Reference Temperature	35	°C
	TempCoeff	Rate Temperature Coefficient	0.0667	-
	MM_C	Molar mass of carbon	12.011	g/mol
	MM_H	Molar mass of hydrogen	1.0079	g/mol
	MM_O	Molar mass of oxygen	15.999	g/mol
	MM_N	Molar mass of nitrogen	14.007	g/mol
	MM_P	Molar mass of phosphorous	30.974	g/mol
	MM_S	Molar mass of sulfur	32.065	g/mol
	MW_[Comp_Index]	Array components providing the molar mass of each	Vector parameters	g/mol
	COD_per_mol_[Comp_Index]	Array components providing the COD of each		gCOD/mol
Stoichiometric Parameters (including elemental composition parameters)	*gam_o	Electron donating capacity (EDC) of organism mass	Calculated Parameters	e-/mol
	*gam_f	EDC of fermentable organics		e-/mol
	*gam_e	EDC of endogenous residue		e-/mol
	*gam_bp	EDC of the biodegradable particulate portion of biomass decay		e-/mol
	*gam_bps	EDC of the biodegradable particulate influent organics		e-/mol
	*gam_us	EDC of the unbiodegradable soluble organics		e-/mol
	*gam_up	EDC of the unbiodegradable particulate organics		e-/mol
	Stoi_H2O_decay	Coefficient of water in the decay process		g/mol
	Stoi_H_decay	Coefficient of H+ in the decay process		g/mol
	Stoi_CO3_decay	Coefficient of CO32- in the decay process		g/mol
	Stoi_NH4_decay	Coefficient of NH4+ in the decay process		g/mol
	Stoi_PO4_decay	Coefficient of PO43- in the decay process		g/mol
	Parameters	Descriptions		Units

Stoi_SO4_decay	Coefficient of SO42- in the decay process		<i>g/mol</i>
Stoi_ER_decay	Coefficient of X_U_Org in the decay process		<i>g/mol</i>
f_XU_Bio_lysis	The unbiodegradable fraction of biomass that accumulates on lysis with death regeneration model	0.08	-
Y_AC	Acetogenesis biomass yield	0.0397	<i>molOrg/molsub</i>
Y_AD	Lo H2 Acidogenesis biomass yield	0.0895	<i>molOrg/molsub</i>
Y_AH	Hi H2 Acidogenesis biomass yield	0.0895	<i>molOrg/molsub</i>
Y_AM	Acetoclastic Methanogenesis biomass yield	0.0393	<i>molOrg/molsub</i>
Y_HM	Hydrogenotrophic Methanogenesis biomass yield	0.04	<i>molOrg/molsub</i>
i_H_Org_mol_perC	H/C : organisms	1.4	<i>dUnit/dUnit</i>
i_HF_mol_perC	H/C : fermentable soluble	2.01	<i>dUnit/dUnit</i>
i_HU_mol_perC	H/C: unbiodegradable soluble	1.646	<i>dUnit/dUnit</i>
i_H_XBInf_mol_perC	H/C: PS biodegradable particulate	2.19	<i>dUnit/dUnit</i>
i_H_XBOrg_mol_perC	H/C: biodegradable particulate	1.463	<i>dUnit/dUnit</i>
i_H_XUInf_mol_perC	H/C: unbiodegradable particulate	1.482	<i>dUnit/dUnit</i>
i_H_XUOrg_mol_perC	H/C: endogenous residue	1.482	<i>dUnit/dUnit</i>
i_K_PP_mol_perP	Molar fraction of K/P in polyphosphate	0.3151	<i>dUnit/dUnit</i>
i_Mg_PP_mol_perP	Molar fraction of Mg/P in polyphosphate	0.3167	<i>dUnit/dUnit</i>
i_N_Org_mol_perC	N/C : organisms	0.2	<i>dUnit/dUnit</i>
i_N_SF_mol_perC	N/C: fermentable soluble	0.119	<i>dUnit/dUnit</i>
i_N_SU_mol_perC	N/C: unbiodegradable soluble	0.062	<i>dUnit/dUnit</i>
i_N_XBInf_mol_perC	N/C: PS biodegradable particulate	0.0643	<i>dUnit/dUnit</i>
i_N_XBOrg_mol_perC	N/C: biodegradable particulate	0.229	<i>dUnit/dUnit</i>
i_N_XUInf_mol_perC	N/C: unbiodegradable particulate	0.113	<i>dUnit/dUnit</i>
i_N_XUOrg_mol_perC	N/C: endogenous residue	0.113	<i>dUnit/dUnit</i>
i_O_Org_mol_perC	O/C : organisms	0.4	<i>dUnit/dUnit</i>
i_O_SF_mol_perC	O/C : fermentable soluble	0.592	<i>dUnit/dUnit</i>
i_O_SU_mol_perC	O/C: unbiodegradable soluble	0.593	<i>dUnit/dUnit</i>
i_O_XBInf_mol_perC	O/C: PS biodegradable particulate	0.653	<i>dUnit/dUnit</i>
i_O_XBOrg_mol_perC	O/C: biodegradable particulate	0.355	<i>dUnit/dUnit</i>
i_O_XUInf_mol_perC	O/C: unbiodegradable particulate	0.472	<i>dUnit/dUnit</i>
i_O_XUOrg_mol_perC	O/C: endogenous residue	0.472	<i>dUnit/dUnit</i>
i_P_Org_mol_perC	P/C : organisms	0	<i>dUnit/dUnit</i>
i_P_SF_mol_perC	P/C: fermentable soluble	0.012	<i>dUnit/dUnit</i>
i_P_SU_mol_perC	P/C: unbiodegradable soluble	0.02	<i>dUnit/dUnit</i>
i_P_XBInf_mol_perC	P/C: PS biodegradable particulate	0.0097	<i>dUnit/dUnit</i>
i_P_XBOrg_mol_perC	P/C: biodegradable particulate	0.031	<i>dUnit/dUnit</i>
i_P_XUInf_mol_perC	P/C: unbiodegradable particulate	0.022	<i>dUnit/dUnit</i>
Parameters	Descriptions	Values	Units

	i_P_XUOrg_mol_perC	P/C: endogenous residue	0.022	dUnit/dUnit
Kinetic Parameters	KS_AC	Half saturation coefficient for acetogens	0.089	g/m3
	KS_AD	Half saturation coefficient for acidogens	0.78	g/m3
	KS_AM	Half saturation coefficient for acetoclastic methanogens	0.013	g/m3
	KS_HM	Half saturation coefficient for hydrogenotrophic methanogens	0.156	g/m3
	KS_BInf_AD_hyd	Half saturation coefficient for X_B_Inf (Primary sludge)	10.124	gCOD/gCOD
	KS_BOrg_AD_hyd	Half saturation coefficient for X_B_Org (organics from biomass death)	10.37	gCOD/gCOD
	K_CO2	Rate constant for CO2 exchange	0.1	1/d
	K_I_H2	Inhibition coefficient for H2 in acidogenesis	1.25	g/m3
	K_I_H_AM	H+ inhibition for acetoclastic methanogens	1.15E-06	mol/kg
	K_I_H_HM	H+ inhibition for hydrogenotrophic methanogens	0.00053	mol/kg
	Kdis_stru	Dissolution of struvite	300	1/d
	Kdis_cap	Dissolution of calcium phosphate	150	1/d
	Kdis_mgkp	Dissolution of K-struvite	100	1/d
	Kdis_cal	Dissolution of calcite	0.5	1/d
	Kdis_mag	Dissolution of magnesite	50	1/d
	Kdis_newb	Dissolution of newberyite	0.05	1/d
	b_AC	Decay rate constant for acetogens	0.015	1/d
	b_AD	Decay rate constant for acidogens	0.041	1/d
	b_AM	Decay rate constant for acetoclastic methanogens	0.037	1/d
	b_HM	Decay rate constant for hydrogenotrophic methanogens	0.01	1/d
	b_OHO_AD	Decay rate constant for OHOs in AD	20	1/d
	b_PAO_AD	Decay rate constant for PAOs in AD	20	1/d
	kH_F_AD_hyd	Hydrolysis rate constant for FBSO	10	1/d
	kH_PHA_AD_hyd	Hydrolysis rate constant for poly-hydroxy-alkanoate (PHA)	5	1/d
	kH_PP_AD_hyd	Hydrolysis rate constant for polyphosphate (PP)	1	1/d
	kM_BInf_AD_hyd	Hydrolysis rate constant for X_B_Inf	2.004	1/d
	kM_BOrg_AD_hyd	Hydrolysis rate constant for X_B_org	1.95	1/d
	kM_fPP_PAO_PHAstor	Maximum rate for PP release with anaerobic PHA storage	0.03	1/d
	mu_AC	Max specific growth rate for acetogens	1.15	1/d
	mu_AD	Max specific growth rate for acidogens	0.8	1/d
	mu_AM	Max specific growth rate for acetoclastic methanogens	4.39	1/d
	mu_HM	Max specific growth rate for hydrogenotrophic methanogens	1.2	1/d
Influent Fractionation parameters in	f_U_Inf	Unbiodegradable particulate fraction of organic feed VSS	0.15	-
	f_U_Org	Unbiodegradable endogenous residue fraction of inoculum seed sludge VSS	0.95	-
	f_Biomass	Live organism fraction of biodegradable portion of dead biomass	0.113	-
	f_AD	Acidogenic fraction of live organisms	0.66505	-
	f_AC	Methanogenic acetogen fraction of live organisms	0.00284	-
	f_AM	Acetoclastic methanogen fraction of live organisms	0.19535	-
	f_HM	Hydrogenotrophic methanogen fraction of live organisms	0.13676	-

The items marked with * in Table 3.6 are calculated with Equation 3.4 below which is the electron donating capacity (EDC, γ_o) the expressions used are given here.

3.7 EXTENSIONS MADE TO UCTSDM3P MODEL

Table 3.7 and Figure 3.9 (below) provide an overview of the processes included in the UCTSDM3P model, further explanations of the model processes can be found in Ikumi (2011) and Ghoor (2020). In Table 3.7 (above), processes 1 to 3 and 9 to 17 are essentially the same as in UCTADM1, except that they have additional terms to account for the P content of organics, biomass, and polyphosphate (PP). Reactions 4 and 5 are added merely because the OHOs and PAOs are additional components of the new model; the lysis (death) reactions have the same stoichiometry for all the organism groups, but their rates may be different (Botha, 2015).

Table 3.7: Stoichiometric Processes of the UCTSDM3P Model	
1	Hydrolysis of fermentable soluble organics (FBSO)
2	Hydrolysis of biodegradable particulate organics (BPO) produced by dead biomass
3	Hydrolysis of (BPO) from primary sludge (PS)
4	Lysis of ordinary heterotrophic organisms (OHOs)
5	Lysis of phosphorus accumulating organisms (PAOs)
6	Release of polyphosphate (PP) with uptake of poly-hydroxyalkanoate (PHA)
7	Release of PP in PAOs
8	Release of PHA in PAOs
9	Low hydrogen partial pressure (pH ₂) Acidogenesis
10	High pH ₂ Acidogenesis
11	Lysis of acidogens
12	Acetogenesis
13	Lysis of acetogens
14	Acetoclastic methanogenesis
15	Lysis of acetoclastic methanogens
16	Hydrogenotrophic methanogenesis
17	Lysis of hydrogenotrophic methanogens

The study by Ghooor (2020) included modifications to the UCTSDM3P model. These included the extension of organic material elemental compositions to include sulfur, hence the current generic organics form in UCTSDM3P (and PWM_SA as a whole) is $C_xH_yO_zN_aP_bS_c$. Further, the model has been extended to cater for biological sulfate reduction reactions expected in augmented bio-sulfate potential tests, in case these are utilized in future to avoid the erroneous gas (methane and carbon dioxide) measurements required in the ABMP test. To ensure confidence in the model utilization, the current UCTSDM3P model underwent rigorous stoichiometric and kinetic checks, mass balance verification method proposed by Hauduc *et al.* (2010) and extensive calibration processes (Ikumi *et al.*, 2015; Ghooor *et al.*, 2020) that include running sensitivity analysis (the standard regression coefficient (SRC) together with the Morris Screening methods) to determine the most influential model parameters. The verification concluded that all processes in the AD model were found to be 100.00% mass balanced on all the elementals (CHONPS) and COD. Figure 3.9 gives a comprehensive relationship of all the processes involved in a three-phase PWM-SA model.

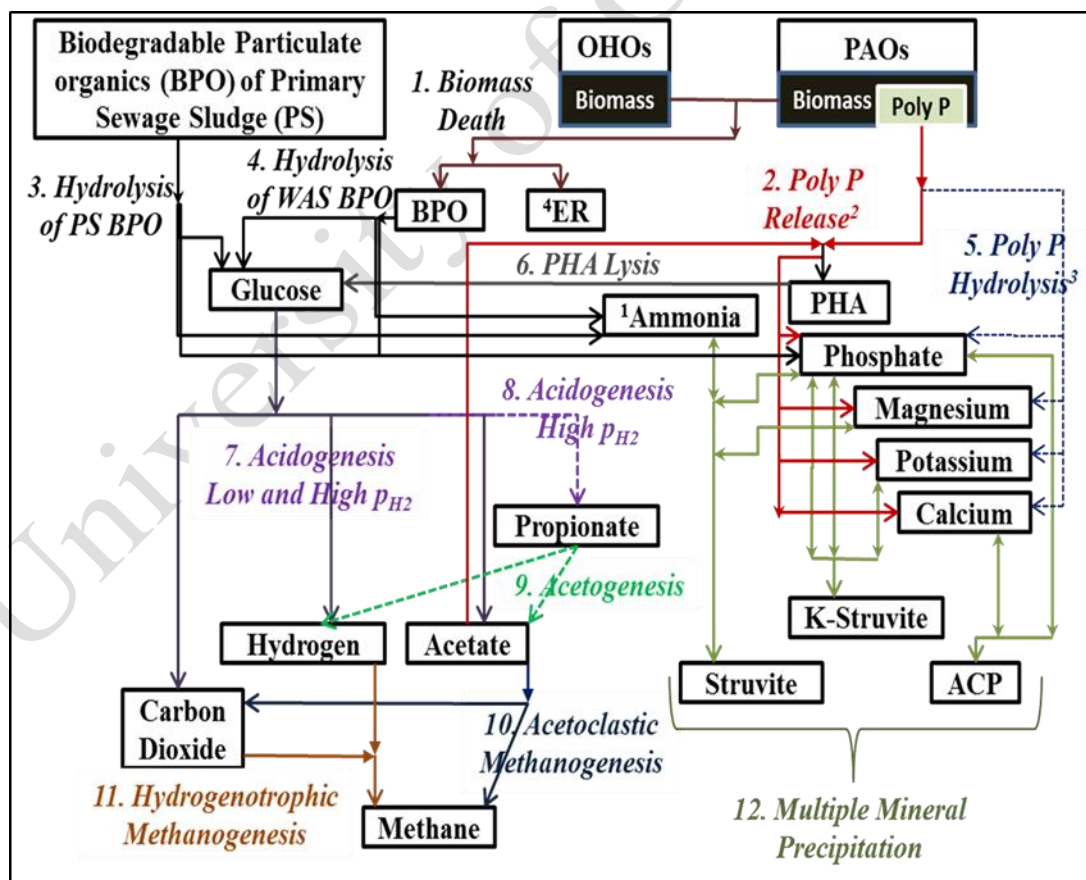


Figure 3.9: Overview of the PWM_SA Three Phase Process Scheme (Ikumi, 2011)

The outcome of the sensitivity analysis highlighted the maximum specific growth rates, retention factor and half-saturation coefficients as the most important parameters to calibrate in the model (Ghoor, 2020). The important parameters determined from the sensitivity analysis were then subjected to a series of steps to calibrate them to model AD dynamics such as impending digester failure and digester start-up. This is required because, while AD has numerous benefits including low energy requirements and low sludge yield, it is notorious for being susceptible to failure and is regarded as unstable and sensitive, and not operated at optimal level. With an improved, calibrated AD model, a better understanding of AD dynamics during failure is possible (Ghoor, 2020).

As hinted in Section 3.5, the process of calibrating the UCTPSU model involves (i) running the raw wastewater through a settleometer to divide the settleable solids of the raw wastewater into the 5 TSS settling velocity groups (where solids in each column are known to settle at a distinct settling velocity), (ii) feeding the solids collected in each of the 5 columns of the settleometer to ABMP test reactors and (iii) analysis of the results from the ABMP reactors to determine (a) hydrolysis kinetic constants, (b) unbiodegradable fraction of solids (hence the TSS can be separated according to UPO, BPO and ISS) and (c) the elemental composition of the BPO, which is obtained by running parameter estimation simulations the ABMP (using UCTSDM3P to virtually replicate the batch AD conditions). Hence the improved UCTSDM3P model was used as a facilitating tool in effecting the UCTPSU calibration.

3.8 DEVELOPMENT OF A PRIMARY SEDIMENTATION UNIT MODEL

3.8.1 DESCRIPTION UCTPSU MODEL

The PST model was developed in two phases (1) discrete PST model and (2) flocculent PST model. Influent settleable solids removals under discrete conditions of a virtual PST were developed in Microsoft Excel. This was performed for steady state conditions and were aimed at mimicking correct proportions of UPO, BPO and ISS (Wentzel *et al.*, 2006; Ikumi *et al.*, 2014) and removals, using raw wastewater (raw WW) and settled WW characteristics from WRC (1984) and Ekama (2017). The particle settling velocity distribution (PSVD) concept of Bachis *et al.* (2015) was adapted to this discrete model. As such, the TSS was divided into five settling velocity groups (Section 3.2.1 shows how the settling velocities were determined) and each TSS settling velocity group was further split into UPO, BPO and ISS settling fractions. It was

found that; the UPO and ISS were removed in greater proportions in the fastest groups and subsequently decreased towards the slowest settling groups Ekama (2017).

On the other hand, the BPO proportions were removed in low proportions in the fastest groups and progressively increased towards the slowest settling groups. The model was verified through strict material mass balances between its inputs and outputs (Polorigni, 2020). Furthermore, the simulations results matched the given data at steady state. These results reflected accurately the percentage removals observed in the experimental studies conducted by Wentzel *et al.* (2006) and Ikumi *et al.* (2014), towards describing the PST reality. Polorigni (2020) also reported that UPO, BPO and ISS settling proportions as well as settling velocities, were used as input parameters into the UCTPSU model (see Tables 3.8 and 5.2). Figure 3.10 shows the 5 sub-components for each of the primary sludge fractionations and each of these sub-components is based on the derived 5 settling velocity groups.

```

32  TYPE UCTPSU_subComponents
33  "The sub components considered in the UCTPSU model"
34  = ENUM {
35      X_ISS1,    //1
36      X_ISS2,    //2
37      X_ISS3,    //3
38      X_ISS4,    //4
39      X_ISS5,    //5
40      X_U_Inf1,  //6
41      X_U_Inf2,  //7
42      X_U_Inf3,  //8
43      X_U_Inf4,  //9
44      X_U_Inf5,  //10
45      X_B_Inf1,  //11
46      X_B_Inf2,  //12
47      X_B_Inf3,  //13
48      X_B_Inf4,  //14
49      X_B_Inf5,  //15
50  };
51
52
53  #endif // PWM_SA
54
55  #endif // WWTP_UCTPSU_modified_definitions
56

```

Figure 3.10: Modified UCTPSU definitions (Polorigni, 2020).

Table 3.8 presents the settling fraction parameters corresponding to each PS fractionation and their respective settling velocity groups and is similar to the list of sub-components showed in Figure 3.10. For example, Alpha_1 is described as X_ISS in settling velocity class 1, and Theta_B refers to X_B_Inf component in settling velocity class 5.

Table 3.8: Set of Settling Fraction Parameters					
Components	Class 1	Class 2	Class 3	Class 4	Class 5
X_ISS	Alpha_I	Beta_I	Gamma_I	Lambda_I	Theta_I
X_U_Inf	Alpha_U	Beta_U	Gamma_U	Lambda_U	Theta_U
X_B_Inf	Alpha_B	Beta_B	Gamma_B	Lambda_B	Theta_B

3.8.2 UCTPSU MODEL MODIFICATIONS

The physical process primary settling tank model of Poliorigni (2020) has been extended in this study to include two stoichiometric bioprocesses (i) hydrolysis of influent biodegradable particulate organics of primary sludge (BPO_PS) to form fermentable soluble organics (FSO) and (ii) the sequential hydrolysis of FSO to volatile fatty acids (VFAs). These two bioprocesses were included to cater for cases whereby the PST units installed at wastewater treatment plants are made to function as fermenters (i.e., when the solid retention times of the PST are lengthened to allow for these bioprocesses take place).

3.8.2.1 HYDROLYSIS

Hydrolysis processes are considered as surface reactions, which occur when the slowly biodegradable substrates are enmeshed with the organisms, which provide hydrolytic enzymes (Dold *et al.*, 1980; Henze *et al.*, 1995). The hydrolysis reaction is modelled such that BPO of PST settled sludge (PS) is enmeshed with some organism mass (with the anaerobic environment, it is assumed that the same biomass that mediates hydrolysis in AD, i.e. acidogenic microorganisms, is present), where it is broken down to fermentable biodegradable soluble organics (FSO; denoted as S_f in PWM_SA). The addition of hydrolysis process to the UCTPSU model is similar to the hydrolysis process in UCTSDM3P. In the UCTSDM3P, a COD balance is maintained between the reactant (BPO_{PS}; denoted as X_{B_Inf} in PWM_SA) and the product (FSO), despite its probability of having a different composition (different X, Y, Z, A, B in $C_{X_f}H_{Y_f}O_{Z_f}N_{A_f}P_{B_f}$) to the BPO ($C_{X_ps}H_{Y_ps}O_{Z_ps}N_{A_ps}P_{B_ps}$). Hence:

Where gam_{ps} and gam_f are electron donating capacities of BPO and FSO, determined from their elemental composition values (see Equations 3.6 and 3.7),

$$BPO_{PS}(mgCOD/l) = FSO(mgCOD/l) \text{ and}$$

$$BPO_{PS}[mol/l] = \frac{gam_{ps}}{gam_f} FSO[mol/l] \quad (3.6)$$

During hydrolysis, the release or uptake of carbonates (CO_3^{2-}), ammonia (NH_4^+), phosphates F (PO_4^{3-}), water (H_2O) and protons (H^+) was similarly included by using the principle of strict mass balance for C, N, P, O and H respectively. This resulted in the following molar stoichiometry Equation 3.7; the stoichiometric coefficients are multiplied with their component molar masses to convert the equation to mass concentration stoichiometry that is fitting with the units used in the PWM_SA model).

$$\begin{aligned}
 & C_{X_{PS}} H_{Y_{PS}} O_{Z_{PS}} N_{A_{PS}} P_{B_{PS}} + \left\{ \left(\frac{gam_{ps}}{gam_f} \right) \cdot (Z_f - 3X_f - 4B_f) - (Z_{ps} - 3X_{ps} - 4B_{ps}) \right\} H_2O \\
 & \rightarrow \left(\frac{gam_{ps}}{gam_f} \right) C_{X_f} H_{Y_f} O_{Z_f} N_{A_f} P_{B_f} + \left\{ A_{ps} - \left(\frac{gam_{ps}}{gam_f} \right) \cdot A_f \right\} NH_4^+ + \left\{ B_{ps} - \left(\frac{gam_{ps}}{gam_f} \right) \cdot \right. \\
 & B_f \left. \right\} PO_4^{3-} + \left\{ X_{ps} - \left(\frac{gam_{ps}}{gam_f} \right) \cdot X_f \right\} CO_3^{2-} + \left\{ 8B_{ps} - 2Z_{ps} + 6X_{ps} + Y_{ps} - 4A_{ps} - (8B_f - \right. \\
 & 2Z_f + 6X_f + Y_f - 4A_f) \cdot \left. \left(\frac{gam_{ps}}{gam_f} \right) \right\} H^+ \quad (3.7)
 \end{aligned}$$

The kinetics rate at which this hydrolysis process occurs is modelled using the saturation kinetics formulation:

$$r_{HYD} = \left(\frac{k_M \cdot \left(\frac{c[X_{B_Inf}]}{Z_{AD}} \right)}{K_S + \left(\frac{c[X_{B_Inf}]}{Z_{AD}} \right)} \right) \cdot Z_{AD} \quad [\text{gCOD}/(\text{l.d})] \quad (3.8)$$

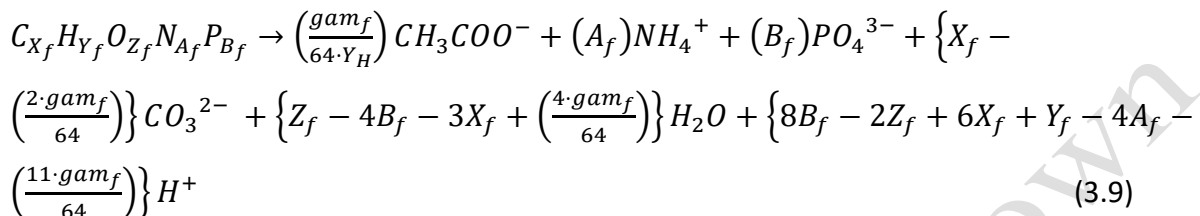
As notable, this kinetic formulation includes acidogenic biomass concentration (Z_{AD}) and incorporates a maximum rate of hydrolysis (k_M) under conditions of high substrate/biomass concentration ratio (X_{B_Inf}/Z_{AD}), hence is based on the quantity of BPO (X_{B_Inf}) attached to the organic biomass active sites, whereby the rate of hydrolysis reaches a maximum at saturation of the active sites of the acidogens.

The K_S parameter is the substrate and acidogenic biomass concentration ratio, at which the specific hydrolysis rate is half its upper limit (k_M) at saturation. In order to use the above process formulations, the kinetic constants (k_M and K_S) have to be determined experimentally (see Chapter 5).

3.8.2.2 FERMENTATION

The process of fermentation is modelled to involve the conversion of fermentable biodegradable soluble organics (FSO) to acetate (S_{VFA} ; taken to represent the volatile fatty acids) accompanied with the release of excess nutrients (in the form of NH_4^+ and PO_4^{3-}).

Similar to the hydrolysis process, a COD mass balance is observed such that the COD of FSO used is equitable to the COD of acetate generated. Thereafter, the CO_3^{2-} , NH_4^+ , PO_4^{3-} , H_2O and H^+ produced are determined using C, N, P, O and H mass balances respectively over the stoichiometric reaction. The molar stoichiometric process is as shown by the Equation 3.9 below:



The FSO, as a soluble component is assumed to be the same concentration throughout the PST reactor and the fermentation kinetics are modelled using the first order kinetic formulation. This is a simple kinetic formulation that assumes the process kinetic rate (i.e. fermentation) is directly proportional to the concentration of available substrate, i.e.:

$$\text{state.Kinetics}[FSO_{Hyd}] = Kh_{fs} * C[S_F] \quad (3.10)$$

Where kh_{fs} is the first order kinetic rate constant for fermentation (1/d) and $C[S_F]$ is the mass concentration (mg/l) of FSO.

3.9 MASS BALANCE VERIFICATION AND MODEL CALIBRATION

Mass balance is achieved when the sum of stoichiometry products equals zero and this was observed for COD and CHONP mass balance. All processes which were part of PWM_SA (Ikumi *et al.*, 2015) and its extensions (including UCTPSU and the modifications made to UCTSDM3P) were found to be 100.00% mass balanced on all the elements (CHONPS), COD and charge (i.e. in Ekama and Ikumi (2019), for verification of PWM_SA; Ghoor (2020), for verification of extended UCTSDM3P, and Polorigni (2020), for verification of UCTPSU). Appendix I shows the mass balance results for the new extensions (UCTPSU model).

Part of the basis of this study is to present the model calibration process for UCTSPU, which included two main stages by performing a sensitivity analysis through (a) conducting an uncertainty propagation by a Monte Carlo (MC) simulation of the model by random sampling of parameter values and (b) determining the standard regression coefficients (SRC) due to

each parameter by fitting a multivariate linear model to the output of the MC simulation (Martin *et al.*, 2010; Neumann, 2012) (see Sections 5.5.1 and 5.5.2).

Following the sensitivity analysis, the experimental data from the settleometer and augmented batch tests are used to determine significant parameters (see Table 5.10 for the UCTPSU model parameters), including the unbiodegradable fraction of the sludge (f'_{sup}), the BPO hydrolysis kinetics and the BPO elemental composition, of the UCTPSU model (see Chapters 4 - 6).

3.10 EXPERIMENTAL SYSTEMS RECONCILIATION

The process of generating data that could be used towards calibrating the UCTPSU model required linking the settleometer and steady-state AD experiments to the ABMP experiment (see Figure 3.1). The AD system effluent is used to supply the cultured seed inoculum to be used in the control ABMP reactor (as explained in Section 3.3.2). In the settleometer, the settled PS in each of the PVC columns are fed (as substrates) into their respective ABMP test reactors (the test reactors contain both the seed inoculum and substrate in equal proportion). The utilized substrates were separately collected from the influent channel to the settleometer (i.e. raw wastewater collected from the PDWWTW inlet works), each of the settleometer tubes (where the substrates are respectively influenced by the settling velocity groups in each tube, and effluent channel from the settleometer (i.e. the wastewater flowing out of the settleometer). These substrates and the seed inoculum (in equal proportion) were used to determine TSS fractionations, elemental mass compositions (EMCs), hydrolysis rate constants, and fractions of the unbiodegradable particulate organics (f'_{sup}).

The determined ABMP effluent data is analyzed and used as input to a parameter estimation exercise (the University of Cape Town sludge Digestion Model 3 (UCTSDM3) is tailored to virtually replicate the ABMP test, fed the ABMP effluent and simulated backwards to determine the ABMP influent characteristics; see chapter 4 for further descriptions of this procedure). From these integrated experimental systems, the data that comprehensively characterizes the PS (i.e., the estimated component settling velocities, biodegradability, BPO hydrolysis rate constants and, BPO elemental composition) are used to calibrate the University of Cape Town Primary Sedimentation Unit (UCTPSU) model.

The modelling software WEST® (Vanhooren *et al.*, 2003) was employed as the simulation platform in this project to simulate UCTPSU model. In addition to WEST® simulation platform, Microsoft Excel and R-Studio software were used as data-processing and data-analyzing platforms (see Chapters 4 - 5).

3.11 CONCLUSION

This chapter has described the sequence of experiments required to calibrate the modified UCTPSU model using the pilot-scale systems of settleometer, AD_SS and ABMP. This chapter has established the procedures followed for each system and briefed on the most important laboratory measurements required for the next chapters involving model description and modifications. The Chapter also described the PWM_SA model, which integrates sub-models for AS and AAD (ASM23P), AD (UCTSDM3P) and the developed physical processes PST model (UCTSPU) as a third sub-model for PWM_SA. The basis of this study was identified to include (i) modification of the UCTPSU model by inclusion of biochemical processes that would allow it to function as a fermenter (i.e., when the solids retention time in the PST is lengthened) and (ii) the presentation of a calibration procedure for the UCTPSU model. This calibration process includes performing a sensitivity analysis and analyzing experimental data generated by measurements from the settleometer that are linked to augmented batch test (see Sections 5.5.1, 4.2 and 4.3). The reason for presenting this calibration procedure is that these 'measured' parameters are deemed to require direct experimental determination, specific to a given system, to ensure their accuracy and enable correct prediction of the PST performance at a plant-wide context. The next chapter will therefore detail the global sensitivity analysis (GSA) as part of the calibration procedure and provide the results obtained from running the experimental set up and the findings from the analysis of these results towards determination of the required UCTPSU parameter values.

CHAPTER 4.0: EXPERIMENTAL RESULTS

4.1 INTRODUCTION

This chapter briefly discusses the results derived from experimental set up described in Chapter 3 (i.e. comprising the settleometer, laboratory scale anaerobic digestion reactor operated at a steady-state (AD_SS), and augmented bio-methane potential (ABMP) test reactors). Interpretations of the results will be directed towards calibration of the University of Cape Town Primary Sedimentation Unit model, UCTPSU). The settleometer with its increasing inner diameter (from smallest to largest pipe) distributes the raw wastewater settleable particulates across the polyvinyl chloride (PVC) columns with respect to their characteristic settling velocity group. The particulates collected at the bottom of each settleometer column (i.e., for each categorized settling velocity group) are transferred to ABMP reactors to generate data that allows for calculation of the unbiodegradable fraction of organics, the elemental composition of the biodegradable particulate organics (BPO) and the hydrolysis kinetic constants of BPO. Equations 4.8 and 4.9 below show how the settling velocities of the settleable particulates are determined according to the diameters of the settleometer columns in which they are collected. The Sections below describe the methods used for determination of the parameters used for defining elemental compositions of BPO (i.e., x , y , z , a and b of $C_xH_yO_zN_aP_b$; see Section 4.2.3 and the BPO-hydrolysis kinetic constants (k_M and K_S ; Section 4.2.5 shows how these kinetic constants are determined from ABMP test results).

4.2 SETTLEOMETER RESULT

The sludge settleability device (settleometer, see Section 3.2) is operated to run on the principles stipulated by Moosbrugger *et al.* (1994). The device was operated at the Inlets unit of Potsdam Wastewater Treatment Works (PDWWTW) to determine the settling rates of the influent wastewater that settled in each of the 5 polyvinyl chloride (PVC) columns (with increasing inner diameter) of the settleometer device. The settleometer effluent (overflow) volume was calculated by multiplying the constant settleometer effluent flow rate by the length of time taken in the experiment to catch the settleometer effluent (See Equation 4.1 below). Following the procedures given in Section 3.2, Table 4.1 depicts the flow rate, internal

column diameters and volumes, up-flow velocity profile and mass balances for test run 3. Appendix A for provides the full result report (Runs 1 – 4). For the purpose accuracy, only the 3rd and 4th settleometer runs will be discussed.

$$Vol_{effluent} = Q_{effluent} * \Delta t_{effluent} \quad (4.1)$$

Where: $Vol_{effluent}$ is the effluent volume (l)

$Q_{effluent}$ (l/min) is the effluent flowrate measured with the help of a calibrated measuring cylinder and stopwatch, and

$\Delta t_{effluent}$ represents the difference between the completion time of settleometer run and time effluent flow was caught by the collecting drum.

The total volume of the settleometer PVC columns was determined by adding the individual volumes of the PVC columns (See Equation 6.2).

$$Vol_{settleometer} = Vol_{PVC1} + Vol_{PVC2} + Vol_{PVC3} + Vol_{PVC4} + Vol_{PVC5} \text{ (l)} \quad (4.2)$$

Where $Vol_{settleometer}$ is the aggregate inner volumes of the settleometer columns and,

$Vol_{PVC1 \text{ to } 5}$ is the measured inner volume of PVC columns 1 to 5

Since mass and volume is conserved in the system, the total influent volume of wastewater pumped through the settleometer for 120 mins is assumed to be the addition of its effluent volume and total volume of the remaining sewage contents in the settleometer (i.e. the volume of settleable sewage sludge that remains in the settleometer columns) and was not dispatched as part of the settleometer effluent (See Equation 4.3).

$$Vol_{influent} = Vol_{settleometer} + Vol_{effluent} \quad (4.3)$$

The influent raw wastewater (M_{RWW_i}) and settled wastewater (i.e. settleometer effluent or overflow mass, M_{SWW_i}) used in the settleometer experiment were determined by multiplying the influent raw wastewater and settled wastewater concentrations by their corresponding volumes determined in Equations 4.1 and 4.3 above.

$$M_{RWW_i} = i * Vol_{influent} \text{ (mg)} \quad (4.4)$$

$$M_{SWW_i} = i * Vol_{effluent} \text{ (mg)} \quad (4.5)$$

Where 'i' represents the measured concentrations (mg/l) i.e. can represent COD, TKN, FSA, TP, OP, TSS, VSS and ISS concentrations.

Table 4. 1: Summary of Settleometer Readings

Test Analysis	Units	Test Run 3								
		1	2	3	4	5	M_TSi	M_RWWi	M_SWWi	MBi
Flow	<i>l/min</i>	-	-	-	-	-	-	0.85	0.85	100
Time	<i>min</i>	-	-	-	-	-	-	120	64	-
Volume	<i>l</i>	1.8	4.3	6.2	9.5	14.5	36.3	90.4	54.1	100
COD (unf)	<i>mg/l</i>	3440	4600	5600	4520	1920	131472	193454.3	43279.4	90.3
COD (filt)	<i>mg/l</i>	840	840	840	840	840	30492	75935.3	43820.4	97.9
TKN	<i>mg/l</i>	147	178	193	183	114	5617	11352.3	5551.7	98.4
TKN (filt)	<i>mg/l</i>	94	94	94	94	94	3400	8466.8	5169.2	101.2
FSA	<i>mg/l</i>	79	79	79	79	79	2870	7146.1	4073.7	97.2
TP	<i>mg/l</i>	18	25	30	26	15	785	2236.2	1338.2	95.0
TP (filt)	<i>mg/l</i>	11	11	11	11	11	394	980.1	555.2	96.8
OP	<i>mg/l</i>	9	9	9	9	9	325	809.1	454.4	96.3
TSS	<i>mg/l</i>	934	4414	2328	1794	382	57677	85879.2	15472.4	85.2
TSS	<i>mg</i>	1681	18980	14434	17043	5539	-	-	-	-
% TSS	%	2	22	17	20	6	67	1.0	18.01	85.2
VSS	<i>mg/l</i>	800	1814	2090	1614	282	41620.2	59121.08	11901.8	90.5
VSS	<i>mg</i>	1440	7800	12958	15333	4089	-	-	-	-
% VSS	%	2	13	22	26	7	70.4	1.0	20.1	90.5
VSS/TSS	<i>no unit</i>	0.857	0.411	0.898	0.900	0.738	0.722	-	-	-
ISS	<i>mg/l</i>	134	2600	238	180	100	16057	26758.2	3570.6	73.4
ISS	<i>mg</i>	241.2	11180	1476	1710	1450	-	-	-	-
ID	<i>mm</i>	45.2	67.6	86.4	105.6	134.4	-	-	-	-
V _s	<i>m²</i>	0.002	0.004	0.006	0.009	0.014	-	-	-	-
	<i>m³/min</i>	0.001	0.001	0.001	0.001	0.001	-	-	-	-
	<i>m³/hr</i>	0.051	0.051	0.051	0.051	0.051	-	-	-	-
	<i>m/hr</i>	31.61	14.13	8.65	5.79	3.57	-	-	-	-
M_TSi	Mass of total settleable solids (in <i>mg</i>) in the measured ' <i>l</i> ' concentration									
M_RWWi	Mass of influent raw wastewater (in <i>mg</i>) in the measured ' <i>l</i> ' concentration									
M_SWWi	Mass of settled (overflow) wastewater (in <i>mg</i>) in the measured ' <i>l</i> ' concentration									
MBi	Mass balance across the device for the measured ' <i>l</i> ' concentration									
ID	Internal column diameter (<i>mm</i>)									
V _s	Settling velocities									

The sum total mass of the calculated 'i' concentrations in each PVC column (M_{TS_i}) can be determined by adding the multiplications of each PVC volume by its measured 'i' concentration (as shown in Equation 4.6).

$$M_{TS_i} = (i_1 * Vol_{PVC1}) + (i_2 * Vol_{PVC2}) + (i_3 * Vol_{PVC3}) + (i_4 * Vol_{PVC4}) + (i_5 * Vol_{PVC5}) \quad (4.6)$$

To verify the performance of the settleometer device, mass balance must be achieved across the device (this means flow and mass must be conserved in the system, from the influent through to the effluent). Mass balance (MB_i) of each concentration was determined as shown in Equation 4.7 below.

$$MB_i = \frac{M_{TS_i} + M_{SWW_i}}{M_{RWW_i}} * 100\% \quad (4.7)$$

Where MB_i is the mass balance 'i' across settleometer.

To calculate settling velocities (V_{Sn}) in PVC columns, the inner diameter of each column was used to determine their respective surface areas (A_{SPVCn}) as shown in Equation 4.8 and the measured flow rate was divided by respective PVC surface area (see Equation 4.9).

$$A_{SPVCn} = 0.25 * PI * ID_{PVCn}^2 \quad (4.8)$$

$$V_{Sn} = \frac{Q_{effluent}}{A_{SPVCn}} \quad (4.9)$$

Where: n represents the particular PVC column number (i.e. n = 1, 2, 3, 4, 5)

From Table 4.1 (above), the following observations were recorded:

1. The flow is conserved. Unlike the regular settleometer test where a pre-determined influent volume was given, the influent volume could not be directly determined. It was calculated by adding the overflow (caught settled wastewater into a receiving container till the run was completed) volume and the 5 PVC volumes. This means that mass (volume) flow-in must equal mass (volume) flow-out and was determined by using the aggregate effluent flows measured at specific interval of time until the run was completed. This also means that the flow is assumed to be independent of frictional forces and gravitational forces (which if accounted for will give different influent and effluent flow rates) with respect to the primary sewage sludge (PSS) and PVC column.
2. Density of the influent wastewater was fractionated across the settleometer system (starting from the smallest inner diameter to the largest) and results from the varying

settling velocity that was determined and observed to reduce across the settleometer system ((from 31.81 m/h to 3.57 m/h).

3. For each test analysis (described in sections 3.4.3.1 – 3.4.3.6), M_{TS_i} was calculated by summing the multiplications of each laboratory analysis by their corresponding column volumes, M_{RWW} was calculated by multiplying the corresponding influent laboratory analysis by the influent volume, and M_{SWW} was also calculated by multiplying the corresponding effluent laboratory analysis by the effluent volume.
4. The laboratory analysis on the filtered samples (including filtered COD, FSA, and OP) in each of the columns is assumed to be uniform (i.e. expected to be the same on the settleometer influent, underflow and overflow) due to the solubility inherent characteristic.
5. The percentage sludge mass (% TSS) retained in each column was determined by respectively dividing each of the retained sludge masses by influent sludge mass. The TSS mass retained in each column appeared to reduce from second column to the last (largest) column but was not consistent as the 3rd column retained TSS lower than the 4th column. However, for VSS and ISS masses, it was observed to record consistent increment from column 1 to 5 and dropped in column 5.

To check the reliability and accuracy of the settleometer system, materials mass balance needed to be done. Mass balance is applied under a steady state condition to ensure that the flux of the materials entering the settleometer system equals the flux of material exiting the settleometer system. Ikumi (2011) reported that material mass balances within the range of 90% - 100% are indicative of accurate and reliable experimental measurements (i.e. such mass balances accommodate a margin of ± 0.1 error) and also stated that mass balances ranging from 80% - 120% (i.e. margin of ± 0.2 error) can be acceptable if the reasons are determined. The determined COD, TKN, TP and VSS mass balance (as shown in Table 4.1) are consistent and within the acceptable range (90 % – 110 %) except for the TSS and ISS masses which are 85.2% and 73.4%. The TSS and ISS mass balances are considered to have been influenced by the operation and testing tool errors (say, the laboratory centrifuge if the centrifuged sample is not all collected). It can be observed that mass of sludge removed from the system increased with decreasing settling velocity, causing increment in tube sludge bed which infers that sludge age will be increased. Hence, there will be record of reduced biodegradables, and

reduced available biomass to mediate hydrolysis and bio-kinetic processes (for reducing up-flow velocity). These plots can be described to show the settling profile of the sludge at different hydraulic settling velocities. Test run 4 (see Table 4.2 below) can also be evaluated for consistency if similar trend is observed.

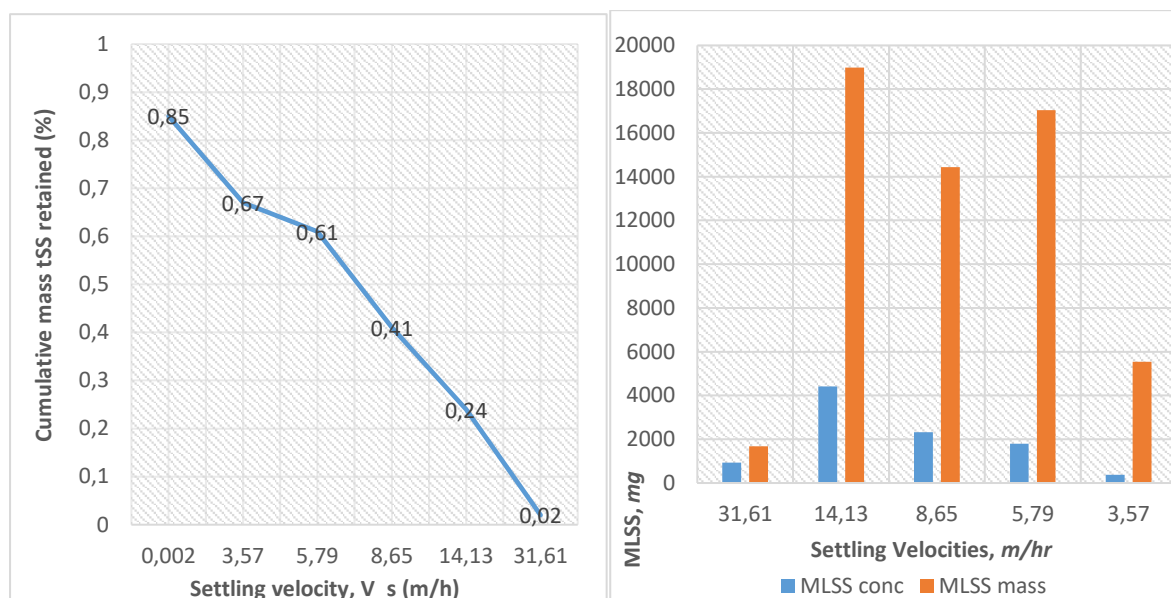


Figure 4.1 (a & b, above): Cumulative TSS Mass Retained and sludge profile in Test Run 3

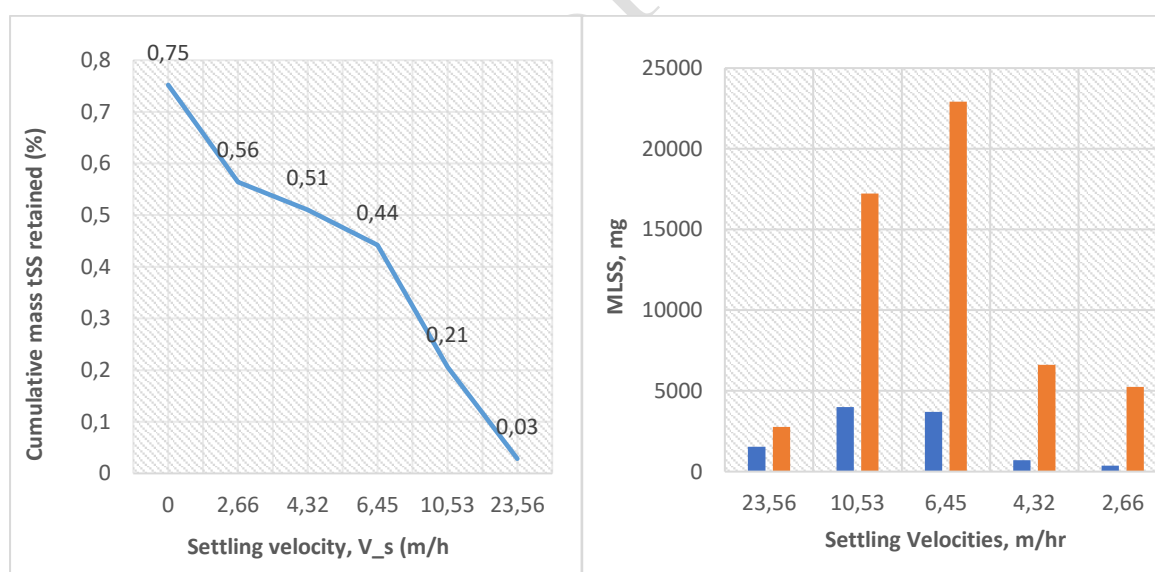


Figure 4.2 (a & b): Cumulative TSS Mass Retained and sludge profile in Test Run 4

Similar result discussion can be done for test run 4 but at this point, observing the data trend for internal consistency was important and the following can be said of the 4th settleometer test run (as shown in Table 4.2, below):

Table 4. 2: Summary of Settleometer Readings for test Run 4

Test Analysis	Units	Test Run 4								
		1	2	3	4	5	M_TSi	M_RWWi	M_SWWi	MBi
Flow	l/min	-	-	-	-	-	-	0.8453	0.8453	100
Time	min	-	-	-	-	-	-	120	64	-
Volume	l	1.8	4.3	6.2	9.5	14.5	36.3	90.4	54.1	100.0
COD (unf)	mg/l	2880	6880	4400	2440	1640	109008.0	139735.2	54243.0	116.9
COD (filt)	mg/l	473	473	473	473	473	17169.9	38029.0	19404.0	96.0
TKN	mg/l	81	272	0	112	95	3766.0	8460.0	4223.0	94.0
TKN (filt)	mg/l	51	51	51	51	51	1834.6	4063.4	2160.9	98.3
FSA	mg/l	69	69	69	69	69	2488.7	5512.2	2820.2	96.3
TP	mg/l	21	34	33	15	13	718.0	1333.3	584.0	97.7
TP (filt)	mg/l	10	10	10	10	10	365.9	810.5	417.2	96.6
OP	mg/l	8.5	8.5	8.5	8.5	8.5	306.7	679.4	399.1	103.9
TSS	mg/l	1536	4006	3698	696	362	54779.2	97123.2	18257.4	75.2
TSS	mg	2765	17226	22928	6612	5249	-	-	-	-
% TSS	%	5	31	42	12	10	-	1.0	18.0	85.2
VSS	mg/l	1238	3492	3212	522	272	46061.4	77184.0	12612.6	76.0
VSS	mg	2228	15016	19914	4959	3944	-	-	-	-
% VSS	%	4.84	32.60	43.23	10.77	8.56	70.4	1	20.1	90.53
VSS/TSS	no unit	0.81	0.87	0.87	0.75	0.75	0.8	-	-	-
ISS	mg/l	298	514	486	174	90	8717.8	19939.2	5644.8	72.1
ISS	mg	536.4	2210.2	3013.2	1653	1305	-	-	-	-
ID	mm	45.2	67.6	86.4	105.6	134.4	-	-	-	-
V _s	m ²	0.0016	0.0035	0.0058	0.0088	0.0142	-	-	-	-
	m ³ /min	0.0008	0.0008	0.0008	0.0008	0.0008	-	-	-	-
	m ³ /hr	0.0507	0.0507	0.0507	0.0507	0.0507	-	-	-	-
	m/hr	23.56	10.53	6.45	4.32	2.66	-	-	-	-
M_TSi	Mass of total settleable solids (in mg) in the measured 'I' concentration									
M_RWWi	Mass of influent raw wastewater (in mg) in the measured 'I' concentration									
M_SWWi	Mass of settled (overflow) wastewater (in mg) in the measured 'I' concentration									
MBi	Mass balance across the device for the measured 'I' concentration									
ID	Internal column diameter (mm)									
V _s	Settling velocities									

1. The settling velocity profile reduced across the settleometer system from the smallest pipe (23.56 m/h) to the largest pipe (2.66 m/h). This means PSS was still fractionated according to particle size and density.
2. The measured filtered COD, FSA and OP were observed to drop relative to the settleometer test run 3. The reason given for the drop in soluble concentration is because of the reduction in organic load at the time of the day when the settleometer test was run (3:30 pm).
3. The two runs (3 and 4) show similar trend except that for test run 4, there was no outlier in the reducing TSS concentration from PVC columns 2 to 5. A similar trend was recorded for its VSS and ISS except for the PVC column 3 of VSS that spiked up rather than reduced. The observed spike might have been because of the sudden discharge (as against gentle discharge) of the samples from each column with causing an efflux of neighboring settled columns.
4. Like test run 3, mass balance was also attained for COD, TKN, TP, TSS and VSS. However (for both runs), the ISS was not well accounted for in its mass balance. This calls for more experimental research work to understand the dynamics of ISS concentration in primary settling tank (and WRRF, in total).

4.3 AUGMENTED BIOMETHANE POTENTIAL TESTS

4.3.1 THE STEADY-STATE AD SYSTEM RESULTS

As a source of the required seed inoculum for the proposed ABMP test, an AD system was operated at steady state (see Section 3.4.1). Table 4.3 (below) provides the average measured data for the AD system - this data was necessary to determine the characteristics of the seed inoculum used for the ABMP test as shown in Section 4.4.

Table 4. 3: Experimental Run of Anaerobic Digestion at a Steady-State Condition		
Test Analysis	Units	Average Values
Mixed Liquor Settleable Solids (MLSS)	mgMLSS/l	16782
Mixed Liquor Volatile Settleable Solids (MLVSS)	mgMLVSS/l	12614
Mixed Liquor Inorganic Settleable Solids MLISS	mgMLISS/l	4168
Influent COD (St_i)	mgCOD/l	52600
Effluent COD (St_e)	mgCOD/l	28525

Table 4.3 is a summary of experimental data measured by Mazivila *et al.* (2020) on an operating 20 l completely mixed mesophilic (35 °C) anaerobic digesters for 68 d fed with primary sludge from PDWWTW.

4.3.2 AUGMENTED BIO-METHANE POTENTIAL (ABMP) TEST RESULTS

The ABMP reactors was run for sludge age of 52 days (the point where little or no obvious biodegradation of the samples except the inoculum was observed). After the 52 days there was no further biogas production and the only organics left in the test batches are unbiodegradable particulate organics (UPO). Results obtained from the ABMP tests performed on the control (inoculum) sample and test samples (containing both the inoculum seed and substrates from the 5-PVC column settleometer) are shown in Tables 4.4 and 4.5 (below).

From Table 4.4 (below), the categories of labels used to describe different sample represents the samples in each settleometer columns (say, 1 to 5, interpreted as column 1 to 5). For each column, a duplicate sample was also tested, which resulted into naming each column with alpha-numeric symbols such as T1a and T1b.

Table 4.4: Summary of Results from ABMP									
ABMP Reactor set up		Period, t	Variables						
			COD	FSA	OP	VSS	ISS	H2CO3Alk	pH
Measured Control ABMP values	C1	t = 0	13440	322	6	6798	1668	1958	7.97
		t = end	10360	547	6	5202	1186	2516	7.21
	C2	t = 0	13440	322	6	6798	1668	1958	7.89
		t = end	7736	547	4	4632	230	1911	7.51
	CAv	t = 0	13440	322	6	6798	1668	1958	7.93
		t = end	11900	435	6	6000	1427	2237	7.57
Column1 Measured Test ABMP Values	T1a	t = 0	16900	322	8	8966	1872	2094	7.89
		t = end	11056	547	5	5716	1366	2953	7.28
	T1b	t = 0	16900	322	8	8966	1872	2094	7.89
		t = end	9288	563	4	4538	1450	2468	7.51
	T1Ave	t = 0	16900	322	8	8966	1872	2094	7.89
		t = end	10172	547	5	5127	1408	2711	7.4
Column2 Measured Test ABMP Values	T2a	t = 0	16940	351	10	8984	1128	2156	7.79
		t = end	11220	520	6	6540	1112	2704	7.2
	T2b	t = 0	16940	351	10	8584	1128	2156	7.79
		t = end	8056	567.7	2.71	3268	1054	2546	7.58
	T2Ave	t = 0	16940	351	10	8784	1128	2156	7.79
		t = end	9638	544	4	4904	1083	2625	7.39
Column3 Measured Test ABMP Values	T3a	t = 0	16820	346	10	8124	2116	2027	7.68
		t = end	10780	531	5	5552	1316	2598	7.25
	T3b	t = 0	16820	346	10	8124	2116	2027	7.68
		t = end	9060	610	2.13	3756	1348	2692	7.57
	T3Ave	t = 0	16820	346	10	8124	2116	2027	7.68
		t = end	9920	571	4	4654	1332	2645	7.41
Column4 Measured Test ABMP Values	T4a	t = 0	16140	347	11	8268	2172	2008	7.73
		t = end	11044	526	6	6438	1972	2744	7.28
	T4b	t = 0	16140	347	11	8268	2172	2008	7.73
		t = end	9588	614.8	2.68	5038	1640	2853	7.6
	T4Ave	t = 0	16140	347	11	8268	2172	2008	7.73
		t = end	10316	570	4	5738	1806	2799	7.44
Column n5	T5a	t = 0	19000	10	11	8522	2238	2061	7.62
		t = end	10640	0	7	6154	1642	2603	7.2

	ABMP Reactor set up	Period, t	Variables						
			COD	FSA	OP	VSS	ISS	H2CO3Alk	pH
	T5b	t = 0	19000	317	11	8522	2238	2061	7.62
		t = end	9040	592	3	4482	1256	2436	7.67
	T5Ave	t = 0	19000	164	11	8522	2238	2061	7.62
		t = end	9840	592	5	5318	1449	2520	7.44
	C1	t = 0	6720	161	3	3399	834	979	7.97
		t = end	5180	273.5	3	2601	593	1258	7.21
	C2	t = 0	6720	161	3	3399	834	979	7.89
		t = end	3868	273.5	2	2316	115	955.5	7.51
CAv	t = 0	6720	161	3	3399	834	979	7.93	
	t = end	5950	217.25	3	3000	713.5	1118.5	7.36	
Calculated Substrate concentrations in ABMP Test Samples	T1a - C1	t = 0	10180	161	5	5567	1038	1115	
		t = end	5876	289.5	2	3115	773	1695	
	T1b - C2	t = 0	10180	161	5	5567	1038	1115	
		t = end	5420	273.5	2	2222	1335	1512	
	T1Ave - CA	t = 0	10180	190	5	5567	1038	1115	
		t = end	4222	302.75	1.5	2127	694.5	1592	
	T2a - C1	t = 0	10220	189.7	7	5585	294	1177	
		t = end	6040	294.2	3	3939	519	1446	
	T2b - C2	t = 0	10220	189.85	6.85	5185	294	1177	
		t = end	4188	270.35	0.71	952	939	1590.5	
	T2Ave - CA	t = 0	10220	185	6.925	5385	294	1177	
		t = end	3688	313.75	1.355	1904	369.5	1506	

ABMP Reactor set up	Period, t	COD	FSA	OP	VSS	ISS	H2CO3Alk
T3a - C1	t = 0	10100	185.3	7	4725	1282	1048
	t = end	5600	336.5	2	2951	723	1340
T3b - C2	t = 0	10100	185.15	6.7	4725	1282	1048
	t = end	5192	297	0.13	1440	1233	1736.5
T3Ave - CA	t = 0	10100	186	6.85	4725	1282	1048
	t = end	3970	308.75	0.565	1654	618.5	1526.5
T4a - C1	t = 0	9420	185.6	8	4869	1338	1029
	t = end	5864	341.3	3	3837	1379	1486
T4b - C2	t = 0	9420	185.8	8.4	4869	1338	1029
	t = end	5720	296.9	0.68	2722	1525	1897.5
T4Ave - CA	t = 0	9420	-151	8.2	4869	1338	1029
	t = end	4366	-217.25	1.34	2738	1093	1680
T5a - C1	t = 0	12280	156.2	8	5123	1404	1082
	t = end	5460	318.5	4	3553	1049	1345
T5b - C2	t = 0	12280	2.6	8.3	5123	1404	1082
	t = end	5172	318.5	0.56	2166	1141	1481
T5Ave - CAve	t = 0	12280	2.6	8.15	5123	1404	1082
	t = end	3890	374.75	1.78	2318	736	1401

The number represented the column while each of the lower-case alphabets represent each sample taken from the column. An average value was also estimated from the duplicates tested in each column. This implies that for each column, there are 3 values to be determined

for wet chemistry analysis conducted on them (i.e., if COD was tested in PVC column 1, the COD test will be determined by using duplicate samples fetched from the column and the average value will also be calculated).

Table 4.5: Summary of ABMP Samples Characteristics at last day (52 nd d) for Settleometer Batch 3						
Samples	CH ₄	f'_{Sup}	f'_{Sbp}	VSS/TSS_day52	VSS/COD	$f_{\text{i,at}}$
Control_1, C1	28	0.77	0.23	0.81	0.50	0.19
Control_2, C2	0	0.58	0.42	0.76	0.60	0.24
Control_Ave, CAve	14	0.67	0.33	0.79	0.54	0.21
PVC_1a, T1a	202	0.65	0.35	0.81	0.52	0.19
PVC_1b, T1b	0	0.55	0.45	0.76	0.49	0.24
PVC_1Ave, T1Ave	98	0.60	0.40	0.79	0.50	0.22
PVC_2a, T2a	0	0.66	0.34	0.86	0.58	0.15
PVC_2b, T2b	0	0.48	0.52	0.76	0.41	0.24
PVC_2Ave, T2Ave	0	0.57	0.43	0.82	0.51	0.18
PVC_3a, T3a	12	0.64	0.36	0.81	0.52	0.19
PVC_3b, T3b	0	0.54	0.46	0.74	0.41	0.26
PVC_3Ave, T3Ave	2	0.59	0.41	0.78	0.47	0.22
PVC_4a, T4a	50	0.68	0.32	0.77	0.58	0.23
PVC_4b, T4b	0	0.59	0.41	0.75	0.53	0.25
PVC_4Ave, T4Ave	23	0.64	0.36	0.76	0.56	0.24
PVC_5a, T5a	38	0.56	0.44	0.79	0.58	0.21
PVC_5b, T5b	86	0.48	0.52	0.78	0.50	0.22
PVC_5Ave, T5Ave	62	0.52	0.48	0.79	0.54	0.21
$f_{\text{i,at}}$	Fraction of inorganic settleable solids with respect to total settleable solids					
f'_{Sup} & f'_{Sbp}	Corresponding feed fractions of ABMP organics (COD) that are unbiodegradable and biodegradable particulates					
CH ₄ _day52	Methane gas produced at the end of ABMP test runs					
PVC	Polyvinyl chloride					

Table 4.5 shows the interpretation of ABMP test results calculated from each PVC column samples and inoculum.

Therefore, we can simply interpret what each letter means from Table 4.4 i.e. first sample (a) of test (T represents the settled organics) was taken from the columns (I = 1, 2, 3, 4, 5) and mixed with control (C1, the inoculum seed) to begin the biodegradation test; duplicate sample (b) for each column was also mixed with a duplicate control (C2, same inoculum seed) and both were examined for laboratory analysis and the outputs from both samples were averaged (such as T1Ave and CAve). The difference in between test (T) and control (C) reveals the actual influent biodegradable organic material available (either a fermentable soluble organic or influent BPO_PS or both). Table 4.7 gives an overview of the elemental mass composition derived from the ABMP tests.

The following observations can be highlighted from the summarized data in Tables 4.4 and 4.5 (above):

1. The ABMP was relatively maintained at favorable buffer environment (alkalinity < 3000 mg/l, pH 7 - 8) appropriate for the inoculum (anaerobic digester biomass cultured under steady state condition) to function well.
2. High COD removal trend was observed from control reactors up to the PVC (poly vinyl chloride) column 2 reactors (see Appendix C for all chart descriptions of analyzed ABMP data). Just after 20 d, the methane yield began to deplete which implies that the biodegradable organics of the control and test samples are left with small concentration. The orthophosphate concentration was observed to deplete instead of increasing. During the digestion process, the organic-bound P in the substrates was expected to be released orthophosphate (OP), hereby increasing the overall OP in each ABMP reactor. This, however, was not observed - the Organically bound P for the PSS biodegradable organics is usually very small and experimental errors significantly influence the outcome. However, the molar fraction of P in sewage biodegradable organics is often assumed to be zero due to its low values. Although at 1st d, it was observed that OP concentration increased from inoculum batch to the last test batch (PVC column 5 samples).
3. As intuitively expected, the free and saline ammonia (FSA) concentrations measured from 0 – 52 d increased. This implies there was successful release of the Organic N bound in the substrates (FBSO and BPO) as FSA during the substrate digestion process.
4. The ISS concentrations measured at the end of ABMP tests were found to be internally consistent per sample type. The ISS concentration difference (with respect to the inoculum

sample) was observed to be less than 350 *mg/l* except for PVC column 4 sample that recorded the highest ISS concentration. This implies that the settling velocity in PVC column 4 settled more ISS proportions (see f_{i_at} in Table 4.5).

5. Very low COD removal was observed at day 52 due to high depletion of BPO in the reactors. This phase signifies limiting point of further methane gas yield as the only organics remaining is UPO (see Table 4.5).
6. Figure 4.3 describes samples (settlemeter and AD) COD biodegradation over long sludge age of 52 days. The essence of the sludge age was to ensure under favorable operating conditions, the remaining organics in ABMP reactors are only unbiodegradable. It illustrates the corresponding CODs in each PVC columns of the settlemeter and AD_SS. Besides higher values corresponding to high electron donor capacity, it also indicates the organic concentrations (soluble and particulates) of the ABMP samples (inoculum and test batches). See Appendix C for complete ABMP data charts and corresponding tables.
7. The trend line in Figure 4.4 shows that the fraction of unbiodegradable particulate organic COD (f'_{sup}) slowly declines with the increased column diameter. This could possibly mean that UPO proportions of TSS are lower for the TSS with reduced settling velocities (i.e., the less dense settleable solids). Also, knowing the f'_{sup} values allows for estimation of the exact BPO fraction in each PVC column (see Table 4.5), hence up-flow velocities in the settlemeter can be related to estimate the corresponding UPO and BPO.

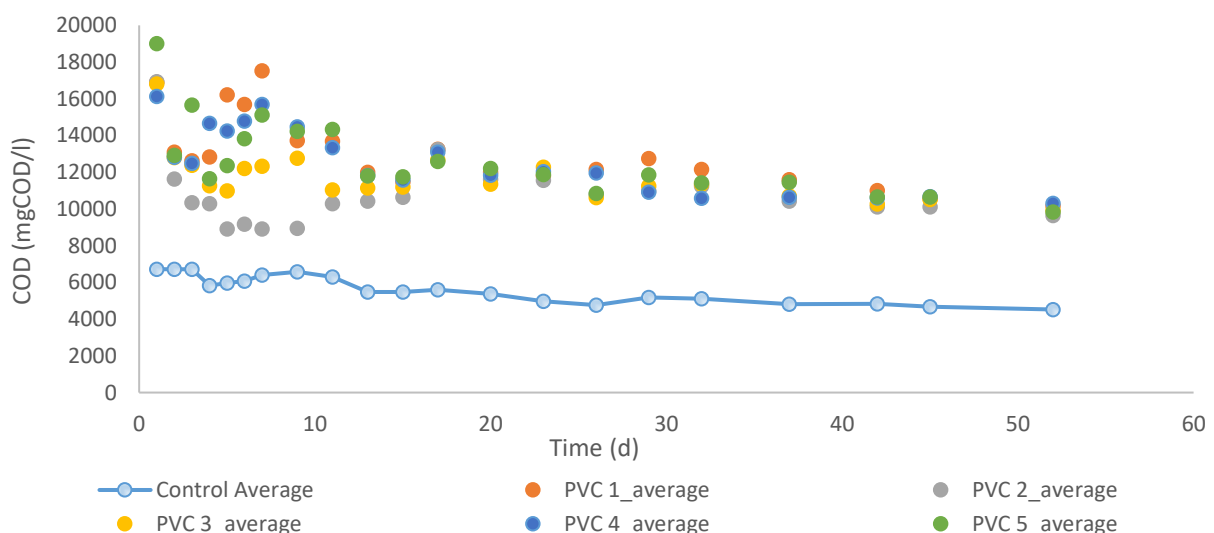


Figure 4. 3: Chemical Oxygen Demand Chart of ABMP Test for 52 days

8. According to Polorigni (2020), TSS (which is ISS + VSS) fractionation is made up of 3 components and they are ISS, UPO, and BPO (whereby the UPO and BPO (organic material) can either be determined using the VSS or COD data and these are well represented by f'_{sup} and f'_{sbp}). Although the sum of the fractions, f'_{sup} and f'_{sbp} equal one (which represents the total VSS) but if directly added with fi_{at} (without considering the VSS/TSS ratio), it does not give the actual TSS concentration. Therefore, the VSS/TSS ratio is applied to account for the equivalent VSS in each total COD fed to ABMP reactors. The VSS/TSS ratio measured at the end of ABMP test was used to account for the residual UPO and BPO. The actual percentage of residual UPO and BPO with respect to the VSS/TSS ratio, f'_{sup} and f'_{sbp} are determined as follows in Equation 4.10:

$$TSS = VSS + ISS \quad (4.10)$$

In terms of TSS, it can be expressed as sum of ratios as shown in Equation 6.11,

$$1 = VSS/TSS + ISS/TSS \quad (4.11)$$

Where: ISS/TSS is expressed as fi_{at}

The two addition components in Equation 4.11 have been determined as shown in Table 4.5. Knowing these values, we can now determine the equivalent VSS concentrations in terms of UPO and BPO by multiplying each of the fractions (f'_{sup} and f'_{sbp}) by VSS/TSS ratio, i.e.:

$$UPO\ VSS = f'_{sup} * VSS/TSS \quad (4.12)$$

$$f'_{sbp} = 1 - f'_{sup} \quad (4.13)$$

$$BPO\ VSS = f'_{sbp} * VSS/TSS \quad (4.14)$$

$$\text{Therefore, } VSS = UPO\ VSS + BPO\ VSS \quad (4.15)$$

Where: ISS is inorganic settleable solids

VSS is volatile settleable solids

TSS is total settleable solids

UPO VSS is the equivalent VSS concentration of unbiodegradable particulate COD.

BPO VSS is the equivalent VSS concentration of biodegradable particulate COD.

From Equation 4.15, the TSS fractionations (ISS, UPO, and BPO) can now be calculated (in percentage) to show the proportions represented in each PVC columns of settleometer device. Table 4.6 gives a summary of the TSS fractionations with respect to settling velocities recorded in the settleometer experimental test. It shows the proportions of TSS components

in each PVC columns where UPO represents the largest TSS component that settles while ISS represents the smallest component. Also, the settling velocity does not assert if there is meant to be a clear-cut increase or decrease in TSS components from PVC columns 1 to 5. Nonetheless, the computed TSS proportion can be accepted to imitate a real primary settling tank in terms of settling TSS components.

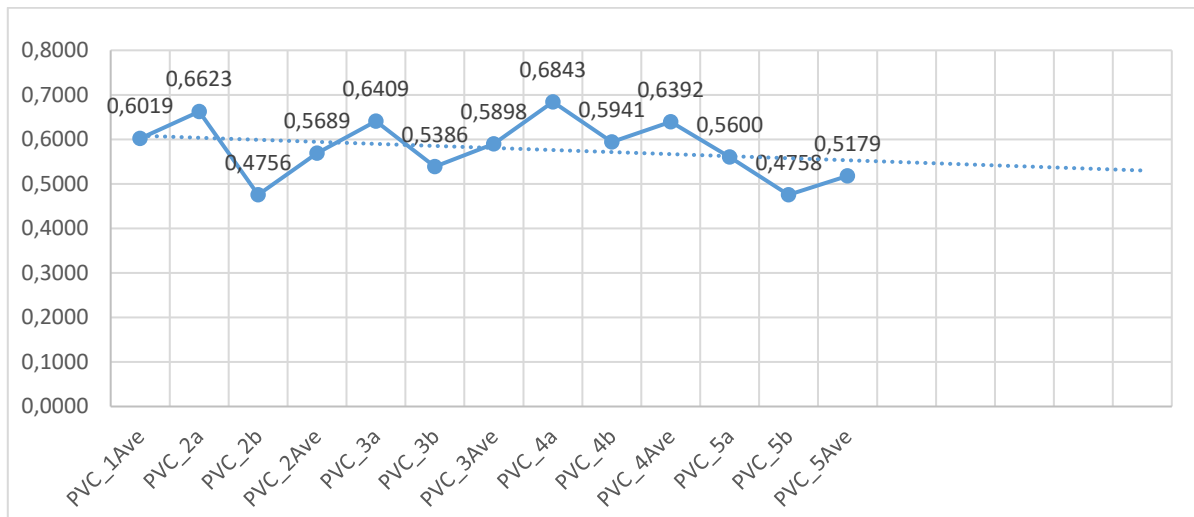


Figure 4. 4: f_{Sup} chart in ABMP reactors

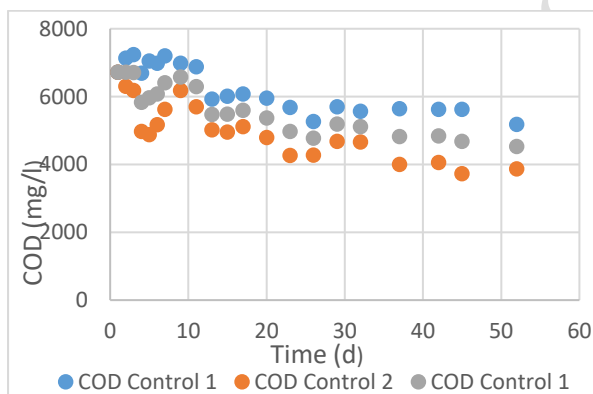


Figure 4.5: Control Total COD

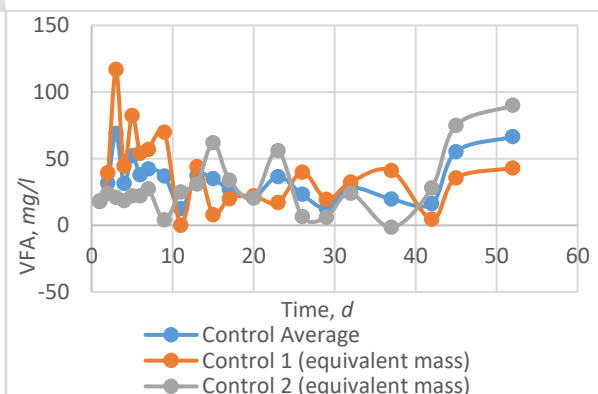


Figure 4.6: Control Total Soluble COD (VFA)

Figures 4.5 – 4.6 (above) respectively show the total COD and soluble COD in ABMP control reactor (for steady state reactor parameters).

4.4 PARAMETER ESTIMATION FOR ABMP CONTROL EXPERIMENT

Parameter estimation is a process that compares the experimentally measured variables with the corresponding model-predicted variables. The parameter estimation process uses the collected experimental data as an objective for the simulated data. The simulation adjusts the

input parameters, such as substrate composition and hydrolysis rate, until the observed experimental data is achieved at the same time-steps.

Table 4.6: TSS fractionation from ABMP Experimental Readings at day 52					
Samples	Settling vel., V_s	ISS	UPO	BPO	TSS
Control_1	-	18.57%	62.8%	18.7%	100.00%
Control_2	-	24.44%	43.5%	32.1%	100.00%
Control_Ave	-	21.44%	52.9%	25.7%	100.00%
PVC_1a	31.608	19.29%	52.8%	27.9%	100.00%
PVC_1b	31.608	24.22%	41.7%	34.1%	100.00%
PVC_1Ave	31.608	21.55%	47.2%	31.2%	100.00%
PVC_2a	14.131	14.53%	56.6%	28.9%	100.00%
PVC_2b	14.131	24.39%	36.0%	39.7%	100.00%
PVC_2Ave	14.131	18.09%	46.6%	35.3%	100.00%
PVC_3a	8.6506	19.16%	51.8%	29.0%	100.00%
PVC_3b	8.6506	26.41%	39.6%	34.0%	100.00%
PVC_3Ave	8.6506	22.25%	45.9%	31.9%	100.00%
PVC_4a	5.7909	23.45%	52.4%	24.2%	100.00%
PVC_4b	5.7909	24.56%	44.8%	30.6%	100.00%
PVC_4Ave	5.7909	23.94%	48.6%	27.4%	100.00%
PVC_5a	3.575	21.06%	44.2%	34.7%	100.00%
PVC_5b	3.575	21.89%	37.2%	40.9%	100.00%
PVC_5Ave	3.575	21.41%	40.7%	37.9%	100.00%
ISS	Inorganic Settleable Solids				
UPO	Unbiodegradable Particulate Organics				
BPO	Biodegradable Particulate Organics				
TSS	Total Settleable Solids				
PVC_i	Where (i = 1, 2, 3, 4 and 5) represent the settleometer columns				
a, b	Either of the two represents the first fetched sample (say, a) and the other is a duplicate				
Ave	Means taking the average of a particular sample and its duplicate from each PVC column.				

Table 4.6 summarizes the TSS fractionations in the biodegradation test run in ABMP reactors showing the percentage of TSS proportions in the settleometer PVC columns with respect to their settling velocities.

The set of parameters that allows for the closest match between the model-predicted variables and experimentally measured variables is identified, according to the minimum error calculated in the simulation platform. Therefore, to find a composition that better fits the observed experimental data, parameter estimation (PE) was conducted on a virtual ABMP experimental reactor that was simulated using the UCTSDM3P model.

Therefore, the observed experimental data from the ABMP Control experiments were set as the objective variables for the parameter estimation procedure. The parameters that were used as the unknowns were the H, O, N and P terms of the biodegradable particulate organics in the PSS (i.e., the parameterized molar fractions of its elemental formulation). Five observed or known variables were set as the simulation objectives: total COD, FSA, OP, VSS, and the H_2CO_3 Alk concentrations (see Appendix F for set of known variables used for control and test samples; Tables 4.7 – 4.8 below, list out the known variables from which variables of key interest were selected).

Table 4.7 Measured Variables from Control Sample 1 (C1) used for Parameter Estimation								
#.t, h	.AD_1.COD_total	.AD_1.FSA	.AD_1.OP	.AD_1.VSS	.AD_1.ISSm	.AD_1.H2CO3alkalinity	.AD_1.VFA	.AD_1.p_H_s
0	6720	155	3	3399	834	979	18	7.93
24	7135	175	4	3542	1011	1006	40	7.49
48	7240	169	4	3689	988	1070	117	7.42
72	6691	167	5	3181	927	1058	45	7.40
96	7045	157	2	3266	905	1140	83	7.37
120	6984	141	4	3166	813	1045	54	7.42
144	7194	170	5	3247	910	1098	57	7.43
168	6978	161	4	3139	780	1021	70	7.36
216	6882	199	3	2857	697	0	0	7.32
264	5927	192	2	3291	1156	1111	44	7.38
312	6012	200	4	3283	1123	1174	8	7.31
360	6076	187	2	3160	776	1169	20	7.32
408	5948	197	4	3377	1129	1200	22	7.30
480	5678	208	3	2772	758	1191	17	7.32
552	5266	189	3	3222	1039	1213	40	7.35
624	5698	205	3	3255	1111	1191	20	7.33
696	5570	223	3	2963	762	1246	33	7.33
768	5642	230	2	3097	814	1286	41	7.42
888	5618	229	3	3050	1062	1252	5	7.43
1008	5620	249	3	2799	739	1274	36	7.43
1080	5180	248	3	2601	593	1258	43	7.36

The PE tool in WEST[®] software (where the virtual ABMP reactor is simulated using the UCTSDM3P model) ran hundreds of iterations until the correct combination of parameters that achieved the desired results with the lowest error was determined.

The third table (see Appendix F) that was also recorded for controls calculated the average of each variables in both data. Each of these data in the control batches are the equivalent value (i.e. the actual value was halved and one-half was used for the ABMP test). The calculated composition of nitrogen in the organics appeared accurate, since both the generated alkalinity and the ammonia in the experiment released are well predicted, as observed in Figures 4.7 and 4.8 (respectively). The drop in the measured ammonia concentration in the ABMP control experiment may be due to experimental error, such as a new mixture of boric acid, or a different normality of the acid used for titration. The chosen P value appears too low as the release of OP is not well predicted, as observed in Figure 4.9. The simulated

concentration of VSS utilized during the experiment appears to match the observed change in VSS relatively well, as observed in Figure 4.10.

Table 4.8 Measured Variables from Control Sample 2 (C2) used for Parameter Estimation								
#.t, h	.AD_1.COD_total	.AD_1.FSA	.AD_1.OP	.AD_1.VSS	.AD_1.ISSm	.AD_1.H2CO3alkalinity	.AD_1.VFA	.AD_1.p_H_s
0	6720	155	3	3399	834	979	18	7.89
24	6300	156	3	3503	832	883	24	7.42
48	6182	151	4	3127	732	882	21	7.42
72	4969	134	3	2776	676	890	19	7.34
96	4874	136	2	2241	576	941	22	7.34
120	5166	157	3	2974	576	941	22	7.43
144	5619	145	3	3322	741	942	28	7.33
168	6179	182	3	2648	866	951	4	7.24
216	5698	176	3	2685	695	965	25	7.19
264	5014	180	3	2774	592	992	31	7.23
312	4952	169	4	3026	655	1064	62	7.25
360	5115	158	2	2681	823	945	34	7.20
408	4790	169	4	2744	661	972	21	7.23
480	4266	179	3	2318	691	1027	56	7.23
552	4274	162	3	2376	587	1019	7	7.27
624	4674	183	3	2489	588	994	6	7.28
696	4658	184	3	2614	687	1036	24	7.22
768	3996	192	4	2021	929	966	-2	7.27
888	4056	193	2	1983	646	1016	28	7.36
1008	3730	206	2	1741	559	1061	75	7.30
1080	3868	199	2	2316	548	1020	90	7.28

As predicted, due to the gas measurement error associated with the experimental BMP, the simulated CH₄ release was higher than the observed CH₄ release, as observed in Figure 4.11. Besides the VFA's inconsistent trend, its accumulation did not match the observed ABMP data well. The haphazard trend of this intermediate product, VFA, is subjected to its recurrent sequestration by inherent acetoclastic methanogens (AM) under a favorable pH condition. This therefore explains that the presence of uninhibited AM is responsible for the inconsistent VFA. The KS_AM value determined in the steady state model may not be accurate, as the rate of the reaction may be affected in a different way. The rate can be adjusted in the ABMP model and inputted back into the steady state model to check for consistency. The VFA data is shown in Figure 4.6. The worst prediction of the ABMP simulation was the operating pH, which is shown in Figure 4.12. The simulated pH dropped far below the observed pH values.

This indicated that the elemental composition determined was incorrect. This issue was resolved by conducting a parameter estimation on the ABMP control reactor, such that a new elemental composition that matched the measured data was determined.

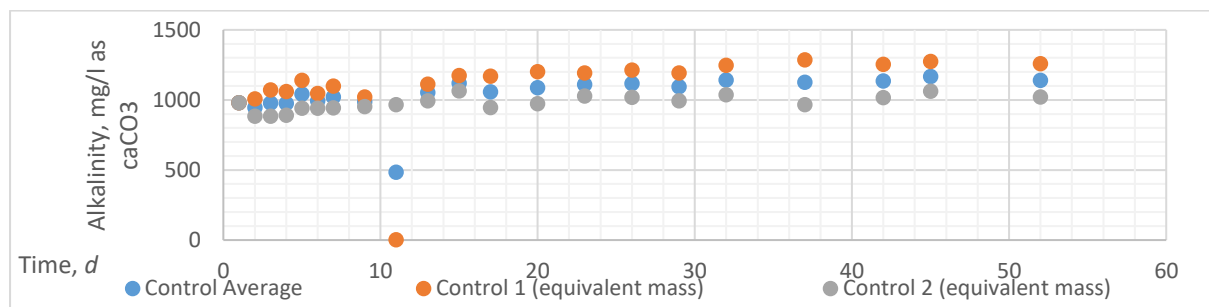


Figure 4.7: Control Carbonate Alkalinity

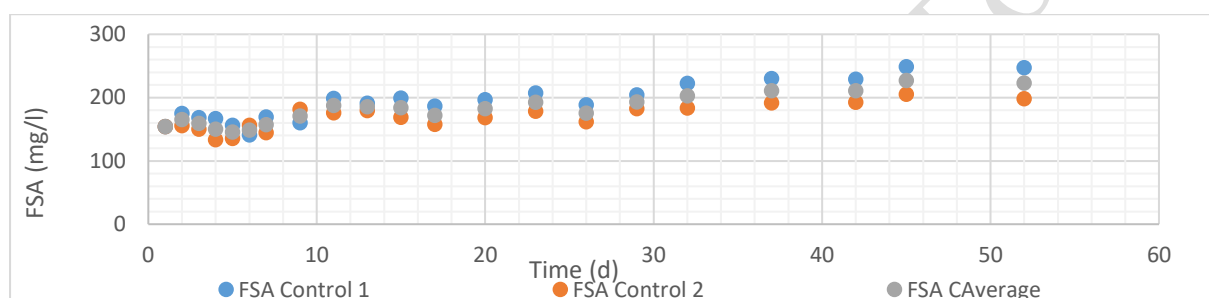


Figure 4.8: Control FSA

Figures 4.7 – 4.8 (above) respectively show H_2CO_3 Alk and FSA in ABMP control reactor for steady-state reactor parameters

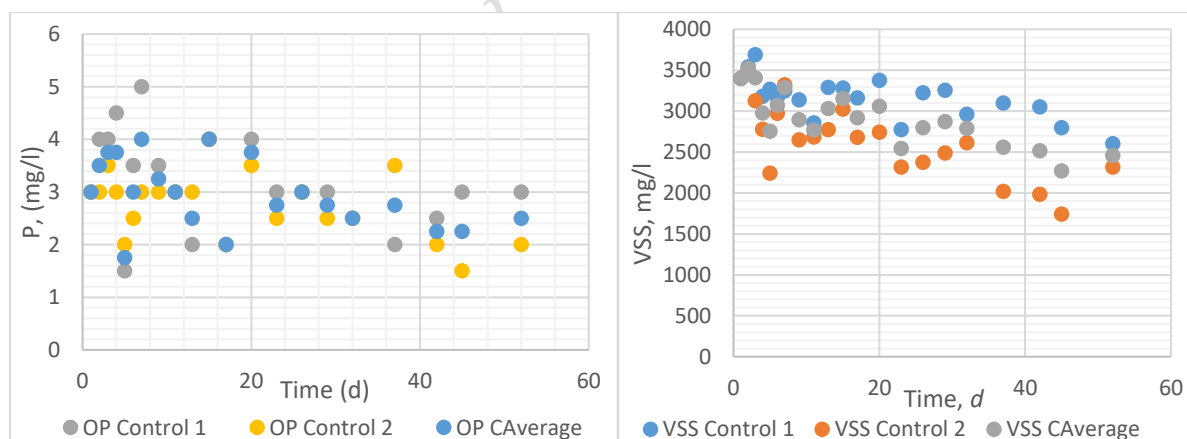


Figure 4.9: Control OP

Figure 4.10: Control VSS

Figures 4.9 – 4.10 respectively show OP and VSS in ABMP control reactor for steady-state reactor parameters

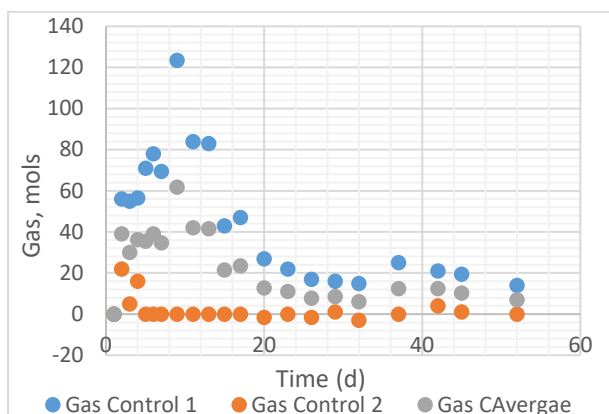


Figure 4.11: Control CH4

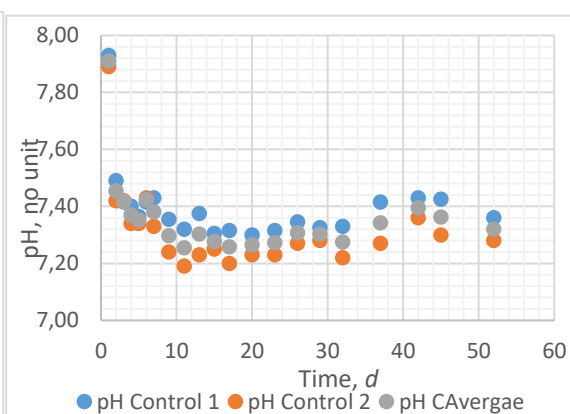


Figure 4.12: Control pH

Figures 4.11 – 4.12 respectively show Methane yield and pH in ABMP control reactor for steady-state reactor parameters

4.5 PROCEEDINGS FOR PARAMETER ESTIMATION OF ABMP TEST EXPERIMENTS

Same procedures followed for the ABMP control experiment were relatively applied to the ABMP test experiment except for two differences. Unlike in the control experiments where the equivalent of actual concentrations are used, the whole concentration for each of the variables is used up (since that will be the justifying procedure to confirm complete biodegradation of the settled bio-organics. Also, since the mixture of both control and test samples will be required for the ABMP test, the actual substrate concentration at time $t = 0$ is estimated by subtracting the equivalent biomass variables from the test batches (also at time, $t = 0$). For example,

Initial condition: time, $t = 0 \text{ h}$

COD Biomass (inoculum) concentration in control batch 1 = 6720 mgCOD/l

COD Test concentration in test batch 1 (i.e in PVC_1a) = 16900 mgCOD/l

COD substrate in test batch 1 = (COD Test – COD Biomass) Concentration

$$= 16900 - 6720$$

$$= 10180 \text{ mgCOD/l}$$

Similar calculations were done per time-steps as observed in the tables (from time 0 h to desired end time), and that was how the actual variable concentrations across all the PVC columns (1 to 5) were determined except for the pH values.

Using Table 4.9 (below) as a guide to calculating the in-situ variables. All columns (except 3, 6, 9, 12, and 15, which were only subtracted with CAve) were separately subtracted with the underlying controls (C1, C2 and CAve).

Table 4.9 Summary of How Substrate Concentrations Were Determined															
S/N	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Tests	T1a	T1b	T1Ave	T2a	T2b	T2Ave	T3a	T3b	T3Ave	T4a	T4b	T4Ave	T5a	T5b	T5Ave
Controls	- C1	- C1	- CAve	- C1	- C1	- CAve	- C1	- C1	- CAve	- C1	- C1	- CAve	- C1	- C1	- CAve
	- C2	- C2		- C2	- C2		- C2	- C2		- C2	- C2		- C2	- C2	
	- CAve	- CAve		- CAve	- CAve		- CAve	- CAve		- CAve	- CAve		- CAve	- CAve	

For example, the first substrate with reference to control batch 1 (per time) is calculated by finding the difference between the test and control batch and this was done for each determined variable (see Section 3.3.2 and Appendix F for the 35 tables recorded).

4.6 CONCLUSION

The settleometer, AD_SS and ABMP experimental results have been presented in this chapter, i.e.: (i) The settleometer test described the sludge settleability characteristics under 5 settling velocity groups accounting for the TSS components in each settling group. (ii) An AD system that was run at steady state and served as the inoculum source (biomass) for ABMP tests. (iii) The ABMP tests, after being seeded with sludge from the steady state AD (which contained the biomass inoculum), utilized samples of sludge that settled in the settleometer columns. These results will be further analyzed and discussed to determine important parameters that influence UCTPSU (generally, PWM_SA) model components and variables. These parameters include: UPO, BPO and ISS proportions of TSS from different settling velocity groups (classified according to the settling velocity of particles that settled in the 5 different columns of the settleometer), the elemental mass composition of BPO and kinetic rate constants for the hydrolysis of BPO. Appendices A – C summarize the three systems' results and lab measurements.

CHAPTER 5.0: MODELLING AND CALIBRATION

5.1 INTRODUCTION

This chapter consolidates the data from the ABMP tests (Chapter 4) together with a developed anaerobic digestion (AD) model to determine the elemental mass compositions of biodegradable solids that were collected in the 5 different columns of the settleometer described in the experimental set up (see chapter 3) and also gives a detailed description of the global sensitivity analysis employed to calibrate the University of Cape Town Primary Sedimentation Unit (UCTPSU) model. The chapter is divided into three main sections (i) determination of the masses in the control and test ABMP reactors, prior to parameter estimation, (ii) implementation of parameter estimation (PE) procedure using the measured ABMP data and the AD model (UCTSDM3P; Ikumi *et al.*, 2015) to determine the substrate elemental composition, and global sensitivity analysis for UCTPSU model.

5.2 DETERMINATION OF CONTROL AND TEST MASSES PRIOR TO AUGMENTED BIOCHEMICAL METHANE POTENTIAL (ABMP) PARAMETER ESTIMATION PROCESS

The UCTSDM3P model was used to simulate a virtual replica of the ABMP test described in Section 4.4. To begin simulating the ABMP experiment, the initial and final masses of the control ABMP and the test ABMP are added as input to the virtually replicated ABMP reactors. The method used in determining these masses is outlined in Figure 5.1 (below). With the assumption that all biodegradable organics have been utilised and converted to methane by the end of the ABMP test, the unbiodegradable fraction of the organics from the inoculum and feed is estimated. With the biodegradable and unbiodegradable masses known for the seed sludge and substrate, the intuitive knowledge of how the substrate is transformed during the AD is required to simulate the parameter estimation correctly: essentially it is important to note that the organics (measured as chemical oxygen demand, COD and volatile suspended solids, VSS) shall be utilised (i.e. decreased through biodegradation) and converted to methane while the ammonia (FSA), orthophosphate (OP) and alkalinity is expected to increase via release of nitrogen (N) and Phosphorus (P) bound in the

biodegradable particulate organic (BPO) material as the BPO gets degraded. Table 5.1 below shows the calculated control and test masses prior to the parameter estimation process.

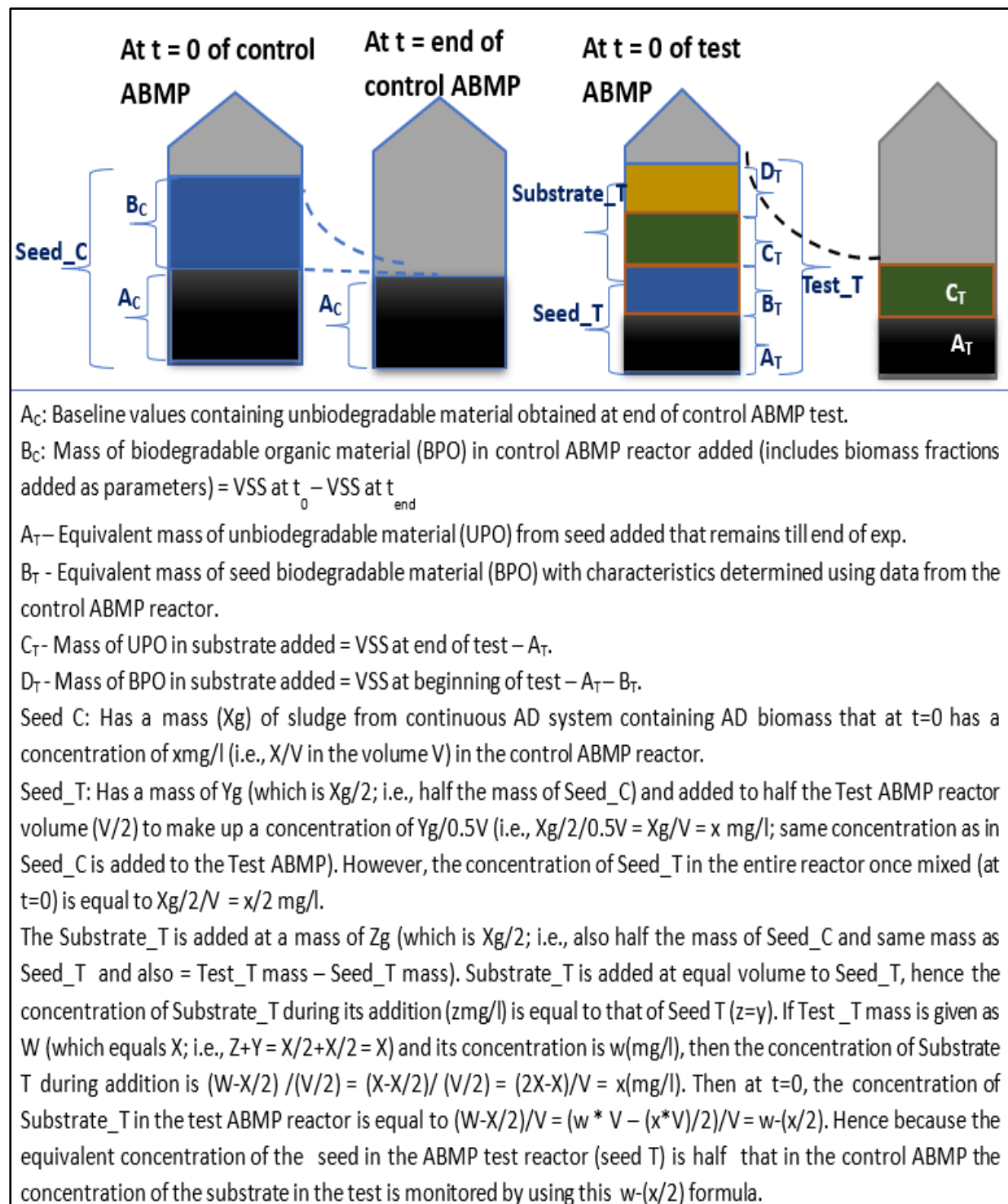


Figure 5.1: Determination of Biodegradable and Unbiodegradable Massed using Augmented Batch Tests

Table 5.1: Calculation of Control and Test Masses Prior to Parameter Estimation				
Samples	UPO	BPO	Total VSS	Units
Seed_C1	5202	1596	6798	mgVSS/l
Seed_C2	4632	2166	6798	mgVSS/l
Seed_T1	2601	798	3399	mgVSS/l
Seed_T2	2316	1083	3399	mgVSS/l
Substrate_T1a	5716	3250	8966	mgVSS/l
Equi_Sub_T1a	2858	1625	4483	mgVSS/l
ABMP_T1a_blend_mass	-	-	6306	mgVSS
Substrate_T1b	4538	4428	8966	mgVSS/l
Equi_Sub_T1b	2269	2214	4483	mgVSS/l
ABMP_T1b_blend_mass	-	-	6306	mgVSS
Substrate_T2a	6540	2444	8984	mgVSS/l
Equi_Sub_T2a	3270	1222	4492	mgVSS/l
ABMP_T2a_blend_mass	-	-	7891	mgVSS
Substrate_T2b	3268	5316	8584	mgVSS/l
Equi_Sub_T2b	1634	2658	4292	mgVSS/l
ABMP_T2b_blend	-	-	7691	mgVSS
Substrate_T3a	5552	2572	8124	mgVSS/l
Equi_Sub_T3a	2776	1286	4062	mgVSS/l
ABMP_T3a_blend	-	-	7461	mgVSS
Substrate_T3b	3756	4368	8124	mgVSS/l
Equi_Sub_T3b	1878	2184	4062	mgVSS/l
ABMP_T3b_blend	-	-	7461	mgVSS
Substrate_T4a	6438	1830	8268	mgVSS/l
Equi_Sub_T4a	3219	915	4134	mgVSS/l
ABMP_T4a_blend	-	-	7533	mgVSS
Substrate_T4b	5038	3230	8268	mgVSS/l
Equi_Sub_T4b	2519	1615	4134	mgVSS/l
ABMP_T4b_blend	-	-	7533	mgVSS
Substrate_T5a	6154	2368	8522	mgVSS/l
Equi_Sub_T5a	3077	1184	4261	mgVSS/l
ABMP_T5a_blend	-	-	7660	mgVSS
Substrate_T5b	4482	4040	8522	mgVSS/l
Equi_Sub_T5b	2241	2020	4261	mgVSS/l
ABMP_T5b_blend	-	-	7660	mgVSS

Prior to calculating the control and test masses initialized for parameter estimation purpose, the volume of seed and substrate used in the ABMP test for both main and duplicate samples were recorded. To determine these masses, the stated procedures in Figure 5.1 were carefully followed using the ABMP data on volatile settleable solids (VSS). Table 5.2 highlights the volumes used in each sample.

Table 5.2: Volume Estimates for Control and Test Mass Initialisation					
	volume	Sample		Duplicate	
		Seed	Substrate	Seed	Substrate
control	/	2	2	1	1
PVC_1	/	0.8	0.8	0.8	0.8
PVC_2	/	1	1	1	1
PVC_3	/	1	1	1	1
PVC_4	/	1	1	1	1
PVC_5	/	1	1	1	1

With these known volumes and ABMP_VSS concentrations (BPO and UPO), the masses (as shown in Table 5.1) were determined by multiplying the VSS concentrations by their respective volumes.

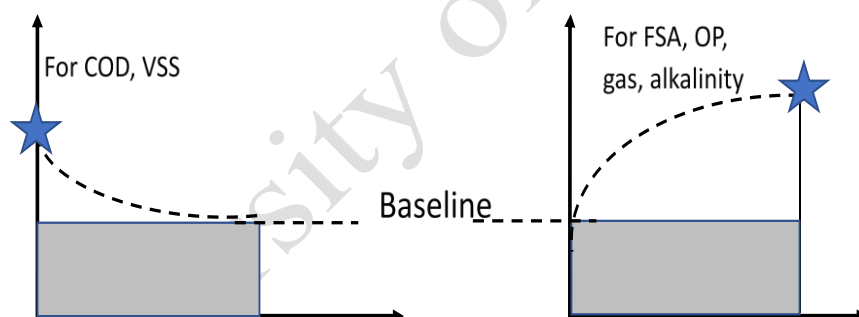


Figure 5. 2: Expected Trend of Variables Measured in Augmented Batch Tests

The ABMP test that virtually replicates the ones run experimentally (i.e., including both the control (run with inoculum only) and the test (with both inoculum and organics) are simulated. The test simulation is subsequent to the control, to allow for the 'initial parameters' (i.e., the elemental composition of the seed sludge, whereby the x , y , z , a and b values of $C_xH_yO_zN_aP_b$ are determined via the PE process described below) to be determined from the control simulation prior to the test ABMP simulation. Performance of PE using the actual test (with inoculum and organics) output data, hence allows for determination of the hydrolysis rate, and composition of the feed organics. Similar to the actual BMP test

procedure, the difference in methane production (or VSS (or COD) removal) by the test and control simulations is attributed to the organics in the feed (see Figure 5.1).

5.3 DETERMINATION OF KINETIC CONSTANTS USING STEADY STATE AD MODEL DATA TO DETERMINE INITIAL ABMP CONTROL VALUES

In order to use the ABMP data to determine the unbiodegradable fraction of sludge and kinetics of hydrolysis, the characteristics of the inoculum seed sludge are required. These characteristics include, amongst other variables, the estimate of the acidogen biomass (Z_{AD}) and the biodegradable particulate organics COD (S_{bp}) concentration of the inoculum seed sludge that was sourced from the steady state AD and added to the control ABMP reactor. Gaszynski *et al.* (2019) indicate that the characteristics of the inoculum seed can be determined with the measured steady state AD influent and effluent concentrations, (see Table 5.4 below) using the following steps:

1. The total COD (S_{ti}) entering the AD is equivalent to the unfiltered organic COD concentration of the PS feed.
2. The total soluble COD (S_{si}) is equivalent to the filtered COD concentration of the PSS feed.
3. The total particulate COD (S_{pi}) is equivalent to the total COD (S_{ti}) minus the total soluble COD (S_{si}).

$$S_{ti} = S_{si} + S_{pi} \quad (5.1)$$

4. The USO COD (S_{usi}) is equal to the effluent filtered COD (S_{se}) concentration minus the effluent VFA COD (S_{bsae}) concentration:

$$S_{se} = S_{usi} + S_{bsae} \quad (5.2)$$

5. The BSO COD (S_{bsi}) is equal to the total soluble COD (S_{si}) concentration minus the USO COD (S_{usi}) concentration:

$$S_{si} = S_{bsi} + S_{usi} \quad (5.3)$$

6. The readily fermentable COD (S_{bsfi}) is equal to the BSO COD (S_{bsi}) concentration minus the influent VFA COD (S_{bsai})

$$S_{bsi} = S_{bsai} + S_{bsfi} \quad (5.4)$$

7. The effluent particulate COD (S_{pe}) is the sum of the UPO COD (S_{upi}), the acidogen biomass (Z_{AD}) and the residual biodegradable organics (S_{bp}).

$$S_{pe} = S_{upi} + Z_{AD} + S_{bp} \quad (5.5)$$

8. The Z_{AD} concentration was determined using the following equations established by Sotemann *et al.* (2005).

- a. Based on a reactor at steady state and a mass balance on the acidogen biomass, the hydrolysis rate of the organics is determined by:

$$r_h = \frac{Z_{AD}}{Y_{AD}} \left(\frac{1}{R} + b_{AD} \right) \quad (5.6)$$

Where: Y_{AD} = Biomass yield (gCOD biomass/ gCOD organics)

R = Sludge age (d)

: b_{AD} = Biomass death rate (1/d)

Table 5.3 Shows AD Biomass Concentration at Sludge of 20 and 67 d		
COD (unfiltered) - influent average	mgCOD/l	55750
COD (unfiltered) - effluent average	mgCOD/l	27113
f_{AD}	no unit	0
Sludge age_20	d	20
Sludge age_67	d	67
YAD	gZAD/gCOD	0.11
bAD	per d	0.04
Biomass, ZAD_20 d	gCOD/l	0.8512
Biomass, ZAD_68 d	gCOD/l	0.4090

- b. Similarly, the hydrolysis rate can also be determined based on a reactor at steady state and a mass balance of the biodegradable organics flowing through the reactor:

$$r_h = \frac{S_{bpi} - S_{bp}}{R} + b_{AD}Z_{AD} \quad (5.7)$$

- c. The concentration of biomass present in the reactor can then be determined by:

$$Z_{AD} = \frac{Y_{AD}(S_{bpi} - S_{bp})}{[1 + b_{AD}R(1 - Y_{AD})]} \quad (5.8)$$

- d. Finally, the COD concentration of methane, if all of it stays dissolved in solution is calculated by:

$$S_m = (1 - Y_{AD}) R r_h \quad (5.9)$$

- e. Using the four equations shown above, the COD concentration of biomass grown inside the reactor can be calculated based on the daily concentration of methane produced by the reaction. Therefore, the Z_{AD} concentration in the effluent stream was calculated by:

$$Z_{AD} = \frac{Y_{AD} S_m}{(1 + b_{AD} R (1 - Y_{AD}) + Y_{AD} R b_{AD}) (1 - Y_{AD})} \quad (5.10)$$

The calculated Z_{AD} is shown in Table 5.4 above

In the UCT AD models (UCTADM (Sötemann *et al.*, 2005); UCTSDM3P (Ikumi *et al.*, 2015)) the hydrolysis of the three different organic materials (proteins, carbohydrates and lipids) of the International Water Association (IWA) ADM1 model (Batstone *et al.*, 2002) is modified to a single hydrolysis process acting on a generic particulate biodegradable organic material representing sewage sludge i.e. $C_xH_yO_zN_A$. With complex organics, like in WWTP sludge, the hydrolysis process is usually the rate-limiting step so that the AD processes that follow it, being much faster, are dealt with stoichiometrically to yield the digester end products, i.e. biomass, CH_4 , CO_2 (dissolved HCO_3^- and gaseous CO_2) and water (Ikumi *et al.*, 2015).

Saturation kinetics formulation is often used in models to represent the utilization of slowly biodegradable particulate organics (BPO) in activated sludge models (Dold *et al.*, 1980; Henze *et al.*, 1987) and hydrolysis of sewage sludge (McCarty, 1974; Ikumi *et al.*, 2014). It includes acidogenic biomass growth (Z_{AD}) and incorporates a maximum rate of hydrolysis under conditions of high substrate/biomass concentration ratio (S_{bp}/Z_{AD}). Saturation kinetics is based on the quantity of BPO (substrate broken down by Z_{AD}) attached to the organic Z_{AD} active sites, whereby the rate of hydrolysis reaches a maximum at saturation of the active sites of the acidogens. This way saturation kinetics is independent of the bulk liquid residual biodegradable COD concentration (S_{bp}), but rather dependent on its concentration with respect to the acidogenic biomass concentration (Z_{AD}). Thus, the saturation kinetic equation used to predict the rate of hydrolysis is:

$$r_{HYD} = \left(\frac{k_M \cdot \left(\frac{S_{bp}}{Z_{AD}} \right)}{K_S + \left(\frac{S_{bp}}{Z_{AD}} \right)} \right) \cdot Z_{AD} \quad [\text{g COD/ (l.d)}] \quad (5.11)$$

Where K_s is the substrate and acidogenic biomass concentration ratio, at which the specific hydrolysis rate is half its upper limit (k_M) at saturation.

The mass balance-based principles (like those used by Sötemann *et al.*, 2005a and Ikumi *et al.*, 2015)) are adopted here to determine the kinetic constants (k_M and K_s) in the hydrolysis rate equations. For completely mixed flow through anaerobic digester conditions, the total COD concentrations (S_{ti}) is fractionated into (i) S_{bp} , (ii) unbiodegradable soluble and particulate COD (S_{us} and S_{up} respectively), (iii) fermentable readily biodegradable organics (FBSO, S_{bsf}) and (iv) volatile fatty acids (VFA, S_{bsa} ; all assumed to be acetate).

Hence in the (i) and effluent (e) of the AD:

$$S_{ti} = S_{bpi} + S_{bsfi} + S_{bsai} + S_{usi} + S_{upi} \quad (5.12)$$

and

$$S_t = S_{bp} + S_{bsf} + S_{bsa} + S_{us} + S_{up} + Z_{AD} \quad (5.13)$$

The S_{bpi} is connected to the residual one (S_{bp} ; i.e., in the effluent) via the volumetric hydrolysis rate (r_{HYD}) derived below.

The derivation of volumetric hydrolyses kinetic rate constants was accomplished using the principle of mass balance over the AD system. For hydrolysis kinetics the components of interest include the BPO and Z_{AD} . Hence using the mass balance principles, the system's change in BPO can be equated to the BPO entering the AD, subtracting the amount exiting the AD and the quantity utilized via hydrolysis, and that generated through death of AD biomass (i.e., Z_{AD}) the so a mass balance on BPO yields:

$$V \cdot \partial S_{bp} = Q_i \cdot \partial t \cdot S_{bpi} - Q_e \cdot \partial t \cdot S_{bpe} - r_{HYD} \cdot V \cdot \partial t + (b_{AD} \cdot Z_{AD}) \cdot V \cdot \partial t \quad (5.14)$$

Where b_{AD} (/d) is the acidogen endogenous respiration rate constant.

In the above Equation 5.14, it is accepted that, negligible endogenous residue (Z_{EAD}) accumulates in the AD.

For AD batch tests, without influent or effluent flow rates (i.e., $Q_i = Q_e = 0$), whereby the change in BPO is a decrease (hence negative) the formulation can be accepted as:

$$-V \cdot \partial S_{bp} = -r_{HYD} \cdot V \cdot \partial t + b_{AD} \cdot Z_{AD_i} \cdot V \cdot \partial t$$

$$\text{Hence, } r_{HYD} \cdot \partial t = \partial S_{bp} + b_{AD} \cdot Z_{AD_i} \cdot \partial t \quad (5.15)$$

Where δS_{bp} equals the S_{bp} at current time (S_{bp_t}) subtracted from the S_{bp} at initial time (S_{bp_ti}) i.e., $S_{bp_ti} - S_{bp_t}$, dividing the above Equation 5.15 by $V \cdot \delta t$, gives:

$$r_{HYD} = b_{AD} \cdot Z_{AD_i} + \frac{(S_{bp_ti} - S_{bp_t})}{\delta t} \quad [\text{gCOD}/(\text{l.d})] \quad (5.16)$$

Applying the mass balance to the acidogenic biomass (Z_{AD}) concentration in the flow through AD yields:

$$V \cdot \partial Z_{AD} = Q_i \cdot Z_{AD} \cdot \partial t - Q_e \cdot Z_{AD} \cdot \partial t + Y_{AD} \cdot r_{HYD} \cdot V \cdot \partial t - b_{AD} \cdot Z_{AD_i} \cdot V \cdot \partial t \quad (5.17a)$$

Noting that $Q_i = Q_e = 0$, for AD batch tests, and dividing the above Equation 2.1 by V , gives:

$$\partial Z_{AD} = Y_{AD} \cdot r_{HYD} \cdot \partial t - b_{AD} \cdot Z_{AD_i} \cdot \partial t \quad (5.17b)$$

Hence the Z_{AD} at current time (Z_{AD_t}) should equal the Z_{AD} at initial time (Z_{AD_ti}) added to the change in Z_{AD} over the time (δZ_{AD}), i.e.:

$$Z_{AD} = Z_{AD_i} + \partial Z_{AD} = Z_{AD_i} + (Y_{AD} \cdot r_{HYD} - b_{AD} \cdot Z_{AD_i}) \cdot \partial t \quad (5.18)$$

Equations 5.1 to 5.18 establish the link between the initial and current COD concentration (S_{ti} and S_t) in the batch test and is computed as follows in the simplified model, for the determination of kinetic constants:

1. Coupling the FBSO (S_{bsfi}) with the BPO (S_{bp}) because it is a complex organic that also requires hydrolysis resulting in the generation of Z_{AD} (i.e., $S_{bp} = S_{bp} + S_{bsf}$).
2. The acidogenic biomass (Z_{AD}) concentration, which has the largest yield value (0.089 mgCOD organism/mgCOD substrate) represents the biomass formation of all the AD microorganism groups, i.e. not only the acidogens, (which are known to have much lower, yield values). However, to account for the growth of acetoclastic methanogen (Z_{AM}) and hydrogenotrophic methanogen (Z_{HM}) biomass, hence improve predictions on methane generation and sludge production, Sötemann *et al.* (2005a) increased the yield coefficient (Y_{AD}) from 0.089 to 0.113 (mgCOD organism/mgCOD substrate). Although the Z_{AM} and Z_{HM} have very low yield coefficients ($Y_{AM} = 0.04$, $Y_{HM} = 0.01$), they still contribute to the overall biomass production. Since acidogenesis produces 67% acetic acid for Z_{AM} growth (and 33% hydrogen), 67% of the Y_{AM} value was added to Y_{AD} . The hydrogenotrophic methanogens (Z_{HM}), being a very small part of AD biomass

were neglected in the adjustment of the Y_{AD} . In the ore complex dynamic simulation AD models, all AD biomass growth kinetics are modelled individually.

3. Accepting the S_{usi} (USO) as negligible ($<100 \text{ mgCOD/l}$ in 50000 mgCOD/l). If the USO is significant, then this should be subtracted from both influent and effluent COD concentration to give the total particulate COD in influent and effluent.
4. Assuming S_{bsa} is used up very rapidly and eliminating it from Equation 5.12 because it is dealt with separately.
5. Setting S_{up_ti} (influent UPO COD) = $f_{SL'up} S_{ti}$, where $f_{SL'up}$ is the unbiodegradable COD fraction of the sludge and $S_{up_te} = S_{up_ti}$. Where S_{up_te} is determined as the particulate COD that remains after batch AD has continued for a long solids' retention time (i.e., $> 40d R_s$).

6. Hence, $S_t = S_{bp} + f_{SL'up} \cdot S_{ti} + Z_{AD}$ and therefore,

$$S_{bp} = S_t - f_{SL'up} \cdot S_{ti} - Z_{AD} \quad (5.19)$$

Hence, the best $f_{SL'up}$ estimate is selected that ensures the S_{bp} value of zero (for the long solids retention time) when calibrating the hydrolysis kinetics.

7. Substituting Equation 5.18 for Z_{AD} in 5.19 yields: $S_{bp} = S_t - f_{SL'up} \cdot S_{ti} - Z_{AD_i} - (Y_{AD} \cdot r_{HYD} - b_{AD} \cdot Z_{AD_i}) \cdot \partial t$

$$(5.20)$$

8. Further, substituting Equation 5.16 for r_{HYD} in 5.20 yields:

$$S_{bp_e} = S_t - f_{SL'up} \cdot S_{ti} - Z_{AD_i} - \left(Y_{AD} \cdot \left(b_{AD} \cdot Z_{AD_i} + \frac{(S_{bp_i} - S_{bp_e})}{\partial t} \right) - b_{AD} \cdot Z_{AD_i} \right) \cdot \partial t, \text{ hence}$$

$$S_{bp_e} = \frac{S_t - f_{SL'up} \cdot S_{ti} - Z_{AD_i} - Y_{AD} \cdot b_{AD} \cdot Z_{AD_i} \cdot \partial t - Y_{AD} \cdot S_{bp_i} + b_{AD} \cdot Z_{AD_i} \cdot \partial t}{(1 - Y_{AD})} \quad (5.21)$$

Therefore, with an estimate of $f_{SL'up}$, the COD characteristics (S_{bp_ti} and Z_{AD_ti}) calculated from the parent steady state AD system (See Appendix B for the AD details) and the measured COD from samples withdrawn from the batch AD experiment at given time intervals, S_{bp_t} can be calculated. Then the $f_{SL'up}$ value that, at the longest sludge retention time ($SRT > 40d$) AD batch reactor, yields a calculated S_{bp} of zero is the one selected. With S_{bp_t} known, r_{HYD} and Z_{AD_t} can be calculated from Equations 5.16 and 5.18, respectively. With S_{bp_e} , Z_{AD} and r_{HYD} calculated for each time interval (where there is a corresponding measurement of S_t), the hydrolysis rate kinetic constants (k_M and K_S for saturation hydrolysis kinetics, see Equation 5.11) can be obtained through non-linear regression methods (such as sum of least squares;

Uncini, 2015): via the utilization of curve fitting software (e.g. the R Studio software; an open source statistical package based on the S language). The model to be fitted (i.e. in this case the saturation hydrolysis kinetic formulation) and the model parameters to be estimated (i.e. the k_M and K_S values) are first specified. Thereafter, the R software determines the best parameter values by calculating fitted values for all the data points of the fitting regression model together with the residuals (differences between the fitted and observed values) such the minimum residual sum-of-squares (i.e. calculated from the totaling of residual squares) is obtained. From this process, the kinetic rate constants (k_M and K_S for saturation hydrolysis kinetics) that would provide the closest predictions are selected for application to the AD reactor. Once the kinetic constants have been determined, the calibrated hydrolysis rate equation can be applied to calculate the residual biodegradable organics at a given time (S_{bp_t}). Tables 5.5 – 5.7 show the summary of 3 runs (out of 38 runs conducted) conducted on RStudio software to determine the hydrolysis rate constants (shown at the base of each table). Figures 5.3 – 5.5 also show the plots of the experimentally determined versus predicted hydrolysis rate curve. Out of the 38 runs (including the control runs), 15 runs gave skewed values and were therefore exempted for no further analysis and the following runs were the samples considered for hydrolysis rate predictions: C1, C2, CAve, T1a – C1, T1b – C1, **T1a – C2**, T1b – C2, T1a – CAve, T1Ave – CAve, T2a – C2, **T2a – CAve**, T2Ave – CAve, T3b – C1, T3b – C2, T3a – CA, T3Ave – CAve, T4b – C1, T4a – C2, T4a – CAve, **T4b – CAve**, T5b – C1, T5a – CAve, and T5Ave – CAve. Therefore, the hydrolysis rate constants, EMCs, f'_{sup} of these (23 successful) tested samples along with pre-determined GSA analysis done (by using the SRC method) can now be used to calibrate the University of Cape Town Primary Sedimentation Unit (UCTPSU) model. Kindly note that the three trials (with bold texts) are the samples explained in Tables 5.4 – 5.6 and Figures 5.3 – 5.5. See Appendix H for the complete data set (23 trial tables and plots).

Table 5.4: Measured and predicted hydrolysis rates for run T1a – C2 (by using the hydrolysis rate constants determined from R software)

ABMP_RS (d)	COD	Sbpm	Sbpe	ZAD	rhYd	Sbpe/ZAD (gCOD/gCOD)	Spec rHYD – meas.	Spec rHYD - pred
0	10.18	0.11	-0.79	0.90	0	0		
2	5.07	-4.58	-6.01	1.43	2.64	16.00	1.85	1.89
7	10.637	1.67	1.22	0.45	-0.25	7.10	1.30	1.16
11	9.774	0.73	0.31	0.42	-0.06	3.70	0.68	0.71
17	9.309	0.84	0.66	0.18	-0.05	3.64	0.67	0.70
29	7.594	-0.43	-0.33	-0.10	0.02	3.17	0.58	0.62
32	7.514	-0.49	-0.29	-0.21	0.02	1.39	0.25	0.30
45	7.418	0.34	1.14	-0.80	-0.01	0.36	0.01	0.08

Table 5.5: Measured and predicted hydrolysis rates for run T2a – CAve (by using the hydrolysis rate constants determined from R software)

ABMP_RS (d)	COD	Sbpm	Sbpe	ZAD	rhYd	Sbpe/ZAD (gCOD/gCOD)	Spec rHYD – meas.	Spec rHYD - pred
0.00	10.22	1.70	0.79	0.91	0.00			
2.00	4.01	-4.51	-6.13	1.63	3.50	25.00	2.15	2.22
3.00	2.61	-5.90	-7.67	1.77	2.86	14.03	1.62	1.46
4.00	2.22	-5.41	-7.08	1.67	2.00	10.30	1.20	1.14
5.00	2.34	-5.42	-7.05	1.63	1.61	8.43	0.98	0.96
6.00	2.37	-5.50	-7.11	1.60	1.35	7.23	0.84	0.84
7.00	1.74	-6.47	-8.15	1.69	1.32	6.67	0.78	0.79
23.00	7.56	0.79	0.62	0.17	0.04	3.71	0.27	0.46
32.00	6.71	-0.20	-0.16	-0.04	0.07	2.90	0.22	0.37

Table 5.6; Measured and predicted hydrolysis rates for run T4b – CAve (by using the hydrolysis rate constants determined from R software)

ABMP_RS (d)	COD	Sbpm	Sbpe	ZAD	rhYd	Sbpe/ZAD (gCOD/gCOD)	Spec rHYD – meas.	Spec rHYD - pred
0.00	9.42	0.70	-0.21	0.91	0.00			
2.00	6.53	-2.19	-3.40	1.20	1.63	18.75	1.36	1.28
3.00	6.31	-2.40	-3.59	1.19	1.17	12.00	0.98	1.10
4.00	9.69	1.86	1.25	0.61	-0.33	2.04	0.48	0.37
6.00	9.63	1.55	0.98	0.58	-0.16	1.69	0.29	0.31
15.00	6.63	-0.85	-1.40	0.55	0.12	1.24	0.21	0.24
17.00	7.98	0.38	0.07	0.32	0.02	0.21	0.07	0.05

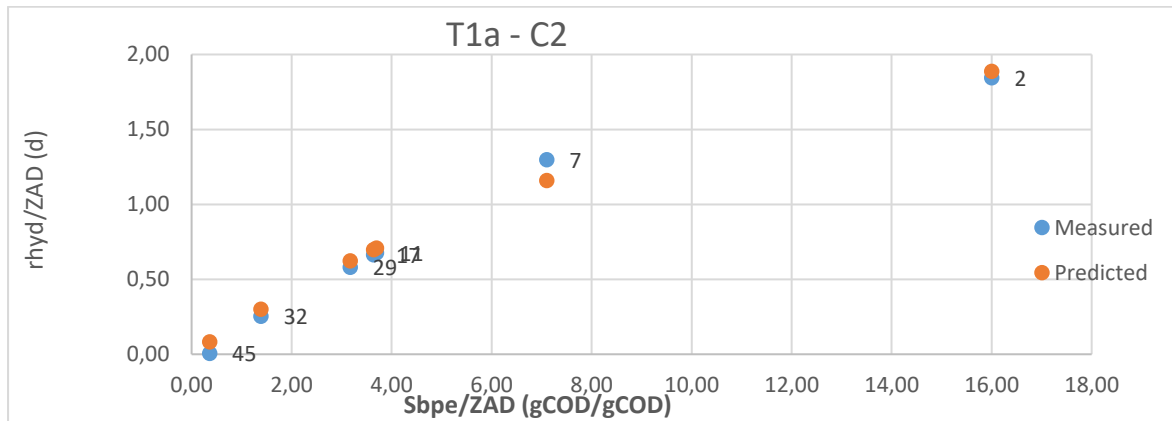


Figure 5.3 (directly above) shows the measurement of specific hydrolysis rate against residual BPO compared with predicted plot (by using the determined k_M of 3.78 and k_S of 16.061).

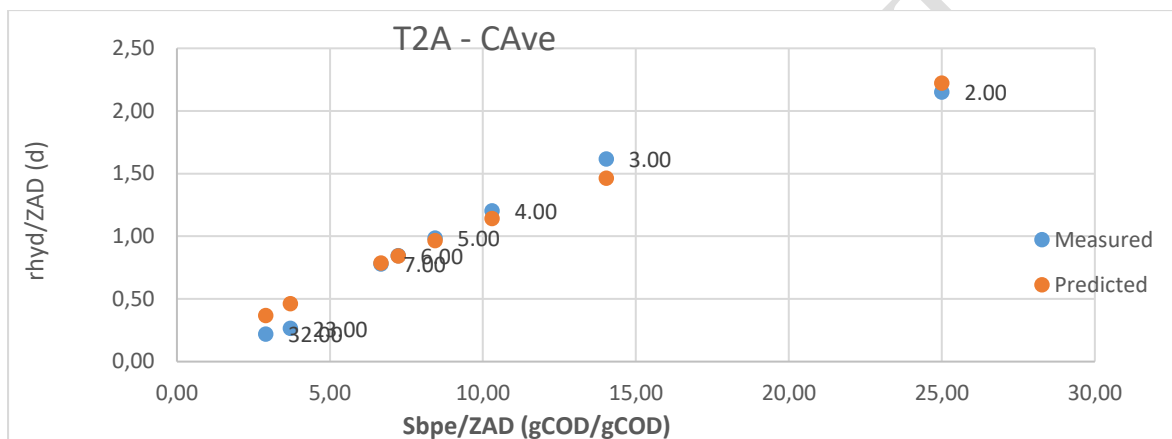


Figure 5.4 (directly above) shows the measurement of specific hydrolysis rate against residual BPO compared with predicted plot (by using the determined k_M of 6.63 and k_S of 49.57).

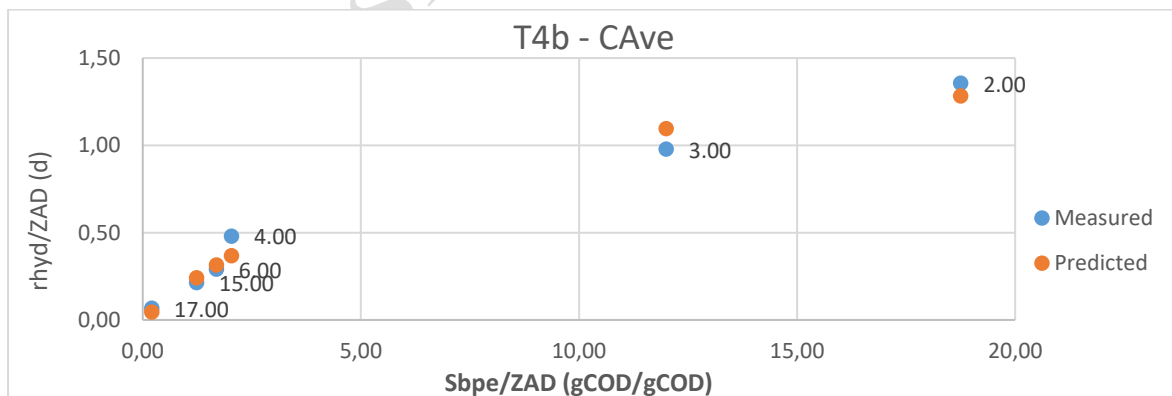


Figure 5.5 (directly above) shows the measurement of specific hydrolysis rate against residual BPO compared with predicted plot (by using the determined k_M of 1.84 and k_S of 8.21).

To find the S_{bpe} in terms of the saturation kinetics with k_M and K_S known, Equation 5.16 for r_{HYD} and Equation 5.18 that defined Z_{AD} are applied to the saturation kinetic Equation 5.21 in the following way:

1. Using the initial concentration at time $t=0$ and the determined k_M and K_S values, the transient terms in the biological kinetic equations with finite difference terms, e.g.

$$\delta S_{bp}/\delta t = (S_{bp \text{ time } 2} - S_{bp \text{ time } 1})/\Delta t \quad (5.22)$$

$$\text{hence } S_{bp \text{ time } 2} = S_{bp \text{ time } 1} + \Delta t (\delta S_{bp}/\delta t) \quad (5.23)$$

where Δt is the time interval between time 2 and time 1.

2. Where $r_{HYD \text{ time } 1}$ is from Equation 5.11 can be given as:

$$r_{HYD \text{ time } 1} = \frac{k_M \cdot \left(\frac{S_{bp \text{ time } 1}}{Z_{AD \text{ time } 1}} \right)}{K_S + \left(\frac{S_{bp \text{ time } 1}}{Z_{AD \text{ time } 1}} \right)} Z_{AD \text{ time } 1} \quad (5.24)$$

And δS_{bp} from Equation 5.16 can be given as:

$$\partial S_{bp} = (r_{HYD} - b_{AD} \cdot Z_{AD_i}) \cdot \partial t \quad (5.25)$$

Substitute the transients in the finite difference equations (e.g. $\delta S_{bp} / \delta t$) by the respective biological kinetic equations, i.e.:

$$Z_{AD \text{ time } 2} = Z_{AD \text{ time } 1} + \partial Z_{AD} = Z_{AD \text{ time } 1} + (Y_{AD} \cdot r_{HYD} - b_{AD} \cdot Z_{AD \text{ time } 1}) \cdot \Delta t \quad (5.26)$$

$$S_{bp \text{ time } 2} = S_{bp \text{ time } 1} + \partial S_{bp} = S_{bp \text{ time } 1} + (r_{HYD} - b_{AD} \cdot Z_{AD \text{ time } 1}) \cdot \Delta t \quad (5.27)$$

3. Write a computer software or spreadsheet to repeat the calculation from the initial conditions by stepping forward in time. This is done by setting the previous step end value equal to the beginning value of the next step. This is done with selected low step length ($\Delta t = 10$ mins, i.e., 5760 steps to make 40 days of integration) to ensure a stable integration.

The procedures that described in this section allows determination of the unbiodegradable particulate COD fraction, $f_{SL'up}$ (also, see Section 4.3.2) and saturation kinetic rate constants for hydrolysis from experimentally measured batch AD results. Having determined the hydrolysis rate constant and f'_{sup} as summarized in Table 5.7 (below), the UCTSDM3P will now be implemented for the ABMP parameter estimation.

5.4 IMPLEMENTATION OF UCTSDM3P FOR ABMP PARAMETER ESTIMATION

A dynamic model for the simulation of augmented biochemical methane potential (ABMP) tests, to estimate the composition of a homogenous biodegradable particulate organic sample has been developed by Botha (2015). According to Botha and Ekama (2015), the same AD model (UCTSDM3P; Ikumi *et al.*, 2015; Ghoor, 2020) is used to simulate ABMP test conditions to determine the composition (x , y , z , a and b in $C_xH_yO_zN_aP_b$) and the hydrolysis kinetic rates for the substrate fed into the AD system. This integration was possible by assuming the substrate is homogeneous and the virtual AD system is run under batch conditions. The following PE procedure as used by Botha and Ekama (2015) was applied towards simulation of the experimental data within the ABMP experimental environment:

Setting the initial values in the 5 l ABMP virtual systems to zero, apart from 5000 ml of water comprising some as the initial reactor contents in order to prevent model errors that would occur due to initialisation equations that require division by mass of water in the system (i.e., the mass of H_2O has to then be > 0). In order to ensure equal volume in the triplicate samples and optimal feed dilution (or potential inhibition of the biological organisms), 5000 ml of water as the initial mass was used in the ABMP test procedure. (Angelidaki *et al.*, 2009; Botha and Ekama, 2015). Figure 5.6 shows the ABMP Configuration for parameter estimation using WEST® simulation platform while Figure 5.7 shows the parameters defined in WEST for proposed simulation.

The AD model simulated under batch (ABMP) conditions required setting the outflow to zero, instantaneous feeding (the whole 5 l volume fed over 1 minute) of the initial digester content, including the concentrations of biomass inoculum (seed) and substrate. Simulating the entrance of digester contents into the batch environment (rather than including them directly as part of initial reactor mass) allowed for parameter controlled fractionation of the initial feed and inoculum components (e.g., the volatile settleable solids (VSS) could be entered directly and divided and distinguished during simulations between its unbiodegradable ($f_{U_Inf} * VSS$) and unbiodegradable ($(1 - f_{U_Inf}) * VSS$) components, using a fractionating parameter (i.e., f_{U_Inf}). This is because the model has limitations in fractionating the declared initial reactor masses but is capable of fractionating influent component concentrations during

simulation. The intrinsic fractionation of initial concentrations into model components that could not be individually measured is the step 1 of parameter estimation. Once the component concentrations are determined, the parameter estimation (PE) function of WEST® simulation platform is used to calculate selected unknown parameters by varying them until the model output is fitting with the measured data (Botha, 2015; Gaszynski *et al.*, 2019). For this to occur, the experimentally measured data is entered into WEST® in a text file that contains the measured ABMP output values of variables such as COD, VSS, ammonia (FSA), orthophosphates (OP), pH and alkalinity (see Figure 5.8 below). The required parameters (those that would define the characteristics of the sludge being digested, i.e.: the y , z , a and b values of $C_1H_yO_zN_aP_b$) are then set as targets for the simulation and given realistic constraints (upper and lower bound values) to adhere to. The simulation then ran multiple iterations (as depicted in Figure 5.9), whereby (through parameter variations within the given constraints) the theoretically predicted variables are adjusted towards meeting the experimentally measured data. The multiple iterations progressed until the parameter values that resulted in the best match between models predicted and experimentally observed variables was achieved.

The ABMP test that virtually replicate the ones run experimentally (i.e., including both the control (run with inoculum only) and the test (with both inoculum and organics) are simulated. The control ABMP is simulated first and the test ABMP is simulated afterwards, using information obtained from the PE performed on the control ABMP. In the simulated control ABMP, the PE and measured output variables are used to determine the unbiodegradable fraction and the elemental composition of biomass in the inoculum seed. To initiate this process the biomass concentration is first estimated. Since the inoculum seed is sourced from the AD system run at steady state (see Section 3.3), the steady state AD equations of Sötemann *et al.* (2005) were used, with a combined AD organism yield (Y_{AD}) value of 0.113, to estimate the biomass concentration (see Equation 5.8). This concentration is entered into the initial values of the simulated ABMP, and parameters added to define the various AD biomass components (i.e., acidogens, acetogens, acetoclastic methanogens and hydrogenotrophic methanogens) as fractions of the total biomass concentration. These parameterised fractions are calibrated using the PE procedure.

The ABMP test simulation is subsequent to the ABMP control simulation, with the ‘initial parameters’ that are associated with the inoculum seed and the biomass present, having already been determined from the ABMP control simulation. From the ABMP test simulation, the unbiodegradable fraction of the substrate and the elemental composition of its BPO can now be calculated, using the same PE exercise described above; i.e., iterations are done towards achieving the best match between the model predicted and measured ABMP test output variable data. The compositions determined by the PE for the biodegradable particulate organics in control sample and each settleometer column samples as detailed in Table 5.7 below (showing the order of increasing column number, from column 1 to column 5): are $C_{2.193}H_{7}O_{0.440}N_{0.215}P_{0.029}$, $C_{2.883}H_{7}O_{1.870}N_{0.372}P_{0.0701}$, $C_{2.909}H_{7}O_{1.843}N_{0.339}P_{0.0004}$, $C_{2.834}H_{7}O_{1.841}N_{0.286}P_{0.00001}$, $C_{2.868}H_{7}O_{1.850}N_{0.312}P_{0.00053}$, $C_{2.881}H_{7}O_{1.848}N_{0.291}P_{0.094}$.

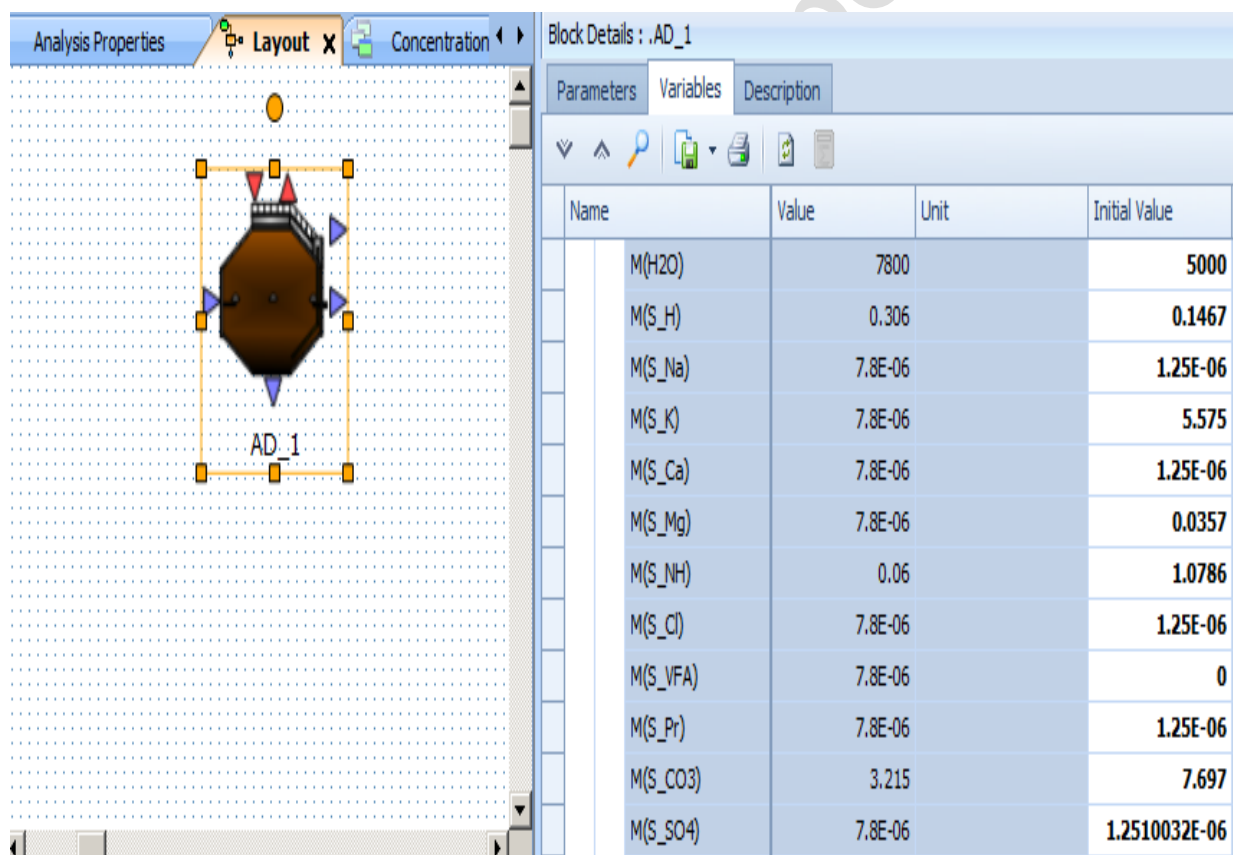


Figure 5.6 (above): ABMP Configuration for Parameter Estimation

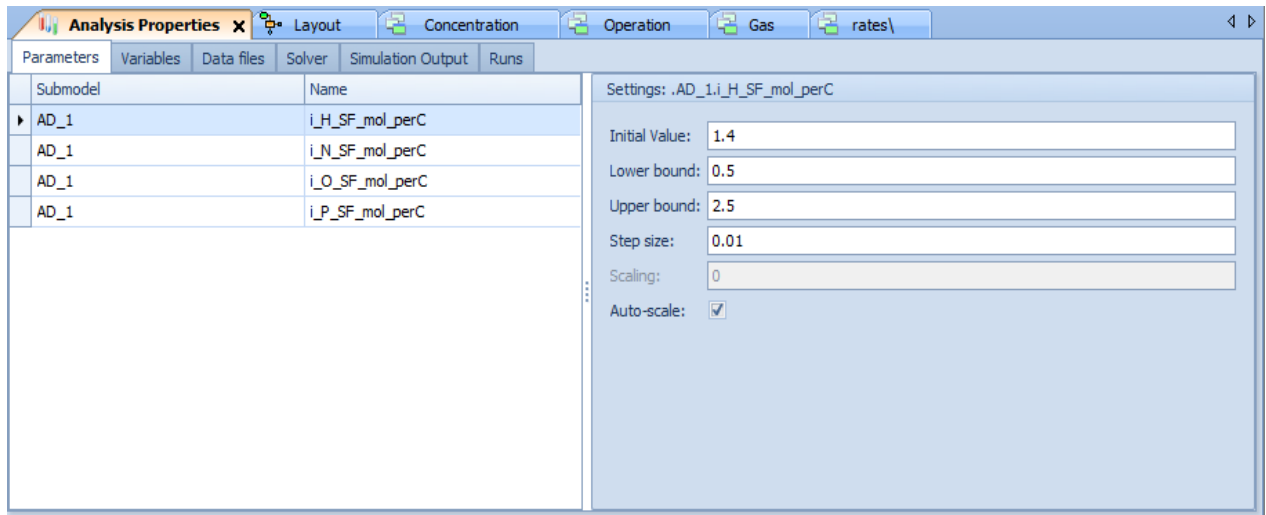


Figure 5.7 (above): Parameter Definition in WEST for Proposed Simulation

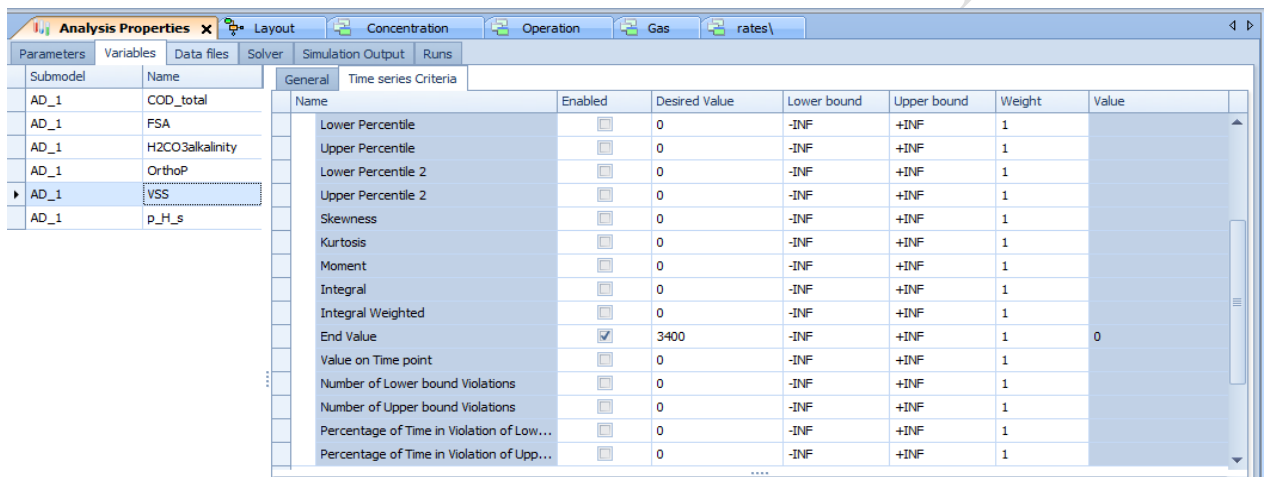


Figure 5.8 (above): Measured Variables for Proposed WEST Simulation

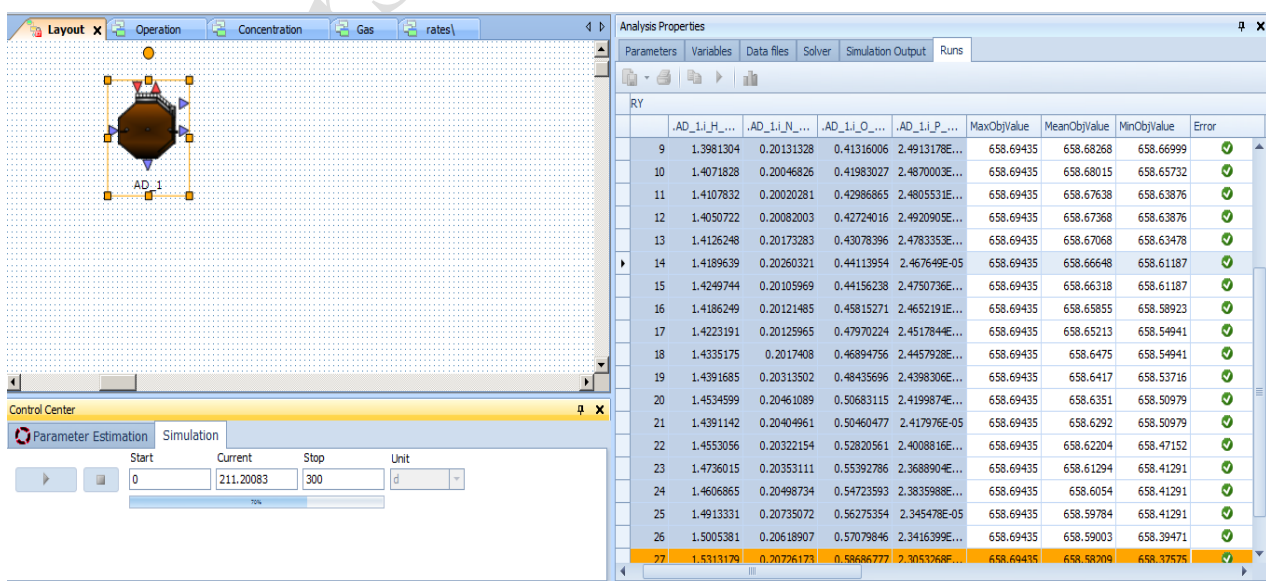


Figure 5.9 (above): WEST iteration process using ABMP Experimental Data

Table 5.7: Summary of ABMP hydrolysis rate constants (k_M and k_S) and f'_{Sup} for 23 successful runs using Settlemeter Run 3 Samples												
X		.i_P_Org_mol_perC	.i_N_Org_mol_perC	.i_O_Org_mol_perC	.i_H_Org_mol_perC	C	k_S	k_M	f'_{Sup}	Settling Vel. (m/h)	Parameters	
2.202		0.000	0.11	0.400	3.179	1	-	-	0.77	-	C1	
2.188		0.040	0.09	0.100	3.200	1	-	-	0.58	-	C2	
2.188		0.000	0.09	0.100	3.199	1	-	-	0.67	-	CAve	
2.801		0.050	0.10	0.650	2.499	1	21.1	8.6	0.58	31.61	T1a - C1	
5.000		0.000	0.20	0.400	1.400	1	552	234.	0.40	31.61	T1b - C1	
2.801		0.050	0.10	0.650	2.499	1	16.0	3.7	0.71	31.61	T1a - C2	
2.984		0.000	0.10	0.649	2.346	1	21.1	8.62	0.53	31.61	T1b - C2	
2.817		0.000	0.10	0.650	2.484	1	14.2	3.9	0.64	31.61	T1a - Cave	
2.813		0.050	0.10	0.648	2.488	1	21.1	8.6	0.55	31.61	T1ave - Cave	
3.063		0.000	0.10	0.639	2.285	1	98.2	8.7	0.72	14.13	T2a - C2	
2.892		0.000	0.16	0.602	2.420	1	49.5	6.6	0.66	14.13	T2a - Cave	
2.811		0.000	0.10	0.645	2.490	1	74.9	140.	0.50	14.13	T2ave - Cave	
5.000		0.000	0.20	0.400	1.400	1	2.72	1.2	0.38	8.65	T3b - C1	
5.000		0.000	0.20	0.400	1.400	1	5.92	3.1	0.51	8.65	T3b - C2	
2.801		0.000	0.10	0.649	2.499	1	5.74	2.3	0.47	8.65	T3a - Cave	
6.080		0.000	0.11	0.619	1.151	1	11.1	1.9	0.53	8.65	T3ave - Cave	
5.000		0.000	0.20	0.410	1.400	1	5.71	2.7	0.47	3.57	T4b - C1	
2.928		0.000	0.10	0.648	2.391	1	16.9	2.0	0.62	3.57	T4a - C2	
4.973		0.000	0.19	0.407	1.407	1	6.82	1.7	0.55	3.57	T4a - Cave	
13.99		0.000	0.32	0.200	0.500	1	2.92	1.3	0.31	14.13	T5a - C1	
4.181		0.000	0.13	0.625	1.674	1	5.80	3.3	0.38	14.13	T5a - Cave	
3.009		0.000	0.10	0.625	2.326	1	17.1	2.2	0.43	14.13	T5ave - Cave	
12.01		0.02	0.20	0.40	1.40	1.	UPO &ER					
4	Charge (e-)						0					

Y		7.00	0.88	0.25	0.00	13.29	51.13	2.08	0.51	0.138	0.2	0.069	0.000
Z		7.00	0.21	0.19	0.08	15.16	42.31	2.86	0.62	0.167	0.0	0.065	0.064
A		7.00	0.21	0.19	0.00	14.72	39.61	2.97	0.66	0.178	0.0	0.070	0.000
B		7.00	1.82	0.28	0.14	14.42	78.08	1.47	0.43	0.090	0.3	0.050	0.056
EDC		7.00	2.00	1.40	0.00	18.80	118.7	1.26	0.50	0.059	0.2	0.165	0.000
MM		7.00	1.82	0.28	0.14	14.42	78.08	1.47	0.43	0.090	0.3	0.050	0.056
f _{cv}		7.00	1.93	0.32	0.00	14.10	78.37	1.43	0.45	0.090	0.3	0.058	0.000
f _c		7.00	1.83	0.28	0.00	13.75	74.17	1.48	0.45	0.095	0.3	0.054	0.000
f _h		7.00	1.82	0.28	0.14	14.46	78.33	1.47	0.43	0.090	0.3	0.050	0.056
f _o		7.00	1.95	0.31	0.00	14.41	79.53	1.44	0.46	0.089	0.3	0.055	0.000
f _n		7.00	1.74	0.47	0.00	13.67	76.27	1.43	0.45	0.093	0.3	0.087	0.000
f _p		7.00	1.81	0.28	0.00	13.76	73.82	1.49	0.45	0.096	0.3	0.054	0.000
MassRatio_SumTotal		7.00	2.00	1.00	0.00	20.00	113.1	1.41	0.53	0.062	0.2	0.124	0.000
		7.00	2.00	1.00	0.00	20.00	113.1	1.41	0.53	0.062	0.2	0.124	0.000
		7.00	1.81	0.28	0.00	13.70	73.84	1.48	0.45	0.096	0.3	0.055	0.000
		7.00	3.76	0.67	0.00	21.76	149.7	1.16	0.48	0.047	0.4	0.064	0.000
		7.00	2.05	1.00	0.00	19.90	113.9	1.39	0.52	0.062	0.2	0.123	0.000
		7.00	1.89	0.29	0.00	14.04	76.71	1.46	0.45	0.092	0.3	0.054	0.000
		7.00	2.02	0.99	0.00	19.87	113.1	1.40	0.52	0.062	0.2	0.123	0.000
		7.00	2.79	4.47	0.00	43.94	282.6	1.24	0.59	0.025	0.1	0.222	0.000
		7.00	2.61	0.58	0.00	16.75	107.2	1.24	0.46	0.066	0.3	0.076	0.000
		7.00	1.88	0.30	0.00	14.35	77.62	1.47	0.46	0.091	0.3	0.056	0.000
		1.00	15.9	14.0	30.9	-	-	-	-	-	-	-	-
		8	99	07	74	-	-	-	-	-	-	-	-
		1	-2	-3	5	-	-	-	-	-	-	-	-

Table 5.8: TSS fractionation from ABMP Experimental Readings showing settling velocities, TSS component concentrations and mass compositions.

PVC_3a	PVC_2Ave	PVC_2b	PVC_2a	PVC_1Ave	PVC_1b	PVC_1a	Control_Ave	Control_2	Control_1	Samples
8.6506	14.131	14.131	14.131	31.608	31.608	31.608	-	-	-	Settling velocity
19.16%	18.09%	24.39%	14.53%	21.55%	24.22%	19.29%	21.44%	24.44%	18.57%	ISS
1961.984	1793.0808	2368.7568	1469.2736	2335.589	2624.9636	2090.6502	907.5552	1034.5452	786.0681	ISS(mg/l)
51.80%	46.60%	36.00%	56.60%	47.20%	41.70%	52.80%	52.90%	43.50%	62.80%	UPO
5304.32	4618.992	3496.32	5723.392	5115.536	4519.446	5722.464	2239.257	1841.355	2658.324	UPO (mg/l)
29.00%	35.30%	39.70%	28.90%	31.20%	34.10%	27.90%	25.70%	32.10%	18.70%	BPO
2969.6	3498.936	3855.664	2922.368	3381.456	3695.758	3023.802	1087.881	1358.793	791.571	BPO (mg/l)
100.00%	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%	TSS
10240	9912	9712	10112	10838	10838	10838	4233	4233	4233	TSS (mg/l)
2.83409	2.90944			2.88274			2.19276			Xave
7	7			7			7			Yave
1.84088	1.84333			1.86977			0.43991			Zave
0.28619	0.33912			0.3723			0.21521			Aave
0.00001	0.00004			0.07013			0.02917			Bave
1	1			1			1			C
2.46993	2.40596			2.42824			3.19233			.i_H_Org_mol_perC
0.64955	0.63357			0.64861			0.20062			.i_O_Org_mol_perC
0.10098	0.11656			0.12915			0.09815			.i_N_Org_mol_perC
0	0.00001			0.02433			0.0133			.i_P_Org_mol_perC

	PVC_5Ave	PVC_5b	PVC_5a	PVC_4Ave	PVC_4b	PVC_4a	PVC_3Ave	PVC_3b
	3.575	3.575	3.575	5.7909	5.7909	5.7909	8.6506	8.6506
	21.41%	21.89%	21.06%	23.94%	24.56%	23.45%	22.25%	26.41%
	2303.716	2355.364	2266.056	2499.336	2564.064	2448.18	2278.4	2704.384
	40.70%	37.20%	44.20%	48.60%	44.80%	52.40%	45.90%	39.60%
	4379.32	4002.72	4755.92	5073.84	4677.12	5470.56	4700.16	4055.04
	37.90%	40.90%	34.70%	27.40%	30.60%	24.20%	31.90%	34.00%
	4078.04	4400.84	3733.72	2860.56	3194.64	2526.48	3266.56	3481.6
	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%
	10760	10760	10760	10440	10440	10440	10240	10240
	2.8807	2.8807	2.8807	2.868	2.868	2.868	2.868	2.868
	7	7	7	7	7	7	7	7
	1.84756	1.84756	1.84756	1.84989	1.84989	1.84989	1.84989	1.84989
	0.29066	0.29066	0.29066	0.31248	0.31248	0.31248	0.31248	0.31248
	0.09389	0.09389	0.09389	0.00053	0.00053	0.00053	0.00053	0.00053
	1	1	1	1	1	1	1	1
	2.42996	2.42996	2.42996	2.44073	2.44073	2.44073	2.44073	2.44073
	0.64136	0.64136	0.64136	0.64501	0.64501	0.64501	0.64501	0.64501
	0.1009	0.1009	0.1009	0.10895	0.10895	0.10895	0.10895	0.10895
	0.03259	0.03259	0.03259	0.00018	0.00018	0.00018	0.00018	0.00018
ISS	Inorganic Settleable Solids							
UPO	Unbiodegradable Particulate Organics							
BPO	Biodegradable Particulate Organics							
TSS	Total Settleable Solids							
PVC_i	Where (i = 1, 2, 3, 4 and 5) represent the settleometer columns							
a, b	Either of the two represents the first fetched sample (say, a) and the other is a duplicate							
Ave	Means taking the average of a particular sample and its duplicate from each PVC column.							

Following the experimentally measured hydrolysis rate and predicted rate constants (see Table 5.7), over 60% of the trials gave acceptable kinetic rate constants across the 5 columns and controls samples. The determined f'_{sup} showed that larger portion of the settled VSS was

unbiodegradable and will therefore increase should PS retention time increase (see Tables 5.7 and 5.8). The biodegradable VSS are the portion of the VSS affected by these two kinetic constants, namely: hydrolysis rate constant for BPO_PS (k_M) and half-saturation coefficient for BPO_PS (k_S). It was observed that the rate constants varied across the trial runs done on the samples, and sludge composition (not concentration) in each trial was reason to have influenced the hydrolysis rates. These findings (hydrolysis rate constants, f'_{sup} and EMCs) will be incomplete if they are not coupled with the sensitivity analysis of the UCTPSU model.

5.5 GLOBAL SENSITIVITY ANALYSIS FOR UCTPSU MODEL

The four primary uses of sensitivity analysis have been outlined by Takács *et al.* (2008):

1. To study the model parameters that require highest priority (i.e. most positive or most negative effect) for rigorous and regular testing.
2. To approve decisions intuitively made for model parameters in prediction of model output variables.
3. Helps in developing a sampling program to gather data for the particular process objective to target the most sensitive model elements (Ikumi, 2011).
4. To assist in examining the strength of assumptions made in model development, by assessing whether the models are overly-dependent on such assumptions, such that parameters value interactions produce extreme model output values (Ikumi *et al.*, 2012).

In this study, sensitivity analysis is performed to identify significant parameters and highlight those required for experimental determination as it relates to the primary settling tank unit. The sensitivity analysis exercise was performed using the Standardised Regression Coefficients (SRC) method, and the theory behind this method and its results are explained using Neumann (2012) proposed objectives.

5.5.1 DETERMINATION OF THE STANDARD REGRESSION COEFFICIENT (SRC)

The sensitivity analysis method applied in this study was the determination of Standard Regression Coefficients (SRC; based on regression). In order to obtain the desired SRC values, the following procedures were followed:

1. Model output variables that required assessment were selected, according to the model calibration objectives. The selected variables are ISS_under, Out_X_B_Inf, Out.X_ISS, Out.X_U_Inf, Out.X_VSS, TSS_Under_s, Under_X_B_Inf, Under_X_U_Inf, Under_X_VSS, and VSS_Under_s (see Table 5. 9 below, for full description). For a system operated at steady state, to assess the uncertainty of these output variables their predicted results after a time equivalent of three sludge ages are the ones captured. Hence the UCTPSU model was run to steady state as shown in Figure 5.10 (below).

Table 5.9 Description of the selected UCTPSU Model Derived Variables for GSA

S/N	Variables	Description
1	ISS_Under	Inorganic settleable solids in the PST underflow
2	Out_X_B_Inf	Influent biodegradable particulate organics in the PST overflow
3	Out.X_ISS	Inorganic settleable solids in the PST overflow
4	Out.X_U_Inf	Influent unbiodegradable particulate organics in the PST overflow
5	Out.X_VSS	Volatile settleable solids in the PST overflow
6	TSS_Under_s	Sub-component total settleable solids in the PST underflow
7	Under_X_B_Inf	Influent biodegradable particulate organics in the PST underflow
8	Under_X_U_Inf	Influent unbiodegradable particulate organics in the PST underflow
9	Under_X_VSS	Volatile settleable solids in the PST underflow
10	VSS_Under_s	Sub-component volatile settleable solids in the PST underflow

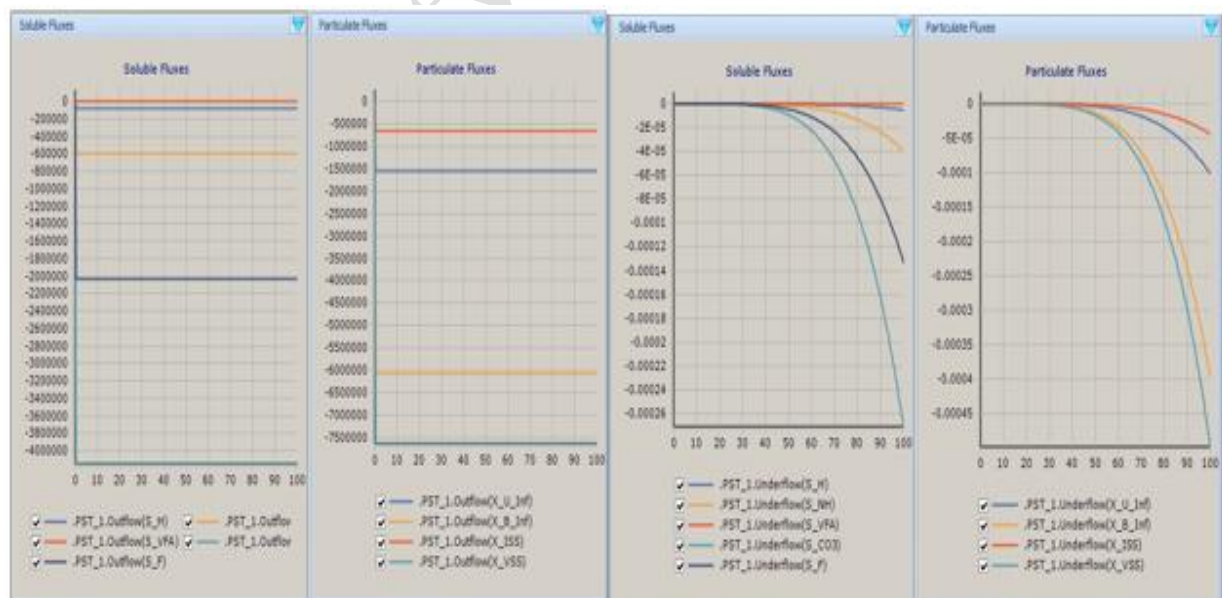


Figure 5.10 the UCTPSU model run at steady state as shown in the outflow fluxes and underflow fluxes of the UCTPSU model.

The underflow, even though shows different outlines for the observed variables, can be said to have similar slopes with increasing retention time at a fixed PST volume. The graph clearly depicts that high magnitude of flow rate was observed from the influent PST (hereby making the retention time almost zero) which however reduced over time. This clearly explains the effect of dynamic flow rate on the retention time and the wastewater characteristics inherent in the PST, and this probably explains the similar slope observed in the underflow PST.

2. For each of the model parameters, value range was specified as obtained from experiment and literature (Ikumi, 2011) and characterised using the method proposed by Brun *et al.* (2002). Brun *et al.* (2002) considered three classes (below) of model parameters relative to their uncertainty degree:

- a. Accurately known – these have a relative uncertainty of 5% (class 1).
- b. Moderately inaccurately known parameters with a relative uncertainty of 20% (class 2).
- c. Very poorly known parameters with a relative uncertainty of 50% (Class 3).

According to Ikumi *et al.* (2015), most kinetic parameters for PW_SA have been classified to class 2, apart from biomass specific growth rate constants which were placed in class 1 and hydrolysis kinetic constants which were placed in class 3. Stoichiometric yield value parameters that belong to the biomass are deemed not to vary significantly for different systems, hence are placed in Class 1. However, stoichiometric influent material characterisation parameters (the X, Y, Z, A and B values in the $C_xH_yO_zN_A P_B$ elemental formulation of each influent component) were all placed into class three since they are mainly specific to the feed source. The parameters (P_i) that were chosen in the UCTPSU model are as shown in the Table 5.10 and Figure 5.11, highlighting 70 parameters in total).

3. To initiate the sensitivity analysis process, uncertainty propagation was conducted by a Monte Carlo (MC) simulation of the model by random sampling of parameter values (Martin *et al.*, 2010). The parameter value ranges (i.e., lower (θ_{i_min}) and upper (θ_{i_max}) prior bounds for the MC simulation were chosen according to the method proposed by Brun *et al.* (2002). These parameters were assumed to be uniformly distributed within their ranges. One thousand (1000) simulations were performed using the WEST® software (Vanhooren *et al.*, 2003), with 1000 sets of random parameter values generated in this way, to provide 1000 sets of values for the selected output variables, which could then be

visualized as histograms or density distributions or characterized in terms of descriptive statistics.

4. At the end 1000 runs of the MC simulation, the results were exported to Microsoft Excel spreadsheet. The mean and standard deviation (SD) for all the MC simulation outputs were determined and these MC simulation data was standardized. The data file was then saved with a different excel format (comma separated values, CSV).

Table 5. 10: Parameters used in simulating the modified UCTPSU Model

S/N	Parameters					
	Type	Name	Description	Initial Value	Units	Class
1	Fractionation	Alpha_B	1st group of BPO settling fraction	0.02	-	1
2		Alpha_I	1st group of ISS settling fraction	0.32	-	1
3		Alpha_U	1st group of UPO settling fraction	0.33	-	1
4		Beta_B	2nd group of BPO settling fraction	0.05	-	1
5		Beta_I	2nd group of ISS settling fraction	0.22	-	1
6		Beta_U	2nd group of UPO settling fraction	0.2	-	1
7		Gamma_B	3rd group of BPO settling fraction	0.1	-	1
8		Gamma_I	3rd group of ISS settling fraction	0.15	-	1
9		Gamma_U	3rd group of UPO settling fraction	0.17	-	1
10		Lambda_B	4th group of BPO settling fraction	0.17	-	1
11		Lambda_I	4th group of ISS settling fraction	0.11	-	1
12		Lambda_U	4th group of UPO settling fraction	0.12	-	1
13		f_U_Inf	Fraction of InfluentVSS_Inf that is unbiodegradable particulate organic substrate	0.15	-	1
14	Composition	ISS_BM	ISS to biomass for Xoh and Xpa	0.15	-	1
15	Settling	X_Lim	Minimal concentration in sludge blanket	900	mgTSS/l	2
16		X_T	Threshold suspended solids concentration	3000	mgTSS/l	2
17	Kinetics	KS_BInf_AD_hyd	Half sat coeff. for BPO_PS (for sewage organics)	10.124	mg/l	2
18		KS_BOrg_AD_hyd	Half sat coeff. for BPO (for organics from biomass death)	10.37	mg/l	2
19		K_ALK	Saturation coeff. for alkalinity (HCO ₃ ⁻)	0.1	mg/l	2
20		TempCoeff	Rate temperature coefficient	0.0667	-	2
21		Tref	System Temperature	30	degC	2
22		kH_F_AD_hyd	Hydrolysis rate constant for FSO	10	1/d	3
23		kM_BInf_AD_hyd	Hydrolysis rate constant for BPO_PS	2.004	1/d	1
24		kM_BOrg_AD_hyd	Hydrolysis rate constant for BPO	1.95	1/d	1
25		Vs_s_X_B_Inf1	Settling velocities for sub_component_X_B_Inf1	127.2	m/hr	2
26		Vs_s_X_B_Inf2	Settling velocities for sub-component_X_B_Inf2	88.8	m/hr	2
27		Vs_s_X_B_Inf3	Settling velocities for sub-component_X_B_Inf3	50.4	m/hr	2
28		Vs_s_X_B_Inf4	Settling velocities for sub-component_X_B_Inf4	21.6	m/hr	2
29		Vs_s_X_B_Inf5	Settling velocities for sub-component_X_B_Inf5	5.5	m/hr	2

30		Vs_s_X_ISS1	Settling velocities for sub-component_X_ISS1	127.2	m/hr	2
31		Vs_s_X_ISS2	Settling velocities for sub-component_X_ISS2	88.8	m/hr	2
32		Vs_s_X_ISS3	Settling velocities for sub-component_X_ISS3	50.4	m/hr	2
33		Vs_s_X_ISS4	Settling velocities for sub-component_X_ISS4	21.6	m/hr	2
34		Vs_s_X_ISS5	Settling velocities for sub-component_X_ISS5	5.5	m/hr	2
35		Vs_s_X_U_Inf1	Settling velocities for sub-component_X_U_Inf1	127.2	m/hr	2
36		Vs_s_X_U_Inf2	Settling velocities for sub-component_X_U_Inf2	88.8	m/hr	2
37		Vs_s_X_U_Inf3	Settling velocities for sub-component_X_U_Inf3	50.4	m/hr	2
38		Vs_s_X_U_Inf4	Settling velocities for sub-component_X_U_Inf4	21.6	m/hr	2
39		Vs_s_X_U_Inf5	Settling velocities for sub-component_X_U_Inf5	5.5	m/hr	2
40	Stoichiometry	i_Ca_PP_mol_perP	Molar fraction of Ca/P in polyphosphate	0.026	dUnit/dUnit	3
41		i_H_Org_mol_perC	H/C : organisms	1.463	dUnit/dUnit	2
42		i_H_SF_mol_perC	H/C : fermentable soluble	2.01	dUnit/dUnit	3
43		i_H_SU_mol_perC	H/C: unbiodegradable soluble	1.646	dUnit/dUnit	2
44		i_H_XBInf_mol_perC	H/C: PS biodegradable particulate	2.19	dUnit/dUnit	3
45		i_H_XBOrg_mol_perC	H/C: biodegradable particulate	1.463	dUnit/dUnit	2
46		i_H_XUInf_mol_perC	H/C: unbiodegradable particulate	1.482	dUnit/dUnit	2
47		i_H_XUOrg_mol_perC	H/C: endogenous residue	1.482	dUnit/dUnit	2
48		i_K_PP_mol_perP	Molar fraction of K/P in polyphosphate	0.31506	dUnit/dUnit	3
49		i_Mg_PP_mol_perP	Molar fraction of Mg/P in polyphosphate	0.31669	dUnit/dUnit	3
50		i_N_Org_mol_perC	N/C : organisms	0.229	dUnit/dUnit	3
51		i_N_SF_mol_perC	N/C: fermentable soluble	0.119	dUnit/dUnit	3
52		i_N_SU_mol_perC	N/C: unbiodegradable soluble	0.062	dUnit/dUnit	3
53		i_N_XBInf_mol_perC	N/C: PS biodegradable particulate	0.0643	dUnit/dUnit	3
54		i_N_XBOrg_mol_perC	N/C: biodegradable particulate	0.229	dUnit/dUnit	3
55		i_N_XUInf_mol_perC	N/C: unbiodegradable particulate	0.113	dUnit/dUnit	3
56		i_N_XUOrg_mol_perC	N/C: endogenous residue	0.113	dUnit/dUnit	3
57		i_O_Org_mol_perC	O/C : organisms	0.355	dUnit/dUnit	3
58		i_O_SF_mol_perC	O/C : fermentable soluble	0.592	dUnit/dUnit	3
59		i_O_SU_mol_perC	O/C: unbiodegradable soluble	0.593	dUnit/dUnit	3
60		i_O_XBInf_mol_perC	O/C: PS biodegradable particulate	0.653	dUnit/dUnit	3
61		i_O_XBOrg_mol_perC	O/C: biodegradable particulate	0.355	dUnit/dUnit	3
62		i_O_XUInf_mol_perC	O/C: unbiodegradable particulate	0.472	dUnit/dUnit	3
63		i_O_XUOrg_mol_perC	O/C: endogenous residue	0.472	dUnit/dUnit	3
64		i_P_Org_mol_perC	P/C : organisms	0.031	dUnit/dUnit	3
65		i_P_SF_mol_perC	P/C: fermentable soluble	0.012	dUnit/dUnit	3
66		i_P_SU_mol_perC	P/C: unbiodegradable soluble	0.02	dUnit/dUnit	3
67		i_P_XBInf_mol_perC	P/C: PS biodegradable particulate	0.0097	dUnit/dUnit	3
68		i_P_XBOrg_mol_perC	P/C: biodegradable particulate	0.031	dUnit/dUnit	3
69		i_P_XUInf_mol_perC	P/C: unbiodegradable particulate	0.022	dUnit/dUnit	3
70		i_P_XUOrg_mol_perC	P/C: endogenous residue	0.022	dUnit/dUnit	3

The standard regression coefficients (SRC_{ij}) due to each parameter quantifies the effect on variable j when parameter i is changed (hence allows prioritisation of important parameters). The SRC method involves the fitting of a multivariate linear model to the output of the MC simulation (Martin *et al.*, 2010; Neumann *et al.*, 2012).

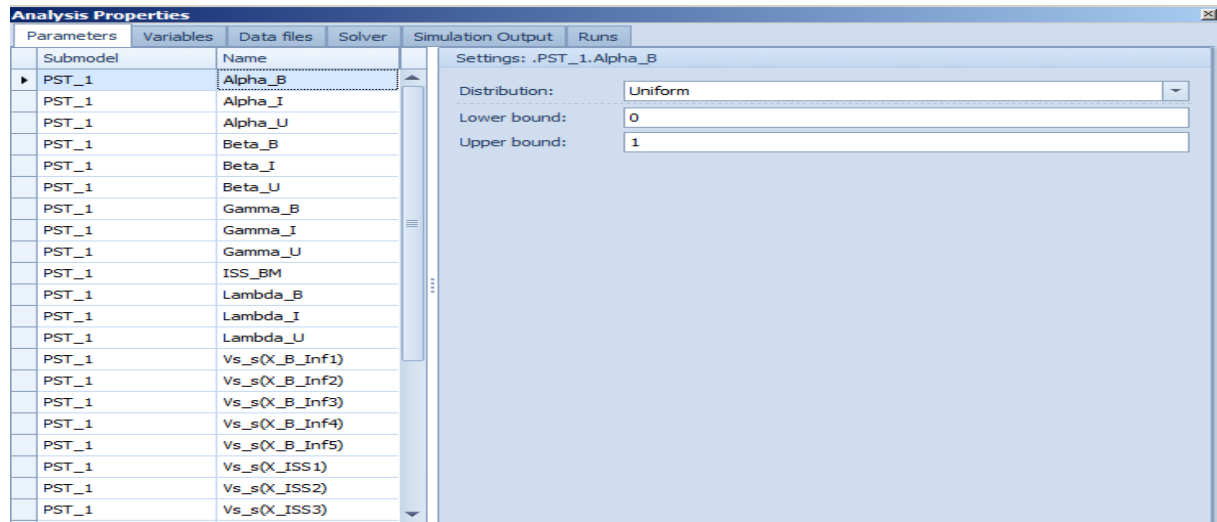


Figure 5.11: GSA Procedure on Uniform Distribution of Value Range for each Parameter

The SRC's multivariate linear regressions relate each output variable (y_j) to all uncertainty parameters (θ_i), to get an Equation of the form:

$$y_j(\theta) = b_{j0} + \sum_{i=1}^r b_{ij} \cdot \theta_i \quad (5.28)$$

The standard regression coefficient is defined as

$$SRC_{ij} = \beta_{ij} = b_{ij} \cdot \frac{\sigma_{y_j}}{\sigma_{\theta_i}}, \quad (5.29)$$

where b_i is the slope obtained from linear regression.

σ_{θ_i} is the standard deviation of the 1000 parameter values generated for parameter i ,

σ_{y_j} is the resulting standard deviation of output variable y_j (Ikumi, 2020).

5. The multivariate linear regression used towards obtaining the required SRC values was performed using the R Studio software (R-Development Core Team, 2011), with the standardized output variables and uncertainty parameters imported from the CSV files. The R Studio program was also applied to find the coefficient of determination (R^2) for each of the selected variables. This procedure is important to determine the extent of confidence in the calculated values (see Appendix E for summary of the results obtained for each of the variables using R Studio). Where the R^2 was above 0.7, a valid measure of sensitivity is deemed to be achieved, while a Lower R^2 (i.e. < 0.7) indicates that the SRC is

being used outside the applied value range, and as a result, some important parameters may not have been accounted for (Neumann, 2012; Saltelli *et al.*, 2004). Also, the extent of impact of each model parameter on the model output variables is comparatively determined using a line graph to depict the parameters that most or least affect the variable outputs. The simultaneously performed multivariate linear regression related each single output variable (Y) to all uncertainty parameters to get Equation 5.30 below:

$$y(i) = f(p_1, P_2, \dots, P_{70}) = b_o + \sum_{i=1}^N b_i * p_i \quad (5.30)$$

Where, b_i is the slope obtained from relating a variable to each individual parameter

b_o is the single intercept obtained for each variable plotted against all parameters in the multivariate linear regression

b_i represents the coefficients obtained by taking the mean and standard deviation of the 1000 outputs from each of the variables.

5.5.2 STANDARDISED REGRESSION COEFFICIENT (SRC) RESULTS

Using Neumann (2012) proposed interpretation, the analysed (via SRC) parameters would be classified into kinetics (process-rate parameters) and stoichiometric (non-kinetic parameters used in determining the input component characteristics). The discussion of the SRC results will be centred on the UCTPSU model parameters whose coefficient of determination (R^2) exceeds 0.7. Also, only parameters that caused significant changes (most important, positively, or negatively) in the above variables will be prioritized. This implies that, for the given virtual experiment, other non-influential parameters can be placed anywhere within their value range (without causing any significant change in the variable outputs).

Table 5.11 gives a summary of the influential parameters on each of the selected model variables showing their corresponding coefficients R^2 (for the most and the least important parameters of the UCTPSU selected variables), mean, kinetic sum, stoichiometry sum, Standard Deviation (SD), and coefficient of variation. Table 5.11 also discuss the relevant UCTPSU model output variables and the model parameters identified to be of importance. These include (i) Inorganic settleable solids in the underflow, (ii) Sub-Component Total Settleable Solids in the Underflow, and (iii) Sub-Component Volatile Settleable Solids in the Underflow.

Table 5.11: Summary of Results for UCTPSU Uncertainty and Sensitivity Analysis using SRC Method																	
Variables	Standardized Regression Coefficient, (β)				Highest β 2 value	R^2	Kinetic (SRC ²)	Stoich. (SRC ²)	Total (SRC ²)	Mean β 2	Std Dev. (β 2)	Coeff. of Variation					
	Most Positive		Most Negative														
ISS_unde	Vs_s	X_	ISS1	0.42	X_T	-0.04										0.30	3
Out_X_B_Inf		X_Lim		0.05	kH_F_AD_	-0.07										0.776	
Out_X_ISS		X_Lim		0.05	kH_F_AD_hy	-0.07										0.776	
Out_X_U_Inf		X_Lim		0.05	kH_F_AD_hy	-0.07										0.776	
Out_X_VSS		X_Lim		0.05	kH_F_AD_hy	-0.07										0.776	
TSS_Under_s	Vs_s_X_B_Inf5			0.76	i_P_XBORG_mol_perC	-0.01	Vs_s_X_B_Inf5									0.190	
Under_X_B_Inf		X_Lim		0.05	kH_F_AD_hy	-0.07										0.803	
Under_X_ISS		X_Lim		0.05	kH_F_AD_hy	-0.07										0.803	
Under_X_U_Inf		X_Lim		0.05	kH_F_AD_hy	-0.07										0.803	
Under_X_VSS	X_Lim			0.05	kH_F_AD_hy	-0.07										0.803	
VSS_Under_s	kM_BOrg_AD_hy			0.76													
					Gamma_I	-0.01											
	kM_BOrg_AD_hy			0.579													
				0.97													
				0.93													
				0.07													
				1.00													
				0.01													
				0.08													
				0.188													

5.5.2.1 INORGANIC SETTLEABLE SOLIDS IN THE UNDERFLOW (ISS_UNDER)

Figure 5.11 shows how ISS_Under has various important model parameters that affect its output (positively and negatively). The retained ISS_Under comes from fractionated influent TSS that is further classified into 5 sub-components with each having unique settling velocities. The identified significant parameters that positively affect ISS_Under (in decreasing order of influence) are Vs_s_X_ISS_1, Vs_s_X_ISS_3, Alpha_I, Vs_s_X_ISS_4, Vs_s_X_ISS_2, Vs_s_X_ISS_5, Beta_I and Gamma_I (all stoichiometric parameters). There is no clear explanation on why the ISS settling velocities in the sub-components (5 to 1) are not progressive except for the observed trend (showing that the higher settling velocity retained more ISS_Under, except for Vs_s_X_ISS_2). Also, X_T, i_O_XUOrg_mol_perC and Alpha_B, add up to the important parameters that influence ISS_Under, with more focus on X_T as the significant parameter with the most negative influence. Intuitively, it can be established that certain TSS concentration must be set below which possibly retained ISS_Under will reduce. This can be practically influenced by the wastewater source and PST operating conditions on-site. Appendix E provides a complete overview of all the GSA results.

5.5.2.2 SUB-COMPONENT TOTAL SETTLEABLE SOLIDS IN THE UNDERFLOW (TSS_UNDER_s)

It appeared that the settling velocity groups for influent biodegradable particulate organics in sub-components 3 to 5 (Vs_s_X_B_Inf_3, Vs_s_X_B_Inf_4, and Vs_s_X_B_Inf_5) are the top parameters that positively affect TSS_Under_s with Vs_s_X_B_Inf_5 being the most significant. These parameters are stoichiometric and inform more on careful parameter setting in the UCTPSU model. It implies that the largest TSS_Under_s is achieved at a settling velocity that does not disrupts the settling of TSS at the PST underflow. It also infers that TSS concentration increased as the settling velocities decreased (from sub-components 3 to 5). Model parameter numbers 49 to 67 (in Figure 5.4) also influence TSS_Under_s concentration, hence moderately defined within its value range with little or no negative impact on the output variable TSS_Under_s. The top parameter with the most negative impact on TSS_Under_s is i_P_XBOrg_mol_perC with -0.0865% impact and is therefore non-influential.

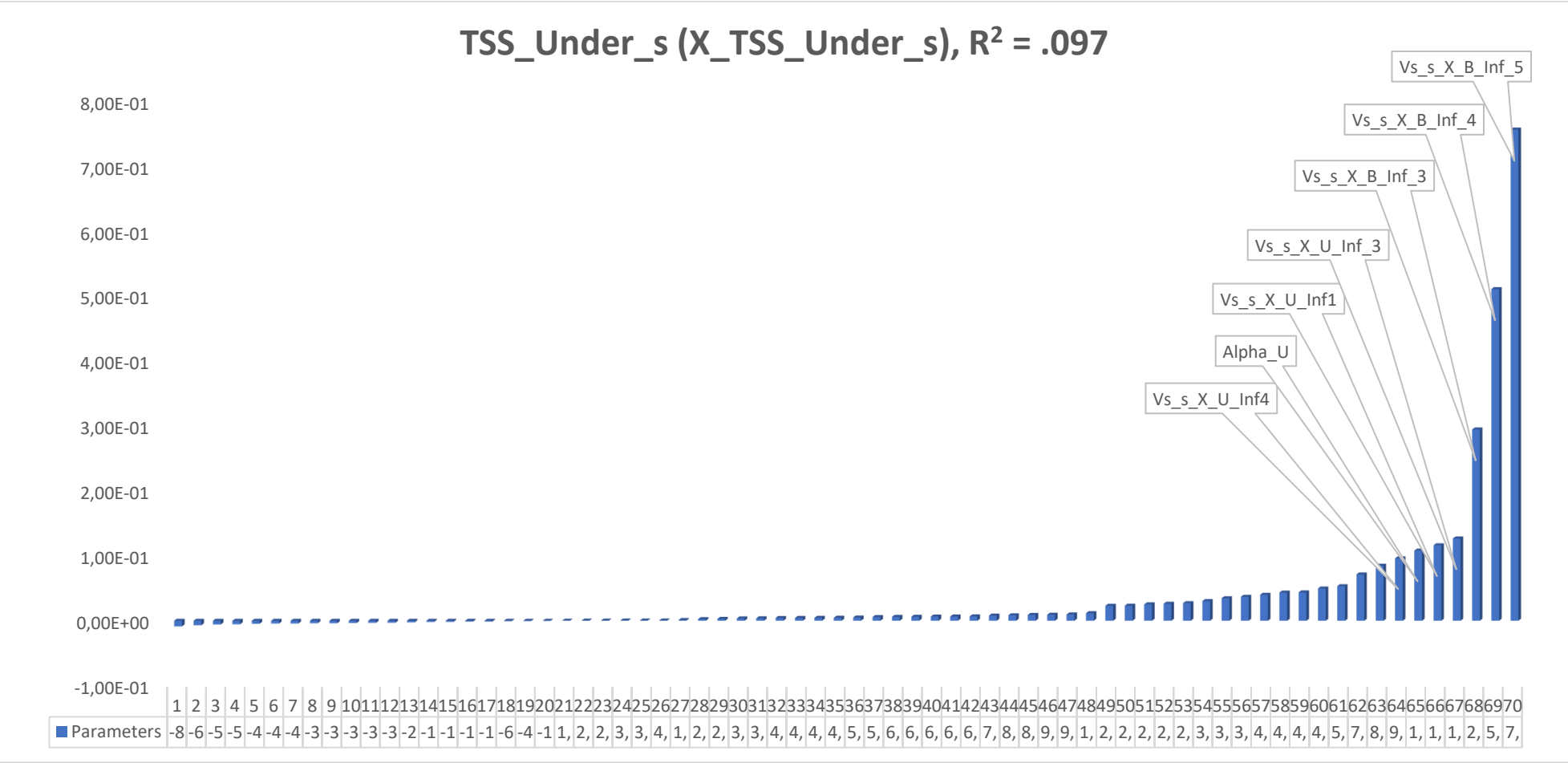


Figure 5.13: SRC Analysis of TSS_Under_s Tested against UCTPSU Model Parameters from most negative to most positive value of parameters

5.5.2.3 SUB-COMPONENT VOLATILE SETTLEABLE SOLIDS IN THE UNDERFLOW (VSS_UNDER_s)

Unlike in X_ISS and TSS_Under_s. kinetic parameters were observed to be the significant parameters that positively affected VSS_Under_s. These parameters (as shown in Figure 5.14) include hydrolysis rate constants of biomass (kM_BOrg_AD_hyd, the most significant parameter), influent biodegradable particulate organics (kM_BInf_AD_hyd) and fermentable soluble organics (kH_F_AD_hyd). The importance of kM_BOrg_AD_hyd helps to explain biomass growth due to VSS_Under_s breakdown. When kM_BOrg_AD_hyd is high, (i.e. food-to-mechanism ratio), it means the hydrolysis of the bio-organics will be slow since little inherent organisms initially existed. This hydrolyzing organism readily sequesters the fermentable soluble but slowly hydrolyze BPO_PS (the biodegradable component of VSS_Under_s i.e. with respect to its generic stoichiometry). The biomass also facilitates the tracking of the energy (CH₄ and CO₂), materials (Orthophosphate, FSA and H₂CO₃ Alk) and charge produced. These bioprocesses occur in the anaerobic environment of the organics (underflow_UCTPSU model). When both soluble and particulate organics are no longer available to sequester, endogenous process will begin with the biomass eating itself (through hydrolysis process) which occurs at a very slow rate.

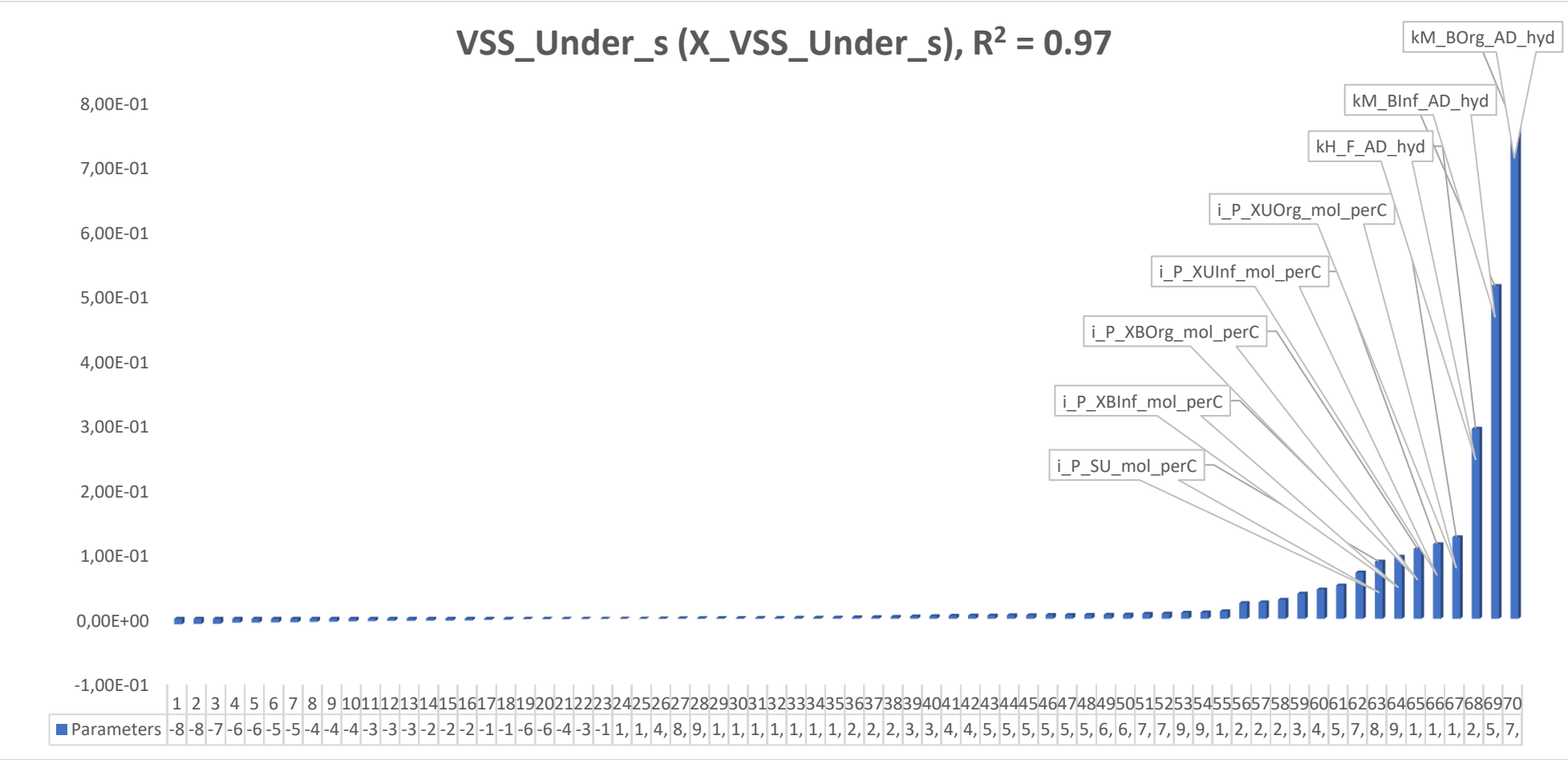


Figure 5.14: SRC Analysis of VSS_Under_s Tested against UCTPSU Model Parameters from most negative to most positive value of parameters

5.6 CONCLUSION

In this chapter, the control and test masses, kinetic rate constants (i.e. the hydrolysis rate constants of both fermentable soluble and influent biodegradable particulate organics) and implementation of UCTSDM3P, required for the ABMP parameter estimation were completed. A summary of successful test runs selected 22 out of the 35 tests samples (i.e. over 60% of the runs gave acceptable kinetic rate constants across the 5-column and controls samples) and that was based on their hydrolysis rate constants (listed in Table 5.7). The selection was possible by applying R Studio software to run a least-square approximation on the residual COD concentrations and rate of hydrolysis, to help determine the kinetic parameters (k_M and k_S). The determined parameters were used to check if the calculated specific hydrolysis rate correlates with the measured specific hydrolysis rate (see Section 5.3). Hence, the determined important parameters required to calibrate the UCTPSU model have been summarized in Tables 5.7 and 5.8 describing settling velocity groups, fraction of the unbiodegradable particulate organic COD (f'_{sup}), the elemental mass compositions of the influent biodegradable particulate organics (BPO_PS) and kinetic rate constants for the hydrolysis of BPO_PS.

General Sensitivity Analysis (GSA) was also performed on the UCTPSU model using the SRC method. This method revealed the most important UCTPSU model output variables (ISS_Under, TSS_Under_s and VSS_Under_s). The SRC method also determined the top parameters that significantly affected these three (3) outputs variables. These variables were affected by stoichiometric parameters (i.e. ISS_Under_s was significantly influenced by Γ_I , β_I , $V_{s_X_ISS_5}$, $V_{s_X_ISS_2}$, $V_{s_X_ISS_4}$, α_I , $V_{s_X_ISS_3}$, and $V_{s_X_ISS_1}$, and TSS_Under_s was also significantly influenced by $V_{s_X_B_Inf_3}$, $V_{s_X_B_Inf_4}$, and $V_{s_X_B_Inf_5}$) except for the VSS_Under_s. Kinetic parameters ($k_{H_F_AD_hyd}$, $k_{M_BInf_AD_hyd}$ and $k_{M_BOrg_AD_hyd}$) were the top influencing parameters that significantly affected the VSS_Under_s variable at the slightest possible change in value. Hence, these consolidated findings (settling velocities of the organics, TSS fractionations (UPO, BPO, and ISS), elemental mass compositions of the organics, fractions of unbiodegradable particulate organics, hydrolysis rate constants) helped to achieve calibration of the UCTPSU model.

CHAPTER 6.0: CONCLUSION AND RECOMMENDATIONS

Towards the data-driven approach to modelling the primary sedimentation unit process, in a plant-wide context, the calibration of a developed University of Cape Town Primary Sedimentation Unit model (UCTPSU) involved (i) the performance of sensitivity analysis to identify the most significant parameters that impact variables of importance in UCTPSU, (ii) performance of settleometer experiments on the raw sewage to separate the primary sludge into settling velocity groups (represented by the 5 different PVC columns of the settleometer device), (iii) performing augmented bio-methane potential (ABMP) test on the sludge collected from the 5 PVC columns of the settleometer and (iv) using the calibrated anaerobic digestion model (UCTSDM3P; Ikumi et al, 2015; Ghoor, 2020) to perform parameter estimation, via iterative simulations in the WEST[®] software. The findings of this calibration process include:

A. SETTLEOMETER, AD_SS AND ABMP TEST RESULTS

- The determination of settling velocities from the settleometer columns. Readings were taken from the settleometer runs 3 and 4, with each showing decreasing settling velocity from the smallest diameter column to the largest diameter column. Settleometer run 3 had the following settling velocities (in m/hr): 31.61, 14.13, 8.65, 5.79 and 3.57 while settling velocities (in m/hr) determined from 4th settleometer run are 23.56, 10.53, 6.45, 4.32, and 2.66. This settling velocity profiles shows that primary sewage sludge was fractionated according to particle size and density.
- In each of the experimental systems, mass was conserved for COD, TKN, TP, TSS and VSS as depicted in their respective mass balance calculation
- The total settleable solid (TSS) components and their proportions in each settleometer columns were estimated (as provided in Table 6.6). With the aid of the ABMP reactor, it was determined (in Table 6.5) that the unbiodegradable particulate organics (UPO) forms the largest total settleable solid (TSS) component removed from the PST underflow followed by biodegradable particulate organics (BPO).
- The unbiodegradable particulate organic COD (f'_{sup}) were determined. Also, the f'_{sup} fractions slightly decreased with respect to the velocity group profile. This could mean that the UPO proportions of TSS are lower for the TSS with reduced settling velocities (see Figure 6.4 and Table 6.6).

B. GENERAL SENSITIVITY ANALYSIS (GSA) USING STANDARDISED REGRESSION COEFFICIENT (SRC) METHOD

- Three different output variables from the University of Cape Town Primary Sedimentation Unit (UCTPSU) model were determined to be the most important and they are ISS_Under, TSS_Under_s, and VSS_Under_s.
- Top parameters that significantly influenced the three most important UCTPSU model output variables were determined. These variables were affected by stoichiometric parameters (i.e. ISS_Under_s was significantly influenced by Γ_I , β_I , $V_{s,s}X_{ISS_5}$, $V_{s,s}X_{ISS_2}$, $V_{s,s}X_{ISS_4}$, α_I , $V_{s,s}X_{ISS_3}$, and $V_{s,s}X_{ISS_1}$, and TSS_Under_s was also significantly influenced by $V_{s,s}X_{B_Inf_3}$, $V_{s,s}X_{B_Inf_4}$, and $V_{s,s}X_{B_Inf_5}$) except for the VSS_Under_s. Kinetic parameters ($k_{H_F_AD_hyd}$, $k_{M_BInf_AD_hyd}$ and $k_{M_BOrg_AD_hyd}$) were the top influencing parameters that significantly affected the VSS_Under_s variable at the slightest possible change in value.

C. UCTSDM3P MODEL IMPLEMENTATION FOR UCTPSU MODEL CALIBRATION

- The elemental mass compositions of the utilized substrates (collected from the 3rd settleometer runs i.e. from its columns) and the biomass (collected from the steady-state anaerobic digestion) were determined (as summarized in Table 7.8). These parameters are $i_{H_Org_mol_perC}$, $i_{O_Org_mol_perC}$, $i_{N_Org_mol_perC}$, and $i_{P_Org_mol_perC}$ and their stoichiometry values are respectively highlighted in Table 7.8. These values are system-oriented therefore inapplicable universally.
- Hydrolysis rate constants were separately evaluated for each control and batch test, to closely ensure that the experimentally measured and the predicted hydrolysis rates are relatively close. The selection of successful control and batch test were based on the relative closeness in the experimentally measured and predicted hydrolysis rate. These kinetic rate constants are listed in Table 7.7.

Hence, the reached findings (hydrolysis rate constants, f'_{sup} and EMCs) along with the sensitivity analysis (see Sections 5.3 – 5.4) can now be coupled into the UCTPSU model to achieve calibration of the model.

6.1 RECOMMENDATIONS

The UCTPSU model calibration was completed by consolidating the experimental and simulation results. Nonetheless, some major aspects of the work can be further investigated in future studies.

Such study works include:

1. Settleometer on-site test on industrial wastewater for comparative study on the impact of settling velocity groups on municipal and industrial wastewater. This study will assist to investigate the effect of settling velocity and sludge characteristics (accounting for wastewater source) on total settleable solid proportions. In addition, the impact of temperature on sludge settleability should also be investigated on-site and in the water quality laboratory.
2. A once-off investigation on the primary sludge types across all the Western Cape wastewater treatment works, conducting AD_SS with full characterisation profile recorded (for future referencing). The findings will serve to update past literature data on experimental AD_SS in Cape Town and also highlight the new developments that can be added to existing simulation tools like the WEST® (Vanhooren *et al.*, 2003).
3. Having determined and observed the wastewater characteristics from the settleometer pilot-plant, extensive study is highly recommended to investigate the inorganic settleable solids in raw wastewater, primary sludge, and wastewater. This investigation is important to account for the missing ISS concentration across the settleometer, hence, affecting its mass balance.
4. An extension on the calibrated UCTPSU model should be investigated by accounting for sulphur elemental mass and metals in the primary sludge. This can begin by studying the existing works on the augmented bio-sulfuric potential removal. The study will further improve the validity and significance of the UCTPSU model as a major control unit in the PWM_SA (Ikumi *et al.*, 2015) and also accommodate every possible elemental mass composition.
5. To further validate the sensitivity analysis (SRC method) employed on the UCTPSU model variables, the Morris Screening (MS) method should also be applied to verify the SRC method applied. Applying the MS method would not only validate similar significant model parameters determined by the SRC method but also reflect the missing model parameters not covered by the SRC method.
6. A comparative study of the impact of calibrated and non-calibrated UCTPSU model on the plant-wide model of South Africa (PWM_SA, Ikumi *et al.*, 2015) should be conducted to justify the

significance of UCTPSU model calibration. The study should be based on the overall assessment of effluent quality, operation cost, and nutrient and energy recovery rates.

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APPENDICES

APPENDIX A: SETTLEOMETER

APPENDIX B: STEADY-STATE ANAEROBIC DIGESTION RESULTS

APPENDIX C: AUGMENTED BIO-METHANE POTENTIAL TEST RESULTS

APPENDIX D: BIOPROCESS STOICHIOMETRY EQUATIONS

APPENDIX E: GENERAL SENSITIVITY ANALYSIS

APPENDIX F: PARAMETER ESTIMATION PROCEDURES

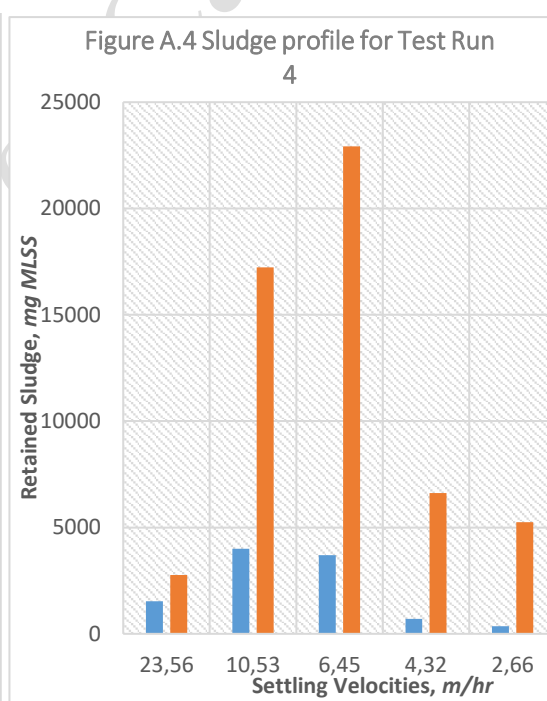
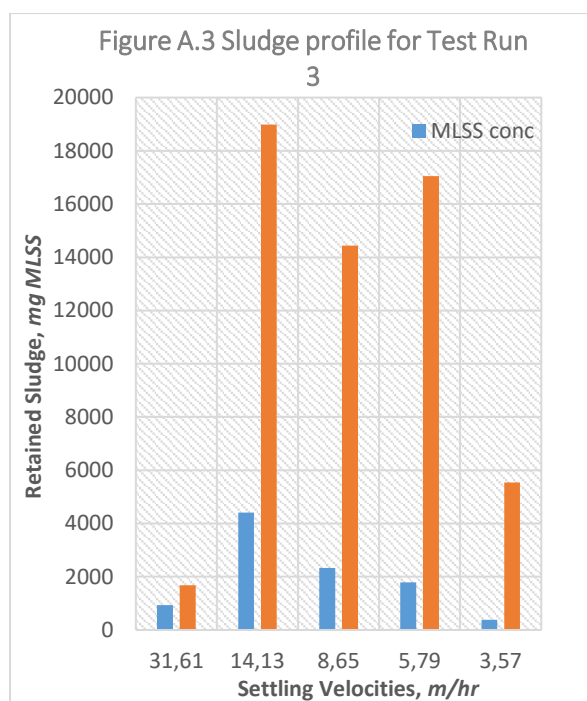
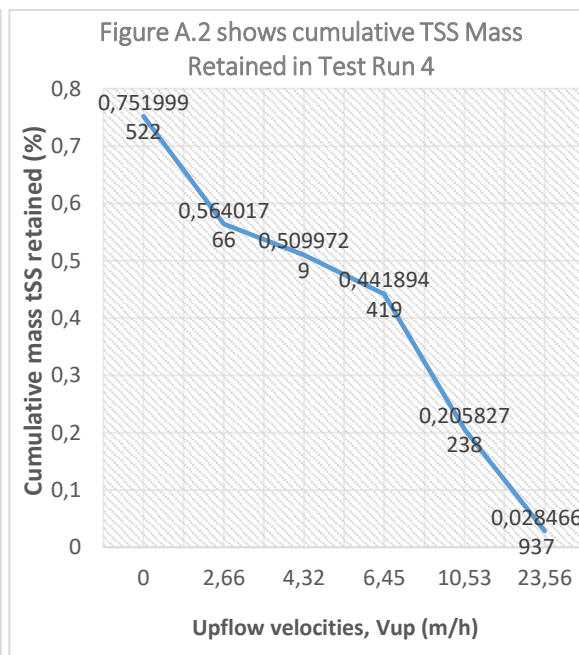
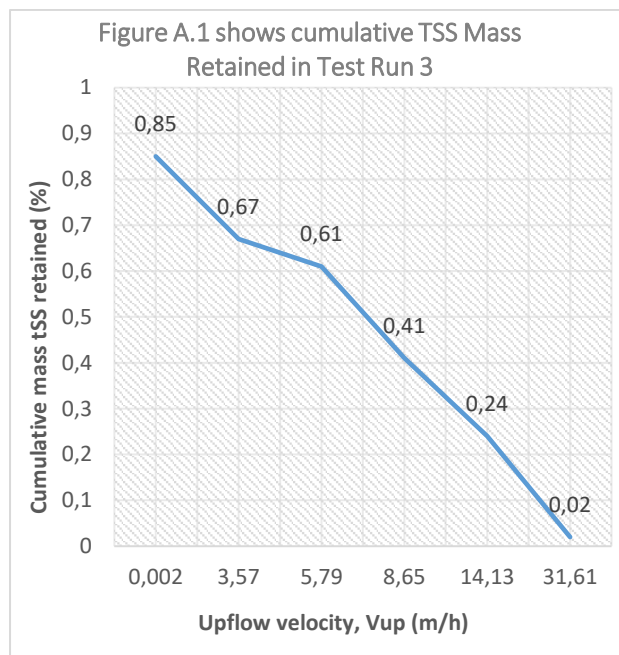
APPENDIX G: ELEMENTAL MASS COMPOSITIONS

APPENDIX H: HYDROLYSIS

APPENDIX I: MASS BALANCE: UCTPSU MODEL VERIFICATION RESULTS

University of Cape Town

APPENDIX A: SETTLEOMETER READINGS FOR TEST RUNS 3 AND 4



Figures A.3 – A.4 represent sludge concentrations and sludge mass against their respective up-flow velocities, it can be observed that mass of sludge removed from the system increased with increasing up-flow velocity, causing reduction in tube sludge bed which infers that sludge age will be reduced. Hence, there will record of reduced biodegradables, and reduced available biomass to mediate hydrolysis and bio-kinetic processes.

Table A.1 Settlemeter Experimental Tests and Readings: Settlemeter Experimental Readings

Dates, Batches and Test Categories		Units	2019/10/15								2019/10/15											
			Run 3								Run 4											
			Blank	Influent	1	2	3	4	5	Effluent	Blank	Inf_0min	Inf_30min	Inf_60min	Inf_90min	Inf_120min	1	2	3	4	5	Effluent
Q	Average flow	l/min	-							-												
COD (unfil.)	Normality	N	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
	Vol_sample, Vs	ml	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10
	Dil. factor, DF	no unit	-	5	20	20	20	20	20	5	-	5	5	5	5	5	20	20	20	20	20	5
	Titra Vol1, TV1	ml	24.8	13.9	20.2	18.5	17.3	19.2	22	20.4	24.8	15.7	15.9	15.9	16.1	16.5	20.8	15.7	18.9	21.7	22.3	18.4
	Titra Vol1, TV2	ml	24.1	13.6	20.1	18.9	17.6	18.4	22.1	20.5	24.1	14.9	15.6	15.9	16.5	14.6	20.9	16	19	21.1	22.5	18.2
	Average Vol, TVAvg	ml	24.45	13.75	20.15	18.7	17.45	18.8	22.05	20.45	24.45	15.3	15.75	15.9	16.3	15.55	20.85	15.85	18.95	21.4	22.4	18.3
	Calc. COD	mgCOD/l	-	2140	3440	4600	5600	4520	1920	800	-	1830	1740	1710	1630	1780	2880	6880	4400	2440	1640	1230
COD (fil.)	Normality	N	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
	Vol_sample, Vs	ml	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10
	Dil. factor, DF	no unit	-	5	-	-	-	-	-	5	-	5	5	5	5	5	-	-	-	-	-	5
	Dates, Batches and Test Categories	Units	Blank	Influent	1	2	3	4	5	Effluent	Blank	Inf_0min	Inf_30min	Inf_60min	Inf_90min	Inf_120min	1	2	3	4	5	Effluent

			TKN (Unfilt.)																TKN (filt.)				
Titra Vol1, TV1	ml	23.8	19.5	-	-	-	-	-	-	-	19.9	23.8	21.3	21.8	21.7	21.7	21	-	-	-	-	-	21.7
Titra Vol1, TV2	ml	24	19.9	-	-	-	-	-	-	19.8	24	21.6	21.6	21.75	21.8	21.1	21	-	-	-	-	-	21.7
Average Vol, TVAvg	ml	23.9	19.7	-	-	-	-	-	-	19.85	23.9	21.45	21.7	21.75	21.75	21.05	21	-	-	-	-	-	21.7
Calc. COD	mgCOD/l	-	840	-	-	-	-	-	-	810	-	490	440	435	430	570	-	-	-	-	-	-	440
Normality	N	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	
Vol_sample, Vs	ml	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	
Dil. factor, DF	no unit	-	2	2	5	5	5	5	2	2	-	2	2	2	2	2	5	10	10	10	5	2	
Titra Vol1, TV1	ml	-	46.5	52.6	25.1	27.6	26.2	40.3	33.1	-	40.3	39.3	36	36.6	34.8	12.4	19.9	19.9	17	34.1	36		
Titra Vol1, TV2	ml	-	43.2	-	25.8	27.5	-	40.9	40.2	-	42.5	40.1	33.2	-	36.4	10.8	18.9	23.1	15.1	-	32.4		
Average Vol, TVAvg	ml	-	44.85	52.6	25.45	27.55	26.2	40.6	36.65	-	41.4	39.7	34.6	36.6	35.6	11.6	19.4	21.5	16.05	34.1	34.2		
Calc. TKN	mgTKN/l	-	125.58	147.28	178.15	192.85	183.4	113.68	102.62	-	115.92	111.16	96.88	102.48	99.68	81.2	271.6	301	112.35	95.48	95.76		
Normality	N	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001		
Vol_sample, Vs	ml	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10		
Dil. factor, DF	no unit	-	1	-	-	-	-	-	1	-	2	2	2	2	2	5	10	10	5	2	2		
Titra Vol1, TV1	ml	-	67.3	-	-	-	-	-	66.3	-	-	-	-	-	17.6	-	-	-	-	-	19.1		

Table A.2 Summary of Settleometer Experimental Readings												
Dates, Batches and Test Categor ies		Test Run 3						Test Run 4				
		2019/10/15						2019/10/15				
FSA	TKN (filt)	TKN	COD (filt)	COD	Volume	Discharge	Measured	Test	mg/l	mg/l	l/min	Units
mg/l	mg/l	mg/l	mg/l	mg/l	l	min	l/min					
79.05	93.66	147.28	840	3440	1.8	-	-	1				
79.05	93.66	178.15	840	4600	4.3	-	-	2				
79.05	93.66	192.85	840	5600	6.2	-	-	3				
79.05	93.66	183.4	840	4520	9.5	-	-	4				
79.05	93.66	113.68	840	1920	14.5	-	-	5				
2869.515	3399.858	5617.479	30492	131472	36.3	0	0	M_TS _i				
7146.05676	8466.78907	11352.3315	75935.328	193454.288	90.3992	120	0.8453	M_RWW _i				
4073.67	5169.179	5551.66	43820.35	43279.36	54.0992	64	0.8453	M_SWW _i				
97.16	101.21	98.39	97.86	90.33	100	-	100	MB _i				
68.56	50.54	81.2	473	2880	1.8		-	1				
68.56	50.54	271.6	473	6880	4.3		-	2				
68.56	50.54	0	473	4400	6.2		-	3				
68.56	50.54	112.35	473	2440	9.5		-	4				
68.56	50.54	95.48	473	1640	14.5		-	5				
2488.728	1834.602	3765.825	17169.9	109008	36.3		0	M_TS _i				
5512.224	4063.416	8460.0096	38029.2	139735.2	80.4	120	0.63	M_RWW _i				
2820.195	2160.9	4223.016	19404	54243	44.1	70	0.63	M_SWW _i				
96.31	98.33	94.43	96.17	116.83	100		100	MB _i				

V _{up}	Internal	VFA	direct pH	Alk	ISS	VSS	TSS	OP	TP (flit)	TP
zw	ww	mg/l	no unit	mg/l as	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l
0.002	45.2	195.17	6.95	-	134	800	934	8.95	10.84211	17.8948
0.0032	67.6	195.17	6.86	-	2600	1814	4414	8.95	10.84211	25.3945
0.006	86.4	195.17	6.74	-	238	2090	2328	8.95	10.84211	29.6055
0.009	105.6	195.17	6.96	-	180	1614	1794	8.95	10.84211	25.7895
0.014	134.4	201.22	6.97	-	100	282	382	8.95	10.84211	14.8422
-	-	7172.396	-	0	16056.8	41620.2	57677	324.885	393.568593	785.17324
-	-	17643.2118	7.08	28657.4503	26758.1632	59121.0768	85879.24	809.07284	980.118070	2236.18693
-	-	10885.84	7.08	12793.92	3570.547	11901.82	15472.37	454.4333	555.2287	1338.241
-	-	102.352322	-	44.64	73.35	90.53	85.18	96.32	96.80	94.96
0.002	45.2	186.22	6.80	-	298	1238	1536	8.45	10.081	20.811
0.004	67.6	186.22	6.61	-	514	3492	4006	8.45	10.081	34.054
0.006	86.4	186.22	7.05	-	486	3212	3698	8.45	10.081	33.243
0.009	105.6	186.22	6.71	-	174	522	696	8.45	10.081	14.7295
0.0142	134.4	186.22	6.97	-	90	272	362	8.45	10.081	12.973
-	-	6759.786	-	0	8717.8	46061.4	54779.2	306.735	365.9403	718.03735
-	-	14972.088	6.73	15573.9624	19939.2	77184	97123.2	679.38	810.5124	1333.33366
-	-	18406.02	6.69	14896.1	5644.8	12612.6	18257.4	399.105	417.164	584.0251
-	-	168.08	-	95.65	72.03	76.02	75.20	103.89	96.62	97.65

	m/min	m/hr	$m3/hr$	$m3/min$
	0.53	31.61	0.050718	0.0008
	0.24	14.13	0.050718	0.0008
	0.14	8.65	0.050718	0.0008
	0.10	5.79	0.050718	0.0008
	0.06	3.57	0.050718	0.0008
	-	-	-	-
	-	-	-	-
	-	-	-	-
	-	-	-	-
	0.39	23.56	0.0378	0.0006
	0.18	10.53	0.0378	0.0006
	0.11	6.45	0.0378	0.0006
	0.07	4.32	0.0378	0.0006
	0.04	2.66	0.0378	0.0006
	-	-	-	-
	-	-	-	-
	-	-	-	-
	-	-	-	-
M_{TS_i}		Mass of total settleable solids (in mg) in the measured ' I ' concentration		
M_{RWW_i}		Mass of influent raw wastewater (in mg) in the measured ' I ' concentration		
M_{SWW_i}		Mass of settled (overflow) wastewater (in mg) in the measured ' I ' concentration		
MB_i		Mass balance across the device for the measured ' I ' concentration		
ID		Internal column diameter (mm)		
V_{up}		Upflow velocities		

Table A.3 Summary of Settling Fractions for Test Run 3 showing fluxes of TSS components							
Groups		1	2	3	4	5	Total
Average Settling velocities		V1	V2	V3	V4	V5	-
	m/hr	31.61	14.13	8.65	5.79	3.57	-
	m/min	0.527	0.236	0.144	0.097	0.06	-
Settling fractions		F1	F2	F3	F4	F5	-
ISS		0.201	0.169	0.207	0.223	0.200	1.000
UPO		0.206	0.203	0.200	0.212	0.178	1.000
BPO		0.191	0.216	0.195	0.167	0.232	1.000
Maximum settling (in fluxes)							
ISS	mgISS/min	3226.6	2708.6	3331.4	3584.5	3205.7	16056.8
UPO	mgVSS/min	4490.5	4433.5	4366.9	4623.7	3872.1	21786.7
BPO	mgVSS/min	3780.1	4276.9	3864.9	3319.71	4591.9	19833.4
TSets	mgTSS/min	11497.3	11418.9	11563.2	11527.9	11669.7	57677
Fractions of TSusps		0.199	0.198	0.200	0.200	0.202	1
Note: All acronyms have been established in the body of the study and abbreviation							

Table A.4 Summary of Sludge Profile for Test Runs 3 & 4																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
	Influent	Effluent	Tube 5	Tube 4	Tube 3	Tube 2	Tube 1	Test Run 3								Test Run 4																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
								mm	l	mg/l	mg	mg	%	%	m/h	mg/l	mg	%	mg/l	mg	%	l	mg/l	mg	mg	%	mg	m/h	mg/l	mg	%	mg/l	mg	%																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
Mass TSS 85.2%	-	-	134.4	105.6	86.4	67.6	45.2																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		

APPENDIX B: STEADY-STATE ANAEROBIC DIGESTION RESULTS

Table B.1: Result of AD at Steady States		05-Aug-19	06-Aug-19	07-Aug-19	08-Aug-19	09-Aug-19	19-Aug-19	20-Aug-19	21-Aug-19	22-Aug-19	23-Aug-19	24-Aug-19	25-Aug-19	26-Aug-19	27-Aug-19	28-Aug-19	29-Aug-19	30-Aug-19	31-Aug-19	01-Sep-19	02-Sep-19	03-Sep-19	04-Sep-19	05-Sep-19	06-Sep-19
Tested daily	Effluent (ml)	800	800	800	800	800	1000	10	10	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000
	Effluent pH	6.46	6.75	6.67	7.20	6.73	6.50	6.82	6.73	6.72	6.77	6.76	6.70	6.67	6.9	6.96	6.99	7.04	7.07	7.1	7.08	7.08	7.1	7.15	7.14
	Influent (ml)	800	800	800	800	800	1000	0	0	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000
	Influent pH	6.19	6.16	6.18	6.17	6.21	6.25	-	-	6.18	-	6.16	5.70	5.77	5.75	5.82	5.88	5.83	6.06	6.01	6.06	6.16	6.16	6.26	6.08
	NaHCO ₃ added (g)	15.21	14.02	14.43	0.00	10.03	14.97	0	0	10.04	0	0	15.56	15.07	10.009	1.0243	1.0196	0	0	0	0	0	0	0	0
	Influent pH after adding NaHCO ₃ (to be fed to the digester)	7.67	7.68	7.66	6.17	7.63	7.67	0.00	0.00	6.67	-	-	7.43	7.47	7.04	6.29	6.18	5.83	6.06	6.01	6.06	6.16	6.16	6.26	6.08
	Effluent pH after feeding (after 20-30minutes)	-	-	7.17	-	7.04	6.70	-	-	6.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Effluent pH (after 24 hours)	6.75	6.67	7.20	6.73	-	6.82	6.73	6.72	6.77	6.76	6.70	6.67	6.9	6.96	6.99	7.04	7.07	7.1	7.08	7.08	7.1	7.15	7.14	7.13
	Gas count						90	93	89	100	82	95	96	191	188	210	228	250	280	305	292	357	375	384	394
Once/Twice a week	Mixed Liquor Settleable Solids (MLSS)																								
	MLSS (mgMLSS/l)			12118			7484			12974		11428				12346		18446				12380			15040
	MLVSS (mgMLVSS/l)			8100			5528			7636		7864				7750		12844				8158			9624
	MLISS (mgMLISS/l)			4018			1956			5338		3564			4596			5602				4222			5416
	Chemical Oxygen Demand																								
	Influent (COD (mgCOD/l)			29360			10675			22975		22500				30900		43200				43700			45600
	Effluent ((COD (mgCOD/l)			12800			12540			13260		11760				12200		11227				13160			13160
	5-Point Titration																								
	Alkalinities (mg CaCO ₃ /l) (Effluent)		2618				643					3060				3956						3853			3765
	VFA (Effluent)		1544				467					1732				1805						1224			674
	H2CO3 Alkalinity to VFA Ratio		1.6962 : 1				1.3783 : 1					1.7663 : 1				2.1914 : 1						3.149 : 1			5.589 : 1
			2 : 1				1 : 1					2 : 1				2 : 1						3 : 1			6 : 1

Table B.1 Continuation: Result of AD at Steady States		07-Sep-19	08-Sep-19	09-Sep-19	10-Sep-19	11-Sep-19	12-Sep-19	13-Sep-19	14-Sep-19	15-Sep-19	16-Sep-19	17-Sep-19	18-Sep-19	19-Sep-19	20-Sep-19	21-Sep-19	23-Sep-19	24-Sep-19	25-Sep-19	26-Sep-19	27-Sep-19	28-Sep-19	29-Sep-19	30-Sep-19	01-Oct-19
Tested daily	Effluent (ml)	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000
	Effluent pH	7.1	7.1	7.1	7.1	7.1	7.0	7.0	7.0	7.0	7.0	7.0	7.0	7.0	7.0	7.0	7.1	7.1	7.0	7.1	7.1	7.0	7.1	7.1	7.1
	Influent (ml)	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000
	Influent pH	6.15	6.08	6.08	6.15	6.08	6.15	5.97	5.96	6.04	5.99	6.09	6.05	5.89	5.73	5.72	5.54	5.68	5.96	6.2	6.22	6.15	6.16	6.1	6.13
	NaHCO ₃ added (g)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	Influent pH after adding NaHCO ₃ (to be fed to the digester)	6.15	6.08	6.08	6.15	6.08	6.15	5.97	5.96	6.04	5.99	6.09	6.05	5.89	5.73	5.72	5.54	5.68	5.96	6.2	6.22	6.15	6.16	6.1	6.13
	Effluent pH after feeding (after 20-30minutes)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Effluent pH (after 24 hours)	7.13	7.14	7.11	7.12	7.08	7.07	7.09	7.08	7.07	7.05	7.08	7	7.08	7.07	7.16	7.1	7.07	7.11	7.1	7.08	7.1	7.11	7.12	7.21
	Gas count	407	383	336	358	356	351	374	367	388	390	416	405	417	411	417	302	377	403	410	439	461	448	456	446
Once/Twice a week	Mixed Liquor Settleable Solids (MLSS)																								
	MLSS (mgMLSS/l)								16752						14468			16950		15004					18408
	MLVSS (mgMLVSS/l)								11022						10300			11716		10850					14108
	MLISS (mgMLISS/l)								5730						4168			5234		4154					4300
	Chemical Oxygen Demand																								
	Influent (COD (mgCOD/l)								60600						58400			54400							78600
	Effluent ((COD (mgCOD/l)								20000						23900			21200							24900
	5-Point Titration																								
	Alkalinities (mg CaCO ₃ /l) (Effluent)	5007															3521	3893	4047	4364	3964	3321		3712	3802
	VFA (Effluent)	548															576	171	138	496	669	787		371	326
	H ₂ CO ₃ Alkalinity to VFA Ratio	9:1417 : 1															6:1153 : 1	22:709 : 1	29:359 : 1	8:79 : 1	5:92 : 1	4:2177 : 1		10:1	11:655 : 1
		9 : 1															6 : 1	23 : 1	29 : 1	9 : 1	6 : 1	4 : 1		10 : 1	12 : 1

Table B.1 Continuation: Result of AD at Steady States		02-Oct	03-Oct	04-Oct	05-Oct	06-Oct	07-Oct	08-Oct	09-Oct	10-Oct	11-Oct	12-Oct	13-Oct	14-Oct	15-Oct	16-Oct	17-Oct	18-Oct	19-Oct	20-Oct	21-Oct
Tested daily	Effluent (ml)	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	800	200	200	200	400
	Effluent pH	7.21	7.2	7.21	7.23	7.21	7.23	7.14	7.42	7.31	7.2	7.22	7.16	7.15	7.13	7.17	7.13	6.99	7.21	7.45	7.33
	Influent (ml)	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	800	200	200	200	400
	Influent pH	6.4	6.38	6.45	6.3	6.3	6.44	6.15	6.25	6.35	5.96	5.81	5.8	5.78	5.65	5.61	5.76	5.8	5.77	5.83	5.83
	NaHCO ₃ added (g)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	Influent pH after adding NaHCO ₃ (to be fed to the digester)	6.4	6.38	6.45	6.3	6.3	6.44	6.15	6.25	6.35	5.96	5.81	5.8	5.78	5.65	5.61	5.76	5.8	5.77	5.83	5.83
	Effluent pH after feeding (after 20-30minutes)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Effluent pH (after 24 hours)	7.2	7.2	7.2	7.2	7.2	7.1	7.4	7.3	7.2	7.2	7.1	7.1	7.1	7.1	7.1	6.9	7.2	7.4	7.3	-
	Gas count	478	458	457	442	471	467	452	487	509	469	435	476	396	446	434	428	383	422	429	283
Once/Twice a week	Mixed Liquor Settleable Solids (MLSS)																				
	MLSS (mgMLSS/l)		14594				18170				18962				16782						
	MLVSS (mgMLVSS/l)		10682				14244				13206				12614						
	MLISS (mgMLISS/l)		3912				3926				5756				4168						
	Chemical Oxygen Demand																				
	Influent (COD (mgCOD/l)		73867				80320								64800				52600	52600	53000
	Effluent ((COD (mgCOD/l)		625				26100								25800				27150	29900	25600
	5-Point Titration																				
	Alkalinities (mg CaCO ₃ /l) (Effluent)		4314	4114	3655	3925	3107	3806				3720			3818		3769	3601		3496	3379
	VFA (Effluent)		472	244	255	227	157	139				184			250		379	634		66	5
	H ₂ CO ₃ Alkalinity to VFA Ratio		9.14 : 1	16.89 : 1	14.33 : 1	17.30 : 1	19.79 : 1	27.39				20.21			15.26		9.94	5.68		53.20	615.20
			9 : 1	17 : 1	14 : 1	17 : 1	20 : 1	27 : 1				20 : 1			15 : 1		10 : 1	6 : 1		53 : 1	615 : 1

APPENDIX C: ABMP (CONTROL AND TEST SAMPLES) RESULTS

Table C.1 Control and Test Masses Prior to Parameter Estimation				
Samples	UPO	BPO	Total	Units
Seed_C1	5202	1596	6798	mgVSS/l
Seed_C2	4632	2166	6798	mgVSS/l
Seed_T1	2601	798	3399	mgVSS/l
Seed_T2	2316	1083	3399	mgVSS/l
Substrate_T1a	5716	3250	8966	mgVSS/l
Equi_Sub_T1a	2858	1625	4483	mgVSS/l
ABMP_T1a_blend_mass	-	-	6306	mgVSS
Substrate_T1b	4538	4428	8966	mgVSS/l
Equi_Sub_T1b	2269	2214	4483	mgVSS/l
ABMP_T1b_blend_mass	-	-	6306	mgVSS
Substrate_T2a	6540	2444	8984	mgVSS/l
Equi_Sub_T2a	3270	1222	4492	mgVSS/l
ABMP_T2a_blend_mass	-	-	15782	mgVSS
Substrate_T2b	3268	5316	8584	mgVSS/l
Equi_Sub_T2b	1634	2658	4292	mgVSS/l
ABMP_T2b_blend	-	-	7691	mgVSS
Substrate_T3a	5552	2572	8124	mgVSS/l
Equi_Sub_T3a	2776	1286	4062	mgVSS/l
ABMP_T3a_blend	-	-	14922	mgVSS
Substrate_T3b	3756	4368	8124	mgVSS/l
Equi_Sub_T3b	1878	2184	4062	mgVSS/l
ABMP_T3b_blend	-	-	7461	mgVSS
Substrate_T4a	6438	1830	8268	mgVSS/l
Equi_Sub_T4a	3219	915	4134	mgVSS/l
ABMP_T4a_blend	-	-	15066	mgVSS
Substrate_T4b	5038	3230	8268	mgVSS/l
Equi_Sub_T4b	2519	1615	4134	mgVSS/l
ABMP_T4b_blend	-	-	7533	mgVSS
Substrate_T5a	6154	2368	8522	mgVSS/l
Equi_Sub_T5a	3077	1184	4261	mgVSS/l
ABMP_T5a_blend	-	-	15320	mgVSS
Substrate_T5b	4482	4040	8522	mgVSS/l
Equi_Sub_T5b	2241	2020	4261	mgVSS/l
ABMP_T5b_blend	-	-	7660	mgVSS

Table C.1: ABMP Data for Control and Test Samples (each with a duplicate and average reading as conducted in WQL, UCT)																						
Samples	Days	1	2	3	4	5	6	7	9	11	13	15	17	20	23	26	29	32	37	42	45	52
ABMP_Control_1	Gas	0	112	110	113	142	156	139	247	168	166	86	94	54	44	34	32	30	50	42	39	28
	COD	13440	14270	14480	13382	14090	13968	14388	13956	13764	11854	12024	12152	11896	11356	10532	11396	11140	11284	11236	11240	10360
	FSA	309	350	337	334	313	282	339	321	398	383	399	373	394	415	378	409	445	460	458	498	495
	TP	149	155	129	164	149	153	164	147	167	136	149	141	114	106	148	148	141	113	109	113	98
	OP	6	8	8	9	3	7	10	7	6	4	8	4	8	6	6	6	5	4	5	6	6
	TSS	8466	9016	9354	8216	8342	7958	8314	7838	7108	8894	8812	7872	9012	7060	8522	8732	7450	7822	8224	7076	6388
	VSS	6798	7084	7378	6362	6532	6332	6494	6278	5714	6582	6566	6320	6754	5544	6444	6510	5926	6194	6100	5598	5202
	ISS	1668	2022	1976	1854	1810	1626	1820	1560	1394	2312	2246	1552	2258	1516	2078	2222	1524	1628	2124	1478	1186
	CO3 Alk	1958	2012	2140	2116	2279	2089	2196	2041	0	2221	2347	2338	2400	2382	2425	2381	2492	2571	2504	2548	2516
	pH	7.97	7.55	7.47	7.45	7.44	7.43	7.43	7.36	7.36	7.31	7.24	7.25	7.22	7.19	7.26	7.24	7.17	7.24	7.28	7.27	7.21
ABMP_Control_2	Gas	0	44	10	32	0	0	0	0	0	0	0	0	-3	0	-3	2	-6	0	8	2	0
	COD	13440	12600	12364	9938	9748	10332	11238	12358	11396	10028	9904	10230	9580	8532	8548	9348	9316	7992	8112	7460	7736
	FSA	309	312	301	267	271	313	290	363	352	359	338	316	337	357	324	365	367	384	386	411	397
	TP	149	151	149	130	126	141	144	178	154	140	147	106	127	123	102	124	111	88	144	83	87
	OP	6	6	7	6	4	5	6	6	6	6	8	4	7	5	6	5	5	7	4	3	4
	TSS	8466	8670	7718	6904	5634	7430	8376	6686	6554	6858	7698	6684	6870	5810	5928	6352	7086	5334	5084	4578	6130
	VSS	6798	7006	6254	5552	4482	5948	6644	5296	5370	5548	6052	5362	5488	4636	4752	4978	5228	4042	3966	3482	4632
	ISS	1668	1664	1464	1352	1152	1482	1732	1390	1184	1310	1646	1322	1382	1174	1176	1374	1858	1292	1118	1096	1498
	CO3 Alk	1958	1766	1764	1780	1882	1884	1902	1930	1984	2127	1889	1944	2054	2037	1987	2071	1931	2032	2121	2040	1911
	pH	7.89	7.43	7.36	7.35	7.29	7.40	7.43	7.35	7.28	7.44	7.37	7.38	7.38	7.44	7.43	7.41	7.49	7.59	7.58	7.58	7.51
ABMP_Control_Avera	Gas	0	78	60	72.5	71	78	69.5	123.5	84	83	43	47	25.5	22	15.5	17	12	25	25	20.5	14
	COD	13440	13435	13422	11660	11919	12150	12813	13157	12580	10941	10964	11191	10738	9944	9540	10372	10228	9638	9674	9350	9048
	FSA	309	331	319	300.5	292	297.5	314.5	342	375	371	368.5	344.5	365.5	386	351	387	406	422	422	454.5	446
	TP	149	153	139	147	138	147	154	163	161	138	148	124	121	115	125	136	126	101	127	98	93
	OP	6	7	8	8	4	6	8	7	6	5	8	4	8	6	6	6	5	6	5	5	5
	TSS	8466	8843	8536	7560	6988	7694	8345	7262	6831	7876	8255	7278	7941	6435	7225	7542	7268	6578	6654	5827	6259

	VSS	6798	7045	6816	5957	5507	6140	6569	5787	5542	6065	6309	5841	6121	5090	5598	5744	5577	5118	5033	4540	4917
	ISS	1668	1843	1720	1603	1481	1389	1651	1646	1392	1748	1778	1599	1790	1449	1626	1699	1449	1743	1708	1298	1141
	CO3	1958.00	1889.0	1952.0	1948.0	2080.5	1985.5	2040.	1971.50	965.00	2102.	2237.0	2113.5	2172.0	2218.0	2231.0	2184.0	2281.5	2251.0	2268.0	2334.5	2278.0
	Alk		0	0	0	0	0	00			50	0	0	0	0	0	0	0	0	0	0	0
	pH	7.93	7.49	7.42	7.40	7.37	7.42	7.43	7.36	7.32	7.38	7.31	7.32	7.30	7.32	7.35	7.33	7.33	7.42	7.43	7.43	7.36
ABMP_Column_la	Gas	0	296	326	236	259	5	186	357	186	188	102	106	74	26	40	55	36	31	18	8	101
	COD	16900	11370	13166	11296	15298	14238	16256	16162	15472	13152	12532	14424	12596	12340	12072	12268	12172	11608	11072	11148	11056
	FSA	322	380	381	369	329	307	358	416	452	474	462	441	451	460	425	478	509	502	496	505	547
	TP	178	132	121	164	174	178	165	175	187	102	143	142	135	131	152	135	135	126	127	106	99
	OP	8	11	15	6	2	5	10	6	6	5	9	4	6	5	5	5	5	6	6	5	5
	TSS	10838	8676	9712	7588	11344	9782	10856	9482	9338	9262	9826	9524	10148	9090	9262	10524	10368	9924	6970	6700	7082
	VSS	8966	6942	7994	5938	8238	7244	9196	7254	7422	7520	7552	7598	7622	6744	7286	7508	6892	6800	5662	4964	5716
	ISS	1872	1734	1718	1650	3106	2538	1660	2228	1916	1742	2274	1926	2526	2346	1976	3016	3476	3124	1308	1736	1366
	CO3	2094	2268	2243	2301	2352	2420	2478	2448	0	2589	2616	2711	2934	2809	2824	2790	2803	2892	2885	2682	2953
	Alk																					
	pH	7.89	7.42	7.42	7.34	7.34	7.43	7.33	7.24	7.19	7.23	7.25	7.20	7.23	7.23	7.27	7.28	7.22	7.27	7.36	7.30	7.28
ABMP_Column_lb	Gas	0	0	137	84	70	66	26	101	75	2	12	16	-4	-4	-2	-3	-5	-10	0	5	-3
	COD	16900	14840	12070	14392	17122	17154	18794	11288	11908	10844	10420	12094	11388	11272	12244	13220	12128	11576	10952	9996	9288
	FSA	322	376	380	344	334	348	361	422	454	476	453	399	430	460	412	484	522	488	483	516	563
	TP	138	176	170	156	161	168	168	183	183	156	138	136	147	158	127	145	141	123	169	103	100
	OP	8	10	12	4	3	8	8	6	4	5	8	3	7	5	3	4	5	4	3	3	4
	TSS	10838	9890	6936	8976	9818	7648	9200	7372	6746	7326	7170	7452	8116	7432	8402	8412	8330	8094	7430	5876	5988
	VSS	8966	7950	5756	7074	7786	6122	7302	6146	5582	6072	5902	5886	6642	5692	6814	6966	6266	5798	5356	4520	4538
	ISS	1872	1940	1180	1902	2032	1526	1898	1226	1164	1254	1268	1566	1474	1740	1588	1446	2064	2296	2074	1356	1450
	CO3	2094	2234	2338	2346	2419	2381	2350	2639	2721	2542	2694	2688	2673	2759	2847	2818	2880	2933	2752	2529	2468
	Alk																					
	pH	7.89	7.43	7.36	7.35	7.29	7.40	7.43	7.35	7.28	7.44	7.37	7.38	7.38	7.44	7.43	7.45	7.41	7.49	7.59	7.58	7.51
ABMP_Column_1_Averag	Gas	0	148	232	160	165	36	106	229	131	95	57	61	35	11	19	26	16	11	9	7	49
	COD	16900	13105	12618	12844	16210	15696	17525	13725	13690	11998	11476	13259	11992	11806	12158	12744	12150	11592	11012	10572	10172
	FSA	322	378	381	357	332	328	360	419	453	475	458	420	441	460	419	481	516	495	490	511	555
	TP	158	154	146	160	168	173	173	174	179	172	120	140	145	147	129	149	138	125	148	105	100
	OP	8	11	14	5	3	7	9	6	5	5	9	4	7	5	4	5	5	5	5	4	5
	TSS	10838	9283	8324	8282	10581	8715	10028	8427	8042	8294	8498	8488	9132	8261	8832	9468	9349	9009	7200	6288	6535
	VSS	8966	7446	6875	6506	8012	6683	8249	6700	6502	6796	6727	6742	7132	6218	7050	7237	6579	6299	5509	4742	5127

	ISS	1872	1837	1449	1776	2569	2032	1779	1727	1540	1498	1771	1746	2000	2043	1782	2231	2770	2710	1691	1546	1408
	CO3 Alk	2094	2251	2291	2324	2386	2401	2414	2544	1361	2566	2655	2700	2804	2784	2836	2804	2842	2913	2819	2606	2711
	pH	7.89	7.43	7.39	7.35	7.32	7.42	7.38	7.30	7.24	7.34	7.31	7.29	7.31	7.34	7.35	7.37	7.32	7.38	7.48	7.44	7.40
ABMP_Column_2a	Gas	0	319	383	336	252	226	191	389	256	182	182	150	17	48	28	25	13	48	41	36	-3
	COD	16940	10730	9318	8048	8298	8446	8148	8276	10204	9630	10284	14618	12472	12534	11352	11860	11824	11296	11316	11464	11220
	FSA	351	389	437	355	343	365	372	405	452	460	438	417	417	417	428	461	490	497	486	512	520
	TP	171	122	144	154	144	158	136	158	134	109	103	143	123	114	122	126	114	105	125	103	102
	OP	10	8	14	5	4	6	13	9	7	7	10	4	7	9	6	5	5	8	7	6	6
	TSS	10112	8342	6148	6562	5218	5186	4732	5342	6868	7072	6818	8164	8640	8752	8144	8346	8340	7954	7414	7668	7652
	VSS	8984	7018	4950	5512	4140	3966	3718	4208	5468	5620	5420	6768	6974	6876	6458	6832	6836	6432	5968	6060	6540
	ISS	1128	1324	1198	1050	1078	1220	1014	1134	1400	1452	1398	1396	1666	1876	1686	1514	1504	1522	1446	1608	1112
	CO3 Alk	2156	2203	2261	2300	2418	2438	2424	2346	0	2518	2420	2584	2644	2689	2691	2686	2844	2816	2755	2699	2704
	pH	7.79	7.27	7.30	7.29	7.29	7.31	7.35	7.24	7.19	7.16	7.21	7.24	7.23	7.21	7.32	7.28	7.24	7.26	7.31	7.29	7.20
ABMP_Column_2b	Gas	0	73	141	111	95	65	44	101	67	74	6	21	-6	-7	-7	-3	-5	-14	2	6	-3
	COD	16940	12550	11380	12532	9536	9892	9684	9616	10362	11214	10988	11870	10748	10580	10240	10116	10672	9576	8908	8776	8056
	FSA	351	391	431	332	322	343	367	404	445	489	457	411	443	476	456	486	509.7	492.8	476.6	547.9	567.7
	TP	149	174	189	161	169	159	160	190	178	123	161	157	155	140	110	152	116	107	150	102	92
	OP	10	12	15	3	3	7	10	9	5	5	7	3	8	5	5	4	4.9	3.15	2.5	1.9	2.71
	TSS	9712	8872	8186	7480	6410	7006	5512	5668	5946	7566	7630	7726	7612	8264	7386	7050	6792	5884	5122	4730	4322
	VSS	8584	6964	6314	5814	4958	5976	4460	4550	4834	5846	5930	6014	5878	6298	5636	5312	5150	4342	3940	3554	3268
	ISS	1128	1908	1872	1666	1452	1030	1052	1118	1112	1720	1700	1712	1734	1966	1750	1738	1642	1542	1182	1176	1054
	CO3 Alk	2156	2249	2158	2326	2362	2403	2419	2656	2632	2682	2624	2672	2770	2736	2819	2821	2938	2813	2692	2613	2546
	pH	7.79	7.36	7.22	7.23	7.26	7.37	7.39	7.29	7.26	7.34	7.34	7.31	7.35	7.37	7.35	7.41	7.40	7.50	7.58	7.58	7.58
ABMP_Column_2_Average	Gas	0	196	262	224	174	146	118	245	162	128	94	86	6	21	11	11	4	17	22	21	-3
	COD	16940	11640	10349	10290	8917	9169	8916	8946	10283	10422	10636	13244	11610	11557	10796	10988	11248	10436	10112	10120	9638
	FSA	351	390	434	343	332	354	369	404	449	474	447	414	430	447	442	474	500	495	481	530	544
	TP	160	148	167	158	157	159	148	174	156	116	132	150	139	127	116	139	115	106	138	103	97
	OP	10	10	14	4	3	6	12	9	6	6	8	3	8	7	6	4	5	6	5	4	4
	TSS	9912	8607	7167	7021	5814	6096	5122	5505	6407	7319	7224	7945	8126	8508	7765	7698	7566	6919	6268	6199	5987
	VSS	8784	6991	5632	5663	4549	4971	4089	4379	5151	5733	5675	6391	6426	6587	6047	6072	5993	5387	4954	4807	4904
	ISS	1128	1616	1535	1358	1265	1125	1033	1126	1256	1586	1549	1554	1700	1921	1718	1626	1573	1532	1314	1392	1083

	CO3 Alk	2156	2226	2210	2313	2390	2421	2422	2501	1316	2600	2522	2628	2707	2713	2755	2754	2891	2815	2724	2656	2625
	pH	7.79	7.32	7.26	7.26	7.28	7.34	7.37	7.27	7.23	7.25	7.28	7.28	7.29	7.29	7.34	7.35	7.32	7.38	7.45	7.44	7.39
ABMP_Column_3a	Gas	0	368	412	249	193	195	168	218	119	222	187	101	34	49	39	23	18	24	26	24	6
	COD	16820	11580	11396	9634	9576	10846	11032	11466	11040	10610	10188	13592	12196	13812	11492	11816	11648	11608	11236	11240	10780
	FSA	346	392	435	366	330	376	379	423	445	454	429	413	431	449	402	464	481	466	488	505	531
	TP	176	146	130	173	173	169	176	178	158	115	118	125	170	162	125	116	119	133	137	103	112
	OP	10	16	13	6	5	11	13	11	7	5	10	7	6	9	7	7	5	7	7	6	5
	TSS	10240	7156	7270	6654	6684	6902	6624	7644	7308	7642	7144	9222	8964	9710	9112	8570	8622	9608	8086	8036	6868
	VSS	8124	5518	5686	5074	5150	5414	5298	5974	5906	6180	5720	7496	7320	7296	7384	6874	7024	7012	6420	6468	5552
	ISS	2116	1638	1584	1580	1534	1488	1326	1670	1402	1462	1424	1726	1644	2414	1728	1696	1598	2596	1666	1568	1316
	CO3 Alk	2027	2184	2227	2299	2443	2354	2401	2760	0	2466	2553	2556	2523	2722	2761	2635	2556	2714	2533	2732	2598
	pH	7.68	7.29	7.41	7.23	7.29	7.33	7.36	7.18	7.21	7.20	7.23	7.21	7.24	7.21	7.29	7.25	7.22	7.26	7.33	7.29	7.25
ABMP_Column_3b	Gas	0	124	163	102	41	0	0	100	60	49	-15	6	-2	-3	-3	-2	-5	-7	0	2	-4
	COD	16820	14010	13352	12904	12392	13574	13612	14056	11054	11676	12192	11778	10520	10740	9752	10680	11044	9812	9320	9796	9060
	FSA	346	408	421	325	320	368	353	405	442	432	442	417	457	497	421	471	487.6	501.5	501.3	564.4	610
	TP	144	174	166	162	174	187	168	168	172	167	146	154	162	144	156	139	112	107	150	104	102
	OP	10	13	14	5	3	7	9	6	5	5	8	4	7	6	5	3	5.5	3.5	2.38	2.68	2.13
	TSS	10240	10390	9424	9110	8254	7596	8458	7962	8270	8076	8522	7538	7138	7004	6984	7702	8058	6438	6344	5186	5104
	VSS	8124	7686	7374	7018	6472	5638	6556	6208	6518	6302	6518	5984	5548	5414	5378	5834	6256	4932	4910	4044	3756
	ISS	2116	2704	2050	2092	1782	1958	1902	1754	1752	1774	2004	1554	1590	1590	1606	1868	1802	1506	1434	1142	1348
	CO3 Alk	2027	2172	2251	2372	2319	2528	2404	2585	3040	2615	2611	2671	2592	2816	2675	2705	2756	2801	2721	2656	2692
	pH	7.68	7.33	7.31	7.26	7.25	7.38	7.37	7.29	7.23	7.36	7.35	7.37	7.39	7.40	7.42	7.46	7.42	7.56	7.63	7.57	7.57
ABMP_Column_3_Average	Gas	0	246	288	176	117	98	84	159	90	136	86	54	16	23	18	11	7	9	13	13	1
	COD	16820	12795	12374	11269	10984	12210	12322	12761	11047	11143	11190	12685	11358	12276	10622	11248	11346	10710	10278	10518	9920
	FSA	346	400	428	346	325	372	366	414	444	443	435	415	444	473	411	468	484	484	495	535	571
	TP	160	160	148	168	174	178	172	173	165	141	132	140	166	153	141	128	116	120	144	104	107
	OP	10	15	14	5	4	9	11	9	6	5	9	6	6	7	6	5	5	5	5	4	4
	TSS	10240	8773	8347	7882	7469	7249	7541	7803	7789	7859	7833	8380	8051	8357	8048	8136	8340	8023	7215	6611	5986
	VSS	8124	6602	6530	6046	5811	5526	5927	6091	6212	6241	6119	6740	6434	6355	6381	6354	6640	5972	5665	5256	4654
	ISS	2116	2171	1817	1836	1658	1723	1614	1712	1577	1618	1714	1640	1617	2002	1667	1782	1700	2051	1550	1355	1332
	CO3 Alk	2027	2178	2239	2336	2381	2441	2403	2673	1520	2541	2582	2614	2558	2769	2718	2670	2656	2758	2627	2694	2645

	pH	7.68	7.31	7.36	7.25	7.27	7.36	7.37	7.24	7.22	7.28	7.29	7.29	7.32	7.31	7.36	7.36	7.32	7.41	7.48	7.43	7.41
ABMP_Column_4a	Gas	0	410	482	373	284	229	157	188	102	191	195	126	99	57	65	37	31	7	4	17	25
	COD	16140	13720	12456	13638	14188	15324	14378	14434	13976	12432	11992	13646	12036	13596	12992	11508	11216	11264	10892	10976	11044
	FSA	347	393	437	366	319	377	392	417	465	463	445	441	449	456	438	482	487	506	501	517	526
	TP	159	159	131	179	162	178	166	161	161	171	167	132	128	121	130	123	121	115	143	109	112
	OP	11	15	15	6	3	8	12	10	7	3	9	6	7	7	7	5	5	8	7	6	6
	TSS	10440	9080	9180	11234	10432	10154	9272	9660	9358	8822	8722	9042	9660	10926	10728	8824	8574	7930	7694	8330	8410
	VSS	8268	6624	7060	7788	7170	6944	7150	7712	7502	7164	6782	7112	7386	7686	6882	6792	6780	6250	6094	6260	6438
	ISS	2172	2456	2120	3446	3262	3210	2122	1948	1856	1658	1940	1930	2274	3240	3846	2032	1794	1680	1600	2070	1972
	CO3 Alk	2008	2308	2407	2304	2387	2419	2514	2502	0	2482	2658	2692	2666	2653	2809	2756	2697	2873	2781	2776	2744
	pH	7.73	7.27	7.25	7.20	7.27	7.28	7.18	7.20	7.19	7.20	7.22	7.21	7.17	7.23	7.31	7.42	7.41	7.40	7.40	7.37	7.28
ABMP_Column_4b	Gas	0	0	107	139	104	92	76	114	46	28	-15	25	-8	-9	-6	-3	-7	-9	0	5	-2
	COD	16140	11930	12528	15680	14306	14262	17028	14518	12690	11232	11180	12538	11648	10464	10944	10316	9972	10024	10320	10364	9588
	FSA	347	407	440	328	374	384	384	421	490	468	460	439	462	486	451	520	516.6	528.1	496.7	560.8	614.8
	TP	154	177	150	143	174	176	168	181	188	148	159	168	161	160	169	125	114	114	159	108	108
	OP	11	13	13	3	4	7	10	7	9	5	9	4	7	7	6	6	5.9	5.4	4.13	3.63	2.68
	TSS	10440	8326	10262	12380	13020	10578	11344	10402	8942	8742	8418	7682	8012	6708	8348	6526	5854	6172	6256	6888	6678
	VSS	8268	6764	7702	8388	9178	8084	7768	7090	6508	6470	6144	5982	6062	5228	6362	4998	4752	5006	4980	5214	5038
	ISS	2172	1562	2560	3992	3842	2494	3576	3312	2434	2272	2274	1700	1950	1480	1986	1528	1102	1166	1276	1674	1640
	CO3 Alk	2008	2256	2292	2364	2531	2515	2559	2610	0	2650	2707	2577	2812	2813	2867	2849	2788	2859	2897	2838	2853
	pH	7.73	7.27	7.25	7.22	7.26	7.35	7.30	7.28	7.25	7.34	7.29	7.22	7.26	7.26	7.30	7.37	7.39	7.47	7.64	7.60	7.60
ABMP_Column_4 Average	Gas	0	205	295	256	194	161	117	151	74	110	90	76	46	24	30	17	12	-1	2	11	12
	COD	16140	12825	12492	14659	14247	14793	15703	14476	13333	11832	11586	13092	11842	12030	11968	10912	10594	10644	10606	10670	10316
	FSA	347	400	439	347	347	381	388	419	478	466	452	440	456	471	444	501	502	517	499	539	570
	TP	157	168	141	161	168	177	167	171	175	160	163	150	145	141	150	124	118	115	151	109	110
	OP	11	14	14	4	4	8	11	9	8	4	9	5	7	7	6	5	5	7	6	5	4
	TSS	10440	8703	9721	11807	11726	10366	10308	10031	8942	8782	8570	8362	8836	8817	9538	7675	8574	7051	6975	7609	7544
	VSS	8268	6694	7381	8088	8174	7514	7459	7401	7005	6817	6463	6547	6724	6457	6622	5895	5766	5628	5537	5737	5738
	ISS	2172	2009	2340	3719	3552	2852	2849	2630	2145	1965	2107	1815	2112	2360	2916	1780	1448	1423	1438	1872	1806
	CO3 Alk	2008	2282	2350	2334	2459	2467	2537	2556	0	2566	2683	2635	2739	2733	2838	2803	2743	2866	2839	2807	2799
	pH	7.73	7.27	7.25	7.21	7.27	7.32	7.24	7.24	7.22	7.27	7.26	7.22	7.22	7.25	7.31	7.40	7.40	7.44	7.52	7.49	7.44
A	Gas	0	72	162	349	195	135	120	180	104	225	246	128	63	27	24	23	20	34	33	41	19

	COD	19000	11140	16634	11482	11260	12632	13818	12980	12088	9954	10468	13130	12174	12142	11452	11976	11848	11872	10912	10864	10640
	FSA	10	72	162	349	195	135	120	180	104	225	246										
	TP	176	140	128	166	157	179	163	149	107	175	114	173	166	119	132	125	121	110	113	118	101
	OP	11	13	8	3	4	8	16	11	7	8	12	8	5	7	7	5	6	11	9	8	7
	TSS	10760	9348	9294	8292	8252	8014	8760	8046	8562	7992	8252	9100	9044	8700	8836	8734	8710	8406	7910	7694	7796
	VSS	8522	7388	7592	6352	6356	6234	6628	6230	6810	6392	6444	7398	7344	8680	6890	7164	7024	6840	6404	6058	6154
	ISS	2238	1960	1702	1940	1896	1780	2132	1816	1752	1600	1808	1702	1700	1823	1946	1570	1686	1566	1506	1636	1642
	CO3 Alk	2061	2195	2180	2235	2137	2257	2337	2517	0	2381	2516	2439	2461	2572	2579	2635	2662	2606	2559	2588	2603
	pH	7.62	7.32	7.22	7.33	7.37	7.37	7.37	7.35	7.20	7.24	7.25	7.24	7.18	7.22	7.19	7.23	7.25	7.30	7.26	7.16	7.20
ABMP_Column_5b	Gas	0	80	170	52	60	76	67	125	72	60	14	43	37	32	25	33	25	44	50	56	43
	COD	19000	14700	14696	11822	13470	15020	16414	15488	16576	13660	13052	12054	12244	11604	10232	11740	11004	11048	10400	10448	9040
	FSA	317	388	405	340	325	358	351	371	446	432	436	409	447	484	428	482	497	505	467	494	592
	TP	141	163	156	166	183	164	163	159	192	164	126	144	168	157	155	143	120	114	155	108	99
	OP	11	12	11	7	3	7	12	6	5	5	10	4	6	5	6	4	5	4	3	3	3
	TSS	10760	9974	11344	10108	10964	10222	8018	11050	11796	11456	10448	8044	9676	9338	8400	8650	8938	8274	7536	7146	5738
	VSS	8522	7714	8442	7576	7676	7614	6228	8284	8984	9068	8176	6670	7344	6268	6576	6750	7062	6452	5852	5424	4482
	ISS	2238	2260	2902	2532	3288	2608	1790	2766	2812	2388	2272	1374	2332	3070	1824	1900	1876	1822	1684	1722	1256
	CO3 Alk	2061	2217	2471	2327	2384	2330	2229	2479	0	2392	2555	2444	2609	2815	2740	2653	2746	2751	2825	2508	2436
	pH	7.62	7.30	7.32	7.31	7.29	7.38	7.36	7.35	7.34	7.34	7.40	7.40	7.39	7.42	7.48	7.53	7.51	7.55	7.74	7.66	7.67
ABMP_Column_5_Average	Gas	0	76	166	201	128	106	94	153	88	143	130	86	50	30	25	28	23	39	42	49	31
	COD	19000	12920	15665	11652	12365	13826	15116	14234	14332	11807	11760	12592	12209	11873	10842	11858	11426	11460	10656	10656	9840
	FSA	164	230	284	345	260	247	235	276	275	328	341	409	447	484	428	482	497	505	467	494	592
	TP	159	152	142	166	170	172	163	154	150	170	120	159	167	138	144	134	121	112	134	113	100
	OP	11	12	10	5	3	8	14	9	6	7	11	6	6	6	6	4	6	7	6	5	5
	TSS	10760	9661	10319	9200	9608	9118	8389	9548	10179	9724	9350	8572	9360	9019	8618	8692	8824	8340	7723	7420	6767
	VSS	8522	7551	8017	6964	7016	6924	6428	7257	7897	7730	7310	7034	7344	7474	6733	6957	7043	6646	6128	5741	5318
	ISS	2238	2110	2302	2236	2592	2194	1961	2291	2282	1994	2040	1538	2016	2447	1885	1735	1781	1694	1595	1679	1449
	CO3 Alk	2061	2206	2326	2281	2261	2294	2283	2498	0	2387	2536	2442	2535	2694	2660	2644	2704	2679	2692	2548	2520
	pH	7.62	7.31	7.27	7.32	7.33	7.38	7.37	7.35	7.27	7.29	7.33	7.32	7.29	7.32	7.34	7.38	7.38	7.43	7.50	7.41	7.44

Table C.2: Summary of ABMP Reactor Mass Compositions , Mass Ratios, and Molar Mass														
fs'up	fp	fn	fo	fh	fc	fcv	MM	EDC	B	A	Z	Y	X	Parameters
0.7708	0.00	0.07	0.28	0.14	0.52	2.08	51.1	13.2	0.00	0.25	0.88	7.00	2.20	C1
0.5755	0.06	0.07	0.08	0.17	0.62	2.87	42.3	15.1	0.08	0.19	0.21	7.00	2.18	C2
0.6732	0.00	0.07	0.09	0.18	0.66	2.97	39.6	14.7	0.00	0.19	0.21	7.00	2.18	CA
0.5772	0.06	0.05	0.37	0.09	0.43	1.48	78.0	14.4	0.14	0.28	1.82	7.00	2.80	T1a - C1
0.4035	0.00	0.17	0.27	0.06	0.51	1.27	118.	18.8	0.00	1.40	2.00	7.00	5.00	T1b - C1
0.7060	0.06	0.05	0.37	0.09	0.43	1.48	78.0	14.4	0.14	0.28	1.82	7.00	2.80	T1a - C2
0.5324	0.00	0.06	0.40	0.09	0.46	1.44	78.3	14.1	0.00	0.32	1.93	7.00	2.98	T1b - C2
0.6416	0.00	0.05	0.39	0.10	0.46	1.48	74.1	13.7	0.00	0.28	1.83	7.00	2.81	T1a - Cave
0.4679	0.00	0.13	0.37	0.08	0.43	1.20	86.8	12.9	0.00	0.78	1.98	7.00	3.08	T1b - Cave
0.5548	0.06	0.05	0.37	0.09	0.43	1.48	78.3	14.4	0.14	0.28	1.82	7.00	2.81	T1ave - Cave
0.5909	0.00	0.05	0.40	0.09	0.46	1.48	75.3	13.9	0.00	0.28	1.86	7.00	2.87	T2a - C1
0.2814	0.00	0.12	0.28	0.06	0.53	1.42	112.	20.0	0.00	0.99	1.97	7.00	4.98	T2b - C1
0.7193	0.00	0.05	0.39	0.09	0.46	1.45	79.5	14.4	0.00	0.31	1.95	7.00	3.06	T2a - C2
0.4097	0.00	0.12	0.29	0.06	0.53	1.40	113.	19.9	0.00	1.00	2.05	7.00	5.00	T2b - C2
0.6551	0.00	0.09	0.37	0.09	0.46	1.43	76.2	13.6	0.00	0.47	1.74	7.00	2.89	T2a - Cave
0.3455	0.00	0.12	0.29	0.06	0.53	1.40	113.	19.9	0.00	1.00	2.05	7.00	5.00	T2b - Cave
0.5003	0.00	0.05	0.39	0.10	0.46	1.49	73.8	13.7	0.00	0.28	1.81	7.00	2.81	T2ave - Cave
0.5544	0.00	0.05	0.40	0.09	0.46	1.47	75.6	13.9	0.00	0.28	1.87	7.00	2.87	T3a - C1
0.3841	0.00	0.12	0.28	0.06	0.53	1.41	113.	20.0	0.00	1.00	2.00	7.00	5.00	T3b - C1
0.6843	0.00	0.05	0.39	0.10	0.46	1.48	74.2	13.7	0.00	0.28	1.83	7.00	2.82	T3a - C2

Table C.2 Continuation: Summary of ABMP Reactor Mass Compositions , Mass Ratios, and Molar Mass

fS'up	fp	fn	fo	fh	fc	fcv	MM	EDC	B	A	Z	Y	X	Parameter
0.514	0.00	0.12	0.28	0.06	0.53	1.41	113.1	20.00	0.000	1.00	2.00	7.0	5.0	T3b - C2
0.4693	0.00	0.05	0.39	0.10	0.46	1.48	73.84	13.70	0.00001	0.28	1.81	7.0	2.80	T3a - Cave
0.5992	0.00	0.12	0.28	0.06	0.53	1.41	113.12	20.00	0.00013	1.00	2.00	7.0	5.00	T3b - Cave
0.5342	0.00	0.06	0.40	0.05	0.49	1.16	149.77	21.76	0.00015	0.67	3.76	7.0	6.08	T3ave - Cave
0.6225	0.00	0.08	0.38	0.09	0.45	1.44	75.27	13.52	0.00004	0.40	1.78	7.0	2.82	T4a - C1
0.4679	0.00	0.12	0.29	0.06	0.53	1.40	113.92	19.90	0.00013	1.00	2.05	7.0	5.00	T4b - C1
0.6225	0.00	0.05	0.40	0.09	0.46	1.46	76.71	14.04	0.00057	0.29	1.89	7.0	2.92	T4a - C2
0.6072	0.00	0.05	0.39	0.10	0.46	1.49	73.77	13.74	0.00000	0.28	1.81	7.0	2.80	T4b - C2
0.5452	0.00	0.12	0.29	0.06	0.53	1.41	113.10	19.87	0.00012	0.99	2.02	7.0	4.97	T4a - Cave
0.6845	0.00	0.05	0.40	0.09	0.46	1.48	74.78	13.83	0.00001	0.28	1.84	7.0	2.84	T4b - Cave
0.6148	0.00	0.05	0.40	0.09	0.46	1.46	76.94	14.07	0.00202	0.29	1.90	7.0	2.93	T4ave - Cave
0.4446	0.00	0.22	0.16	0.02	0.59	1.24	282.63	43.94	0.00002	4.47	2.79	7.0	13.9	T5a - C1
0.3143	0.00	0.05	0.40	0.09	0.46	1.43	81.25	14.49	0.00019	0.31	2.02	7.0	3.11	T5b - C1
0.5514	0.06	0.05	0.37	0.09	0.43	1.47	78.75	14.49	0.1413	0.28	1.83	7.0	2.82	T5a - C2
0.4211	0.00	0.18	0.17	0.07	0.59	1.61	107.60	21.66	0.00015	1.38	1.12	7.0	5.26	T5b - C2
0.3794	0.00	0.08	0.39	0.07	0.47	1.25	107.25	16.75	0.00011	0.58	2.61	7.0	4.18	T5a - Cave
0.4863	0.06	0.05	0.37	0.09	0.43	1.48	78.20	14.43	0.14028	0.28	1.82	7.0	2.80	T5b - Cave
0.4328	0.00	0.06	0.39	0.09	0.47	1.48	77.62	14.35	0.00001	0.30	1.88	7.0	3.01	T5ave - Cave

Table C.3: Summary of ABMP Data Showing Substrate Concentrations and Variables									
ABMP Reactor set up		Period, t	Variables						
			COD	FSA	OP	VSS	ISS	H2CO3Alk	pH
Measured Control ABMP values	Control 1	t = 0	13440	322	6	6798	1668	1958	7.97
		t = end	10360	547	6	5202	1186	2516	7.21
	Control 2	t = 0	13440	322	6	6798	1668	1958	7.89
		t = end	7736	547	4	4632	230	1911	7.51
	Control Average	t = 0	13440	322	6	6798	1668	1958	7.93
		t = end	11900	435	6	6000	1427	2237	7.57
Column1 Measured Test ABMP Values	T1a	t = 0	16900	322	8	8966	1872	2094	7.89
		t = end	11056	547	5	5716	1366	2953	7.28
	T1b	t = 0	16900	322	8	8966	1872	2094	7.89
		t = end	9288	563	4	4538	1450	2468	7.51
	T1Ave	t = 0	16900	322	8	8966	1872	2094	7.89
		t = end	10172	547	5	5127	1408	2711	7.4
Column2 Measured Test ABMP Values	T2a	t = 0	16940	351	10	8984	1128	2156	7.79
		t = end	11220	520	6	6540	1112	2704	7.2
	T2b	t = 0	16940	351	10	8584	1128	2156	7.79
		t = end	8056	567.7	2.71	3268	1054	2546	7.58
	T2Ave	t = 0	16940	351	10	8784	1128	2156	7.79
		t = end	9638	544	4	4904	1083	2625	7.39
Column3 Measured Test ABMP Values	T3a	t = 0	16820	346	10	8124	2116	2027	7.68
		t = end	10780	531	5	5552	1316	2598	7.25
	T3b	t = 0	16820	346	10	8124	2116	2027	7.68
		t = end	9060	610	2.13	3756	1348	2692	7.57
	T3Ave	t = 0	16820	346	10	8124	2116	2027	7.68
		t = end	9920	571	4	4654	1332	2645	7.41
Column4 Measured Test ABMP Values	T4a	t = 0	16140	347	11	8268	2172	2008	7.73
		t = end	11044	526	6	6438	1972	2744	7.28
	T4b	t = 0	16140	347	11	8268	2172	2008	7.73
		t = end	9588	614.8	2.68	5038	1640	2853	7.6
	T4Ave	t = 0	16140	347	11	8268	2172	2008	7.73
		t = end	10316	570	4	5738	1806	2799	7.44
Column5 Measured Test ABMP Values	T5a	t = 0	19000	10	11	8522	2238	2061	7.62
		t = end	10640	0	7	6154	1642	2603	7.2
	T5b	t = 0	19000	317	11	8522	2238	2061	7.62
		t = end	9040	592	3	4482	1256	2436	7.67
	T5Ave	t = 0	19000	164	11	8522	2238	2061	7.62
		t = end	9840	592	5	5318	1449	2520	7.44
		t = 0	6720	161	3	3399	834	979	7.97

Equivalent Control concentrations relative to Test ABMPs	Control 1 (C1)	t = end	5180	273.5	3	2601	593	1258	7.21
	Control 2 (C2)	t = 0	6720	161	3	3399	834	979	7.89
		t = end	3868	273.5	2	2316	115	955.5	7.51
	Control Avg. (CA)	t = 0	6720	161	3	3399	834	979	7.93
		t = end	5950	217.25	3	3000	713.5	1118.5	7.36
Calculated Substrate concentrations in ABMP Test Samples	T1a - C1	t = 0	10180	161	5	5567	1038	1115	
		t = end	5876	289.5	2	3115	773	1695	
	T1b - C2	t = 0	10180	161	5	5567	1038	1115	
		t = end	5420	273.5	2	2222	1335	1512.5	
	T1Ave - CA	t = 0	10180	190	5	5567	1038	1115	
		t = end	4222	302.75	1.5	2127	694.5	1592	
	T2a - C1	t = 0	10220	189.7	7	5585	294	1177	
		t = end	6040	294.2	3	3939	519	1446	
	T2b - C2	t = 0	10220	189.85	6.85	5185	294	1177	
		t = end	4188	270.35	0.71	952	939	1590.5	
	T2Ave - CA	t = 0	10220	185	6.925	5385	294	1177	
		t = end	3688	313.75	1.355	1904	369.5	1506.5	
	T3a - C1	t = 0	10100	185.3	7	4725	1282	1048	
		t = end	5600	336.5	2	2951	723	1340	
	T3b - C2	t = 0	10100	185.15	6.7	4725	1282	1048	
		t = end	5192	297	0.13	1440	1233	1736.5	
	T3Ave - CA	t = 0	10100	186	6.85	4725	1282	1048	
		t = end	3970	308.75	0.565	1654	618.5	1526.5	
	T4a - C1	t = 0	9420	185.6	8	4869	1338	1029	
		t = end	5864	341.3	3	3837	1379	1486	
	T4b - C2	t = 0	9420	185.8	8.4	4869	1338	1029	
		t = end	5720	296.9	0.68	2722	1525	1897.5	
	T4Ave - CA	t = 0	9420	-151	8.2	4869	1338	1029	
		t = end	4366	-217.25	1.34	2738	1092.5	1680	
	T5a - C1	t = 0	12280	156.2	8	5123	1404	1082	
		t = end	5460	318.5	4	3553	1049	1345	
	T5b - C2	t = 0	12280	2.6	8.3	5123	1404	1082	
		t = end	5172	318.5	0.56	2166	1141	1480.5	
	T5Ave - CA	t = 0	12280	2.6	8.15	5123	1404	1082	
		t = end	3890	374.75	1.78	2318	735.5	1401	

Table C.4.1 ABMP Test for Column 1						Rhyd/Z_AD	
Tests	Time (d)	Sbpe	Z_AD	rhYd	Sbpe/Z_AD (gCOD/gCOD)	Measured	Predicted
T1b – C1 KM (8.619) kS (21.103)	0	2.530735	0.909265				
	7	0.99688	0.85112	0.256402	2.17	0.703984	0.803645
	9	1.4525	0.7335	0.157084	1.980231	0.64242	0.739394
	11	0.965616	0.722384	0.179563	1.336709	0.43365	0.513424
	13	0.577944	0.700056	0.187495	0.825568	0.267828	0.324489
	20	0.16472	0.51528	0.155581	0.319671	0.103707	0.128614
	42	0.010807	-0.19481	0.097278	0.06	0.019465	0.024436
T1a – C2 KM (3.784) kS (16.061)	0	-0.79926	0.909265				
	2	-6.01219	1.432191	2.643743	16	1.845943	1.8884
	7	1.218177	0.449823	-0.25093	7.1	1.298057	1.159984
	11	0.305289	0.420711	-0.06313	3.7	0.676452	0.708507
	17	0.662001	0.181999	-0.04868	3.637394	0.665006	0.698732
	29	-0.32694	-0.10306	0.020993	3.172434	0.58	0.624147
	32	-0.28726	-0.20674	0.02128	1.389433	0.254023	0.301289
	45	1.135375	-0.79737	-0.00571	0.36	0.007164	0.082957
T1a – CAve KM (3.963) kS (14.213)	0	2.06	0.909265	0			
	2	-5.1194	1.654403	3.626981	18.52	2.192321	2.242225
	4	-3.12714	1.363143	1.334066	6.9	1.49	1.295159
	6	-0.28821	0.976209	0.428648	2.462906	0.439095	0.585305
	9	0.857452	0.747548	0.170896	1.147021	0.228609	0.29594
	11	0.804616	0.687384	0.151406	1.17055	0.220264	0.301549
	17	1.412738	0.420262	0.075354	0.83	0.179303	0.218659
Units	Days	(gCOD)	(gCOD)	(gCOD/l/d)	(gCOD/gCOD)	gCOD/(gCOD.l.d)	

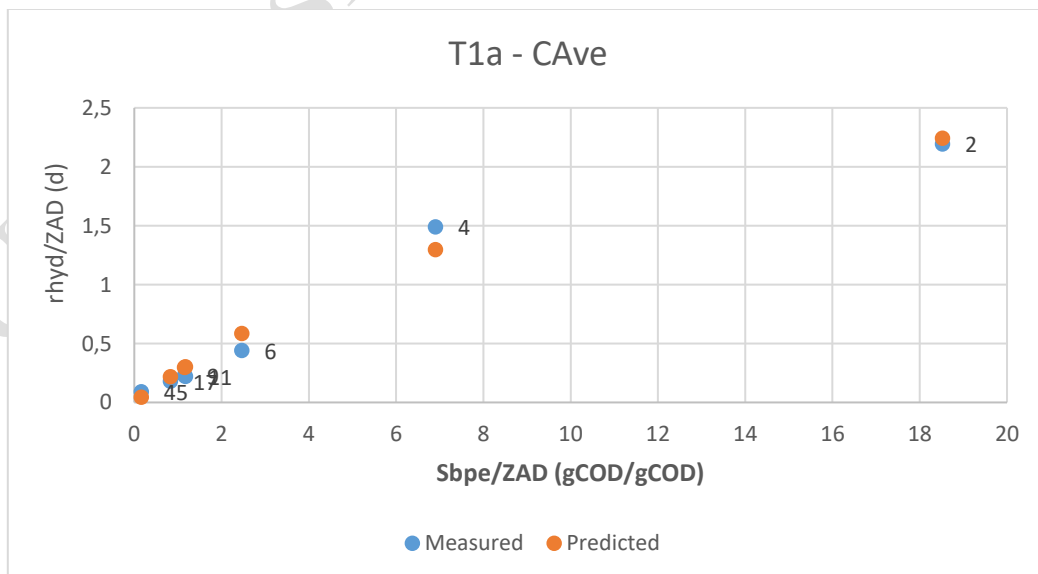
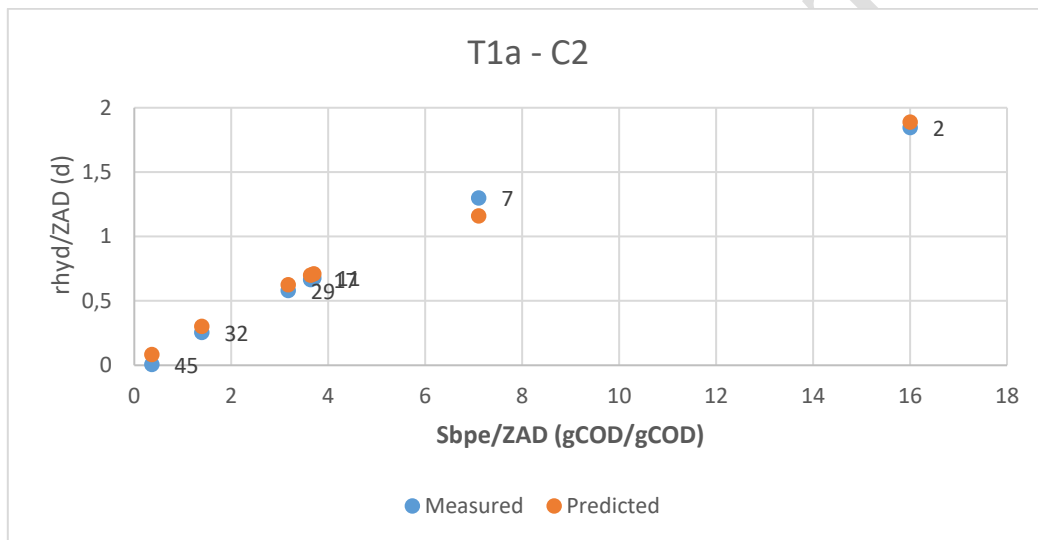
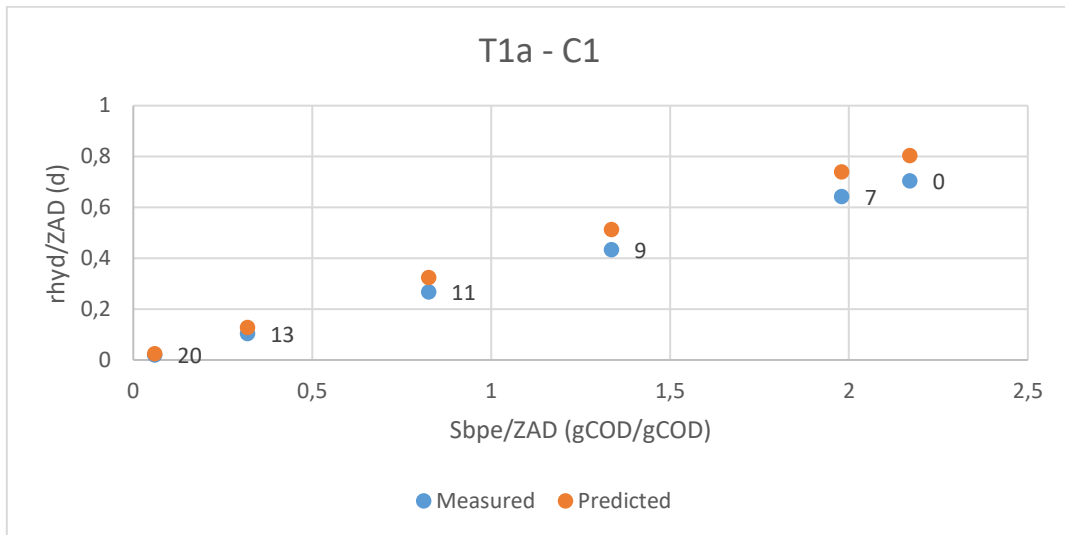


Table C.4.2 ABMP Test for Column 2						Rhyd/Z_AD	
Tests	Time (d)	Sbpe	Z_AD	rhYd	Sbpe/Z_AD (gCOD/gCOD)	Measured	Predicted
T2a – C2 KM (8.744) kS (98.298)	0	-0.009	0.91	0			
	2	-5.99	1.52	3.03	28	2.1	1.94
	3	-7.28	1.63	2.46	15	1.3	1.16
	9	-8.22	1.54	0.95	7.6	0.6	0.63
	11	-4.89	1.10	0.48	6.40	0.44	0.53
	29	-0.042	-0.046	0.038	5.4	0.38	0.455
	45	2.236	-0.832	-0.013	0.34	0.0152	0.030
T2a – CAve KM (6.631) kS (49.566)	0	0.790	0.909	0			
	2	-6.130	1.625	3.49	25	2.152	2.223
	3	-7.670	1.766	2.858	14.03	1.618	1.463
	4	-7.078	1.667	2.005	10.3	1.203	1.140
	5	-7.05	1.63	1.61	8.43	0.98	0.96
	6	-7.11	1.60	1.35	7.2	0.84	0.84
	7	-8.15	1.69	1.32	6.67	0.78	0.79
	23	0.62	0.17	0.04	3.71	0.27	0.46
	32	-0.16	-0.04	0.07	2.9	0.22	0.37
T2Ave – CAve KM (140.81) kS (74.96)	0	2.00	0.91				
	2	-3.91	1.51	2.98	1.07	1.98	1.97
	3	-5.31	1.63	2.47	0.81	1.51	1.50
	4	-3.35	1.38	1.378	0.54	1.00	1.00
	5	-5.15	1.55	1.47	0.51	0.95	0.90
	6	-5.09	1.51	1.22	0.431	0.81	0.81
	7	-6.09	1.59	1.19	0.40	0.75	0.75
	9	-6.37	1.55	0.97	0.33	0.62	0.63
	11	-4.13	1.24	0.59	0.26	0.480	0.48
	13	-2.05	0.94	0.35	0.20	0.37	0.38
	15	-1.77	0.84	0.29	0.18	0.34	0.35
	20	-0.23	0.50	0.15	0.16	0.30	0.30
	23	0.72	0.29	0.09	0.17	0.32	0.32
	26	0.43	0.23	0.100	0.23	0.43	0.40
Units	Days	(gCOD)	(gCOD)	(gCOD/l/d)	(gCOD/gCOD)	gCOD/(gCOD.l.d)	Units

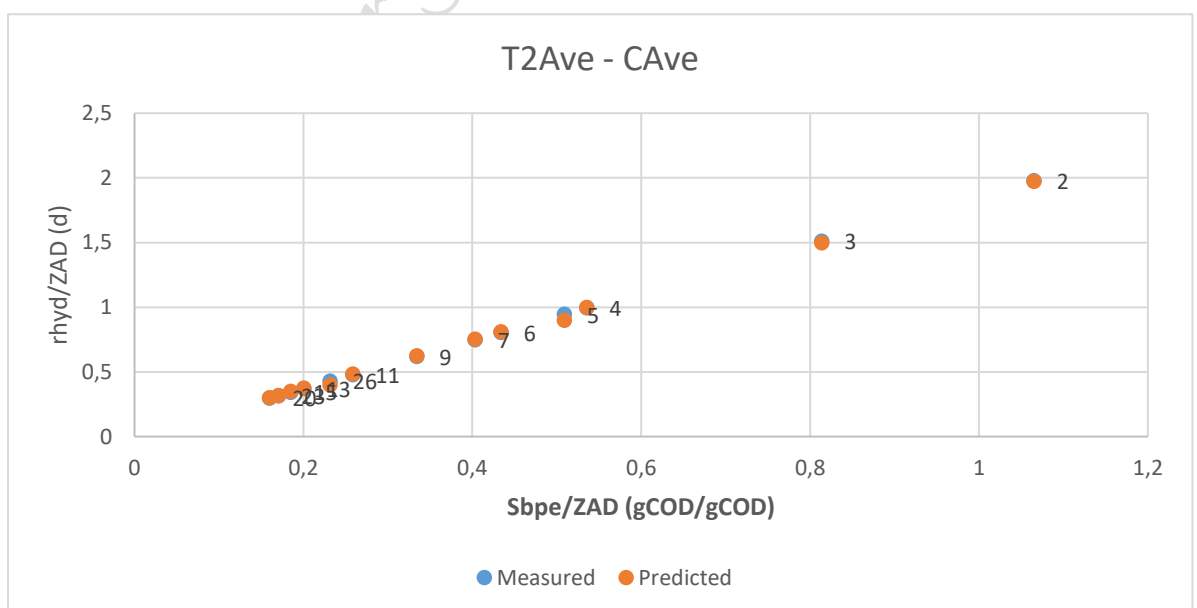
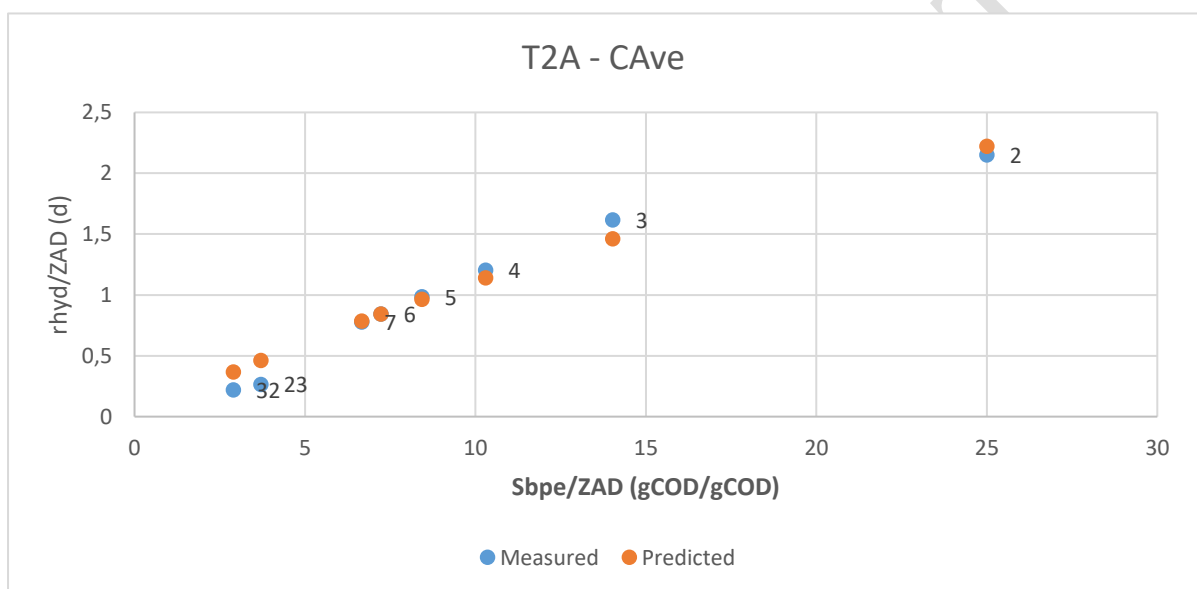
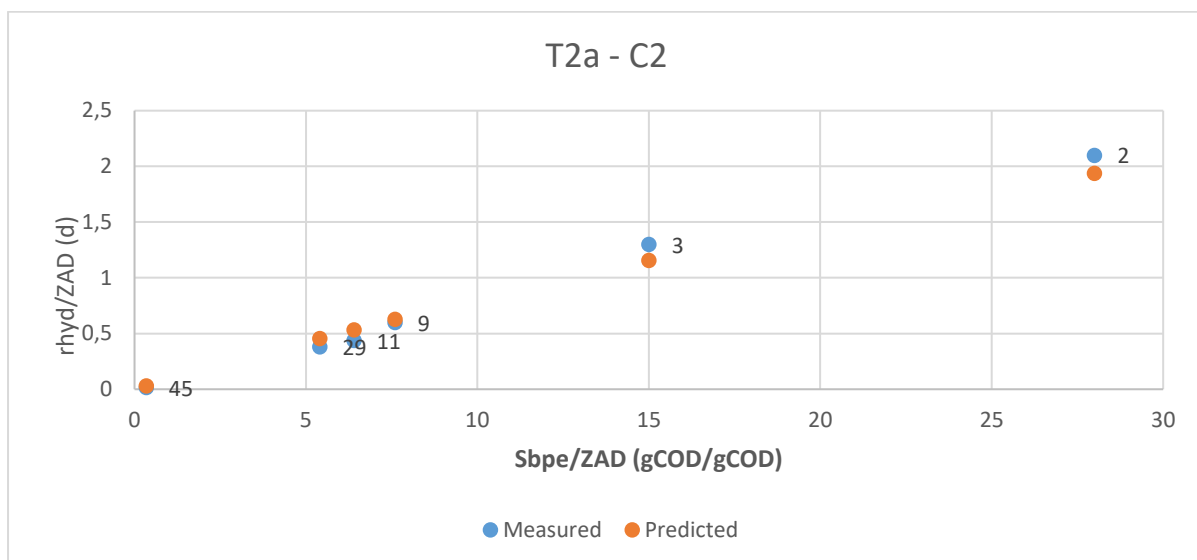


Table C.4.3 ABMP Test for Column 3						Rhyd/Z_AD	
Tests	Time (d)	Sbpe	Z_AD	rhYd	Sbpe/Z_AD (gCOD/gCOD)	Measured	Predicted
T3b – C1 KM (1.278) kS (2.728)	0	4.6	0.9	0			
	3	-0.40	1.37	1.69	1.7	0.52	0.49
	9	1.21	0.99	0.41	1.22	0.37	0.40
	13	1.05	0.88	0.31	1.19	0.36	0.39
	17	0.97	0.75	0.25	1.09	0.33	0.36
	23	0.92	0.56	0.20	0.65	0.35	0.25
	37	0.48	0.15	0.15	0.21	0.02	0.09
T3b – C2 KM (3.139) kS (5.926)	0	1.07	0.91	0			
	2	-1.07	1.08	1.11	3.02	1.02	1.06
	3	-1.51	1.10	0.89	1.63	0.82	0.68
	4	0.75	0.81	0.12	0.93	0.39	0.43
	15	0.4	0.49	0.08	0.82	0.29	0.38
	26	-0.41	0.22	0.09	0.53	0.24	0.26
	37	0.69	-0.27	0.05	0.26	0.17	0.13
T3a – CAve KM (2.335) kS (5.743)	0	2.47	0.91	0			
	3	-3.01	1.43	1.86	4.91	0.97	1.08
	5	-3.43	1.41	1.22	3.7	0.86	0.91
	15	-1.12	0.82	0.28	0.94	0.34	0.33
	17	0.44	0.58	0.16	0.76	0.27	0.27
	29	0.15	0.21	0.12	0.71	0.39	0.26
T3Ave – CAve KM (1.936) kS (11.149)	0	1.67	0.91	0			
	9	-2.79	1.35	2.27	64.63	1.68	1.65
	11	-3.21	1.36	1.66	21	1.22	1.27
	13	-2.43	1.24	1.06	9	0.86	0.87
	15	-3.01	1.27	0.97	7.27	0.77	0.76
	20	0.05	0.23	0.10	0.21	0.43	0.04
Units	Days	(gCOD)	(gCOD)	(gCOD/l/d)	(gCOD/gCOD)	gCOD/(gCOD. l.d)	Units

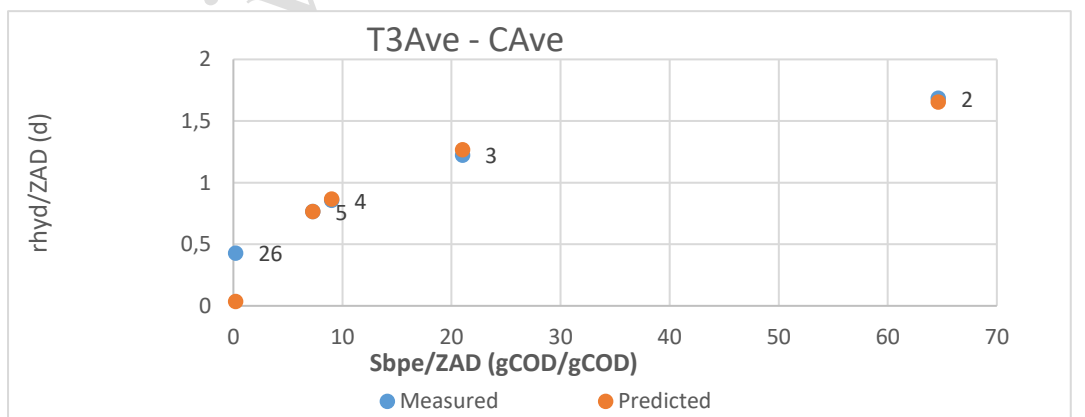
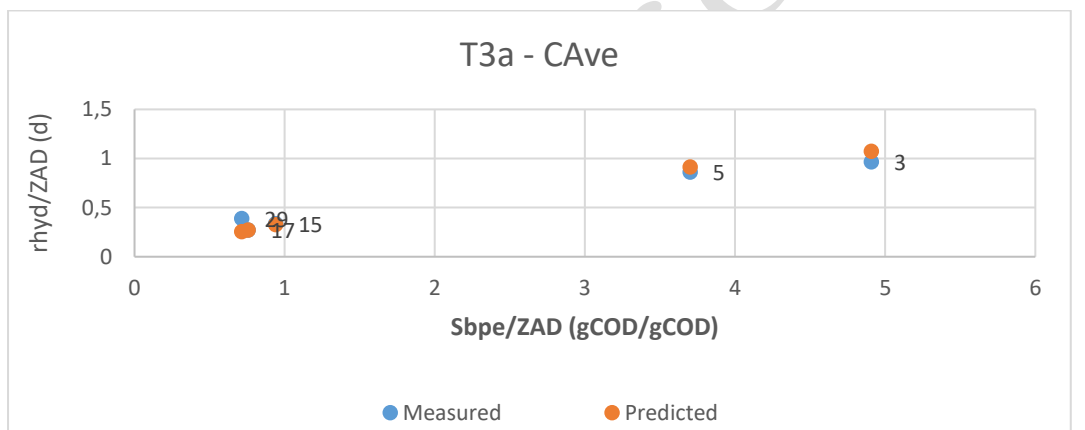
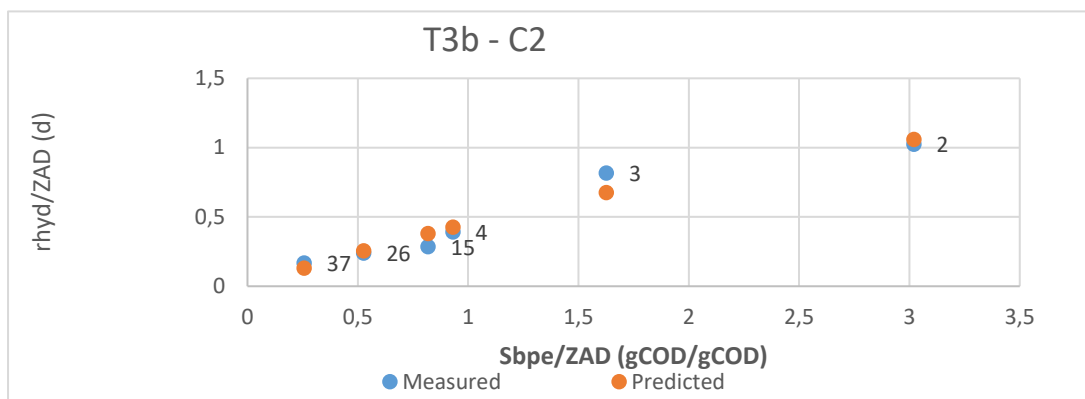
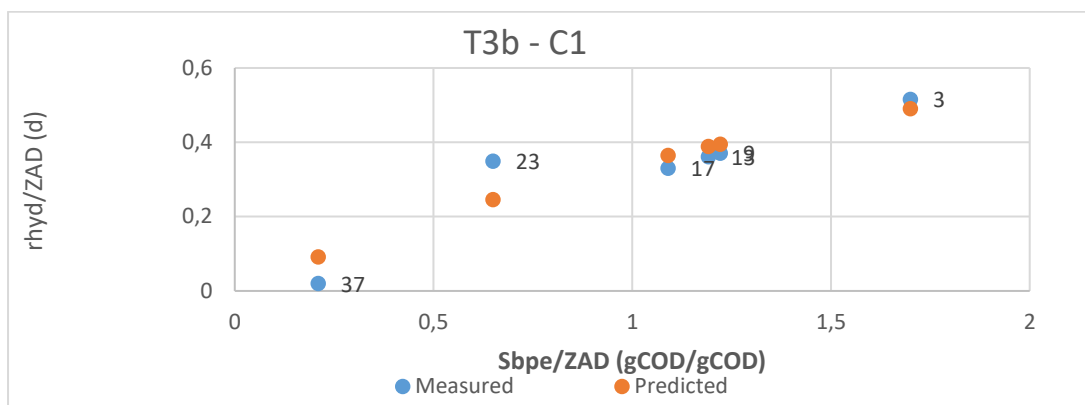


Table C.4.4 ABMP Test for Column 4						Rhyd/Z_AD	
Tests	Time (d)	Sbpe	Z_AD	rhYd	Sbpe/Z_AD (gCOD/gCOD)	Measured	Predicted
T4b – C1 KM (2.737) kS (57.715)	0	2.59	0.91				
	2	-3.02	1.48	2.84	13	1.92	1.90
	3	-2.54	1.39	1.75	4.96	1.26	1.27
	4	2.29	0.81	0.11	2.82	0.84	0.90
	6	0.10	0.99	0.45	0.10	0.46	0.05
	9	0.52	0.85	0.27	0.61	0.32	0.26
	20	0.01	0.54	0.17	0.02	0.31	0.01
T4a – C2 KM (2.032) kS (16.922)	0	-1.51	0.91	0			
	6	1.30	0.39	-0.43	36	1.37	1.38
	29	-1.04	-0.10	0.02	10.03	0.86	0.76
	32	-1.22	-0.18	0.03	6.68	0.46	0.58
	42	0.15	-0.67	-0.00	3.28	0.35	0.33
	52	1.12	-1.11	-0.01	0.6	0.04	0.07
T4a – CAve KM (1.748) kS (6.828)	0	1.39	0.91				
	2	-2.74	1.31	2.10	39.63	1.60	1.49
	3	-3.19	1.33	1.56	21	1.18	1.32
	5	-0.07	0.91	0.33	3.45	0.53	0.59
	11	-1.06	0.82	0.26	2.4	0.53	0.45
	17	0.58	0.44	0.08	1.32	0.29	0.28
	32	-0.56	0.07	0.10	0.65	0.28	0.15
	37	-0.07	-0.15	0.08	0.44	0.09	0.11
T3b– CAve KM (1.844) kS (8.208)	0	-0.21	0.91				
	2	-3.40	1.20	1.63	18.75	1.36	1.28
	3	-3.59	1.19	1.17	12	0.98	1.10
	4	1.25	0.61	-0.33	2.04	0.48	0.37
	6	0.98	0.58	-0.16	1.69	0.29	0.31
	15	-1.40	0.55	0.12	1.24	0.21	0.24
	17	0.07	0.32	0.02	0.21	0.07	0.05
Units	Days	(gCOD)	(gCOD)	(gCOD/l/d)	(gCOD/gCOD)	gCOD/(gCOD.l.d)	Units

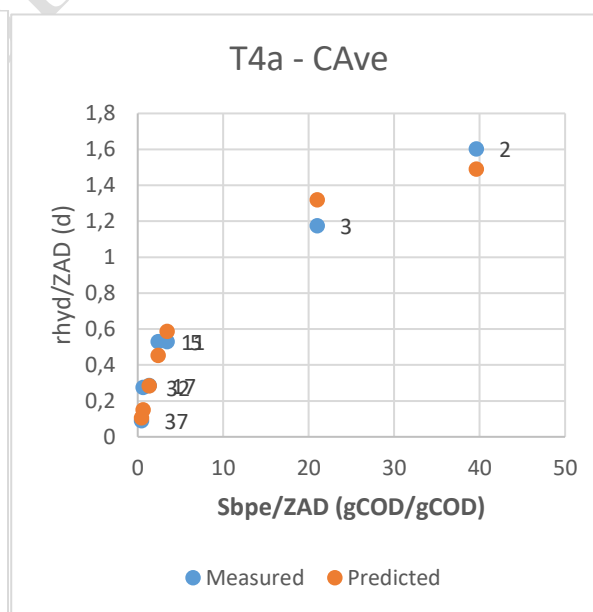
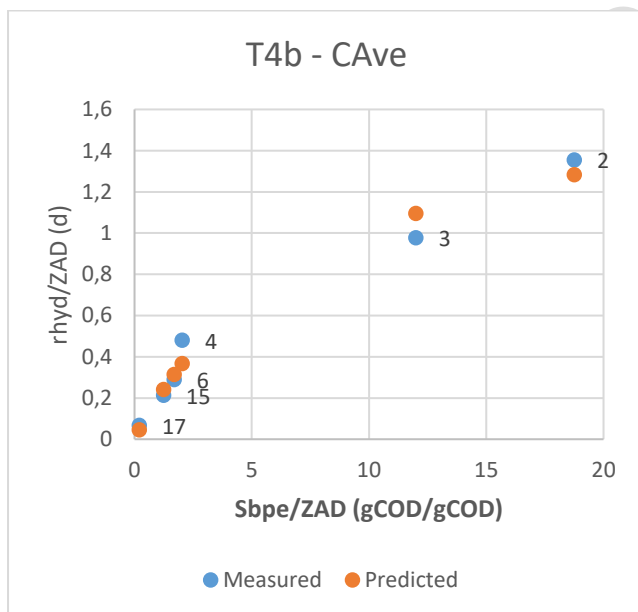
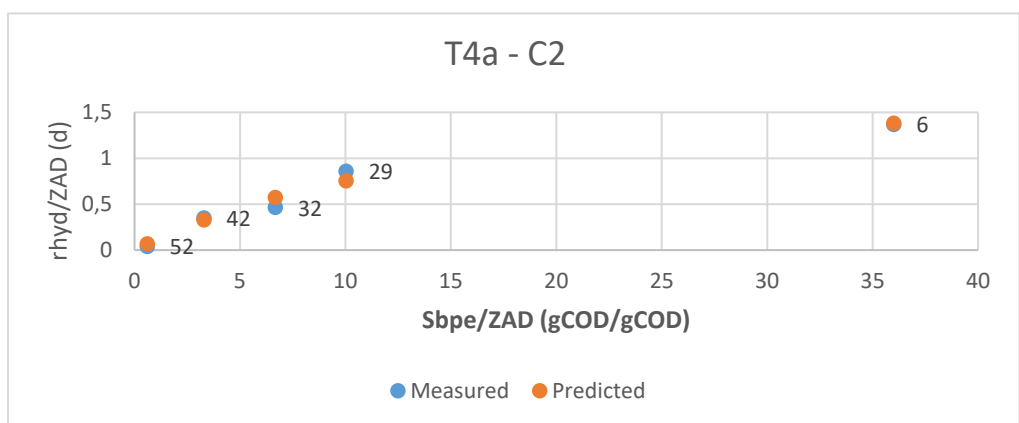
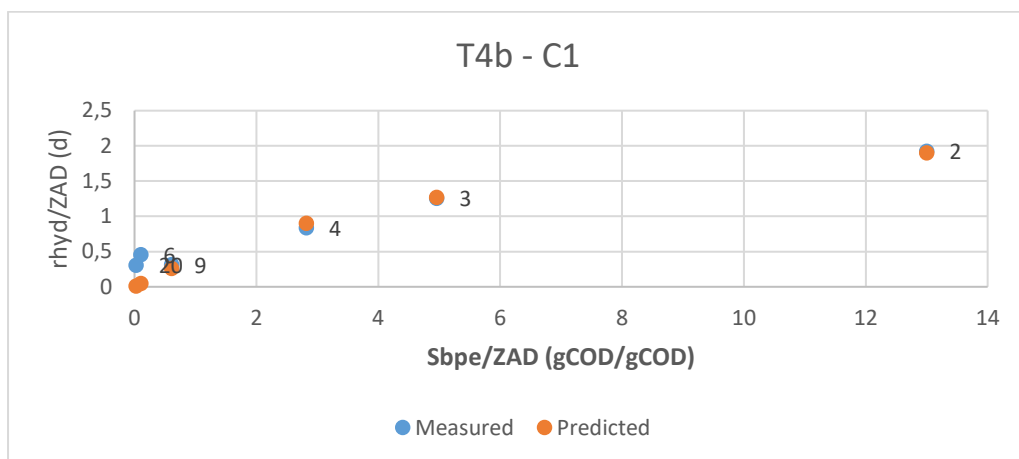


Table C.4.5 ABMP Test for Column 5						Rhyd/Z_AD	
Tests	Time (d)	Sbpe	Z_AD	rhYd	Sbpe/Z_AD (gCOD/gCOD)	Measured	Predicted
T5b – C1 KM (1.362) kS (2.928)	0	5.81	0.90	0			
	6	0.95	1.26	0.85	2.7	0.67	0.65
	7	2.08	1.09	0.57	1.90	0.52	0.54
	9	1.60	1.08	0.50	1.48	0.47	0.46
	15	1.25	0.93	0.34	1.35	0.37	0.43
	20	0.67	0.83	0.29	0.81	0.32	0.30
	23	0.67	0.73	0.26	0.92	0.36	0.33
	26	0.16	0.69	0.25	0.24	0.09	0.10
T5a – CAve KM (3.343) kS (5.808)	0	4.655304	0.904696				
	2	-2.59	1.66	3.66	7.82	2.21	1.92
	3	0.43	1.28	1.45	5.81	1.3	1.67
	5	-2.15	1.51	1.40	3.4	1.23	1.23
	6	-0.53	1.29	0.90	1.36	0.51	0.63
	7	0.36	1.16	0.65	0.31	0.49	0.17
	13	-0.67	1.08	0.45	0.48	0.41	0.25
	20	0.13	0.76	0.26	0.18	0.39	0.10
	26	0.26	0.55	0.21	0.10	0.35	0.06
	37	0.89	0.11	0.14	0.06	0.26	0.04
T5Ave – CAve KM (2.276) kS (17.163)	0	4.11	0.90	0			
	2	-2.67	1.60	3.420	143.4401	2.14	2.03
	4	-2.02	1.47	1.57	24	1.07	1.33
	5	-1.47	1.37	1.15	10.4	0.84	0.86
	11	0.22	0.98	0.39	1.69	0.62	0.20
	13	-0.70	1.02	0.41	1.37	0.40	0.17
	20	0.24	0.68	0.23	0.35	0.34	0.05
	29	0.59	0.35	0.16	0.06	0.34	0.01
Units	Days	(gCOD)	(gCOD)	(gCOD/l/d)	(gCOD/gCOD)	gCOD/(gCOD.l.d)	Units

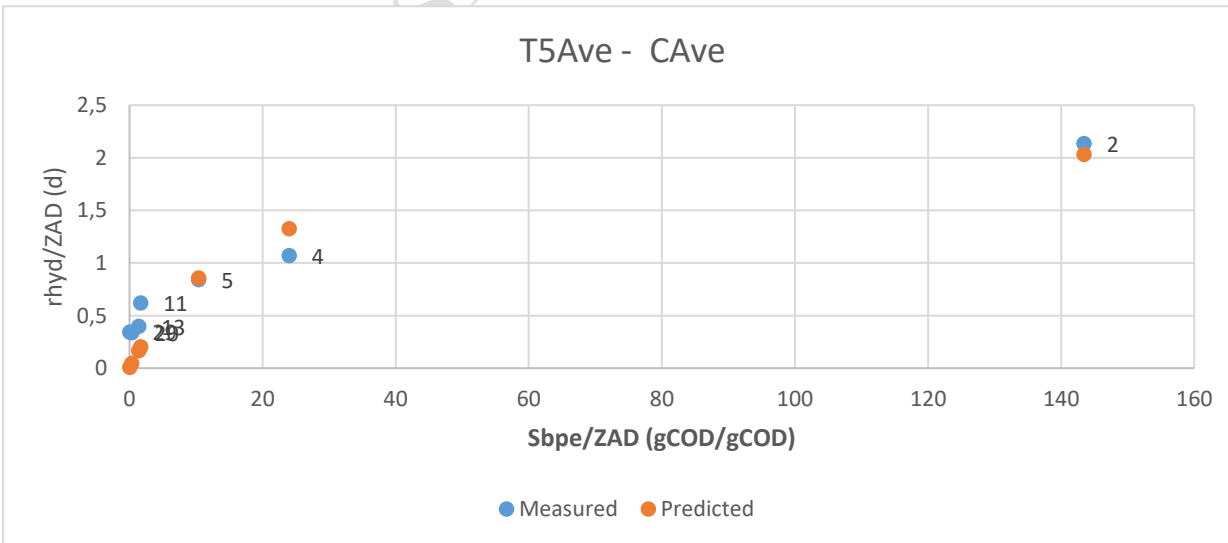
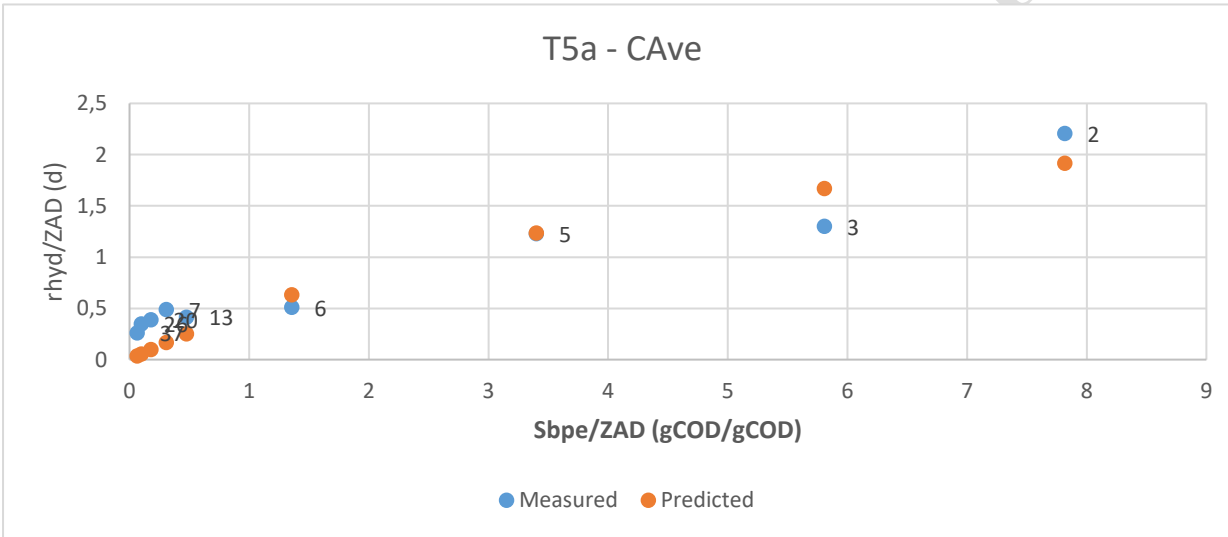
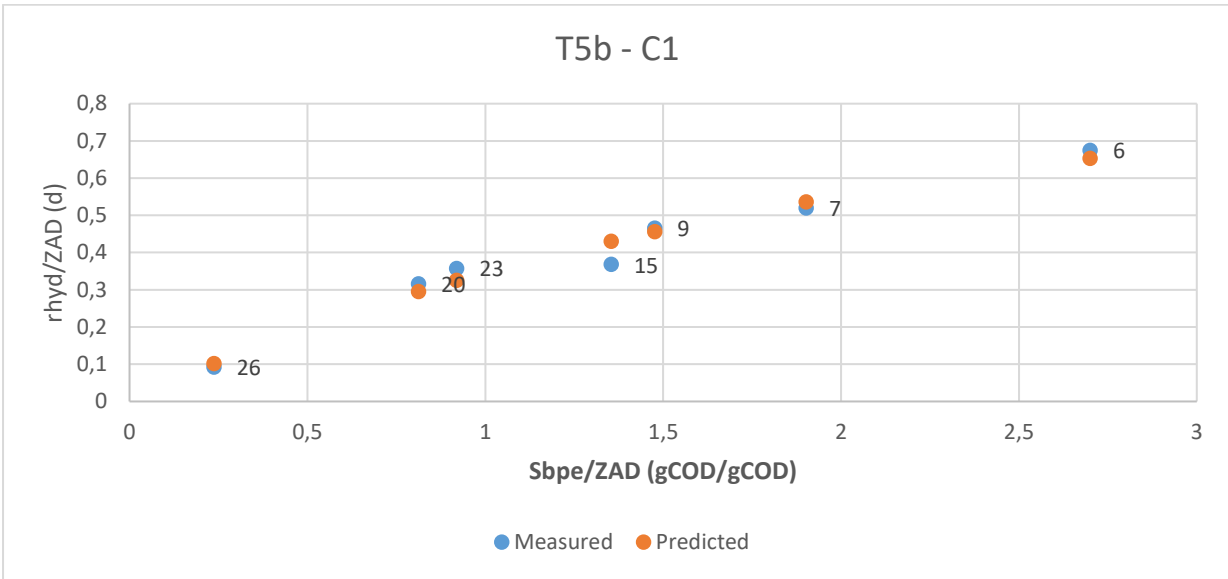


Table C.5.1 Residual Biodegradable Particulate Concentration (Sbp) for PVC Column 1				
Time	T1a - C1	T1b - C1	T1a - Cave	T1Ave - Cave
d	gCOD/l	gCOD/l	gCOD/l	gCOD/l
0	2.53	3.552819	2.06	1.25
5		3.26		
7	1.00			
9			0.86	
11	0.97		0.80	
13	0.58			
17				0.32
20	0.16			
23				0.31
32		1.96		
42	0.01			

Table C.5.2 Residual Biodegradable Particulate Concentration (Sbp) for PVC Columns 2 and 3					
Time	T2a - Cave	T3b - C1	T3b - C2	T3a - Cave	T3Ave - Cave
d	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l
0	0.79	4.57	1.07	2.47	1.67
4			0.75		
9		1.21	0.86		
11			0.80		
13		1.05			
15			0.40		
17		0.97		0.44	
23	0.62	0.92			
26					0.05
29				0.15	
37		0.48			

Table C.5.3 Residual Biodegradable Particulate Concentration (Sbp) for PVC Column 4				
Time	T4b - C1	T4a - C2	T4a - Cave	T4b - Cave
d	gCOD/l	gCOD/l	gCOD/l	gCOD/l
0	2.60		1.39	
4	2.29			1.25
6		1.30		0.98
9	0.52			
17			0.58	0.07
20	0.01			
42		0.15		

Table C.5.4 Residual Biodegradable Particulate Concentration (Sbp) for PVC Column 5			
Time	T5b - C1	T5a - CAve	T5Ave - CAve
d	gCOD/l	gCOD/l	gCOD/l
0	5.81	4.66	4.11
3		0.43	
7	2.08	0.36	
9	1.60		
11			0.22
15	1.25		
20	0.67	0.13	0.24
23	0.67		
26	0.163087		
42		0.147973	

Table C.6 Measured COD Removal for Columns 1 – 2 (%)														
Time	T1a - C1	T1b - C1	T1a - C2	T1b - C2	T1a - Cave	T1b - Cave	T1ave - Cave	T2a - C1	T2b - C1	T2a - C2	T2b - C2	T2a - Cave	T2b - Cave	T2ave - Cave
(d)	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l
2		24.31				20.21			47.2				43.1	
3	41.8					47.35								
4				7.43		15.89	31.10		43.02		26.1		34.56	
5	18.93				8.27									
6	28.74				19.81									
7					3.25									
9		57.66	1.94	49.81	5.86	53.73	29.80							
11		50.63	3.99	39.00	9.80	44.81	27.31							
13	29.03	51.70	20.06	42.73	24.54	47.21	35.88		48.46		39.49			
15		56.70	25.54	46.29	30.74	51.49	41.12		51.51		41.1			
17		40.88		31.44	13.28	36.16	24.72	16.48	43.48	7.04	34.04	11.76	38.76	25.26
20		46.56	23.32	35.19	29.01	40.87	34.94	36.31	53.24	24.93	41.87	30.62	47.55	39.09
23		45.04	20.69	31.18	27.62	38.11	32.87	33.05	52.24	19.17	38.37	26.11	45.3	35.71
26	33.14	31.45	23.40	21.71	28.27	26.58	27.42	40.61	51.53	30.86	41.79	35.74	46.66	41.2
29	35.46		25.40		30.43	21.08	25.76	39.86	56.99	29.8	46.94	34.83	51.96	43.4
32	35.15	35.58	26.19	26.62	30.67	31.1002	30.88409	38.96	50.28	30	41.32	34.48	45.8	40.14
37	41.39	41.70	25.22	25.54	33.31	33.62	33.47	44.85	61.75	28.68	45.58	36.77	53.66	45.22
42	46.42	47.60	31.08	32.25	38.75	39.93	39.34	44.42	68.07	29.08	52.73	36.75	60.4	48.58
45				38.45	36.41	47.73	42.07	42.99	69.39	24.42	50.83	33.7	60.11	46.91
52				46.76	35.83	53.20	44.52	41.06	72.14	28.17	59.25	34.62	65.7	50.16
fSup	0.58	0.40	0.71	0.53	0.64	0.47	0.56	0.59	0.28	0.72	0.41	0.66	0.35	0.50

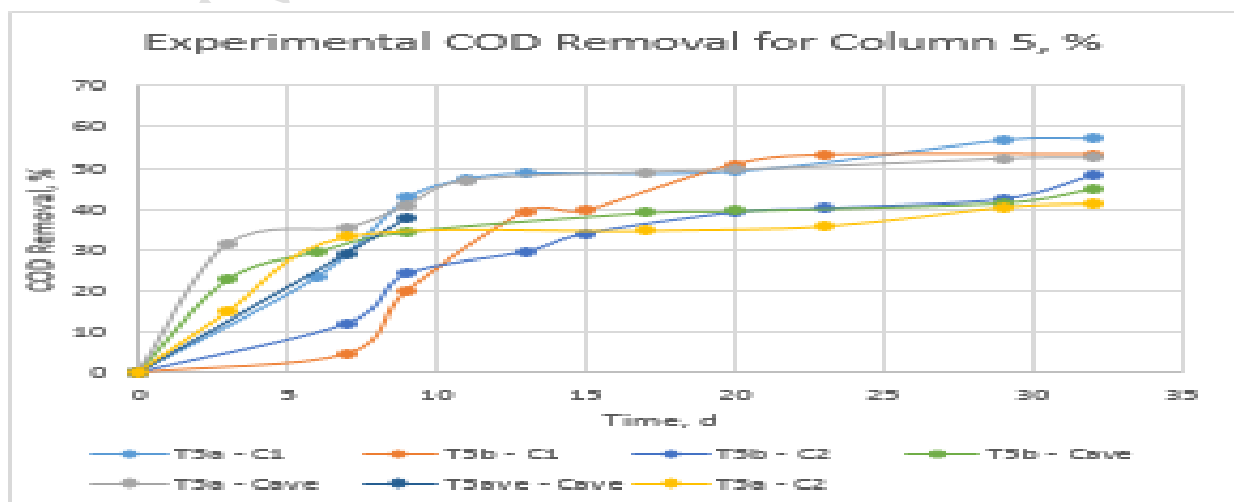
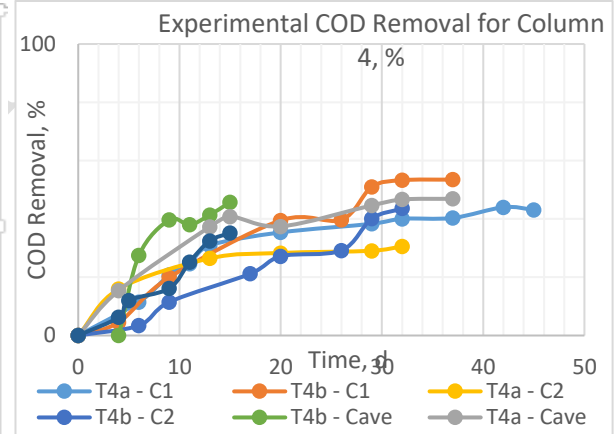
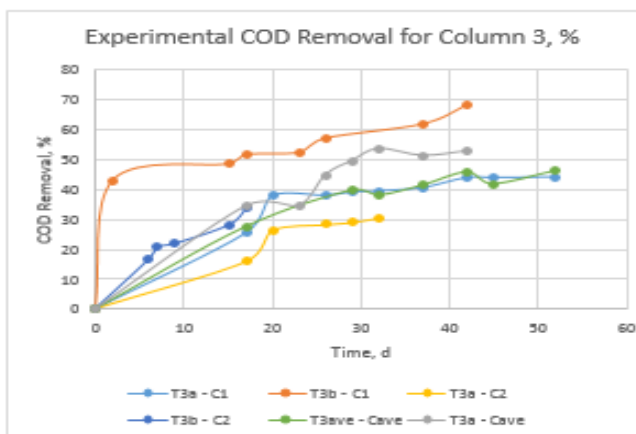
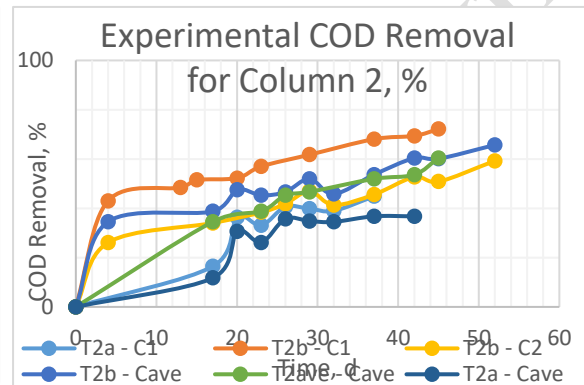
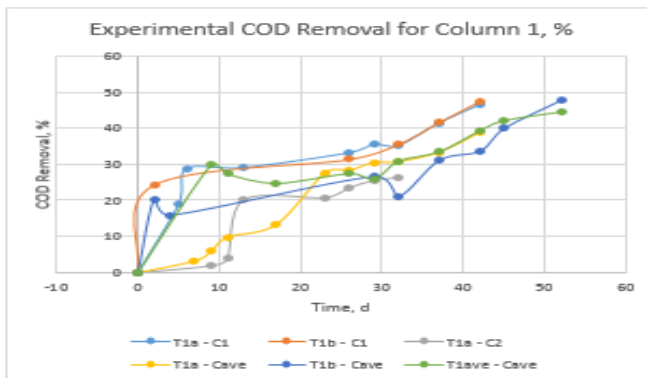
Table C.6 Continuation: Measured COD Removal for Columns 3 – 4 (%)

Time	T3a - C1	T3b - C1	T3a - C2	T3b - C2	T3a - Cave	T3b - Cave	T3ave - Cave	T4a - C1	T4b - C1	T4a - C2	T4b - C2	T4a - Cave	T4b - Cave	T4ave - Cave
(d)	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l
2		31.68					39.51			21.23				
4									4.58	7.97		15.41	0	6.27
5									22.92					12.02
6				16.62		30.02		11.46	22.74		3.44		0.65	7.45
7				20.7		33.37		23.74			0			
9				21.84	42.41	34.56		20.85	19.96		11.48		14.38	16.16
11								24.69			25.8		21.21	25.23
13						39.01		30.94		21.25		37.31	29.64	32.47
15		38.51		28.09		37.94						40.83	31.54	35.2
17	25.38		15.94	33.76	34.29	24.85	29.57				21.2		17.68	
20	37.84		26.46		46.07	34.7		35.37	39.49	23.08	27.2	37.43	27.22	31.28
23	19.31	49.49	5.44	35.62	34.4	20.53	27.47						19.88	
26	38.06	55.15	28.31	45.4	46.6	36.86			39.72		29.19		20.6	
29	39.12	50.28	29.06		44.7	34.64	39.67	38.32	50.98	27.45	40.11	44.65	35.62	39.21
32	39.51		30.55		42.48	33.52	38	40.06	53.27	30.38	43.59	46.67	38.74	41.83
37	40.61	58.25	24.44	42.08	49.43	33.26	41.35	40.32	53.48		36.01	46.9		38.16
42	44.03	62.85	28.68	47.5	53.44	38.09	45.77	44.01	50.08					38.76
45	44.01	58.19	25.44		51.1	32.53	41.82	43.14	49.64					
52	44.2	61.1	31.32	48.21	52.65	39.76	46.21	37.75	53.21					38.51
fSup	0.55445	0.38415	0.68435	0.51405	0.46930	0.59920	0.53425	0.62250	0.46794	0.62250	0.60721	0.54522	0.68450	0.614862
5	8	6	9	7	8	7	5	1	5	9	3	1		

Table C.6 Continuation: Measured COD Removal for Column 5 (%)

Time	T5a - C1	T5b - C1	T5a - C2	T5b - C2	T5a - Cave	T5b - Cave	T5ave - Cave
(d)	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l	gCOD/l
0	0	0	0	0	0	0	0
3	23.5		14.89		31.39	22.78	
6						29.48	
7		24.92	33.23	12.09	35.49		29.08
9		30.7	0	24.19	40.91	34.41	37.66
11			0		39.33	29.69	
13		37.03		29.59			48.4
15		42.67		34.04			48.88
17	42.56		34.73		46.94	39.11	
20	49.3	48.73	39.87	39.3	49.01	39.58	44.3
23	47.36	51.74	35.86	40.24	49.55	38.05	43.8

26	49.63	59.56	41.55		54.59		50.55
29	48.88	50.8	40.54	42.46		41.5	45.67
32	48.88	55.75	41.45	48.32	52.31	44.89	48.6
37	49.27	55.98	35.86		52.62		45.92
42	56.89	61.06	44.17	48.34	58.97	46.25	52.61
45	57.3	60.68		45.29	58.99	43.6	51.29
52	55.54	68.57	44.85	57.88	62.05	51.37	56.71
fSup	0.444625	0.314332	0.551466	0.421173	0.379479	0.486319	0.432899



APPENDIX D: STOICHIOMETRY BIOPROCESS EQAUTIONS FOR BPO_PS SUB-COMPONENTS IN UCTPSU MODEL

Stoichiometric Modifications for UCTPSU Model		
Processes	Components	Relationships
FSO_Hyd	[H ₂ O]	$\left[parameters.MW_{[H_2O]} * parameters.i_{OSF_{mol_{perc}}} - 3 - 4 * parameters.i_{PSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right]$
	[S _H]	$\left[parameters.MW_{[S_H]} * \left(3 * i_{PSF_{mol_{perc}}} + 2 - parameters.i_{NSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right) \right]$
	[S _{NH}]	$\left[parameters.MW_{[S_{NH}]} * parameters.i_{NSF_{mol_{perc}}} \right]$
	[S _{CO₂}]	$\left[parameters.MW_{CO_2} * (1 - 0.25 * parameters.gam_f) \right]$
	[S _{PO₄}]	$\left[parameters.MW_{[S_{PO_4}]} * parameters.i_{PSF_{mol_{perc}}} \right]$
	[S _{Gl_u}]	$\left[parameters.MW_{[S_{Glu]} * parameters.gam_f / 24 \right]$
	[S _F]	- $\left[parameters.MW_{S_F} \right]$
BPO_PS_Hyd1	[H ₂ O]	$\left[parameters.MW_{[H_2O]} * parameters.i_{OSF_{mol_{perc}}} - 3 - 4 * parameters.i_{PSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right]$
	[S _H]	$\left[parameters.MW_{[S_H]} * \left(3 * i_{PSF_{mol_{perc}}} + 2 - parameters.i_{NSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right) \right]$
	[S _{NH}]	$\left[parameters.MW_{[S_{NH}]} * parameters.i_{NSF_{mol_{perc}}} \right]$
	[S _{CO₂}]	$\left[parameters.MW_{CO_2} * (1 - 0.25 * parameters.gam_f) \right]$
	[S _{PO₄}]	$\left[parameters.MW_{[S_{PO_4}]} * parameters.i_{PSF_{mol_{perc}}} \right]$
	[S _{Gl_u}]	$\left[parameters.MW_{[S_{Glu]} * parameters.gam_f / 24 \right]$
	[BPO_PS_Hyd1]	- $\left[parameters.MW_{BPO_PS_Hyd1} \right]$
BPO_PS_Hyd2	[H ₂ O]	$\left[parameters.MW_{[H_2O]} * parameters.i_{OSF_{mol_{perc}}} - 3 - 4 * parameters.i_{PSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right]$
	[S _H]	$\left[parameters.MW_{[S_H]} * \left(3 * i_{PSF_{mol_{perc}}} + 2 - parameters.i_{NSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right) \right]$
	[S _{NH}]	$\left[parameters.MW_{[S_{NH}]} * parameters.i_{NSF_{mol_{perc}}} \right]$
	[S _{CO₂}]	$\left[parameters.MW_{CO_2} * (1 - 0.25 * parameters.gam_f) \right]$
	[S _{PO₄}]	$\left[parameters.MW_{[S_{PO_4}]} * parameters.i_{PSF_{mol_{perc}}} \right]$
	[S _{Gl_u}]	$\left[parameters.MW_{[S_{Glu]} * parameters.gam_f / 24 \right]$
	[BPO_PS_Hyd2]	- $\left[parameters.MW_{BPO_PS_Hyd2} \right]$
BPO_PS_Hyd3	[H ₂ O]	$\left[parameters.MW_{[H_2O]} * parameters.i_{OSF_{mol_{perc}}} - 3 - 4 * parameters.i_{PSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right]$
	[S _H]	$\left[parameters.MW_{[S_H]} * \left(3 * i_{PSF_{mol_{perc}}} + 2 - parameters.i_{NSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right) \right]$
	[S _{NH}]	$\left[parameters.MW_{[S_{NH}]} * parameters.i_{NSF_{mol_{perc}}} \right]$
	[S _{CO₂}]	$\left[parameters.MW_{CO_2} * (1 - 0.25 * parameters.gam_f) \right]$
	[S _{PO₄}]	$\left[parameters.MW_{[S_{PO_4}]} * parameters.i_{PSF_{mol_{perc}}} \right]$
	[S _{Gl_u}]	$\left[parameters.MW_{[S_{Glu]} * parameters.gam_f / 24 \right]$
	[BPO_PS_Hyd3]	- $\left[parameters.MW_{BPO_PS_Hyd3} \right]$
BPO_PS_Hyd4	[H ₂ O]	$\left[parameters.MW_{[H_2O]} * parameters.i_{OSF_{mol_{perc}}} - 3 - 4 * parameters.i_{PSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right]$
	[S _H]	$\left[parameters.MW_{[S_H]} * \left(3 * i_{PSF_{mol_{perc}}} + 2 - parameters.i_{NSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right) \right]$
	[S _{NH}]	$\left[parameters.MW_{[S_{NH}]} * parameters.i_{NSF_{mol_{perc}}} \right]$
	[S _{CO₂}]	$\left[parameters.MW_{CO_2} * (1 - 0.25 * parameters.gam_f) \right]$
	[S _{PO₄}]	$\left[parameters.MW_{[S_{PO_4}]} * parameters.i_{PSF_{mol_{perc}}} \right]$
	[S _{Gl_u}]	$\left[parameters.MW_{[S_{Glu]} * parameters.gam_f / 24 \right]$
	[BPO_PS_Hyd4]	- $\left[parameters.MW_{BPO_PS_Hyd4} \right]$
BPO_PS_Hyd5	[H ₂ O]	$\left[parameters.MW_{[H_2O]} * parameters.i_{OSF_{mol_{perc}}} - 3 - 4 * parameters.i_{PSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right]$
	[S _H]	$\left[parameters.MW_{[S_H]} * \left(3 * i_{PSF_{mol_{perc}}} + 2 - parameters.i_{NSF_{mol_{perc}}} - 0.5 * parameters.gam_f \right) \right]$
	[S _{NH}]	$\left[parameters.MW_{[S_{NH}]} * parameters.i_{NSF_{mol_{perc}}} \right]$
	[S _{CO₂}]	$\left[parameters.MW_{CO_2} * (1 - 0.25 * parameters.gam_f) \right]$
	[S _{PO₄}]	$\left[parameters.MW_{[S_{PO_4}]} * parameters.i_{PSF_{mol_{perc}}} \right]$
	[S _{Gl_u}]	$\left[parameters.MW_{[S_{Glu]} * parameters.gam_f / 24 \right]$
	[BPO_PS_Hyd5]	- $\left[parameters.MW_{BPO_PS_Hyd5} \right]$

APPENDIX E: GENERAL SENSITIVITY ANALYSIS

ISS_under					
Residuals	Min	1Q	Median	3Q	Max
	-1.91827	-0.26881	0.03868	0.3475	1.03244
Coefficients					
	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	1.22E-11	1.52E-02	0	1	
Alpha_B	-2.96E-02	1.58E-02	-1.866	0.06234	.
Alpha_I	3.83E-01	1.56E-02	24.542	< 2e-16	***
Alpha_U	7.28E-03	1.57E-02	0.465	0.64207	
Beta_B	7.64E-04	1.59E-02	0.048	0.96158	
Beta_I	1.82E-01	1.58E-02	11.479	< 2e-16	***
Beta_U	9.07E-03	1.56E-02	0.58	0.56186	
Gamma_B	-1.05E-02	1.57E-02	-0.666	0.50572	
Gamma_I	1.02E-01	1.58E-02	6.45E+00	1.82E-10	***
Gamma_U	1.18E-02	1.58E-02	0.743	0.45753	
ISS_BM	1.83E-02	1.57E-02	1.171	0.24198	
KS_BInf_AD_hyd	1.67E-02	1.57E-02	1.064	0.2874	
KS_BOrg_AD_hyd	3.94E-02	1.58E-02	2.5	0.0126	*
K_ALK	-7.35E-03	1.60E-02	-0.461	0.64511	
Lambda_B	-8.48E-03	1.57E-02	-0.54	0.58964	
Lambda_I	-1.24E-02	1.58E-02	-0.787	0.43176	
Lambda_U	-7.50E-03	1.56E-02	-0.482	0.63009	
TempCoeff	1.23E-02	1.58E-02	0.782	0.43465	
Tref	1.93E-02	1.61E-02	1.202	0.2298	
Vs_s_X_B_Inf1	-1.50E-02	1.58E-02	-0.947	0.34412	
Vs_s_X_B_Inf2	-2.69E-02	1.58E-02	-1.705	0.0885	.
Vs_s_X_B_Inf3	2.19E-02	1.58E-02	1.389	0.16508	
Vs_s_X_B_Inf4	-7.60E-03	1.60E-02	-0.476	0.63434	
Vs_s_X_B_Inf5	5.02E-04	1.56E-02	0.032	0.9744	
Vs_s_X_ISS1	4.22E-01	1.57E-02	26.906	< 2e-16	***
Vs_s_X_ISS2	2.71E-01	1.59E-02	17.033	< 2e-16	***
Vs_s_X_ISS3	4.21E-01	1.58E-02	26.616	< 2e-16	***
Vs_s_X_ISS4	3.26E-01	1.56E-02	20.886	< 2e-16	***
Vs_s_X_ISS5	2.24E-01	1.58E-02	14.165	< 2e-16	***
Vs_s_X_U_Inf1	1.59E-02	1.58E-02	1.005	0.31496	
Vs_s_X_U_Inf2	2.77E-03	1.60E-02	0.173	0.86235	
Vs_s_X_U_Inf3	1.13E-02	1.57E-02	0.72	0.47155	
Vs_s_X_U_Inf4	6.79E-03	1.57E-02	0.432	0.666	
Vs_s_X_U_Inf5	1.85E-02	1.59E-02	1.17	0.24239	
X_Lim	2.06E-02	1.59E-02	1.298	0.19457	
X_T	-4.25E-02	1.59E-02	-2.677	0.00756	**
f_U_Inf	9.82E-03	1.57E-02	0.627	0.53067	

i_Ca_PP_mol_perP	2.60E-03	1.57E-02	0.165	0.86883		
i_H_Org_mol_perC	5.47E-03	1.57E-02	0.348	0.72758		
i_H_SF_mol_perC	1.74E-03	1.59E-02	0.109	0.9133		
i_H_SU_mol_perC	-1.22E-02	1.57E-02	-0.781	0.4352		
i_H_XBInf_mol_perC	6.27E-04	1.57E-02	0.04	0.96811		
i_H_XBOrg_mol_perC	-3.65E-03	1.57E-02	-0.233	0.81589		
i_H_XUInf_mol_perC	-2.38E-03	1.57E-02	-0.152	0.87911		
i_H_XUOrg_mol_perC	-1.58E-02	1.57E-02	-1.005	0.31499		
i_K_PP_mol_perP	2.77E-02	1.56E-02	1.773	0.07662		
i_Mg_PP_mol_perP	7.28E-03	1.57E-02	0.462	0.64386		
i_N_Org_mol_perC	1.67E-02	1.60E-02	1.041	0.29824		
i_N_SF_mol_perC	-2.24E-02	1.57E-02	-1.426	0.15423		
i_N_SU_mol_perC	2.47E-02	1.58E-02	1.563	0.11837		
i_N_XBInf_mol_perC	-1.31E-02	1.58E-02	-0.825	0.40951		
i_N_XBOrg_mol_perC	-1.45E-02	1.58E-02	-0.919	0.35846		
i_N_XUInf_mol_perC	-8.24E-03	1.57E-02	-0.524	0.6004		
i_N_XUOrg_mol_perC	1.37E-02	1.58E-02	0.865	0.38724		
i_O_Org_mol_perC	-1.46E-02	1.59E-02	-0.917	0.35923		
i_O_SF_mol_perC	2.72E-03	1.57E-02	0.174	0.86215		
i_O_SU_mol_perC	-1.47E-02	1.58E-02	-0.931	0.35219		
i_O_XBInf_mol_perC	-1.58E-03	1.56E-02	-0.102	0.91912		
i_O_XBOrg_mol_perC	1.90E-03	1.58E-02	0.12	0.90442		
i_O_XUInf_mol_perC	-3.98E-03	1.57E-02	-0.254	0.79963		
i_O_XUOrg_mol_perC	-3.25E-02	1.58E-02	-2.061	0.03963 *		
i_P_Org_mol_perC	3.22E-02	1.56E-02	2.063	0.03938 *		
i_P_SF_mol_perC	1.25E-02	1.57E-02	0.794	0.42719		
i_P_SU_mol_perC	9.26E-03	1.56E-02	0.594	0.55258		
i_P_XBInf_mol_perC	1.22E-02	1.57E-02	0.777	0.43762		
i_P_XBOrg_mol_perC	-5.40E-03	1.58E-02	-0.341	0.73328		
i_P_XUInf_mol_perC	1.87E-03	1.58E-02	0.119	0.90562		
i_P_XUOrg_mol_perC	-3.12E-03	1.58E-02	-0.198	0.84335		
kH_F_AD_hyd	2.16E-03	1.59E-02	0.136	0.89168		
kM_BInf_AD_hyd	4.54E-03	1.58E-02	0.288	0.77379		
kM_BOrg_AD_hyd	-6.62E-03	1.59E-02	-0.417	0.67665		

Signif. codes	0 '***'	0.001 '**'	0.01 '*'	0.05 '.'	0.1 ''	1

Residual standard error: 0.4816 on 929 degrees of freedom

Multiple R-squared: 0.7845, Adjusted R-squared: 0.7683

F-statistic: 48.31 on 70 and 929 DF, p-value: < 2.2e-16

Out_X_B_Inf

Residuals: Min 1Q Median 3Q Max

-5.9661 -0.0634 0.314 0.5054 1.148

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	1.11E-11	3.20E-02	0	1
Alpha_B	2.48E-02	3.33E-02	0.746	0.4558
Alpha_I	1.70E-02	3.28E-02	0.518	0.6044
Alpha_U	1.15E-02	3.29E-02	0.349	0.7269
Beta_B	-1.13E-02	3.33E-02	-0.34	0.7341
Beta_I	-8.62E-03	3.33E-02	-0.259	0.7957
Beta_U	4.63E-03	3.29E-02	0.141	0.8881
Gamma_B	1.26E-02	3.30E-02	0.382	0.7025
Gamma_I	-4.19E-02	3.31E-02	-1.267	0.2055
Gamma_U	-8.37E-03	3.33E-02	-0.252	0.8014
ISS_BM	4.92E-02	3.29E-02	1.495	0.1353
KS_BInf_AD_hyd	1.96E-02	3.29E-02	0.596	0.5513
KS_BOrg_AD_hyd	-1.98E-03	3.31E-02	-0.06	0.9523
K_ALK	2.25E-02	3.35E-02	0.671	0.5025
Lambda_B	1.85E-02	3.30E-02	0.56	0.5755
Lambda_I	-5.11E-02	3.32E-02	-1.538	0.1244
Lambda_U	2.82E-03	3.27E-02	0.086	0.9313
TempCoeff	2.37E-02	3.31E-02	0.714	0.4754
Tref	-3.68E-02	3.38E-02	-1.088	0.2768
Vs_s_X_B_Inf1	-4.09E-02	3.33E-02	-1.229	0.2196
Vs_s_X_B_Inf2	-5.67E-03	3.31E-02	-0.171	0.8642
Vs_s_X_B_Inf3	3.64E-02	3.31E-02	1.098	0.2724
Vs_s_X_B_Inf4	1.04E-02	3.36E-02	0.309	0.7572
Vs_s_X_B_Inf5	-4.54E-02	3.29E-02	-1.381	0.1678
Vs_s_X_ISS1	2.36E-02	3.30E-02	0.715	0.4746
Vs_s_X_ISS2	-2.19E-03	3.34E-02	-0.065	0.9478
Vs_s_X_ISS3	4.06E-02	3.32E-02	1.223	0.2215
Vs_s_X_ISS4	3.29E-02	3.28E-02	1.005	0.3153
Vs_s_X_ISS5	-4.81E-03	3.32E-02	-0.145	0.8849
Vs_s_X_U_Inf1	2.89E-02	3.32E-02	0.869	0.3852
Vs_s_X_U_Inf2	3.45E-02	3.36E-02	1.028	0.3041
Vs_s_X_U_Inf3	1.15E-02	3.29E-02	0.348	0.728
Vs_s_X_U_Inf4	3.71E-02	3.31E-02	1.121	0.2627
Vs_s_X_U_Inf5	4.73E-02	3.33E-02	1.418	0.1566
X_Lim	5.37E-02	3.34E-02	1.607	0.1084
X_T	-4.11E-03	3.34E-02	-0.123	0.9021
f_U_Inf	-3.77E-02	3.29E-02	-1.144	0.253
i_Ca_PP_mol_perP	-1.33E-02	3.31E-02	-0.4	0.6891
i_H_Org_mol_perC	2.05E-02	3.30E-02	0.623	0.5336
i_H_SF_mol_perC	1.75E-02	3.35E-02	0.521	0.6022

i_H_SU_mol_perC	-2.57E-02	3.29E-02	-0.781	0.4352
i_H_XBInf_mol_perC	1.62E-02	3.30E-02	0.49	0.6243
i_H_XBOrg_mol_perC	-1.54E-03	3.30E-02	-0.047	0.9627
i_H_XUInf_mol_perC	3.32E-02	3.29E-02	1.009	0.3131
i_H_XUOrg_mol_perC	-3.86E-02	3.31E-02	-1.168	0.2431
i_K_PP_mol_perP	-1.33E-02	3.29E-02	-0.404	0.6864
i_Mg_PP_mol_perP	-1.19E-03	3.31E-02	-0.036	0.9713
i_N_Org_mol_perC	-1.64E-02	3.37E-02	-0.488	0.6257
i_N_SF_mol_perC	5.10E-02	3.30E-02	1.549	0.1217
i_N_SU_mol_perC	-1.94E-04	3.32E-02	-0.006	0.9953
i_N_XBInf_mol_perC	-1.25E-02	3.33E-02	-0.374	0.7085
i_N_XBOrg_mol_perC	4.01E-02	3.33E-02	1.206	0.2283
i_N_XUInf_mol_perC	1.40E-02	3.31E-02	0.424	0.672
i_N_XUOrg_mol_perC	1.57E-02	3.33E-02	0.471	0.6379
i_O_Org_mol_perC	-8.23E-03	3.35E-02	-0.246	0.8057
i_O_SF_mol_perC	-2.82E-03	3.30E-02	-0.086	0.9318
i_O_SU_mol_perC	-3.45E-02	3.32E-02	-1.04	0.2986
i_O_XBInf_mol_perC	4.85E-02	3.28E-02	1.48	0.1392
i_O_XBOrg_mol_perC	-1.21E-02	3.33E-02	-0.364	0.7159
i_O_XUInf_mol_perC	-5.93E-02	3.30E-02	-1.799	0.0724 .
i_O_XUOrg_mol_perC	-2.80E-02	3.32E-02	-0.845	0.3985
i_P_Org_mol_perC	-1.50E-02	3.28E-02	-0.456	0.6483
i_P_SF_mol_perC	5.39E-03	3.31E-02	0.163	0.8707
i_P_SU_mol_perC	-3.57E-03	3.28E-02	-0.109	0.9132
i_P_XBInf_mol_perC	1.88E-02	3.31E-02	0.568	0.5702
i_P_XBOrg_mol_perC	-1.68E-02	3.33E-02	-0.506	0.6128
i_P_XUInf_mol_perC	4.68E-03	3.32E-02	0.141	0.888
i_P_XUOrg_mol_perC	-8.78E-05	3.32E-02	-0.003	0.9979
kH_F_AD_hyd	-7.06E-02	3.33E-02	-2.118	0.0344 *
kM_BInf_AD_hyd	9.09E-03	3.32E-02	0.274	0.784
kM_BOrg_AD_hyd	1.92E-02	3.34E-02	0.575	0.5657

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.012 on 929 degrees of freedom
Multiple R-squared: 0.0477, Adjusted R-squared: -0.02405
F-statistic: 0.6648 on 70 and 929 DF, p-value: 0.9841

Out.X_ISS

Residuals:	Min	1Q	Median	3Q	Max
	-5.9661	-0.0634	0.314	0.5054	1.148

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	1.21E-11	3.20E-02	0	1
Alpha_B	2.48E-02	3.33E-02	0.746	0.4558
Alpha_I	1.70E-02	3.28E-02	0.518	0.6044
Alpha_U	1.15E-02	3.29E-02	0.349	0.7269
Beta_B	-1.13E-02	3.33E-02	-0.34	0.7341
Beta_I	-8.62E-03	3.33E-02	-0.259	0.7957
Beta_U	4.63E-03	3.29E-02	0.141	0.8881
Gamma_B	1.26E-02	3.30E-02	0.382	0.7025
Gamma_I	-4.19E-02	3.31E-02	-1.267	0.2055
Gamma_U	-8.37E-03	3.33E-02	-0.252	0.8014
ISS_BM	4.92E-02	3.29E-02	1.495	0.1353
KS_BInf_AD_hyd	1.96E-02	3.29E-02	0.596	0.5513
KS_BOrg_AD_hyd	-1.98E-03	3.31E-02	-0.06	0.9523
K_ALK	2.25E-02	3.35E-02	0.671	0.5025
Lambda_B	1.85E-02	3.30E-02	0.56	0.5755
Lambda_I	-5.11E-02	3.32E-02	-1.538	0.1244
Lambda_U	2.82E-03	3.27E-02	0.086	0.9313
TempCoeff	2.37E-02	3.31E-02	0.714	0.4754
Tref	-3.68E-02	3.38E-02	-1.088	0.2768
Vs_s_X_B_Inf1	-4.09E-02	3.33E-02	-1.229	0.2196
Vs_s_X_B_Inf2	-5.67E-03	3.31E-02	-0.171	0.8642
Vs_s_X_B_Inf3	3.64E-02	3.31E-02	1.098	0.2724
Vs_s_X_B_Inf4	1.04E-02	3.36E-02	0.309	0.7572
Vs_s_X_B_Inf5	-4.54E-02	3.29E-02	-1.381	0.1678
Vs_s_X_ISS1	2.36E-02	3.30E-02	0.715	0.4746
Vs_s_X_ISS2	-2.19E-03	3.34E-02	-0.065	0.9478
Vs_s_X_ISS3	4.06E-02	3.32E-02	1.223	0.2215
Vs_s_X_ISS4	3.29E-02	3.28E-02	1.005	0.3153
Vs_s_X_ISS5	-4.81E-03	3.32E-02	-0.145	0.8849
Vs_s_X_U_Inf1	2.89E-02	3.32E-02	0.869	0.3852
Vs_s_X_U_Inf2	3.45E-02	3.36E-02	1.028	0.3041
Vs_s_X_U_Inf3	1.15E-02	3.29E-02	0.348	0.728
Vs_s_X_U_Inf4	3.71E-02	3.31E-02	1.121	0.2627
Vs_s_X_U_Inf5	4.73E-02	3.33E-02	1.418	0.1566
X_Lim	5.37E-02	3.34E-02	1.607	0.1084
X_T	-4.11E-03	3.34E-02	-0.123	0.9021
f_U_Inf	-3.77E-02	3.29E-02	-1.144	0.253
i_Ca_PP_mol_perP	-1.33E-02	3.31E-02	-0.4	0.6891
i_H_Org_mol_perC	2.05E-02	3.30E-02	0.623	0.5336
i_H_SF_mol_perC	1.75E-02	3.35E-02	0.521	0.6022
i_H_SU_mol_perC	-2.57E-02	3.29E-02	-0.781	0.4352
i_H_XBInf_mol_perC	1.62E-02	3.30E-02	0.49	0.6243
i_H_XBOrg_mol_perC	-1.54E-03	3.30E-02	-0.047	0.9627
i_H_XUInf_mol_perC	3.32E-02	3.29E-02	1.009	0.3131

i_H_XUOrg_mol_perC	-3.86E-02	3.31E-02	-1.168	0.2431		
i_K_PP_mol_perP	-1.33E-02	3.29E-02	-0.404	0.6864		
i_Mg_PP_mol_perP	-1.19E-03	3.31E-02	-0.036	0.9713		
i_N_Org_mol_perC	-1.64E-02	3.37E-02	-0.488	0.6257		
i_N_SF_mol_perC	5.10E-02	3.30E-02	1.549	0.1217		
i_N_SU_mol_perC	-1.94E-04	3.32E-02	-0.006	0.9953		
i_N_XBInf_mol_perC	-1.25E-02	3.33E-02	-0.374	0.7085		
i_N_XBOrg_mol_perC	4.01E-02	3.33E-02	1.206	0.2283		
i_N_XUInf_mol_perC	1.40E-02	3.31E-02	0.424	0.672		
i_N_XUOrg_mol_perC	1.57E-02	3.33E-02	0.471	0.6379		
i_O_Org_mol_perC	-8.23E-03	3.35E-02	-0.246	0.8057		
i_O_SF_mol_perC	-2.82E-03	3.30E-02	-0.086	0.9318		
i_O_SU_mol_perC	-3.45E-02	3.32E-02	-1.04	0.2986		
i_O_XBInf_mol_perC	4.85E-02	3.28E-02	1.48	0.1392		
i_O_XBOrg_mol_perC	-1.21E-02	3.33E-02	-0.364	0.7159		
i_O_XUInf_mol_perC	-5.93E-02	3.30E-02	-1.799	0.0724 .		
i_O_XUOrg_mol_perC	-2.80E-02	3.32E-02	-0.845	0.3985		
i_P_Org_mol_perC	-1.50E-02	3.28E-02	-0.456	0.6483		
i_P_SF_mol_perC	5.39E-03	3.31E-02	0.163	0.8707		
i_P_SU_mol_perC	-3.57E-03	3.28E-02	-0.109	0.9132		
i_P_XBInf_mol_perC	1.88E-02	3.31E-02	0.568	0.5702		
i_P_XBOrg_mol_perC	-1.68E-02	3.33E-02	-0.506	0.6128		
i_P_XUInf_mol_perC	4.68E-03	3.32E-02	0.141	0.888		
i_P_XUOrg_mol_perC	-8.78E-05	3.32E-02	-0.003	0.9979		
kH_F_AD_hyd	-7.06E-02	3.33E-02	-2.118	0.0344 *		
kM_BInf_AD_hyd	9.09E-03	3.32E-02	0.274	0.784		
kM_BOrg_AD_hyd	1.92E-02	3.34E-02	0.575	0.5657		

Signif. codes:	0 '***'	0.001 '**'	0.01 '*'	0.05 '.'	0.1 ''	1

Residual standard error: 1.012 on 929 degrees of freedom

Multiple R-squared: 0.0477, Adjusted R-squared: -0.02405

F-statistic: 0.6648 on 70 and 929 DF, p-value: 0.9841

Out.X_U_Inf

Residuals:	Min	1Q	Median	3Q	Max
	-5.9661	-0.0634	0.314	0.5054	1.148

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	1.21E-11	3.20E-02	0	1
Alpha_B	2.48E-02	3.33E-02	0.746	0.4558
Alpha_I	1.70E-02	3.28E-02	0.518	0.6044

Alpha_U	1.15E-02	3.29E-02	0.349	0.7269
Beta_B	-1.13E-02	3.33E-02	-0.34	0.7341
Beta_I	-8.62E-03	3.33E-02	-0.259	0.7957
Beta_U	4.63E-03	3.29E-02	0.141	0.8881
Gamma_B	1.26E-02	3.30E-02	0.382	0.7025
Gamma_I	-4.19E-02	3.31E-02	-1.267	0.2055
Gamma_U	-8.37E-03	3.33E-02	-0.252	0.8014
ISS_BM	4.92E-02	3.29E-02	1.495	0.1353
KS_BInf_AD_hyd	1.96E-02	3.29E-02	0.596	0.5513
KS_BOrg_AD_hyd	-1.98E-03	3.31E-02	-0.06	0.9523
K_ALK	2.25E-02	3.35E-02	0.671	0.5025
Lambda_B	1.85E-02	3.30E-02	0.56	0.5755
Lambda_I	-5.11E-02	3.32E-02	-1.538	0.1244
Lambda_U	2.82E-03	3.27E-02	0.086	0.9313
TempCoeff	2.37E-02	3.31E-02	0.714	0.4754
Tref	-3.68E-02	3.38E-02	-1.088	0.2768
Vs_s_X_B_Inf1	-4.09E-02	3.33E-02	-1.229	0.2196
Vs_s_X_B_Inf2	-5.67E-03	3.31E-02	-0.171	0.8642
Vs_s_X_B_Inf3	3.64E-02	3.31E-02	1.098	0.2724
Vs_s_X_B_Inf4	1.04E-02	3.36E-02	0.309	0.7572
Vs_s_X_B_Inf5	-4.54E-02	3.29E-02	-1.381	0.1678
Vs_s_X_ISS1	2.36E-02	3.30E-02	0.715	0.4746
Vs_s_X_ISS2	-2.19E-03	3.34E-02	-0.065	0.9478
Vs_s_X_ISS3	4.06E-02	3.32E-02	1.223	0.2215
Vs_s_X_ISS4	3.29E-02	3.28E-02	1.005	0.3153
Vs_s_X_ISS5	-4.81E-03	3.32E-02	-0.145	0.8849
Vs_s_X_U_Inf1	2.89E-02	3.32E-02	0.869	0.3852
Vs_s_X_U_Inf2	3.45E-02	3.36E-02	1.028	0.3041
Vs_s_X_U_Inf3	1.15E-02	3.29E-02	0.348	0.728
Vs_s_X_U_Inf4	3.71E-02	3.31E-02	1.121	0.2627
Vs_s_X_U_Inf5	4.73E-02	3.33E-02	1.418	0.1566
X_Lim	5.37E-02	3.34E-02	1.607	0.1084
X_T	-4.11E-03	3.34E-02	-0.123	0.9021
f_U_Inf	-3.77E-02	3.29E-02	-1.144	0.253
i_Ca_PP_mol_perP	-1.33E-02	3.31E-02	-0.4	0.6891
i_H_Org_mol_perC	2.05E-02	3.30E-02	0.623	0.5336
i_H_SF_mol_perC	1.75E-02	3.35E-02	0.521	0.6022
i_H_SU_mol_perC	-2.57E-02	3.29E-02	-0.781	0.4352
i_H_XBInf_mol_perC	1.62E-02	3.30E-02	0.49	0.6243
i_H_XBOrg_mol_perC	-1.54E-03	3.30E-02	-0.047	0.9627
i_H_XUInf_mol_perC	3.32E-02	3.29E-02	1.009	0.3131
i_H_XUOrg_mol_perC	-3.86E-02	3.31E-02	-1.168	0.2431
i_K_PP_mol_perP	-1.33E-02	3.29E-02	-0.404	0.6864
i_Mg_PP_mol_perP	-1.19E-03	3.31E-02	-0.036	0.9713
i_N_Org_mol_perC	-1.64E-02	3.37E-02	-0.488	0.6257

i_N_SF_mol_perC	5.10E-02	3.30E-02	1.549	0.1217
i_N_SU_mol_perC	-1.94E-04	3.32E-02	-0.006	0.9953
i_N_XBInf_mol_perC	-1.25E-02	3.33E-02	-0.374	0.7085
i_N_XBOrg_mol_perC	4.01E-02	3.33E-02	1.206	0.2283
i_N_XUInf_mol_perC	1.40E-02	3.31E-02	0.424	0.672
i_N_XUOrg_mol_perC	1.57E-02	3.33E-02	0.471	0.6379
i_O_Org_mol_perC	-8.23E-03	3.35E-02	-0.246	0.8057
i_O_SF_mol_perC	-2.82E-03	3.30E-02	-0.086	0.9318
i_O_SU_mol_perC	-3.45E-02	3.32E-02	-1.04	0.2986
i_O_XBInf_mol_perC	4.85E-02	3.28E-02	1.48	0.1392
i_O_XBOrg_mol_perC	-1.21E-02	3.33E-02	-0.364	0.7159
i_O_XUInf_mol_perC	-5.93E-02	3.30E-02	-1.799	0.0724
i_O_XUOrg_mol_perC	-2.80E-02	3.32E-02	-0.845	0.3985
i_P_Org_mol_perC	-1.50E-02	3.28E-02	-0.456	0.6483
i_P_SF_mol_perC	5.39E-03	3.31E-02	0.163	0.8707
i_P_SU_mol_perC	-3.57E-03	3.28E-02	-0.109	0.9132
i_P_XBInf_mol_perC	1.88E-02	3.31E-02	0.568	0.5702
i_P_XBOrg_mol_perC	-1.68E-02	3.33E-02	-0.506	0.6128
i_P_XUInf_mol_perC	4.68E-03	3.32E-02	0.141	0.888
i_P_XUOrg_mol_perC	-8.78E-05	3.32E-02	-0.003	0.9979
kH_F_AD_hyd	-7.06E-02	3.33E-02	-2.118	0.0344 *
kM_BInf_AD_hyd	9.09E-03	3.32E-02	0.274	0.784
kM_BOrg_AD_hyd	1.92E-02	3.34E-02	0.575	0.5657

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.012 on 929 degrees of freedom
Multiple R-squared: 0.0477, Adjusted R-squared: -0.02405
F-statistic: 0.6648 on 70 and 929 DF, p-value: 0.9841

Out.X_VSS

Residuals:	Min	1Q	Median	3Q	Max
	-5.9661	-0.0634	0.314	0.5054	1.148

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	1.31E-11	3.20E-02	0	1
Alpha_B	2.48E-02	3.33E-02	0.746	0.4558
Alpha_I	1.70E-02	3.28E-02	0.518	0.6044
Alpha_U	1.15E-02	3.29E-02	0.349	0.7269
Beta_B	-1.13E-02	3.33E-02	-0.34	0.7341
Beta_I	-8.62E-03	3.33E-02	-0.259	0.7957
Beta_U	4.63E-03	3.29E-02	0.141	0.8881

Gamma_B	1.26E-02	3.30E-02	0.382	0.7025
Gamma_I	-4.19E-02	3.31E-02	-1.267	0.2055
Gamma_U	-8.37E-03	3.33E-02	-0.252	0.8014
ISS_BM	4.92E-02	3.29E-02	1.495	0.1353
KS_BInf_AD_hyd	1.96E-02	3.29E-02	0.596	0.5513
KS_BOrg_AD_hyd	-1.98E-03	3.31E-02	-0.06	0.9523
K_ALK	2.25E-02	3.35E-02	0.671	0.5025
Lambda_B	1.85E-02	3.30E-02	0.56	0.5755
Lambda_I	-5.11E-02	3.32E-02	-1.538	0.1244
Lambda_U	2.82E-03	3.27E-02	0.086	0.9313
TempCoeff	2.37E-02	3.31E-02	0.714	0.4754
Tref	-3.68E-02	3.38E-02	-1.088	0.2768
Vs_s_X_B_Inf1	-4.09E-02	3.33E-02	-1.229	0.2196
Vs_s_X_B_Inf2	-5.67E-03	3.31E-02	-0.171	0.8642
Vs_s_X_B_Inf3	3.64E-02	3.31E-02	1.098	0.2724
Vs_s_X_B_Inf4	1.04E-02	3.36E-02	0.309	0.7572
Vs_s_X_B_Inf5	-4.54E-02	3.29E-02	-1.381	0.1678
Vs_s_X_ISS1	2.36E-02	3.30E-02	0.715	0.4746
Vs_s_X_ISS2	-2.19E-03	3.34E-02	-0.065	0.9478
Vs_s_X_ISS3	4.06E-02	3.32E-02	1.223	0.2215
Vs_s_X_ISS4	3.29E-02	3.28E-02	1.005	0.3153
Vs_s_X_ISS5	-4.81E-03	3.32E-02	-0.145	0.8849
Vs_s_X_U_Inf1	2.89E-02	3.32E-02	0.869	0.3852
Vs_s_X_U_Inf2	3.45E-02	3.36E-02	1.028	0.3041
Vs_s_X_U_Inf3	1.15E-02	3.29E-02	0.348	0.728
Vs_s_X_U_Inf4	3.71E-02	3.31E-02	1.121	0.2627
Vs_s_X_U_Inf5	4.73E-02	3.33E-02	1.418	0.1566
X_Lim	5.37E-02	3.34E-02	1.607	0.1084
X_T	-4.11E-03	3.34E-02	-0.123	0.9021
f_U_Inf	-3.77E-02	3.29E-02	-1.144	0.253
i_Ca_PP_mol_perP	-1.33E-02	3.31E-02	-0.4	0.6891
i_H_Org_mol_perC	2.05E-02	3.30E-02	0.623	0.5336
i_H_SF_mol_perC	1.75E-02	3.35E-02	0.521	0.6022
i_H_SU_mol_perC	-2.57E-02	3.29E-02	-0.781	0.4352
i_H_XBInf_mol_perC	1.62E-02	3.30E-02	0.49	0.6243
i_H_XBOrg_mol_perC	-1.54E-03	3.30E-02	-0.047	0.9627
i_H_XUInf_mol_perC	3.32E-02	3.29E-02	1.009	0.3131
i_H_XUOrg_mol_perC	-3.86E-02	3.31E-02	-1.168	0.2431
i_K_PP_mol_perP	-1.33E-02	3.29E-02	-0.404	0.6864
i_Mg_PP_mol_perP	-1.19E-03	3.31E-02	-0.036	0.9713
i_N_Org_mol_perC	-1.64E-02	3.37E-02	-0.488	0.6257
i_N_SF_mol_perC	5.10E-02	3.30E-02	1.549	0.1217
i_N_SU_mol_perC	-1.94E-04	3.32E-02	-0.006	0.9953
i_N_XBInf_mol_perC	-1.25E-02	3.33E-02	-0.374	0.7085
i_N_XBOrg_mol_perC	4.01E-02	3.33E-02	1.206	0.2283

i_N_XUInf_mol_perC	1.40E-02	3.31E-02	0.424	0.672
i_N_XUOrg_mol_perC	1.57E-02	3.33E-02	0.471	0.6379
i_O_Org_mol_perC	-8.23E-03	3.35E-02	-0.246	0.8057
i_O_SF_mol_perC	-2.82E-03	3.30E-02	-0.086	0.9318
i_O_SU_mol_perC	-3.45E-02	3.32E-02	-1.04	0.2986
i_O_XBInf_mol_perC	4.85E-02	3.28E-02	1.48	0.1392
i_O_XBOrg_mol_perC	-1.21E-02	3.33E-02	-0.364	0.7159
i_O_XUInf_mol_perC	-5.93E-02	3.30E-02	-1.799	0.0724 .
i_O_XUOrg_mol_perC	-2.80E-02	3.32E-02	-0.845	0.3985
i_P_Org_mol_perC	-1.50E-02	3.28E-02	-0.456	0.6483
i_P_SF_mol_perC	5.39E-03	3.31E-02	0.163	0.8707
i_P_SU_mol_perC	-3.57E-03	3.28E-02	-0.109	0.9132
i_P_XBInf_mol_perC	1.88E-02	3.31E-02	0.568	0.5702
i_P_XBOrg_mol_perC	-1.68E-02	3.33E-02	-0.506	0.6128
i_P_XUInf_mol_perC	4.68E-03	3.32E-02	0.141	0.888
i_P_XUOrg_mol_perC	-8.78E-05	3.32E-02	-0.003	0.9979
kH_F_AD_hyd	-7.06E-02	3.33E-02	-2.118	0.0344 *
kM_BInf_AD_hyd	9.09E-03	3.32E-02	0.274	0.784
kM_BOrg_AD_hyd	1.92E-02	3.34E-02	0.575	0.5657

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.012 on 929 degrees of freedom

Multiple R-squared: 0.0477, Adjusted R-squared: -0.02405

F-statistic: 0.6648 on 70 and 929 DF, p-value: 0.9841

Under_X_B_Inf

Residuals:	Min	1Q	Median	3Q	Max
	-5.9543	-0.0634	0.3073	0.5015	1.1991

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	7.35E-12	3.20E-02	0	1
Alpha_B	3.27E-02	3.33E-02	0.982	0.3264
Alpha_I	1.96E-02	3.28E-02	0.598	0.5497
Alpha_U	2.43E-02	3.29E-02	0.739	0.46
Beta_B	8.39E-03	3.33E-02	0.252	0.8012
Beta_I	-4.95E-03	3.33E-02	-0.149	0.8818
Beta_U	9.02E-03	3.29E-02	0.274	0.7838
Gamma_B	2.13E-02	3.30E-02	0.647	0.5176
Gamma_I	-3.41E-02	3.31E-02	-1.031	0.3026
Gamma_U	1.55E-03	3.32E-02	0.046	0.9629
ISS_BM	4.82E-02	3.29E-02	1.464	0.1435

KS_BInf_AD_hyd	2.10E-02	3.29E-02	0.637	0.524
KS_BOrg_AD_hyd	-2.45E-03	3.31E-02	-0.074	0.9411
K_ALK	2.36E-02	3.35E-02	0.703	0.4821
Lambda_B	2.59E-02	3.30E-02	0.783	0.4335
Lambda_I	-4.74E-02	3.32E-02	-1.427	0.1538
Lambda_U	6.64E-03	3.27E-02	0.203	0.8391
TempCoeff	2.28E-02	3.31E-02	0.689	0.4912
Tref	-3.73E-02	3.38E-02	-1.105	0.2693
Vs_s_X_B_Inf1	-3.99E-02	3.32E-02	-1.2	0.2306
Vs_s_X_B_Inf2	-6.38E-03	3.31E-02	-0.193	0.8472
Vs_s_X_B_Inf3	4.51E-02	3.31E-02	1.363	0.1731
Vs_s_X_B_Inf4	1.03E-02	3.35E-02	0.308	0.7582
Vs_s_X_B_Inf5	-5.13E-02	3.29E-02	-1.56	0.1191
Vs_s_X_ISS1	2.08E-02	3.29E-02	0.631	0.5282
Vs_s_X_ISS2	-5.06E-03	3.34E-02	-0.151	0.8797
Vs_s_X_ISS3	4.52E-02	3.32E-02	1.363	0.1731
Vs_s_X_ISS4	3.32E-02	3.28E-02	1.014	0.3109
Vs_s_X_ISS5	-7.97E-03	3.32E-02	-0.24	0.8103
Vs_s_X_U_Inf1	2.88E-02	3.32E-02	0.868	0.3857
Vs_s_X_U_Inf2	3.60E-02	3.35E-02	1.074	0.2831
Vs_s_X_U_Inf3	1.82E-02	3.29E-02	0.555	0.5793
Vs_s_X_U_Inf4	3.89E-02	3.30E-02	1.178	0.2391
Vs_s_X_U_Inf5	4.62E-02	3.33E-02	1.387	0.1657
X_Lim	5.20E-02	3.34E-02	1.557	0.1199
X_T	-4.65E-03	3.34E-02	-0.139	0.8892
f_U_Inf	-3.65E-02	3.29E-02	-1.108	0.268
i_Ca_PP_mol_perP	-1.14E-02	3.31E-02	-0.344	0.7311
i_H_Org_mol_perC	2.30E-02	3.30E-02	0.698	0.4856
i_H_SF_mol_perC	1.76E-02	3.35E-02	0.525	0.5995
i_H_SU_mol_perC	-2.85E-02	3.29E-02	-0.865	0.3873
i_H_XBInf_mol_perC	1.69E-02	3.30E-02	0.513	0.6077
i_H_XBOrg_mol_perC	3.32E-04	3.29E-02	0.01	0.9919
i_H_XUInf_mol_perC	3.53E-02	3.29E-02	1.072	0.2838
i_H_XUOrg_mol_perC	-3.86E-02	3.30E-02	-1.168	0.2431
i_K_PP_mol_perP	-1.12E-02	3.29E-02	-0.342	0.7327
i_Mg_PP_mol_perP	3.53E-04	3.31E-02	0.011	0.9915
i_N_Org_mol_perC	-1.59E-02	3.36E-02	-0.473	0.6363
i_N_SF_mol_perC	5.14E-02	3.29E-02	1.562	0.1187
i_N_SU_mol_perC	2.42E-04	3.32E-02	0.007	0.9942
i_N_XBInf_mol_perC	-1.22E-02	3.33E-02	-0.368	0.7131
i_N_XBOrg_mol_perC	4.01E-02	3.33E-02	1.206	0.228
i_N_XUInf_mol_perC	1.45E-02	3.30E-02	0.438	0.6618
i_N_XUOrg_mol_perC	1.59E-02	3.32E-02	0.477	0.6332
i_O_Org_mol_perC	-7.81E-03	3.34E-02	-0.234	0.8153
i_O_SF_mol_perC	-3.59E-03	3.30E-02	-0.109	0.9133

i_O_SU_mol_perC	-3.65E-02	3.31E-02	-1.1	0.2714
i_O_XBInf_mol_perC	4.60E-02	3.28E-02	1.405	0.1603
i_O_XBOrg_mol_perC	-1.35E-02	3.32E-02	-0.406	0.6849
i_O_XUInf_mol_perC	-5.62E-02	3.30E-02	-1.704	0.0886 .
i_O_XUOrg_mol_perC	-2.84E-02	3.32E-02	-0.856	0.3924
i_P_Org_mol_perC	-1.44E-02	3.28E-02	-0.439	0.6607
i_P_SF_mol_perC	5.09E-03	3.31E-02	0.154	0.8778
i_P_SU_mol_perC	-4.45E-03	3.28E-02	-0.136	0.892
i_P_XBInf_mol_perC	2.20E-02	3.31E-02	0.665	0.5065
i_P_XBOrg_mol_perC	-1.65E-02	3.33E-02	-0.496	0.6197
i_P_XUInf_mol_perC	6.16E-03	3.32E-02	0.186	0.8527
i_P_XUOrg_mol_perC	7.82E-05	3.32E-02	0.002	0.9981
kH_F_AD_hyd	-7.46E-02	3.33E-02	-2.241	0.0253 *
kM_BInf_AD_hyd	8.52E-03	3.31E-02	0.257	0.7972
kM_BOrg_AD_hyd	1.85E-02	3.34E-02	0.555	0.5791

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.012 on 929 degrees of freedom

Multiple R-squared: 0.04898, Adjusted R-squared: -0.02268

F-statistic: 0.6835 on 70 and 929 DF, p-value: 0.9775

Under.X_ISS

Residuals:	Min	1Q	Median	3Q	Max
	-5.9543	-0.0634	0.3073	0.5015	1.1991

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	7.35E-12	3.20E-02	0	1
Alpha_B	3.27E-02	3.33E-02	0.982	0.3264
Alpha_I	1.96E-02	3.28E-02	0.598	0.5497
Alpha_U	2.43E-02	3.29E-02	0.739	0.46
Beta_B	8.39E-03	3.33E-02	0.252	0.8012
Beta_I	-4.95E-03	3.33E-02	-0.149	0.8818
Beta_U	9.02E-03	3.29E-02	0.274	0.7838
Gamma_B	2.13E-02	3.30E-02	0.647	0.5176
Gamma_I	-3.41E-02	3.31E-02	-1.031	0.3026
Gamma_U	1.55E-03	3.32E-02	0.046	0.9629
ISS_BM	4.82E-02	3.29E-02	1.464	0.1435
KS_BInf_AD_hyd	2.10E-02	3.29E-02	0.637	0.524
KS_BOrg_AD_hyd	-2.45E-03	3.31E-02	-0.074	0.9411
K_ALK	2.36E-02	3.35E-02	0.703	0.4821
Lambda_B	2.59E-02	3.30E-02	0.783	0.4335

Lambda_I	-4.74E-02	3.32E-02	-1.427	0.1538
Lambda_U	6.64E-03	3.27E-02	0.203	0.8391
TempCoeff	2.28E-02	3.31E-02	0.689	0.4912
Tref	-3.73E-02	3.38E-02	-1.105	0.2693
Vs_s_X_B_Inf1	-3.99E-02	3.32E-02	-1.2	0.2306
Vs_s_X_B_Inf2	-6.38E-03	3.31E-02	-0.193	0.8472
Vs_s_X_B_Inf3	4.51E-02	3.31E-02	1.363	0.1731
Vs_s_X_B_Inf4	1.03E-02	3.35E-02	0.308	0.7582
Vs_s_X_B_Inf5	-5.13E-02	3.29E-02	-1.56	0.1191
Vs_s_X_ISS1	2.08E-02	3.29E-02	0.631	0.5282
Vs_s_X_ISS2	-5.06E-03	3.34E-02	-0.151	0.8797
Vs_s_X_ISS3	4.52E-02	3.32E-02	1.363	0.1731
Vs_s_X_ISS4	3.32E-02	3.28E-02	1.014	0.3109
Vs_s_X_ISS5	-7.97E-03	3.32E-02	-0.24	0.8103
Vs_s_X_U_Inf1	2.88E-02	3.32E-02	0.868	0.3857
Vs_s_X_U_Inf2	3.60E-02	3.35E-02	1.074	0.2831
Vs_s_X_U_Inf3	1.82E-02	3.29E-02	0.555	0.5793
Vs_s_X_U_Inf4	3.89E-02	3.30E-02	1.178	0.2391
Vs_s_X_U_Inf5	4.62E-02	3.33E-02	1.387	0.1657
X_Lim	5.20E-02	3.34E-02	1.557	0.1199
X_T	-4.65E-03	3.34E-02	-0.139	0.8892
f_U_Inf	-3.65E-02	3.29E-02	-1.108	0.268
i_Ca_PP_mol_perP	-1.14E-02	3.31E-02	-0.344	0.7311
i_H_Org_mol_perC	2.30E-02	3.30E-02	0.698	0.4856
i_H_SF_mol_perC	1.76E-02	3.35E-02	0.525	0.5995
i_H_SU_mol_perC	-2.85E-02	3.29E-02	-0.865	0.3873
i_H_XBInf_mol_perC	1.69E-02	3.30E-02	0.513	0.6077
i_H_XBOrg_mol_perC	3.32E-04	3.29E-02	0.01	0.9919
i_H_XUInf_mol_perC	3.53E-02	3.29E-02	1.072	0.2838
i_H_XUOrg_mol_perC	-3.86E-02	3.30E-02	-1.168	0.2431
i_K_PP_mol_perP	-1.12E-02	3.29E-02	-0.342	0.7327
i_Mg_PP_mol_perP	3.53E-04	3.31E-02	0.011	0.9915
i_N_Org_mol_perC	-1.59E-02	3.36E-02	-0.473	0.6363
i_N_SF_mol_perC	5.14E-02	3.29E-02	1.562	0.1187
i_N_SU_mol_perC	2.42E-04	3.32E-02	0.007	0.9942
i_N_XBInf_mol_perC	-1.22E-02	3.33E-02	-0.368	0.7131
i_N_XBOrg_mol_perC	4.01E-02	3.33E-02	1.206	0.228
i_N_XUInf_mol_perC	1.45E-02	3.30E-02	0.438	0.6618
i_N_XUOrg_mol_perC	1.59E-02	3.32E-02	0.477	0.6332
i_O_Org_mol_perC	-7.81E-03	3.34E-02	-0.234	0.8153
i_O_SF_mol_perC	-3.59E-03	3.30E-02	-0.109	0.9133
i_O_SU_mol_perC	-3.65E-02	3.31E-02	-1.1	0.2714
i_O_XBInf_mol_perC	4.60E-02	3.28E-02	1.405	0.1603
i_O_XBOrg_mol_perC	-1.35E-02	3.32E-02	-0.406	0.6849
i_O_XUInf_mol_perC	-5.62E-02	3.30E-02	-1.704	0.0886

i_O_XUOrg_mol_perC	-2.84E-02	3.32E-02	-0.856	0.3924
i_P_Org_mol_perC	-1.44E-02	3.28E-02	-0.439	0.6607
i_P_SF_mol_perC	5.09E-03	3.31E-02	0.154	0.8778
i_P_SU_mol_perC	-4.45E-03	3.28E-02	-0.136	0.892
i_P_XBInf_mol_perC	2.20E-02	3.31E-02	0.665	0.5065
i_P_XBOrg_mol_perC	-1.65E-02	3.33E-02	-0.496	0.6197
i_P_XUInf_mol_perC	6.16E-03	3.32E-02	0.186	0.8527
i_P_XUOrg_mol_perC	7.82E-05	3.32E-02	0.002	0.9981
kH_F_AD_hyd	-7.46E-02	3.33E-02	-2.241	0.0253 *
kM_BInf_AD_hyd	8.52E-03	3.31E-02	0.257	0.7972
kM_BOrg_AD_hyd	1.85E-02	3.34E-02	0.555	0.5791

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.012 on 929 degrees of freedom

Multiple R-squared: 0.04898, Adjusted R-squared: -0.02268

F-statistic: 0.6835 on 70 and 929 DF, p-value: 0.9775

Under.X_U_Inf

Residuals:	Min	1Q	Median	3Q	Max
	-5.9543	-0.0634	0.3073	0.5015	1.1991

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	6.35E-12	3.20E-02	0	1
Alpha_B	3.27E-02	3.33E-02	0.982	0.3264
Alpha_I	1.96E-02	3.28E-02	0.598	0.5497
Alpha_U	2.43E-02	3.29E-02	0.739	0.46
Beta_B	8.39E-03	3.33E-02	0.252	0.8012
Beta_I	-4.95E-03	3.33E-02	-0.149	0.8818
Beta_U	9.02E-03	3.29E-02	0.274	0.7838
Gamma_B	2.13E-02	3.30E-02	0.647	0.5176
Gamma_I	-3.41E-02	3.31E-02	-1.031	0.3026
Gamma_U	1.55E-03	3.32E-02	0.046	0.9629
ISS_BM	4.82E-02	3.29E-02	1.464	0.1435
KS_BInf_AD_hyd	2.10E-02	3.29E-02	0.637	0.524
KS_BOrg_AD_hyd	-2.45E-03	3.31E-02	-0.074	0.9411
K_ALK	2.36E-02	3.35E-02	0.703	0.4821
Lambda_B	2.59E-02	3.30E-02	0.783	0.4335
Lambda_I	-4.74E-02	3.32E-02	-1.427	0.1538
Lambda_U	6.64E-03	3.27E-02	0.203	0.8391
TempCoeff	2.28E-02	3.31E-02	0.689	0.4912
Tref	-3.73E-02	3.38E-02	-1.105	0.2693

Vs_s_X_B_Inf1	-3.99E-02	3.32E-02	-1.2	0.2306
Vs_s_X_B_Inf2	-6.38E-03	3.31E-02	-0.193	0.8472
Vs_s_X_B_Inf3	4.51E-02	3.31E-02	1.363	0.1731
Vs_s_X_B_Inf4	1.03E-02	3.35E-02	0.308	0.7582
Vs_s_X_B_Inf5	-5.13E-02	3.29E-02	-1.56	0.1191
Vs_s_X_ISS1	2.08E-02	3.29E-02	0.631	0.5282
Vs_s_X_ISS2	-5.06E-03	3.34E-02	-0.151	0.8797
Vs_s_X_ISS3	4.52E-02	3.32E-02	1.363	0.1731
Vs_s_X_ISS4	3.32E-02	3.28E-02	1.014	0.3109
Vs_s_X_ISS5	-7.97E-03	3.32E-02	-0.24	0.8103
Vs_s_X_U_Inf1	2.88E-02	3.32E-02	0.868	0.3857
Vs_s_X_U_Inf2	3.60E-02	3.35E-02	1.074	0.2831
Vs_s_X_U_Inf3	1.82E-02	3.29E-02	0.555	0.5793
Vs_s_X_U_Inf4	3.89E-02	3.30E-02	1.178	0.2391
Vs_s_X_U_Inf5	4.62E-02	3.33E-02	1.387	0.1657
X_Lim	5.20E-02	3.34E-02	1.557	0.1199
X_T	-4.65E-03	3.34E-02	-0.139	0.8892
f_U_Inf	-3.65E-02	3.29E-02	-1.108	0.268
i_Ca_PP_mol_perP	-1.14E-02	3.31E-02	-0.344	0.7311
i_H_Org_mol_perC	2.30E-02	3.30E-02	0.698	0.4856
i_H_SF_mol_perC	1.76E-02	3.35E-02	0.525	0.5995
i_H_SU_mol_perC	-2.85E-02	3.29E-02	-0.865	0.3873
i_H_XBInf_mol_perC	1.69E-02	3.30E-02	0.513	0.6077
i_H_XBOrg_mol_perC	3.32E-04	3.29E-02	0.01	0.9919
i_H_XUInf_mol_perC	3.53E-02	3.29E-02	1.072	0.2838
i_H_XUOrg_mol_perC	-3.86E-02	3.30E-02	-1.168	0.2431
i_K_PP_mol_perP	-1.12E-02	3.29E-02	-0.342	0.7327
i_Mg_PP_mol_perP	3.53E-04	3.31E-02	0.011	0.9915
i_N_Org_mol_perC	-1.59E-02	3.36E-02	-0.473	0.6363
i_N_SF_mol_perC	5.14E-02	3.29E-02	1.562	0.1187
i_N_SU_mol_perC	2.42E-04	3.32E-02	0.007	0.9942
i_N_XBInf_mol_perC	-1.22E-02	3.33E-02	-0.368	0.7131
i_N_XBOrg_mol_perC	4.01E-02	3.33E-02	1.206	0.228
i_N_XUInf_mol_perC	1.45E-02	3.30E-02	0.438	0.6618
i_N_XUOrg_mol_perC	1.59E-02	3.32E-02	0.477	0.6332
i_O_Org_mol_perC	-7.81E-03	3.34E-02	-0.234	0.8153
i_O_SF_mol_perC	-3.59E-03	3.30E-02	-0.109	0.9133
i_O_SU_mol_perC	-3.65E-02	3.31E-02	-1.1	0.2714
i_O_XBInf_mol_perC	4.60E-02	3.28E-02	1.405	0.1603
i_O_XBOrg_mol_perC	-1.35E-02	3.32E-02	-0.406	0.6849
i_O_XUInf_mol_perC	-5.62E-02	3.30E-02	-1.704	0.0886
i_O_XUOrg_mol_perC	-2.84E-02	3.32E-02	-0.856	0.3924
i_P_Org_mol_perC	-1.44E-02	3.28E-02	-0.439	0.6607
i_P_SF_mol_perC	5.09E-03	3.31E-02	0.154	0.8778
i_P_SU_mol_perC	-4.45E-03	3.28E-02	-0.136	0.892

i_P_XBInf_mol_perC	2.20E-02	3.31E-02	0.665	0.5065
i_P_XBOrg_mol_perC	-1.65E-02	3.33E-02	-0.496	0.6197
i_P_XUInf_mol_perC	6.16E-03	3.32E-02	0.186	0.8527
i_P_XUOrg_mol_perC	7.82E-05	3.32E-02	0.002	0.9981
kH_F_AD_hyd	-7.46E-02	3.33E-02	-2.241	0.0253 *
kM_BInf_AD_hyd	8.52E-03	3.31E-02	0.257	0.7972
kM_BOrg_AD_hyd	1.85E-02	3.34E-02	0.555	0.5791

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.012 on 929 degrees of freedom

Multiple R-squared: 0.04898, Adjusted R-squared: -0.02268

F-statistic: 0.6835 on 70 and 929 DF, p-value: 0.9775

Under.X_VSS

Residuals:	Min	1Q	Median	3Q	Max
	-5.9543	-0.0634	0.3073	0.5015	1.1991

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	6.35E-12	3.20E-02	0	1
Alpha_B	3.27E-02	3.33E-02	0.982	0.3264
Alpha_I	1.96E-02	3.28E-02	0.598	0.5497
Alpha_U	2.43E-02	3.29E-02	0.739	0.46
Beta_B	8.39E-03	3.33E-02	0.252	0.8012
Beta_I	-4.95E-03	3.33E-02	-0.149	0.8818
Beta_U	9.02E-03	3.29E-02	0.274	0.7838
Gamma_B	2.13E-02	3.30E-02	0.647	0.5176
Gamma_I	-3.41E-02	3.31E-02	-1.031	0.3026
Gamma_U	1.55E-03	3.32E-02	0.046	0.9629
ISS_BM	4.82E-02	3.29E-02	1.464	0.1435
KS_BInf_AD_hyd	2.10E-02	3.29E-02	0.637	0.524
KS_BOrg_AD_hyd	-2.45E-03	3.31E-02	-0.074	0.9411
K_ALK	2.36E-02	3.35E-02	0.703	0.4821
Lambda_B	2.59E-02	3.30E-02	0.783	0.4335
Lambda_I	-4.74E-02	3.32E-02	-1.427	0.1538
Lambda_U	6.64E-03	3.27E-02	0.203	0.8391
TempCoeff	2.28E-02	3.31E-02	0.689	0.4912
Tref	-3.73E-02	3.38E-02	-1.105	0.2693
Vs_s_X_B_Inf1	-3.99E-02	3.32E-02	-1.2	0.2306
Vs_s_X_B_Inf2	-6.38E-03	3.31E-02	-0.193	0.8472
Vs_s_X_B_Inf3	4.51E-02	3.31E-02	1.363	0.1731
Vs_s_X_B_Inf4	1.03E-02	3.35E-02	0.308	0.7582

Vs_s_X_B_Inf5	-5.13E-02	3.29E-02	-1.56	0.1191
Vs_s_X_ISS1	2.08E-02	3.29E-02	0.631	0.5282
Vs_s_X_ISS2	-5.06E-03	3.34E-02	-0.151	0.8797
Vs_s_X_ISS3	4.52E-02	3.32E-02	1.363	0.1731
Vs_s_X_ISS4	3.32E-02	3.28E-02	1.014	0.3109
Vs_s_X_ISS5	-7.97E-03	3.32E-02	-0.24	0.8103
Vs_s_X_U_Inf1	2.88E-02	3.32E-02	0.868	0.3857
Vs_s_X_U_Inf2	3.60E-02	3.35E-02	1.074	0.2831
Vs_s_X_U_Inf3	1.82E-02	3.29E-02	0.555	0.5793
Vs_s_X_U_Inf4	3.89E-02	3.30E-02	1.178	0.2391
Vs_s_X_U_Inf5	4.62E-02	3.33E-02	1.387	0.1657
X_Lim	5.20E-02	3.34E-02	1.557	0.1199
X_T	-4.65E-03	3.34E-02	-0.139	0.8892
f_U_Inf	-3.65E-02	3.29E-02	-1.108	0.268
i_Ca_PP_mol_perP	-1.14E-02	3.31E-02	-0.344	0.7311
i_H_Org_mol_perC	2.30E-02	3.30E-02	0.698	0.4856
i_H_SF_mol_perC	1.76E-02	3.35E-02	0.525	0.5995
i_H_SU_mol_perC	-2.85E-02	3.29E-02	-0.865	0.3873
i_H_XBInf_mol_perC	1.69E-02	3.30E-02	0.513	0.6077
i_H_XBOrg_mol_perC	3.32E-04	3.29E-02	0.01	0.9919
i_H_XUInf_mol_perC	3.53E-02	3.29E-02	1.072	0.2838
i_H_XUOrg_mol_perC	-3.86E-02	3.30E-02	-1.168	0.2431
i_K_PP_mol_perP	-1.12E-02	3.29E-02	-0.342	0.7327
i_Mg_PP_mol_perP	3.53E-04	3.31E-02	0.011	0.9915
i_N_Org_mol_perC	-1.59E-02	3.36E-02	-0.473	0.6363
i_N_SF_mol_perC	5.14E-02	3.29E-02	1.562	0.1187
i_N_SU_mol_perC	2.42E-04	3.32E-02	0.007	0.9942
i_N_XBInf_mol_perC	-1.22E-02	3.33E-02	-0.368	0.7131
i_N_XBOrg_mol_perC	4.01E-02	3.33E-02	1.206	0.228
i_N_XUInf_mol_perC	1.45E-02	3.30E-02	0.438	0.6618
i_N_XUOrg_mol_perC	1.59E-02	3.32E-02	0.477	0.6332
i_O_Org_mol_perC	-7.81E-03	3.34E-02	-0.234	0.8153
i_O_SF_mol_perC	-3.59E-03	3.30E-02	-0.109	0.9133
i_O_SU_mol_perC	-3.65E-02	3.31E-02	-1.1	0.2714
i_O_XBInf_mol_perC	4.60E-02	3.28E-02	1.405	0.1603
i_O_XBOrg_mol_perC	-1.35E-02	3.32E-02	-0.406	0.6849
i_O_XUInf_mol_perC	-5.62E-02	3.30E-02	-1.704	0.0886
i_O_XUOrg_mol_perC	-2.84E-02	3.32E-02	-0.856	0.3924
i_P_Org_mol_perC	-1.44E-02	3.28E-02	-0.439	0.6607
i_P_SF_mol_perC	5.09E-03	3.31E-02	0.154	0.8778
i_P_SU_mol_perC	-4.45E-03	3.28E-02	-0.136	0.892
i_P_XBInf_mol_perC	2.20E-02	3.31E-02	0.665	0.5065
i_P_XBOrg_mol_perC	-1.65E-02	3.33E-02	-0.496	0.6197
i_P_XUInf_mol_perC	6.16E-03	3.32E-02	0.186	0.8527
i_P_XUOrg_mol_perC	7.82E-05	3.32E-02	0.002	0.9981

kH_F_AD_hyd	-7.46E-02	3.33E-02	-2.241	0.0253 *
kM_BInf_AD_hyd	8.52E-03	3.31E-02	0.257	0.7972
kM_BOrg_AD_hyd	1.85E-02	3.34E-02	0.555	0.5791

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.012 on 929 degrees of freedom

Multiple R-squared: 0.04898, Adjusted R-squared: -0.02268

F-statistic: 0.6835 on 70 and 929 DF, p-value: 0.9775

VSS_Under_s

Residuals:	Min	1Q	Median	3Q	Max
	-0.76005	-0.08654	0.02092	0.1113	0.39311

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	-1.84E-12	5.39E-03	0	1	
Alpha_B	3.53E-03	5.60E-03	0.631	0.5285	
Alpha_I	-2.91E-03	5.52E-03	-0.526	0.5991	
Alpha_U	1.08E-01	5.54E-03	19.454	< 2e-16	***
Beta_B	9.24E-03	5.61E-03	1.648	0.0998	.
Beta_I	2.84E-03	5.60E-03	0.508	0.6118	
Beta_U	2.53E-02	5.53E-03	4.582	5.24E-06	***
Gamma_B	4.51E-02	5.55E-03	8.122	1.45E-15	***
Gamma_I	-8.55E-03	5.57E-03	-1.535	0.1251	
Gamma_U	2.92E-02	5.60E-03	5.221	2.20E-07	***
ISS_BM	-5.64E-03	5.54E-03	-1.019	0.3087	
KS_BInf_AD_hyd	1.72E-03	5.54E-03	0.31	0.7565	
KS_BOrg_AD_hyd	-1.05E-04	5.57E-03	-0.019	0.985	
K_ALK	5.36E-03	5.64E-03	0.95	0.3422	
Lambda_B	2.41E-02	5.56E-03	4.34	1.58E-05	***
Lambda_I	-3.00E-04	5.59E-03	-0.054	0.9572	
Lambda_U	-4.09E-04	5.50E-03	-0.074	0.9407	
TempCoeff	4.67E-03	5.58E-03	0.837	0.4026	
Tref	3.97E-03	5.68E-03	0.699	0.4848	
Vs_s_X_B_Inf1	3.88E-02	5.60E-03	6.935	7.61E-12	***
Vs_s_X_B_Inf2	8.82E-02	5.57E-03	15.835	< 2e-16	***
Vs_s_X_B_Inf3	2.94E-01	5.57E-03	52.68	< 2e-16	***
Vs_s_X_B_Inf4	5.14E-01	5.65E-03	91.068	< 2e-16	***
Vs_s_X_B_Inf5	7.61E-01	5.53E-03	137.473	< 2e-16	***
Vs_s_X_ISS1	2.38E-03	5.54E-03	0.428	0.6685	
Vs_s_X_ISS2	-3.27E-03	5.62E-03	-0.581	0.5615	
Vs_s_X_ISS3	-3.72E-03	5.59E-03	-0.665	0.5063	

Vs_s_X_ISS4	-1.80E-03	5.51E-03	-0.326	0.7442	
Vs_s_X_ISS5	1.60E-04	5.59E-03	0.029	0.9771	
Vs_s_X_U_Inf1	1.15E-01	5.59E-03	20.58	< 2e-16	***
Vs_s_X_U_Inf2	7.14E-02	5.64E-03	12.642	< 2e-16	***
Vs_s_X_U_Inf3	1.26E-01	5.54E-03	22.76	< 2e-16	***
Vs_s_X_U_Inf4	9.59E-02	5.56E-03	17.233	< 2e-16	***
Vs_s_X_U_Inf5	5.14E-02	5.61E-03	9.16	< 2e-16	***
X_Lim	-5.45E-03	5.63E-03	-0.969	0.3327	
X_T	-6.66E-04	5.62E-03	-0.119	0.9056	
f_U_Inf	-4.89E-03	5.54E-03	-0.884	0.3771	
i_Ca_PP_mol_perP	1.14E-02	5.57E-03	2.053	0.0404	*
i_H_Org_mol_perC	5.97E-03	5.55E-03	1.075	0.2826	
i_H_SF_mol_perC	9.10E-04	5.64E-03	0.161	0.8719	
i_H_SU_mol_perC	1.53E-03	5.54E-03	0.276	0.7826	
i_H_XBInf_mol_perC	9.68E-03	5.55E-03	1.745	0.0813	.
i_H_XBOrg_mol_perC	8.22E-04	5.54E-03	0.148	0.8822	
i_H_XUInf_mol_perC	-4.03E-03	5.54E-03	-0.728	0.4668	
i_H_XUOrg_mol_perC	6.46E-03	5.56E-03	1.161	0.2459	
i_K_PP_mol_perP	5.38E-03	5.53E-03	0.973	0.3308	
i_Mg_PP_mol_perP	-4.62E-03	5.56E-03	-0.83	0.4069	
i_N_Org_mol_perC	4.93E-03	5.66E-03	0.87	0.3845	
i_N_SF_mol_perC	-6.44E-04	5.54E-03	-0.116	0.9075	
i_N_SU_mol_perC	1.01E-03	5.58E-03	0.181	0.8565	
i_N_XBInf_mol_perC	5.90E-03	5.60E-03	1.054	0.292	
i_N_XBOrg_mol_perC	1.16E-03	5.60E-03	0.207	0.8363	
i_N_XUInf_mol_perC	1.20E-03	5.56E-03	0.216	0.8291	
i_N_XUOrg_mol_perC	5.01E-03	5.60E-03	0.895	0.3708	
i_O_Org_mol_perC	1.01E-03	5.63E-03	0.179	0.8582	
i_O_SF_mol_perC	7.68E-03	5.55E-03	1.384	0.1668	
i_O_SU_mol_perC	1.48E-03	5.58E-03	0.265	0.791	
i_O_XBInf_mol_perC	4.98E-04	5.52E-03	0.09	0.928	
i_O_XBOrg_mol_perC	1.30E-04	5.60E-03	0.023	0.9815	
i_O_XUInf_mol_perC	-1.44E-03	5.55E-03	-0.259	0.796	
i_O_XUOrg_mol_perC	-3.30E-03	5.58E-03	-0.591	0.555	
i_P_Org_mol_perC	-7.83E-03	5.52E-03	-1.417	0.1568	
i_P_SF_mol_perC	-2.73E-03	5.57E-03	-0.49	0.624	
i_P_SU_mol_perC	7.98E-03	5.51E-03	1.448	0.148	
i_P_XBInf_mol_perC	-6.09E-03	5.57E-03	-1.094	0.2744	
i_P_XBOrg_mol_perC	-8.09E-03	5.60E-03	-1.445	0.1489	
i_P_XUInf_mol_perC	-6.01E-03	5.59E-03	-1.076	0.2822	
i_P_XUOrg_mol_perC	6.09E-03	5.59E-03	1.09	0.2759	
kH_F_AD_hyd	2.19E-03	5.60E-03	0.392	0.6955	
kM_BInf_AD_hyd	-2.92E-03	5.58E-03	-0.524	0.6004	
kM_BOrg_AD_hyd	5.77E-03	5.62E-03	1.028	0.3042	

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.1703 on 929 degrees of freedom

Multiple R-squared: 0.973, Adjusted R-squared: 0.971

F-statistic: 479 on 70 and 929 DF, p-value: < 2.2e-16

University of Cape Town

ISS_under					Variables					
Multivariate regression no intercept			Multivariate regression & intercept		Parameters	Number	Name	Parameter		
Std.	β_0^2	SRC (β_0)	Std.	β^2						
0.06234	3.48195	-1.866	1.59E-02	1.81E-03	X_T	1	Alpha_B	Fractionation		
0.00756	7.16632	-2.677	1.58E-02	1.06E-03	i_O_XUOrg_mol_per	2	Alpha_I			
0.03963	4.24772	-2.061	1.58E-02	8.74E-04	Alpha_B	3	Alpha_U			
0.0885	2.90702	-1.705	1.58E-02	7.21E-04	Vs_s_X_B_Inf2	4	Beta_B			
0.15423	2.03347	-1.426	1.57E-02	5.00E-04	i_N_SF_mol_perC	5	Beta_I			
0.31499	1.01002	-1.005	1.57E-02	2.50E-04	i_H_XUOrg_mol_per	6	Beta_U			
0.34412	0.89680	-0.947	1.58E-02	2.24E-04	Vs_s_X_B_Inf1	7	Gamma_B			
0.35219	0.86676	-0.931	1.58E-02	2.16E-04	i_O_SU_mol_perC	8	Gamma_I			
0.35846	0.84456	-0.919	1.59E-02	2.13E-04	i_O_Org_mol_perC	9	Gamma_U			
0.35923	0.84088	-0.917	1.58E-02	2.11E-04	i_N_XBOrg_mol_per	10	Lambda_B			
0.40951	0.68062	-0.825	1.58E-02	1.71E-04	i_N_XBInf_mol_per	11	Lambda_I			
0.43176	0.61936	-0.787	1.58E-02	1.55E-04	Lambda_I	12	Lambda_U			
0.4352	0.60996	-0.781	1.57E-02	1.50E-04	i_H_SU_mol_perC	13	f_U_Inf			
0.50572	0.44355	-0.666	1.57E-02	1.09E-04	Gamma_B	14	ISS_BM	Com- positio n		
0.58964	0.2916	-0.54	1.57E-02	7.18E-05	Lambda_B	15	X_Lim	Settling		
0.6004	0.27457	-0.524	1.57E-02	6.79E-05	i_N_XUInf_mol_per	16	X_T			

Out.X_ISS		Out_X_B_Inf							
Multive	Parameters	Multive regression no intercept			Multive regression & intercept			Parameters	
SRC (β)		Std.	β ₀ ²	SRC (β ₀)	Std.	β ²	SRC (β)		
-7.06E-	kH_F_AD_hyd	0.0344 *	4.49E+00	-2.118	3.33E-02	4.98E-03	-7.06E-	kH_F_AD_hyd	
-5.93E-	i_O_XUInf_mol_perC	0.0724 .	3.24E+00	-1.799	3.30E-02	3.52E-03	-5.93E-	i_O_XUInf_mol_per	
-5.11E-	Lambda_I	0.1244	2.37E+00	-1.538	3.32E-02	2.61E-03	-5.11E-	Lambda_I	
-4.54E-	Vs_s_X_B_Inf5	0.1678	1.91E+00	-1.381	3.29E-02	2.06E-03	-4.54E-	Vs_s_X_B_Inf5	
-4.19E-	Gamma_I	0.2055	1.61E+00	-1.267	3.31E-02	1.76E-03	-4.19E-	Gamma_I	
-4.09E-	Vs_s_X_B_Inf1	0.2196	1.51E+00	-1.229	3.33E-02	1.67E-03	-4.09E-	Vs_s_X_B_Inf1	
-3.86E-	i_H_XUOrg_mol_per	0.2431	1.36E+00	-1.168	3.31E-02	1.49E-03	-3.86E-	i_H_XUOrg_mol_per	
-3.77E-	f_U_Inf	0.253	1.31E+00	-1.144	3.29E-02	1.42E-03	-3.77E-	f_U_Inf	
-3.68E-	Tref	0.2768	1.18E+00	-1.088	3.38E-02	1.35E-03	-3.68E-	Tref	
-3.45E-	i_O_SU_mol_perC	0.2986	1.08E+00	-1.04	3.32E-02	1.19E-03	-3.45E-	i_O_SU_mol_perC	
-2.80E-	i_O_XUOrg_mol_per	0.3985	7.14E-01	-0.845	3.32E-02	7.86E-04	-2.80E-	i_O_XUOrg_mol_per	
-2.57E-	i_H_SU_mol_perC	0.4352	6.10E-01	-0.781	3.29E-02	6.61E-04	-2.57E-	i_H_SU_mol_perC	
-1.68E-	i_P_XBOrg_mol_perC	0.6128	2.56E-01	-0.506	3.33E-02	2.84E-04	-1.68E-	i_P_XBOrg_mol_per	
-1.64E-02	i_N_Org_mol_perC	0.6257	2.38E-01	-0.488	3.37E-02	2.70E-04	-1.64E-02	i_N_Org_mol_perC	
-1.50E-	i_P_Org_mol_perC	0.6483	2.08E-01	-0.456	3.28E-02	2.24E-04	-1.50E-	i_P_Org_mol_perC	
-1.33E-	i_K_PP_mol_perP	0.6864	1.63E-01	-0.404	3.29E-02	1.76E-04	-1.33E-	i_K_PP_mol_perP	

Out.X_U_Inf														
Multive		Multive regression & intercept				Parameters		Multive regression no						
β_0^2	SRC	Std.	β^2	SRC (β)				Std.	β_0^2	SRC	Std.	β^2		
4.48	-2.118	3.33E-02	4.98E-03	-7.06E-	kH_F_AD_hyd			0.0344 *	4.48592	-2.118	3.33E-02	4.98E-03		
3.23	-1.799	3.30E-02	3.52E-03	-5.93E-	i_O_XUInf_mol_perC			0.0724 .	3.23640	-1.799	3.30E-02	3.52E-03		
2.36	-1.538	3.32E-02	2.61E-03	-5.11E-	Lambda_I			0.1244	2.36544	-1.538	3.32E-02	2.61E-03		
1.90	-1.381	3.29E-02	2.06E-03	-4.54E-	Vs_s_X_B_Inf5			0.1678	1.90716	-1.381	3.29E-02	2.06E-03		
1.60	-1.267	3.31E-02	1.76E-03	-4.19E-	Gamma_I			0.2055	1.60528	-1.267	3.31E-02	1.76E-03		
1.51	-1.229	3.33E-02	1.67E-03	-4.09E-	Vs_s_X_B_Inf1			0.2196	1.51044	-1.229	3.33E-02	1.67E-03		
1.36	-1.168	3.31E-02	1.49E-03	-3.86E-	i_H_XUOrg_mol_per			0.2431	1.36422	-1.168	3.31E-02	1.49E-03		
1.30	-1.144	3.29E-02	1.42E-03	-3.77E-	f_U_Inf			0.253	1.30873	-1.144	3.29E-02	1.42E-03		
1.18	-1.088	3.38E-02	1.35E-03	-3.68E-	Tref			0.2768	1.18374	-1.088	3.38E-02	1.35E-03		
1.08	-1.04	3.32E-02	1.19E-03	-3.45E-	i_O_SU_mol_perC			0.2986	1.0816	-1.04	3.32E-02	1.19E-03		
0.71	-0.845	3.32E-02	7.86E-04	-2.80E-	i_O_XUOrg_mol_per			0.3985	0.71402	-0.845	3.32E-02	7.86E-04		
0.60	-0.781	3.29E-02	6.61E-04	-2.57E-	i_H_SU_mol_perC			0.4352	0.60996	-0.781	3.29E-02	6.61E-04		
0.25	-0.506	3.33E-02	2.84E-04	-1.68E-	i_P_XBOrg_mol_per			0.6128	0.25603	-0.506	3.33E-02	2.84E-04		
0.23 814	-0.488	3.37E-02	2.70E-04	-1.64E-02	i_N_Org_mol_perC			0.6257	0.23814 4	-0.488	3.37E-02	2.70E-04		
0.20	-0.456	3.28E-02	2.24E-04	-1.50E-	i_P_Org_mol_perC			0.6483	0.20793	-0.456	3.28E-02	2.24E-04		
0.16	-0.404	3.29E-02	1.76E-04	-1.33E-	i_K_PP_mol_perP			0.6864	0.16321	-0.404	3.29E-02	1.76E-04		

TSS_Under_s			Out.X_VSS								
Multive	Parameters		Multive regression		Multive regression & intercept			Parameters			
SRC (β)			Std.	β ₀ [^]	SRC	Std.	β ²	SRC (β)		Std.	
-8.65E-	i_P_XBOrg_mol_pe		0.03	4.48	-	3.33E-02	4.98E-03	-7.06E-	kH_F_AD_hyd	0.03	
-6.92E-	i_O_XUOrg_mol_pe		0.07	3.23	-	3.30E-02	3.52E-03	-5.93E-	i_O_XUInf_mol_per	0.07	
-5.77E-	i_P_XUInf_mol_per		0.12	2.36	-	3.32E-02	2.61E-03	-5.11E-	Lambda_I	0.12	
-5.42E-	X_T		0.16	1.90	-	3.29E-02	2.06E-03	-4.54E-	Vs_s_X_B_Inf5	0.16	
-4.69E-	i_P_XBInf_mol_per		0.20	1.60	-	3.31E-02	1.76E-03	-4.19E-	Gamma_I	0.20	
-4.28E-	i_H_XUInf_mol_per		0.21	1.51	-	3.33E-02	1.67E-03	-4.09E-	Vs_s_X_B_Inf1	0.21	
-4.18E-	i_P_Org_mol_perC		0.24	1.36	-	3.31E-02	1.49E-03	-3.86E-	i_H_XUOrg_mol_pe	0.24	
-3.78E-	i_Mg_PP_mol_perP		0.25	1.30	-	3.29E-02	1.42E-03	-3.77E-	f_U_Inf	0.25	
-3.77E-	f_U_Inf		0.27	1.18	-	3.38E-02	1.35E-03	-3.68E-	Tref	0.27	
-3.56E-	ISS_BM		0.29	1.08	-1.04	3.32E-02	1.19E-03	-3.45E-	i_O_SU_mol_perC	0.29	
-3.14E-	i_N_SF_mol_perC		0.39	0.71	-	3.32E-02	7.86E-04	-2.80E-	i_O_XUOrg_mol_pe	0.39	
-3.11E-	X_Lim		0.43	0.60	-	3.29E-02	6.61E-04	-2.57E-	i_H_SU_mol_perC	0.43	
-2.40E-	kM_BInf_AD_hyd		0.61	0.25	-	3.33E-02	2.84E-04	-1.68E-	i_P_XBOrg_mol_per	0.61	
-1.87E-03	i_O_XUInf_mol_perC		0.62	0.23	-	3.37E-02	2.70E-04	-1.64E-02	i_N_Org_mol_perC	0.62	57
-1.69E-	Lambda_I		0.64	0.20	-	3.28E-02	2.24E-04	-1.50E-	i_P_Org_mol_perC	0.64	
-1.32E-	i_P_SF_mol_perC		0.68	0.16	-	3.29E-02	1.76E-04	-1.33E-	i_K_PP_mol_perP	0.68	

Under_X_B_Inf							*	*	*		
Multive regression no			Multive regression & intercept			Parameters	Multive regression				
Std.	β ₀ ^{^2}	SRC (β ₀)	Std.	β ^{^2}	SRC (β)						
0.02	5.02	-2.241	3.33E-02	5.56E-03	-7.46E-	KH_F_AD_hyd	0.13	2.26	-	5.74E-03	7.48E-05
0.08	2.90	-1.704	3.30E-02	3.15E-03	-5.62E-	i_O_XUInf_mol_per	0.22	1.45	-	5.73E-03	4.79E-05
0.11	2.43	-1.56	3.29E-02	2.63E-03	-5.13E-	Vs_s_X_B_Inf5	0.31	1.01	-	5.73E-03	3.33E-05
0.15	2.03	-1.427	3.32E-02	2.25E-03	-4.74E-	Lambda_I	0.34	0.88	-	5.76E-03	2.94E-05
0.23	1.44	-1.2	3.32E-02	1.59E-03	-3.99E-	Vs_s_X_B_Inf1	0.41	0.67	-0.82	5.71E-03	2.20E-05
0.24	1.36	-1.168	3.30E-02	1.49E-03	-3.86E-	i_H_XUOrg_mol_pe	0.45	0.56	-	5.69E-03	1.83E-05
0.26	1.22	-1.108	3.38E-02	1.39E-03	-3.73E-	Tref	0.46	0.54	-	5.67E-03	1.74E-05
0.26	1.22	-1.105	3.29E-02	1.33E-03	-3.65E-	f_U_Inf	0.50	0.43	-	5.71E-03	1.43E-05
0.27	1.21	-1.1	3.31E-02	1.33E-03	-3.65E-	i_O_SU_mol_perC	0.50	0.43	-	5.68E-03	1.42E-05
0.30	1.06	-1.031	3.31E-02	1.16E-03	-3.41E-	Gamma_I	0.53	0.39	-	5.68E-03	1.27E-05
0.38	0.74	-0.865	3.29E-02	8.11E-04	-2.85E-	i_H_SU_mol_perC	0.58	0.30	-	5.69E-03	9.87E-06
0.39	0.73	-0.856	3.32E-02	8.05E-04	-2.84E-	i_O_XUOrg_mol_pe	0.59	0.29	-	5.77E-03	9.68E-06
0.61	0.24	-0.496	3.33E-02	2.73E-04	-1.65E-	i_P_XBOrg_mol_per	0.67	0.17	-	5.73E-03	5.76E-06
0.63	0.22	-0.473	3.36E-02	2.53E-04	-1.59E-	i_N_Org_mol_perC	0.74	0.10	-		
63	372				02		23	824	0.329	5.69E-03	3.50E-06
0.66	0.19	-0.439	3.28E-02	2.07E-04	-1.44E-	i_P_Org_mol_perC	0.76	0.08	-	5.74E-03	2.86E-06
0.68	0.16	-0.406	3.32E-02	1.82E-04	-1.35E-	i_O_XBOrg_mol_per	0.81	0.05	-0.23	5.71E-03	1.73E-06

Under.X_U_Inf		Under.X_ISS							
Multive	Parameters	Multive regression no			Multive regression & intercept			Parameters	
SRC (β)		Std.	β ₀ ²	SRC (β ₀)	Std.	β ²	SRC (β)		
-7.46E-	kH_F_AD_hyd	0.02	5.02	-2.241	3.33E-02	5.56E-03	-7.46E-	kH_F_AD_hyd	
-5.62E-	i_O_XUInf_mol_perC	0.08	2.90	-1.704	3.30E-02	3.15E-03	-5.62E-	i_O_XUInf_mol_per	
-5.13E-	Vs_s_X_B_Inf5	0.11	2.43	-1.56	3.29E-02	2.63E-03	-5.13E-	Vs_s_X_B_Inf5	
-4.74E-	Lambda_I	0.15	2.03	-1.427	3.32E-02	2.25E-03	-4.74E-	Lambda_I	
-3.99E-	Vs_s_X_B_Inf1	0.23	1.44	-1.2	3.32E-02	1.59E-03	-3.99E-	Vs_s_X_B_Inf1	
-3.86E-	i_H_XUOrg_mol_perC	0.24	1.36	-1.168	3.30E-02	1.49E-03	-3.86E-	i_H_XUOrg_mol_pe	
-3.73E-	Tref	0.26	1.22	-1.108	3.38E-02	1.39E-03	-3.73E-	Tref	
-3.65E-	f_U_Inf	0.26	1.22	-1.105	3.29E-02	1.33E-03	-3.65E-	f_U_Inf	
-3.65E-	i_O_SU_mol_perC	0.27	1.21	-1.1	3.31E-02	1.33E-03	-3.65E-	i_O_SU_mol_perC	
-3.41E-	Gamma_I	0.30	1.06	-1.031	3.31E-02	1.16E-03	-3.41E-	Gamma_I	
-2.85E-	i_H_SU_mol_perC	0.38	0.74	-0.865	3.29E-02	8.11E-04	-2.85E-	i_H_SU_mol_perC	
-2.84E-	i_O_XUOrg_mol_perC	0.39	0.73	-0.856	3.32E-02	8.05E-04	-2.84E-	i_O_XUOrg_mol_pe	
-1.65E-	i_P_XBOrg_mol_perC	0.61	0.24	-0.496	3.33E-02	2.73E-04	-1.65E-	i_P_XBOrg_mol_pe	
-1.59E-02	i_N_Org_mol_perC	0.63 63	0.22 372	-0.473	3.36E-02	2.53E-04	-1.59E-02	i_N_Org_mol_perC	
-1.44E-	i_P_Org_mol_perC	0.66	0.19	-0.439	3.28E-02	2.07E-04	-1.44E-	i_P_Org_mol_perC	
-1.35E-	i_O_XBOrg_mol_perC	0.68	0.16	-0.406	3.32E-02	1.82E-04	-1.35E-	i_O_XBOrg_mol_pe	

Under.X_VSS										
Multivariate regression no			Multivariate regression & intercept			Parameters		Multivariate regression no		
Std.	β_0^2	SRC (β_0)	Std.	β^2	SRC (β)			Std.	β_0^2	β^2
0.02	5.022	-2.241	3.33E-02	5.56E-03	-7.46E-	kH_F_AD_hyd		0.025	5.02	3.33E-02
0.08	2.903	-1.704	3.30E-02	3.15E-03	-5.62E-	i_O_XUInf_mol_per		0.088	2.90	3.30E-02
0.11	2.433	-1.56	3.29E-02	2.63E-03	-5.13E-	Vs_s_X_B_Inf5		0.119	2.43	3.29E-02
0.15	2.036	-1.427	3.32E-02	2.25E-03	-4.74E-	Lambda_I		0.153	2.03	3.32E-02
0.23	1.44	-1.2	3.32E-02	1.59E-03	-3.99E-	Vs_s_X_B_Inf1		0.230	1.44	3.32E-02
0.24	1.364	-1.168	3.30E-02	1.49E-03	-3.86E-	i_H_XUOrg_mol_per		0.243	1.36	3.30E-02
0.26	1.227	-1.108	3.38E-02	1.39E-03	-3.73E-	Tref		0.268	1.22	3.38E-02
0.26	1.221	-1.105	3.29E-02	1.33E-03	-3.65E-	f_U_Inf		0.269	1.22	3.29E-02
0.27	1.21	-1.1	3.31E-02	1.33E-03	-3.65E-	i_O_SU_mol_perC		0.271	1.21	3.31E-02
0.30	1.062	-1.031	3.31E-02	1.16E-03	-3.41E-	Gamma_I		0.302	1.06	3.31E-02
0.38	0.748	-0.865	3.29E-02	8.11E-04	-2.85E-	i_H_SU_mol_perC		0.387	0.74	3.29E-02
0.39	0.732	-0.856	3.32E-02	8.05E-04	-2.84E-	i_O_XUOrg_mol_per		0.392	0.73	3.32E-02
0.61	0.246	-0.496	3.33E-02	2.73E-04	-1.65E-	i_P_XBOrg_mol_per		0.619	0.24	3.33E-02
0.63	0.223	-0.473	3.36E-02	2.53E-04	-1.59E-	i_N_Org_mol_perC		0.636	0.22	3.36E-02
0.66	0.192	-0.439	3.28E-02	2.07E-04	-1.44E-	i_P_Org_mol_perC		0.660	0.19	3.28E-02
0.68	0.164	-0.406	3.32E-02	1.82E-04	-1.35E-	i_O_XBOrg_mol_per		0.684	0.16	3.32E-02

VSS_Under_s						
Multive regression no		Multive regression & intercept			Parameters	
Std.	β_0^2	SRC	Std.	β^2	SRC (β)	
0.1251	2.35	-	5.57E-03	7.31E-05	-8.55E-	Gamma_I
0.1489	2.08	-	5.60E-03	6.54E-05	-8.09E-	i_P_XBOrg_mol_per
0.1568	2.00	-	5.52E-03	6.12E-05	-7.83E-	i_P_Org_mol_perC
0.2744	1.19	-	5.57E-03	3.71E-05	-6.09E-	Beta_B
0.2822	1.15	-	5.59E-03	3.62E-05	-6.01E-	Beta_I
0.3087	1.03	-	5.54E-03	3.18E-05	-5.64E-	Beta_U
0.3327	0.93	-	5.63E-03	2.97E-05	-5.45E-	Gamma_B
0.3771	0.78	-	5.54E-03	2.40E-05	-4.89E-	Gamma_I
0.4069	0.68	-0.83	5.56E-03	2.13E-05	-4.62E-	Gamma_U
0.4668	0.52	-	5.54E-03	1.63E-05	-4.03E-	ISS_BM
0.5063	0.44	-	5.59E-03	1.38E-05	-3.72E-	KS_BInf_AD_hyd
0.555	0.34	-	5.58E-03	1.09E-05	-3.30E-	KS_BOrg_AD_hyd
0.5615	0.33	-	5.62E-03	1.07E-05	-3.27E-	K_ALK
0.5991	0.27	-	5.58E-03	8.55E-06	-2.92E-	Lambda_B
0.6004	0.27	-	5.52E-03	8.44E-06	-2.91E-	Lambda_I
0.624	0.24	-0.49	5.57E-03	7.45E-06	-2.73E-	Lambda_U

Out_X_B_Inf				ISS_under						Variables				Parameters
Multivariate regression &		Parameters		Multivariate regression no intercept			Multivariate regression & intercept			Parameters				Parameters
β^2	SRC (β)			Std.	β_0^2	SRC	Std. Error	β^2	SRC (β)					Type
1.76E-04	-1.33E-02	i_Ca_PP_mol_perP		0.63009	0.232324	-0.482	1.60E-02	5.77E-05	-7.60E-03	Vs_s_X_B_Inf4	17	KS_BInf_AD_hyd		
1.55E-04	-1.25E-02	i_N_XBInf_mol_perC		0.63434	0.226576	-0.476	1.56E-02	5.62E-05	-7.50E-03	Lambda_U	18	KS_BOrg_AD_hyd		
1.47E-04	-1.21E-02	i_O_XBOrg_mol_perC		0.64511	0.212521	-0.461	1.60E-02	5.40E-05	-7.35E-03	K_ALK	19	K_ALK		
1.28E-04	-1.13E-02	Beta_B		0.67665	0.173889	-0.417	1.59E-02	4.39E-05	-6.62E-03	km_BOrg_AD_hyd	20	TempCoeff		
7.43E-05	-8.62E-03	Beta_I		0.73328	0.116281	-0.341	1.58E-02	2.91E-05	-5.40E-03	i_P_XBOrg_mol_perC	21	Tref		
7.00E-05	-8.37E-03	Gamma_U		0.79963	0.064516	-0.254	1.57E-02	1.59E-05	-3.98E-03	i_O_XUInf_mol_perC	22	kh_F_AD_hyd		
6.77E-05	-8.23E-03	i_O_Org_mol_perC		0.81589	0.054289	-0.233	1.57E-02	1.33E-05	-3.65E-03	i_H_XBOrg_mol_perC	23	km_BInf_AD_hyd		
3.21E-05	-5.67E-03	Vs_s_X_B_Inf2		0.84335	0.039204	-0.198	1.58E-02	9.74E-06	-3.12E-03	i_P_XUOrg_mol_perC	24	km_BOrg_AD_hy		
2.31E-05	-4.81E-03	Vs_s_X_ISS5		0.87911	0.023104	-0.152	1.57E-02	5.68E-06	-2.38E-03	i_H_XUInf_mol_perC	25	Vs_s_X_B_Inf1		
1.69E-05	-4.11E-03	X_T		0.91912	0.010404	-0.102	1.56E-02	2.51E-06	-1.58E-03	i_O_XBInf_mol_perC	26	Vs_s_X_B_Inf2		
1.28E-05	-3.57E-03	i_P_SU_mol_perC		0.9744	0.001024	0.032	1.56E-02	2.52E-07	5.02E-04	Vs_s_X_B_Inf5	27	Vs_s_X_B_Inf3		
7.96E-06	-2.82E-03	i_O_SF_mol_perC		0.96811	0.0016	0.04	1.57E-02	3.93E-07	6.27E-04	i_H_XBInf_mol_perC	28	Vs_s_X_B_Inf4		
4.78E-06	-2.19E-03	Vs_s_X_ISS2		0.96158	0.002304	0.048	1.59E-02	5.84E-07	7.64E-04	Beta_B	29	Vs_s_X_B_Inf5		
3.92E-06	-1.98E-03	KS_BOrg_AD_hyd		0.9133	0.011881	0.109	1.59E-02	3.01E-06	1.74E-03	i_H_SF_mol_perC	30	Vs_s_X_ISS1		
2.37E-06	-1.54E-03	i_H_XBOrg_mol_perC		0.90562	0.014161	0.119	1.58E-02	3.51E-06	1.87E-03	i_P_XUInf_mol_perC	31	Vs_s_X_ISS2		
1.42E-06	-1.19E-03	i_Mg_PP_mol_perP		0.90442	0.0144	0.12	1.58E-02	3.61E-06	1.90E-03	i_O_XBOrg_mol_perC	32	Vs_s_X_ISS3		
3.77E-08	-1.94E-04	i_N_SU_mol_perC		0.89168	0.018496	0.136	1.59E-02	4.66E-06	2.16E-03	kh_F_AD_hyd	33	Vs_s_X_ISS4		
7.71E-09	-8.78E-05	i_P_XUOrg_mol_perC		0.86883	0.027225	0.165	1.57E-02	6.77E-06	2.60E-03	i_Ca_PP_mol_perP	34	Vs_s_X_ISS5		
7.96E-06	2.82E-03	Lambda_U		0.86235	0.029929	0.173	1.57E-02	7.42E-06	2.72E-03	i_O_SF_mol_perC	35	Vs_s_X_U_Inf1		
2.14E-05	4.63E-03	Beta_U		0.86215	0.030276	0.174	1.60E-02	7.66E-06	2.77E-03	Vs_s_X_U_Inf2	36	Vs_s_X_U_Inf2		
2.19E-05	4.68E-03	i_P_XUInf_mol_perC		0.77379	0.082944	0.288	1.58E-02	2.06E-05	4.54E-03	km_BInf_AD_hyd	37	Vs_s_X_U_Inf3		
2.90E-05	5.39E-03	i_P_SF_mol_perC		0.72758	0.121104	0.348	1.57E-02	2.99E-05	5.47E-03	i_H_Org_mol_perC	38	Vs_s_X_U_Inf4		
8.27E-05	9.09E-03	km_BInf_AD_hyd		0.666	0.186624	0.432	1.57E-02	4.61E-05	6.79E-03	Vs_s_X_U_Inf4	39	Vs_s_X_U_Inf5		

Kinetics

Out.X_U_Inf			Out.X_ISS												
Multive	Parameters		Multive regression no intercept				Multive regression & intercept				Parameters		Multive regression no intercept		
SRC (β)			Std. Error	β ⁰ ^2	SRC (β ₀)		Std. Error	β ⁰ ^2	SRC (β)				Std. Error	β ⁰ ^2	SRC (β ₀)
-1.33E-02	i_Ca_PP_mol_perP		0.6891	0.16	-0.4		0.6891	1.76E-02	-1.33E-02		i_Ca_PP_mol_perP		0.6891	1.60E-01	-0.4
-1.25E-02	i_N_XBInf_mol_perC		0.7085	0.139876	-0.374		0.7085	1.55E-02	-1.25E-02		i_N_XBInf_mol_perC		0.7085	1.40E-01	-0.374
-1.21E-02	i_O_XBOrg_mol_perC		0.7159	0.132496	-0.364		0.7159	1.47E-02	-1.21E-02		i_O_XBOrg_mol_perC		0.7159	1.32E-01	-0.364
-1.13E-02	Beta_B		0.7341	0.1156	-0.34		0.7341	1.28E-02	-1.13E-02		Beta_B		0.7341	1.16E-01	-0.34
-8.62E-03	Beta_I		0.7957	0.067081	-0.259		0.7957	7.43E-03	-8.62E-03		Beta_I		0.7957	6.71E-02	-0.259
-8.37E-03	Gamma_U		0.8014	0.063504	-0.252		0.8014	7.00E-03	-8.37E-03		Gamma_U		0.8014	6.35E-02	-0.252
-8.23E-03	i_O_Org_mol_perC		0.8057	0.060516	-0.246		0.8057	6.77E-03	-8.23E-03		i_O_Org_mol_perC		0.8057	6.05E-02	-0.246
-5.67E-03	Vs_s_X_B_Inf2		0.8642	0.029241	-0.171		0.8642	3.21E-03	-5.67E-03		Vs_s_X_B_Inf2		0.8642	2.92E-02	-0.171
-4.81E-03	Vs_s_X_ISS5		0.8849	0.021025	-0.145		0.8849	2.31E-03	-4.81E-03		Vs_s_X_ISS5		0.8849	2.10E-02	-0.145
-4.11E-03	X_T		0.9021	0.015129	-0.123		0.9021	1.69E-03	-4.11E-03		X_T		0.9021	1.51E-02	-0.123
-3.57E-03	i_P_SU_mol_perC		0.9132	0.011881	-0.109		0.9132	1.28E-03	-3.57E-03		i_P_SU_mol_perC		0.9132	1.19E-02	-0.109
-2.82E-03	i_O_SF_mol_perC		0.9318	0.007396	-0.086		0.9318	7.96E-03	-2.82E-03		i_O_SF_mol_perC		0.9318	7.40E-03	-0.086
-2.19E-03	Vs_s_X_ISS2		0.9478	0.004225	-0.065		0.9478	4.78E-03	-2.19E-03		Vs_s_X_ISS2		0.9478	4.23E-03	-0.065
-1.98E-03	KS_BOrg_AD_hyd		0.9523	0.0036	-0.06		0.9523	3.92E-03	-1.98E-03		KS_BOrg_AD_hyd		0.9523	3.60E-03	-0.06
-1.54E-03	i_H_XBOrg_mol_perC		0.9627	0.002209	-0.047		0.9627	2.37E-03	-1.54E-03		i_H_XBOrg_mol_perC		0.9627	2.21E-03	-0.047
-1.19E-03	i_Mg_PP_mol_perP		0.9713	0.001296	-0.036		0.9713	1.42E-03	-1.19E-03		i_Mg_PP_mol_perP		0.9713	1.30E-03	-0.036
-1.94E-04	i_N_SU_mol_perC		0.9953	0.000036	-0.006		0.9953	3.77E-03	-1.94E-04		i_N_SU_mol_perC		0.9953	3.60E-05	-0.006
-8.78E-05	i_P_XUOrg_mol_perC		0.9979	0.000009	-0.003		0.9979	7.71E-03	-8.78E-05		i_P_XUOrg_mol_perC		0.9979	9.00E-06	-0.003
2.82E-03	Lambda_U		0.9313	0.007396	0.086		0.9313	3.27E-02	2.82E-03		Lambda_U		0.9313	7.40E-03	0.086
4.63E-03	Beta_U		0.8881	0.019881	0.141		0.8881	2.14E-03	4.63E-03		Beta_U		0.8881	1.99E-02	0.141
4.68E-03	i_P_XUInf_mol_perC		0.888	0.019881	0.141		0.888	3.32E-02	4.68E-03		i_P_XUInf_mol_perC		0.888	1.99E-02	0.141
5.39E-03	i_P_SF_mol_perC		0.8707	0.026569	0.163		0.8707	2.90E-03	5.39E-03		i_P_SF_mol_perC		0.8707	2.66E-02	0.163
9.09E-03	kM_BInf_AD_hyd		0.784	0.075076	0.274		0.784	3.32E-02	9.09E-03		kM_BInf_AD_hyd		0.784	7.51E-02	0.274

TSS_Under_s			Out_X_VSS													
Multive		Parameters	Multive regression no intercept			Multive regression & intercept			Parameters			Multive regression no intercept				
SRC (β)			Std. Error	β ²	SRC	Std. Error	β ²	SRC (β)			Std. Error	β ²	SRC	Std. Error	β ²	
-1.25E-03		Lambda_U	0.6891	0.16	-0.4	3.31E-02	1.76E-04	-1.33E-02		i_Ca_PP_mol_perP	0.6891	0.16	-0.4	3.31E-02	1.76E-04	
-6.34E-04		i_O_Org_mol_perC	0.7085	0.139876	-0.374	3.33E-02	1.55E-04	-1.25E-02		i_N_XBInf_mol_perC	0.7085	0.13987	-0.374	3.33E-02	1.55E-04	
-4.77E-04		i_N_XBOrg_mol_perC	0.7159	0.132496	-0.364	3.33E-02	1.47E-04	-1.21E-02		i_O_XBOrg_mol_perC	0.7159	0.13249	-0.364	3.33E-02	1.47E-04	
-1.73E-04		i_O_SU_mol_perC	0.7341	0.1156	-0.34	3.33E-02	1.28E-04	-1.13E-02		Beta_B	0.7341	0.1156	-0.34	3.33E-02	1.28E-04	
1.52E-04		i_H_SU_mol_perC	0.7957	0.067081	-0.259	3.33E-02	7.43E-05	-8.62E-03		Beta_I	0.7957	0.06708	-0.259	3.33E-02	7.43E-05	
2.04E-04		Alpha_B	0.8014	0.063504	-0.252	3.33E-02	7.00E-05	-8.37E-03		Gamma_U	0.8014	0.06350	-0.252	3.33E-02	7.00E-05	
2.72E-04		i_N_XUInf_mol_perC	0.8057	0.060516	-0.246	3.35E-02	6.77E-05	-8.23E-03		i_O_Org_mol_perC	0.8057	0.06051	-0.246	3.35E-02	6.77E-05	
3.18E-04		i_O_XBInf_mol_perC	0.8642	0.029241	-0.171	3.31E-02	3.21E-05	-5.67E-03		Vs_s_X_B_Inf2	0.8642	0.02924	-0.171	3.31E-02	3.21E-05	
3.42E-04		i_O_XBOrg_mol_perC	0.8849	0.021025	-0.145	3.32E-02	2.31E-05	-4.81E-03		Vs_s_X_ISS5	0.8849	0.02102	-0.145	3.32E-02	2.31E-05	
4.09E-04		i_H_XBOrg_mol_perC	0.9021	0.015129	-0.123	3.34E-02	1.69E-05	-4.11E-03		X_T	0.9021	0.01512	-0.123	3.34E-02	1.69E-05	
1.10E-03		i_H_SF_mol_perC	0.9132	0.011881	-0.109	3.28E-02	1.28E-05	-3.57E-03		i_P_SU_mol_perC	0.9132	0.01188	-0.109	3.28E-02	1.28E-05	
2.42E-03		kH_F_AD_hyd	0.9318	0.007396	-0.086	3.30E-02	7.96E-06	-2.82E-03		i_O_SF_mol_perC	0.9318	0.00739	-0.086	3.30E-02	7.96E-06	
2.86E-03		Gamma_I	0.9478	0.004225	-0.065	3.34E-02	4.78E-06	-2.19E-03		Vs_s_X_ISS2	0.9478	0.00422	-0.065	3.34E-02	4.78E-06	
3.58E-03		KS_BInf_AD_hyd	0.9523	0.0036	-0.06	3.31E-02	3.92E-06	-1.98E-03		KS_BOrg_AD_hyd	0.9523	0.0036	-0.06	3.31E-02	3.92E-06	
3.77E-03		i_N_SU_mol_perC	0.9627	0.002209	-0.047	3.30E-02	2.37E-06	-1.54E-03		i_H_XBOrg_mol_perC	0.9627	0.00220	-0.047	3.30E-02	2.37E-06	
4.30E-03		KS_BOrg_AD_hyd	0.9713	0.001296	-0.036	3.31E-02	1.42E-06	-1.19E-03		i_Mg_PP_mol_perP	0.9713	0.00129	-0.036	3.31E-02	1.42E-06	
4.41E-03		i_N_XBInf_mol_perC	0.9953	0.000036	-0.006	3.32E-02	3.77E-08	-1.94E-04		i_N_SU_mol_perC	0.9953	0.00003	-0.006	3.32E-02	3.77E-08	
4.51E-03		K_ALK	0.9979	0.000009	-0.003	3.32E-02	7.71E-09	-8.78E-05		i_P_XUOrg_mol_perC	0.9979	0.00000	-0.003	3.32E-02	7.71E-09	
4.65E-03		i_H_XUOrg_mol_perC	0.9313	0.007396	0.086	3.27E-02	7.96E-06	2.82E-03		Lambda_U	0.9313	0.00739	0.086	3.27E-02	7.96E-06	
5.00E-03		kM_BOrg_AD_hyd	0.8881	0.019881	0.141	3.29E-02	2.14E-05	4.63E-03		Beta_U	0.8881	0.01988	0.141	3.29E-02	2.14E-05	
5.71E-03		i_P_XUOrg_mol_perC	0.888	0.019881	0.141	3.32E-02	2.19E-05	4.68E-03		i_P_XUInf_mol_perC	0.888	0.01988	0.141	3.32E-02	2.19E-05	
6.02E-03		TempCoeff	0.8707	0.026569	0.163	3.31E-02	2.90E-05	5.39E-03		i_P_SF_mol_perC	0.8707	0.02656	0.163	3.31E-02	2.90E-05	
6.11E-03		Tref	0.784	0.075076	0.274	3.32E-02	8.27E-05	9.09E-03		kM_BInf_AD_hyd	0.784	0.07507	0.274	3.32E-02	8.27E-05	

Under_X_ISS			Under_X_B_Inf													
Multive	Parameters		Multive regression no intercept				Multive regression & intercept				Parameters		Multive regression no intercept			
SRC (β)			Std. Error	β ⁰ ^2	SRC (β ₀)		Std. Error	β ²	SRC (β)				Std. Error	β ⁰ ^2	SRC (β ₀)	β ²
-1.22E-02	i_N_XBInf_mol_per		0.7131	0.135424	-0.368		3.33E-02	1.50E-04	-1.22E-02		i_N_XBInf_mol_per		0.8254	0.048841	-0.221	1.55E-06
-1.14E-02	i_Ca_PP_mol_perP		0.7311	0.118336	-0.344		3.31E-02	1.29E-04	-1.14E-02		i_Ca_PP_mol_perP		0.9127	0.0121	-0.11	5.77E-03
-1.12E-02	i_K_PP_mol_perP		0.7327	0.116964	-0.342		3.29E-02	1.26E-04	-1.12E-02		i_K_PP_mol_perP		0.9339	0.006889	-0.083	5.74E-03
-7.97E-03	Vs_s_X_ISS5		0.8103	0.0576	-0.24		3.32E-02	6.36E-05	-7.97E-03		Vs_s_X_ISS5		0.9759	0.0009	-0.03	5.72E-03
-7.81E-03	i_O_Org_mol_perC		0.8153	0.054756	-0.234		3.34E-02	6.10E-05	-7.81E-03		i_O_Org_mol_perC		0.9786	0.000729	0.027	5.69E-03
-6.38E-03	Vs_s_X_B_Inf2		0.8472	0.037249	-0.193		3.31E-02	4.07E-05	-6.38E-03		Vs_s_X_B_Inf2		0.9717	0.001296	0.036	5.75E-03
-5.06E-03	Vs_s_X_ISS2		0.8797	0.022801	-0.151		3.34E-02	2.56E-05	-5.06E-03		Vs_s_X_ISS2		0.962	0.002304	0.048	5.71E-03
-4.95E-03	Beta_I		0.8818	0.022201	-0.149		3.33E-02	2.45E-05	-4.95E-03		Beta_I		0.9552	0.003136	0.056	5.66E-03
-4.65E-03	X_T		0.8892	0.019321	-0.139		3.34E-02	2.16E-05	-4.65E-03		X_T		0.9525	0.0036	0.06	5.74E-03
-4.45E-03	i_P_SU_mol_perC		0.892	0.018496	-0.136		3.28E-02	1.98E-05	-4.45E-03		i_P_SU_mol_perC		0.9427	0.005184	0.072	5.69E-03
-3.59E-03	i_O_SF_mol_perC		0.9133	0.011881	-0.109		3.30E-02	1.29E-05	-3.59E-03		i_O_SF_mol_perC		0.8494	0.0361	0.19	5.79E-03
-2.45E-03	KS_BOrg_AD_hyd		0.9411	0.005476	-0.074		3.31E-02	5.98E-06	-2.45E-03		KS_BOrg_AD_hyd		0.6735	0.178084	0.422	5.75E-03
7.82E-05	i_P_XUOrg_mol_pe		0.9981	0.000004	0.002		3.32E-02	6.12E-09	7.82E-05		i_P_XUOrg_mol_pe		0.6163	0.251001	0.501	5.71E-03
2.42E-04	i_N_SU_mol_perC		0.9942	0.000049	0.007		3.32E-02	5.88E-08	2.42E-04		i_N_SU_mol_perC		0.5295	0.395641	0.629	5.69E-03
3.32E-04	i_H_XBOrg_mol_pe		0.9919	0.0001	0.01		3.29E-02	1.10E-07	3.32E-04		i_H_XBOrg_mol_pe		0.511	0.431649	0.657	5.73E-03
3.53E-04	i_Mg_PP_mol_perP		0.9915	0.000121	0.011		3.31E-02	1.25E-07	3.53E-04		i_Mg_PP_mol_perP		0.4518	0.567009	0.753	5.72E-03
1.55E-03	Gamma_U		0.9629	0.002116	0.046		3.32E-02	2.39E-06	1.55E-03		Gamma_U		0.443	0.588289	0.767	5.74E-03
5.09E-03	i_P_SF_mol_perC		0.8778	0.023716	0.154		3.31E-02	2.59E-05	5.09E-03		i_P_SF_mol_perC		0.4361	0.606841	0.779	5.79E-03
6.16E-03	i_P_XUInf_mol_per		0.8527	0.034596	0.186		3.32E-02	3.80E-05	6.16E-03		i_P_XUInf_mol_per		0.4151	0.664225	0.815	5.71E-03
6.64E-03	Lambda_U		0.8391	0.041209	0.203		3.27E-02	4.41E-05	6.64E-03		Lambda_U		0.3858	0.753424	0.868	5.76E-03
8.39E-03	Beta_B		0.8012	0.063504	0.252		3.33E-02	7.05E-05	8.39E-03		Beta_B		0.3197	0.992016	0.996	5.73E-03
8.52E-03	kM_BInf_AD_hyd		0.7972	0.066049	0.257		3.31E-02	7.26E-05	8.52E-03		kM_BInf_AD_hyd		0.2949	1.098304	1.048	5.72E-03
9.02E-03	Beta_U		0.7838	0.075076	0.274		3.29E-02	8.13E-05	9.02E-03		Beta_U		0.2927	1.108809	1.053	5.83E-03

Under_X_VSS	Under_X_U_Inf										
Parameters	Multive regression no intercept			Multive regression & intercept			Parameters				
	Std. Error	β_0^2	SRC	Std. Error	β^2	SRC (β)					
i_N_XBInf_mol_perC	0.7131	0.135424	-0.368	3.33E-02	1.50E-04	-1.22E-02	i_N_XBInf_mol_perC				
i_Ca_PP_mol_perP	0.7311	0.118336	-0.344	3.31E-02	1.29E-04	-1.14E-02	i_Ca_PP_mol_perP				
i_K_PP_mol_perP	0.7327	0.116964	-0.342	3.29E-02	1.26E-04	-1.12E-02	i_K_PP_mol_perP				
Vs_s_X_ISS5	0.8103	0.0576	-0.24	3.32E-02	6.36E-05	-7.97E-03	Vs_s_X_ISS5				
i_O_Org_mol_perC	0.8153	0.054756	-0.234	3.34E-02	6.10E-05	-7.81E-03	i_O_Org_mol_perC				
Vs_s_X_B_Inf2	0.8472	0.037249	-0.193	3.31E-02	4.07E-05	-6.38E-03	Vs_s_X_B_Inf2				
Vs_s_X_ISS2	0.8797	0.022801	-0.151	3.34E-02	2.56E-05	-5.06E-03	Vs_s_X_ISS2				
Beta_I	0.8818	0.022201	-0.149	3.33E-02	2.45E-05	-4.95E-03	Beta_I				
X_T	0.8892	0.019321	-0.139	3.34E-02	2.16E-05	-4.65E-03	X_T				
i_P_SU_mol_perC	0.892	0.018496	-0.136	3.28E-02	1.98E-05	-4.45E-03	i_P_SU_mol_perC				
i_O_SF_mol_perC	0.9133	0.011881	-0.109	3.30E-02	1.29E-05	-3.59E-03	i_O_SF_mol_perC				
KS_BOrg_AD_hyd	0.9411	0.005476	-0.074	3.31E-02	5.98E-06	-2.45E-03	KS_BOrg_AD_hyd				
i_P_XUOrg_mol_perC	0.9981	0.000004	0.002	3.32E-02	6.12E-09	7.82E-05	i_P_XUOrg_mol_perC				
i_N_SU_mol_perC	0.9942	0.000049	0.007	3.32E-02	5.88E-08	2.42E-04	i_N_SU_mol_perC				
i_H_XBOrg_mol_perC	0.9919	0.0001	0.01	3.29E-02	1.10E-07	3.32E-04	i_H_XBOrg_mol_perC				
i_Mg_PP_mol_perP	0.9915	0.000121	0.011	3.31E-02	1.25E-07	3.53E-04	i_Mg_PP_mol_perP				
Gamma_U	0.9629	0.002116	0.046	3.32E-02	2.39E-06	1.55E-03	Gamma_U				
i_P_SF_mol_perC	0.8778	0.023716	0.154	3.31E-02	2.59E-05	5.09E-03	i_P_SF_mol_perC				
i_P_XUInf_mol_perC	0.8527	0.034596	0.186	3.32E-02	3.80E-05	6.16E-03	i_P_XUInf_mol_perC				
Lambda_U	0.8391	0.041209	0.203	3.27E-02	4.41E-05	6.64E-03	Lambda_U				
Beta_B	0.8012	0.063504	0.252	3.33E-02	7.05E-05	8.39E-03	Beta_B				
kM_BInf_AD_hyd	0.7972	0.066049	0.257	3.31E-02	7.26E-05	8.52E-03	kM_BInf_AD_hyd				
Beta_U	0.7838	0.075076	0.274	3.29E-02	8.13E-05	9.02E-03	Beta_U				

VSS_Under_s											
Multivariate regression no intercept				Multivariate regression & intercept				Multivariate regression no intercept			
Std.	β_0^2	SRC	Parameters	Std. Error	β^2	SRC (β)	TempCoeff	Std. Error	β_0^2	SRC (β_0)	Std. Error
0.7442	0.106276	-0.326		5.51E-03	3.24E-06	-1.80E-03		0.7131	0.13542	-0.368	3.33E-02
0.796	0.067081	-0.259		5.55E-03	2.06E-06	-1.44E-03	Tref	0.7311	0.11833	-0.344	3.31E-02
0.9056	0.014161	-0.119		5.62E-03	4.43E-07	-6.66E-04	Vs_s_X_B_Inf1	0.7327	0.11696	-0.342	3.29E-02
0.9075	0.013456	-0.116		5.54E-03	4.15E-07	-6.44E-04	Vs_s_X_B_Inf2	0.8103	0.0576	-0.24	3.32E-02
0.9407	0.005476	-0.074		5.50E-03	1.68E-07	-4.09E-04	Vs_s_X_B_Inf3	0.8153	0.05475	-0.234	3.34E-02
0.9572	0.002916	-0.054		5.59E-03	9.02E-08	-3.00E-04	Vs_s_X_B_Inf4	0.8472	0.03724	-0.193	3.31E-02
0.985	0.000361	-0.019		5.57E-03	1.10E-08	-1.05E-04	Vs_s_X_B_Inf5	0.8797	0.02280	-0.151	3.34E-02
0.9815	0.000529	0.023		5.60E-03	1.69E-08	1.30E-04	Vs_s_X_ISS1	0.8818	0.02220	-0.149	3.33E-02
0.9771	0.000841	0.029		5.59E-03	2.57E-08	1.60E-04	Vs_s_X_ISS2	0.8892	0.01932	-0.139	3.34E-02
0.928	0.0081	0.09		5.52E-03	2.48E-07	4.98E-04	Vs_s_X_ISS3	0.892	0.01849	-0.136	3.28E-02
0.8822	0.021904	0.148		5.54E-03	6.76E-07	8.22E-04	Vs_s_X_ISS4	0.9133	0.01188	-0.109	3.30E-02
0.8719	0.025921	0.161		5.64E-03	8.27E-07	9.10E-04	Vs_s_X_ISS5	0.9411	0.00547	-0.074	3.31E-02
0.8582	0.032041	0.179		5.63E-03	1.01E-06	1.01E-03	Vs_s_X_U_Inf1	0.9981	0.00000	0.002	3.32E-02
0.8565	0.032761	0.181		5.58E-03	1.02E-06	1.01E-03	Vs_s_X_U_Inf2	0.9942	0.00004	0.007	3.32E-02
0.8363	0.042849	0.207		5.60E-03	1.34E-06	1.16E-03	Vs_s_X_U_Inf3	0.9919	0.0001	0.01	3.29E-02
0.8291	0.046656	0.216		5.56E-03	1.44E-06	1.20E-03	Vs_s_X_U_Inf4	0.9915	0.00012	0.011	3.31E-02
0.791	0.070225	0.265		5.58E-03	2.19E-06	1.48E-03	Vs_s_X_U_Inf5	0.9629	0.00211	0.046	3.32E-02
0.7826	0.076176	0.276		5.54E-03	2.34E-06	1.53E-03	X_lim	0.8778	0.02371	0.154	3.31E-02
0.7565	0.0961	0.31		5.54E-03	2.95E-06	1.72E-03	X_T	0.8527	0.03459	0.186	3.32E-02
0.6955	0.153664	0.392		5.60E-03	4.81E-06	2.19E-03	f_U_Inf	0.8391	0.04120	0.203	3.27E-02
0.6685	0.183184	0.428		5.54E-03	5.64E-06	2.38E-03	i_Ca_PP_mol_per	0.8012	0.06350	0.252	3.33E-02
0.6118	0.258064	0.508		5.60E-03	8.08E-06	2.84E-03	i_H_Org_mol_per	0.7972	0.06604	0.257	3.31E-02
0.5285	0.398161	0.631		5.60E-03	1.25E-05	3.53E-03	i_H_SF_mol_perc	0.7838	0.07507	0.274	3.29E-02

ISS_under		Variables				
Multive regression &		Parameters	Number	Name	Type	Parameters
β^2	SRC (β)					
5.29E-05	7.28E-03	i_Mg_PP_mol_perP	40	i_Ca_PP_mol_perP		
5.30E-05	7.28E-03	Alpha_U	41	i_H_Org_mol_perC		
8.23E-05	9.07E-03	Beta_U	42	i_H_SF_mol_perC		
8.58E-05	9.26E-03	i_P_SU_mol_perC	43	i_H_SU_mol_perC		
9.65E-05	9.82E-03	f_U_Inf	44	i_H_XBInf_mol_perC		
1.27E-04	1.13E-02	Vs_s_X_U_Inf3	45	i_H_XBOrg_mol_perC		
1.38E-04	1.18E-02	Gamma_U	46	i_H_XUInf_mol_perC		
1.50E-04	1.22E-02	i_P_XBInf_mol_perC	47	i_H_XUOrg_mol_perC		
1.52E-04	1.23E-02	TempCoeff	48	i_K_PP_mol_perP		
1.56E-04	1.25E-02	i_P_SF_mol_perC	49	i_Mg_PP_mol_perP		
1.87E-04	1.37E-02	i_N_XUOrg_mol_perC	50	i_N_Org_mol_perC		
2.52E-04	1.59E-02	Vs_s_X_U_Inf1	51	i_N_SF_mol_perC		
2.78E-04	1.67E-02	i_N_Org_mol_perC	52	i_N_SU_mol_perC		
2.78E-04	1.67E-02	KS_BInf_AD_hyd	53	i_N_XBInf_mol_perC		
3.36E-04	1.83E-02	ISS_BM	54	i_N_XBOrg_mol_perC		
3.44E-04	1.85E-02	Vs_s_X_U_Inf5	55	i_N_XUInf_mol_perC		
3.73E-04	1.93E-02	Tref	56	i_N_XUOrg_mol_perC		
4.26E-04	2.06E-02	X_Lim	57	i_O_Org_mol_perC		
4.79E-04	2.19E-02	Vs_s_X_B_Inf3	58	i_O_SF_mol_perC		
6.09E-04	2.47E-02	i_N_SU_mol_perC	59	i_O_SU_mol_perC		
7.68E-04	2.77E-02	i_K_PP_mol_perP	60	i_O_XBInf_mol_perC		
1.04E-03	3.22E-02	i_P_Org_mol_perC	61	i_O_XBOrg_mol_perC		
1.55E-03	3.94E-02	KS_BOrg_AD_hyd	62	i_O_XUInf_mol_perC		
1.03E-02	1.02E-01	Gamma_I	63	i_O_XUOrg_mol_perC		
3.31E-02	1.82E-01	Beta_I	64	i_P_Org_mol_perC		
5.01E-02	2.24E-01	Vs_s_X_ISS5	65	i_P_SF_mol_perC		
7.33E-02	2.71E-01	Vs_s_X_ISS2	66	i_P_SU_mol_perC		
1.06E-01	3.26E-01	Vs_s_X_ISS4	67	i_P_XBInf_mol_perC		
1.47E-01	3.83E-01	Alpha_I	68	i_P_XBOrg_mol_perC		
1.77E-01	4.21E-01	Vs_s_X_ISS3	69	i_P_XUInf_mol_perC		
1.78E-01	4.22E-01	Vs_s_X_ISS1	70	i_P_XUOrg_mol_perC		

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Out_X_B_Inf									
Multive regression & intercept			Parameters			Multive regression no intercept			
Std. Error	β^2	SRC (β)				Std. Error	β^2	SRC (β)	Std. Error
3.36E-02	1.08E-04	1.04E-02	33332222			0.64386	0.2134	0.462	1.57E-02
3.29E-02	1.31E-04	1.15E-02	Vs_s_X_U_Inf3			0.64207	0.2162	0.465	1.57E-02
3.29E-02	1.32E-04	1.15E-02	Alpha_U			0.56186	0.3364	0.58	1.56E-02
3.30E-02	1.59E-04	1.26E-02	Gamma_B			0.55258	0.3528	0.594	1.56E-02
3.31E-02	1.96E-04	1.40E-02	i_N_XUInf_mol_perC			0.53067	0.3931	0.627	1.57E-02
3.33E-02	2.45E-04	1.57E-02	i_N_XUOrg_mol_perC			0.47155	0.5184	0.72	1.57E-02
3.30E-02	2.61E-04	1.62E-02	i_H_XBInf_mol_perC			0.45753	0.5520	0.743	1.58E-02
3.28E-02	2.90E-04	1.70E-02	Alpha_I			0.43762	0.6037	0.777	1.57E-02
3.35E-02	3.06E-04	1.75E-02	i_H_SF_mol_perC			0.43465	0.6115	0.782	1.58E-02
3.30E-02	3.42E-04	1.85E-02	Lambda_B			0.42719	0.6304	0.794	1.57E-02
3.31E-02	3.53E-04	1.88E-02	i_P_XBInf_mol_perC			0.38724	0.7482	0.865	1.58E-02
3.34E-02	3.68E-04	1.92E-02	kM_BOrg_AD_hyd			0.31496	1.0100	1.005	1.58E-02
3.29E-02	3.85E-04	1.96E-02	KS_BInf_AD_hyd			0.29824	1.0836	1.041	1.60E-02
3.30E-02	4.22E-04	2.05E-02	i_H_Org_mol_perC			0.2874	1.1320	1.064	1.57E-02
3.35E-02	5.06E-04	2.25E-02	K_ALK			0.24239	1.3689	1.17	1.57E-02
3.30E-02	5.56E-04	2.36E-02	Vs_s_X_ISS1			0.24198	1.3712	1.171	1.59E-02
3.31E-02	5.60E-04	2.37E-02	TempCoeff			0.2298	1.4448	1.202	1.61E-02
3.33E-02	6.17E-04	2.48E-02	Alpha_B			0.19457	1.6848	1.298	1.59E-02
3.32E-02	8.32E-04	2.89E-02	Vs_s_X_U_Inf1			0.16508	1.9293	1.389	1.58E-02
3.28E-02	1.08E-03	3.29E-02	Vs_s_X_ISS4			0.11837	2.4429	1.563	1.58E-02
3.29E-02	1.10E-03	3.32E-02	i_H_XUInf_mol_perC			0.07662	3.1435	1.773	1.56E-02
3.36E-02	1.19E-03	3.45E-02	Vs_s_X_U_Inf2			0.03938	4.2559	2.063	1.56E-02
3.31E-02	1.32E-03	3.64E-02	Vs_s_X_B_Inf3			0.0126	6.25	2.5	1.58E-02
3.31E-02	1.37E-03	3.71E-02	Vs_s_X_U_Inf4			1.82E-10	41.576	6.45E+00	1.58E-02
3.33E-02	1.61E-03	4.01E-02	i_N_XBOrg_mol_perC			< 2e-16	131.76	11.479	1.58E-02
3.32E-02	1.65E-03	4.06E-02	Vs_s_X_ISS3			< 2e-16	200.64	14.165	1.58E-02
3.33E-02	2.23E-03	4.73E-02	Vs_s_X_U_Inf5			< 2e-16	290.12	17.033	1.59E-02
3.28E-02	2.35E-03	4.85E-02	i_O_XBInf_mol_perC			< 2e-16	436.22	20.886	1.56E-02
3.29E-02	2.42E-03	4.92E-02	ISS_BM			< 2e-16	602.30	24.542	1.56E-02
3.30E-02	2.61E-03	5.10E-02	i_N_SF_mol_perC			< 2e-16	708.41	26.616	1.58E-02
3.34E-02	2.89E-03	5.37E-02	X_Lim			< 2e-16	723.93	26.906	1.57E-02

Out_X_ISS								
Multive	Multive regression & intercept			Parameters		Multive regression no intercept		
SRC (β_0)	Std. Error	β^2	SRC (β)			Std. Error	β_0^2	SRC (β_0)
0.309	3.36E-02	1.08E-04	1.04E-02	Vs_s_X_B_Inf4		0.7572	9.55E-02	0.309
0.348	3.29E-02	1.31E-04	1.15E-02	Vs_s_X_U_Inf3		0.728	1.21E-01	0.348
0.349	3.29E-02	1.32E-04	1.15E-02	Alpha_U		0.7269	1.22E-01	0.349
0.382	3.30E-02	1.59E-04	1.26E-02	Gamma_B		0.7025	1.46E-01	0.382
0.424	3.31E-02	1.96E-04	1.40E-02	i_N_XUInf_mol_perC		0.672	1.80E-01	0.424
0.471	3.33E-02	2.45E-04	1.57E-02	i_N_XUOrg_mol_perC		0.6379	2.22E-01	0.471
0.49	3.30E-02	2.61E-04	1.62E-02	i_H_XBInf_mol_perC		0.6243	2.40E-01	0.49
0.518	3.28E-02	2.90E-04	1.70E-02	Alpha_I		0.6044	2.68E-01	0.518
0.521	3.35E-02	3.06E-04	1.75E-02	i_H_SF_mol_perC		0.6022	2.71E-01	0.521
0.56	3.30E-02	3.42E-04	1.85E-02	Lambda_B		0.5755	3.14E-01	0.56
0.568	3.31E-02	3.53E-04	1.88E-02	i_P_XBInf_mol_perC		0.5702	3.23E-01	0.568
0.575	3.34E-02	3.68E-04	1.92E-02	kM_BOrg_AD_hyd		0.5657	3.31E-01	0.575
0.596	3.29E-02	3.85E-04	1.96E-02	KS_BInf_AD_hyd		0.5513	3.55E-01	0.596
0.623	3.30E-02	4.22E-04	2.05E-02	i_H_Org_mol_perC		0.5336	3.88E-01	0.623
0.671	3.35E-02	5.06E-04	2.25E-02	K_ALK		0.5025	4.50E-01	0.671
0.714	3.30E-02	5.56E-04	2.36E-02	Vs_s_X_ISS1		0.4754	5.10E-01	0.714
0.715	3.31E-02	5.60E-04	2.37E-02	TempCoeff		0.4746	5.11E-01	0.715
0.746	3.33E-02	6.17E-04	2.48E-02	Alpha_B		0.4558	5.57E-01	0.746
0.869	3.32E-02	8.32E-04	2.89E-02	Vs_s_X_U_Inf1		0.3852	7.55E-01	0.869
1.005	3.28E-02	1.08E-03	3.29E-02	Vs_s_X_ISS4		0.3153	1.01E+0	1.005
1.009	3.29E-02	1.10E-03	3.32E-02	i_H_XUInf_mol_perC		0.3131	1.02E+0	1.009
1.028	3.36E-02	1.19E-03	3.45E-02	Vs_s_X_U_Inf2		0.3041	1.06E+0	1.028
1.098	3.31E-02	1.32E-03	3.64E-02	Vs_s_X_B_Inf3		0.2724	1.21E+0	1.098
1.121	3.31E-02	1.37E-03	3.71E-02	Vs_s_X_U_Inf4		0.2627	1.26E+0	1.121
1.206	3.33E-02	1.61E-03	4.01E-02	i_N_XBOrg_mol_perC		0.2283	1.45E+0	1.206
1.223	3.32E-02	1.65E-03	4.06E-02	Vs_s_X_ISS3		0.2215	1.50E+0	1.223
1.418	3.33E-02	2.23E-03	4.73E-02	Vs_s_X_U_Inf5		0.1566	2.01E+0	1.418
1.48	3.28E-02	2.35E-03	4.85E-02	i_O_XBInf_mol_perC		0.1392	2.19E+0	1.48
1.495	3.29E-02	2.42E-03	4.92E-02	ISS_BM		0.1353	2.24E+0	1.495
1.549	3.30E-02	2.61E-03	5.10E-02	i_N_SF_mol_perC		0.1217	2.40E+0	1.549
1.607	3.34E-02	2.89E-03	5.37E-02	X_Lim		0.1084	2.58E+0	1.607

Out_X_U_Inf								
Multiple regression no		Multiple regression & intercept			Parameters			
β_0^2	SRC (β_0)	Std. Error	β^2	SRC (β)			Std. Error	β_0^2
0.0954	0.309	3.36E-02	1.08E-04	1.04E-02	Vs_s_X_B_Inf4		0.7572	0.0954
0.1211	0.348	3.29E-02	1.31E-04	1.15E-02	Vs_s_X_U_Inf3		0.728	0.1211
0.1218	0.349	3.29E-02	1.32E-04	1.15E-02	Alpha_U		0.7269	0.1218
0.1459	0.382	3.30E-02	1.59E-04	1.26E-02	Gamma_B		0.7025	0.1459
0.1797	0.424	3.31E-02	1.96E-04	1.40E-02	i_N_XUInf_mol_perC		0.672	0.1797
0.2218	0.471	3.33E-02	2.45E-04	1.57E-02	i_N_XUOrg_mol_per		0.6379	0.2218
0.2401	0.49	3.30E-02	2.61E-04	1.62E-02	i_H_XBInf_mol_perC		0.6243	0.2401
0.2683	0.518	3.28E-02	2.90E-04	1.70E-02	Alpha_I		0.6044	0.2683
0.2714	0.521	3.35E-02	3.06E-04	1.75E-02	i_H_SF_mol_perC		0.6022	0.2714
0.3136	0.56	3.30E-02	3.42E-04	1.85E-02	Lambda_B		0.5755	0.3136
0.3226	0.568	3.31E-02	3.53E-04	1.88E-02	i_P_XBInf_mol_perC		0.5702	0.3226
0.3306	0.575	3.34E-02	3.68E-04	1.92E-02	kM_BOrg_AD_hyd		0.5657	0.3306
0.3552	0.596	3.29E-02	3.85E-04	1.96E-02	KS_BInf_AD_hyd		0.5513	0.3552
0.3881	0.623	3.30E-02	4.22E-04	2.05E-02	i_H_Org_mol_perC		0.5336	0.3881
0.4502	0.671	3.35E-02	5.06E-04	2.25E-02	K_ALK		0.5025	0.4502
0.5097	0.714	3.30E-02	5.56E-04	2.36E-02	Vs_s_X_ISS1		0.4754	0.5097
0.5112	0.715	3.31E-02	5.60E-04	2.37E-02	TempCoeff		0.4746	0.5112
0.5565	0.746	3.33E-02	6.17E-04	2.48E-02	Alpha_B		0.4558	0.5565
0.7551	0.869	3.32E-02	8.32E-04	2.89E-02	Vs_s_X_U_Inf1		0.3852	0.7551
1.0100	1.005	3.28E-02	1.08E-03	3.29E-02	Vs_s_X_ISS4		0.3153	1.0100
1.0180	1.009	3.29E-02	1.10E-03	3.32E-02	i_H_XUInf_mol_perC		0.3131	1.0180
1.0567	1.028	3.36E-02	1.19E-03	3.45E-02	Vs_s_X_U_Inf2		0.3041	1.0567
1.2056	1.098	3.31E-02	1.32E-03	3.64E-02	Vs_s_X_B_Inf3		0.2724	1.2056
1.2566	1.121	3.31E-02	1.37E-03	3.71E-02	Vs_s_X_U_Inf4		0.2627	1.2566
1.4544	1.206	3.33E-02	1.61E-03	4.01E-02	i_N_XBOrg_mol_perC		0.2283	1.4544
1.4957	1.223	3.32E-02	1.65E-03	4.06E-02	Vs_s_X_ISS3		0.2215	1.4957
2.0107	1.418	3.33E-02	2.23E-03	4.73E-02	Vs_s_X_U_Inf5		0.1566	2.0107
2.1904	1.48	3.28E-02	2.35E-03	4.85E-02	i_O_XBInf_mol_perC		0.1392	2.1904
2.2350	1.495	3.29E-02	2.42E-03	4.92E-02	ISS_BM		0.1353	2.2350
2.3994	1.549	3.30E-02	2.61E-03	5.10E-02	i_N_SF_mol_perC		0.1217	2.3994
2.5824	1.607	3.34E-02	2.89E-03	5.37E-02	X_Lim		0.1084	2.5824

Out_X_VSS							
Multive regression no		Multive regression & intercept			Parameters	Std. Error	
$\beta_0^{\wedge}2$	SRC (β_0)	Std. Error	$\beta^{\wedge}2$	SRC (β)			
0.0954	0.309	3.36E-02	1.08E-04	1.04E-02	Vs_s_X_B_Inf4	0.7572	
0.1211	0.348	3.29E-02	1.31E-04	1.15E-02	Vs_s_X_U_Inf3	0.728	
0.1218	0.349	3.29E-02	1.32E-04	1.15E-02	Alpha_U	0.7269	
0.1459	0.382	3.30E-02	1.59E-04	1.26E-02	Gamma_B	0.7025	
0.1797	0.424	3.31E-02	1.96E-04	1.40E-02	i_N_XUInf_mol_perC	0.672	
0.2218	0.471	3.33E-02	2.45E-04	1.57E-02	i_N_XUOrg_mol_perC	0.6379	
0.2401	0.49	3.30E-02	2.61E-04	1.62E-02	i_H_XBInf_mol_perC	0.6243	
0.2683	0.518	3.28E-02	2.90E-04	1.70E-02	Alpha_I	0.6044	
0.2714	0.521	3.35E-02	3.06E-04	1.75E-02	i_H_SF_mol_perC	0.6022	
0.3136	0.56	3.30E-02	3.42E-04	1.85E-02	Lambda_B	0.5755	
0.3226	0.568	3.31E-02	3.53E-04	1.88E-02	i_P_XBInf_mol_perC	0.5702	
0.3306	0.575	3.34E-02	3.68E-04	1.92E-02	kM_BOrg_AD_hyd	0.5657	
0.3552	0.596	3.29E-02	3.85E-04	1.96E-02	KS_BInf_AD_hyd	0.5513	
0.3881	0.623	3.30E-02	4.22E-04	2.05E-02	i_H_Org_mol_perC	0.5336	
0.4502	0.671	3.35E-02	5.06E-04	2.25E-02	K_ALK	0.5025	
0.5097	0.714	3.30E-02	5.56E-04	2.36E-02	Vs_s_X_ISS1	0.4754	
0.5112	0.715	3.31E-02	5.60E-04	2.37E-02	TempCoeff	0.4746	
0.5565	0.746	3.33E-02	6.17E-04	2.48E-02	Alpha_B	0.4558	
0.7551	0.869	3.32E-02	8.32E-04	2.89E-02	Vs_s_X_U_Inf1	0.3852	
1.0100	1.005	3.28E-02	1.08E-03	3.29E-02	Vs_s_X_ISS4	0.3153	
1.0180	1.009	3.29E-02	1.10E-03	3.32E-02	i_H_XUInf_mol_perC	0.3131	
1.0567	1.028	3.36E-02	1.19E-03	3.45E-02	Vs_s_X_U_Inf2	0.3041	
1.2056	1.098	3.31E-02	1.32E-03	3.64E-02	Vs_s_X_B_Inf3	0.2724	
1.2566	1.121	3.31E-02	1.37E-03	3.71E-02	Vs_s_X_U_Inf4	0.2627	
1.4544	1.206	3.33E-02	1.61E-03	4.01E-02	i_N_XBOrg_mol_perC	0.2283	
1.4957	1.223	3.32E-02	1.65E-03	4.06E-02	Vs_s_X_ISS3	0.2215	
2.0107	1.418	3.33E-02	2.23E-03	4.73E-02	Vs_s_X_U_Inf5	0.1566	
2.1904	1.48	3.28E-02	2.35E-03	4.85E-02	i_O_XBInf_mol_perC	0.1392	
2.2350	1.495	3.29E-02	2.42E-03	4.92E-02	ISS_BM	0.1353	
2.3994	1.549	3.30E-02	2.61E-03	5.10E-02	i_N_SF_mol_perC	0.1217	
2.5824	1.607	3.34E-02	2.89E-03	5.37E-02	X_Lim	0.1084	

TSS_Under_s							
Multivariate regression no		Multivariate regression & intercept			Parameters	Std.	
β^2	SRC (β_0)	Std. Error	β^2	SRC (β)			
1.2882	1.135	5.74E-03	4.24E-05	6.51E-03	i_N_XUOrg_mol_perC	0.7572	
1.3202	1.149	5.69E-03	4.29E-05	6.55E-03	i_H_Org_mol_perC	0.728	
1.3548	1.164	5.81E-03	4.57E-05	6.76E-03	i_N_Org_mol_perC	0.7269	
1.9460	1.395	5.69E-03	6.30E-05	7.94E-03	i_O_SF_mol_perC	0.7025	
2.2201	1.49	5.67E-03	7.15E-05	8.45E-03	i_K_PP_mol_perP	0.672	
2.5153	1.586	5.66E-03	8.05E-05	8.97E-03	i_P_SU_mol_perC	0.6379	
2.5985	1.612	5.76E-03	8.61E-05	9.28E-03	Beta_B	0.6243	
2.9036	1.704	5.69E-03	9.40E-05	9.70E-03	i_H_XBInf_mol_perC	0.6044	
4.1656	2.041	5.71E-03	1.36E-04	1.17E-02	i_Ca_PP_mol_perP	0.6022	
16.265	4.033	5.70E-03	5.30E-04	2.30E-02	Lambda_B	0.5755	
16.321	4.04	5.75E-03	5.37E-04	2.32E-02	Beta_I	0.5702	
19.333	4.397	5.74E-03	6.36E-04	2.52E-02	Vs_s_X_ISS5	0.5657	
21.344	4.62	5.67E-03	6.87E-04	2.62E-02	Beta_U	0.5513	
22.005	4.691	5.77E-03	7.32E-04	2.71E-02	Vs_s_X_ISS2	0.5336	
27.973	5.289	5.74E-03	9.22E-04	3.04E-02	Gamma_U	0.5025	
37.527	6.126	5.66E-03	1.20E-03	3.47E-02	Vs_s_X_ISS4	0.4754	
41.344	6.43	5.74E-03	1.36E-03	3.69E-02	Vs_s_X_B_Inf1	0.4746	
49.843	7.06	5.67E-03	1.60E-03	4.00E-02	Alpha_I	0.4558	
57.229	7.565	5.73E-03	1.88E-03	4.34E-02	Vs_s_X_ISS3	0.3852	
58.782	7.667	5.70E-03	1.91E-03	4.37E-02	Gamma_B	0.3153	
75.933	8.714	5.69E-03	2.46E-03	4.96E-02	Vs_s_X_ISS1	0.3131	
85.359	9.239	5.75E-03	2.82E-03	5.32E-02	Vs_s_X_U_Inf5	0.3041	
151.46	12.307	5.79E-03	5.08E-03	7.13E-02	Vs_s_X_U_Inf2	0.2724	
219.69	14.822	5.71E-03	7.17E-03	8.47E-02	Vs_s_X_B_Inf2	0.2627	
283.45	16.836	5.71E-03	9.24E-03	9.61E-02	Vs_s_X_U_Inf4	0.2283	
360.96	18.999	5.68E-03	1.17E-02	1.08E-01	Alpha_U	0.2215	
410.38	20.258	5.73E-03	1.35E-02	1.16E-01	Vs_s_X_U_Inf1	0.1566	
496.48	22.282	5.68E-03	1.60E-02	1.27E-01	Vs_s_X_U_Inf3	0.1392	
2651.1	51.489	5.72E-03	8.67E-02	2.94E-01	Vs_s_X_B_Inf3	0.1353	
7765.1	88.12	5.79E-03	2.61E-01	5.11E-01	Vs_s_X_B_Inf4	0.1217	
17756.	133.255	5.68E-03	5.72E-01	7.56E-01	Vs_s_X_B_Inf5	0.1084	

Under_X_B_Inf						
Multive regression no intercept		Multive regression & intercept			Parameters	Std. Error
$\beta_0^{\wedge}2$	SRC (β_0)	Std. Error	$\beta^{\wedge}2$	SRC (β)		
0.094864	0.308	3.35E-02	1.07E-04	1.03E-02	Vs_s_X_B_Inf4	0.2568
0.191844	0.438	3.30E-02	2.09E-04	1.45E-02	i_N_XUInf_mol_perC	0.2506
0.227529	0.477	3.32E-02	2.52E-04	1.59E-02	i_N_XUOrg_mol_perC	0.2446
0.263169	0.513	3.30E-02	2.86E-04	1.69E-02	i_H_XBInf_mol_perC	0.1634
0.275625	0.525	3.35E-02	3.09E-04	1.76E-02	i_H_SF_mol_perC	0.1366
0.308025	0.555	3.29E-02	3.33E-04	1.82E-02	Vs_s_X_U_Inf3	0.113
0.308025	0.555	3.34E-02	3.43E-04	1.85E-02	kM_BOrg_AD_hyd	0.1074
0.357604	0.598	3.28E-02	3.85E-04	1.96E-02	Alpha_I	0.0888
0.398161	0.631	3.29E-02	4.32E-04	2.08E-02	Vs_s_X_ISS1	0.0416
0.405769	0.637	3.29E-02	4.40E-04	2.10E-02	KS_BInf_AD_hyd	5.97E-05
0.418609	0.647	3.30E-02	4.55E-04	2.13E-02	Gamma_B	5.77E-05
0.442225	0.665	3.31E-02	4.83E-04	2.20E-02	i_P_XBInf_mol_perC	1.22E-05
0.474721	0.689	3.31E-02	5.20E-04	2.28E-02	TempCoeff	4.39E-06
0.487204	0.698	3.30E-02	5.29E-04	2.30E-02	i_H_Org_mol_perC	3.13E-06
0.494209	0.703	3.35E-02	5.56E-04	2.36E-02	K_ALK	1.53E-07
0.546121	0.739	3.29E-02	5.91E-04	2.43E-02	Alpha_U	1.33E-09
0.613089	0.783	3.30E-02	6.68E-04	2.59E-02	Lambda_B	2.04E-10
0.753424	0.868	3.32E-02	8.29E-04	2.88E-02	Vs_s_X_U_Inf1	3.25E-12
0.964324	0.982	3.33E-02	1.07E-03	3.27E-02	Alpha_B	9.30E-14
1.028196	1.014	3.28E-02	1.10E-03	3.32E-02	Vs_s_X_ISS4	4.42E-14
1.149184	1.072	3.29E-02	1.25E-03	3.53E-02	i_H_XUInf_mol_perC	< 2e-16
1.153476	1.074	3.35E-02	1.30E-03	3.60E-02	Vs_s_X_U_Inf2	< 2e-16
1.387684	1.178	3.30E-02	1.52E-03	3.89E-02	Vs_s_X_U_Inf4	< 2e-16
1.454436	1.206	3.33E-02	1.61E-03	4.01E-02	i_N_XBOrg_mol_perC	< 2e-16
1.857769	1.363	3.31E-02	2.04E-03	4.51E-02	Vs_s_X_B_Inf3	< 2e-16
1.857769	1.363	3.32E-02	2.05E-03	4.52E-02	Vs_s_X_ISS3	< 2e-16
1.923769	1.387	3.28E-02	2.12E-03	4.60E-02	i_O_XBInf_mol_perC	< 2e-16
1.974025	1.405	3.33E-02	2.13E-03	4.62E-02	Vs_s_X_U_Inf5	< 2e-16
2.143296	1.464	3.29E-02	2.32E-03	4.82E-02	ISS_BM	< 2e-16
2.424249	1.557	3.29E-02	2.64E-03	5.14E-02	i_N_SF_mol_perC	< 2e-16
2.439844	1.562	3.34E-02	2.71E-03	5.20E-02	X_Lim	< 2e-16

Under.X_ISS								
Multive	Multive regression & intercept			Parameters		Std. Error		
	SRC (β_0)	Std. Error	β^2	SRC (β)				
0.308	3.35E-02	1.07E-04	1.03E-02	1.03E-02	Vs_s_X_B_Inf4	0.7582		
0.438	3.30E-02	2.09E-04	1.45E-02	1.45E-02	i_N_XUInf_mol_per	0.6618		
0.477	3.32E-02	2.52E-04	1.59E-02	1.59E-02	i_N_XUOrg_mol_pe	0.6332		
0.513	3.30E-02	2.86E-04	1.69E-02	1.69E-02	i_H_XBInf_mol_per	0.6077		
0.525	3.35E-02	3.09E-04	1.76E-02	1.76E-02	i_H_SF_mol_perC	0.5995		
0.555	3.29E-02	3.33E-04	1.82E-02	1.82E-02	Vs_s_X_U_Inf3	0.5791		
0.555	3.34E-02	3.43E-04	1.85E-02	1.85E-02	KM_BOrg_AD_hyd	0.5793		
0.598	3.28E-02	3.85E-04	1.96E-02	1.96E-02	Alpha_I	0.5497		
0.631	3.29E-02	4.32E-04	2.08E-02	2.08E-02	Vs_s_X_ISS1	0.5282		
0.637	3.29E-02	4.40E-04	2.10E-02	2.10E-02	KS_BInf_AD_hyd	0.524		
0.647	3.30E-02	4.55E-04	2.13E-02	2.13E-02	Gamma_B	0.5176		
0.665	3.31E-02	4.83E-04	2.20E-02	2.20E-02	i_P_XBInf_mol_per	0.5065		
0.689	3.31E-02	5.20E-04	2.28E-02	2.28E-02	TempCoeff	0.4912		
0.698	3.30E-02	5.29E-04	2.30E-02	2.30E-02	i_H_Org_mol_perC	0.4856		
0.703	3.35E-02	5.56E-04	2.36E-02	2.36E-02	K_ALK	0.4821		
0.739	3.29E-02	5.91E-04	2.43E-02	2.43E-02	Alpha_U	0.46		
0.783	3.30E-02	6.68E-04	2.59E-02	2.59E-02	Lambda_B	0.4335		
0.868	3.32E-02	8.29E-04	2.88E-02	2.88E-02	Vs_s_X_U_Inf1	0.3857		
0.982	3.33E-02	1.07E-03	3.27E-02	3.27E-02	Alpha_B	0.3264		
1.014	3.28E-02	1.10E-03	3.32E-02	3.32E-02	Vs_s_X_ISS4	0.3109		
1.072	3.29E-02	1.25E-03	3.53E-02	3.53E-02	i_H_XUInf_mol_per	0.2838		
1.074	3.35E-02	1.30E-03	3.60E-02	3.60E-02	Vs_s_X_U_Inf2	0.2831		
1.178	3.30E-02	1.52E-03	3.89E-02	3.89E-02	Vs_s_X_U_Inf4	0.2391		
1.206	3.33E-02	1.61E-03	4.01E-02	4.01E-02	i_N_XBOrg_mol_pe	0.228		
1.363	3.31E-02	2.04E-03	4.51E-02	4.51E-02	Vs_s_X_B_Inf3	0.1731		
1.363	3.32E-02	2.05E-03	4.52E-02	4.52E-02	Vs_s_X_ISS3	0.1731		
1.387	3.28E-02	2.12E-03	4.60E-02	4.60E-02	i_O_XBInf_mol_per	0.1657		
1.405	3.33E-02	2.13E-03	4.62E-02	4.62E-02	Vs_s_X_U_Inf5	0.1603		
1.464	3.29E-02	2.32E-03	4.82E-02	4.82E-02	ISS_BM	0.1435		
1.557	3.29E-02	2.64E-03	5.14E-02	5.14E-02	i_N_SF_mol_perC	0.1199		
1.562	3.34E-02	2.71E-03	5.20E-02	5.20E-02	X_Lim	0.1187		

Under_X_U_Inf								
Multive	Multive regression & intercept			Parameters				
SRC (β ₀)	Std. Error	β ²	SRC (β)					
0.308	3.35E-02	1.07E-04	1.03E-02	Vs_s_X_B_Inf4			Std. Error	β ₀ ²
0.438	3.30E-02	2.09E-04	1.45E-02	i_N_XUInf_mol_perC			0.7582	0.094864
0.477	3.32E-02	2.52E-04	1.59E-02	i_N_XUOrg_mol_per			0.6618	0.191844
0.513	3.30E-02	2.86E-04	1.69E-02	i_H_XBInf_mol_perC			0.6332	0.227529
0.525	3.35E-02	3.09E-04	1.76E-02	i_H_SF_mol_perC			0.6077	0.263169
0.555	3.29E-02	3.33E-04	1.82E-02	Vs_s_X_U_Inf3			0.5995	0.275625
0.555	3.34E-02	3.43E-04	1.85E-02	kM_BOrg_AD_hyd			0.5791	0.308025
0.598	3.28E-02	3.85E-04	1.96E-02	Alpha_I			0.5793	0.308025
0.631	3.29E-02	4.32E-04	2.08E-02	Vs_s_X_ISS1			0.5497	0.357604
0.637	3.29E-02	4.40E-04	2.10E-02	KS_BInf_AD_hyd			0.5282	0.398161
0.647	3.30E-02	4.55E-04	2.13E-02	Gamma_B			0.524	0.405769
0.665	3.31E-02	4.83E-04	2.20E-02	i_P_XBInf_mol_perC			0.5176	0.418609
0.689	3.31E-02	5.20E-04	2.28E-02	TempCoeff			0.5065	0.442225
0.698	3.30E-02	5.29E-04	2.30E-02	i_H_Org_mol_perC			0.4912	0.474721
0.703	3.35E-02	5.56E-04	2.36E-02	K_ALK			0.4856	0.487204
0.739	3.29E-02	5.91E-04	2.43E-02	Alpha_U			0.4821	0.494209
0.783	3.30E-02	6.68E-04	2.59E-02	Lambda_B			0.46	0.546121
0.868	3.32E-02	8.29E-04	2.88E-02	Vs_s_X_U_Inf1			0.4335	0.613089
0.982	3.33E-02	1.07E-03	3.27E-02	Alpha_B			0.3857	0.753424
1.014	3.28E-02	1.10E-03	3.32E-02	Vs_s_X_ISS4			0.3264	0.964324
1.072	3.29E-02	1.25E-03	3.53E-02	i_H_XUInf_mol_perC			0.3109	1.028196
1.074	3.35E-02	1.30E-03	3.60E-02	Vs_s_X_U_Inf2			0.2838	1.149184
1.178	3.30E-02	1.52E-03	3.89E-02	Vs_s_X_U_Inf4			0.2831	1.153476
1.206	3.33E-02	1.61E-03	4.01E-02	i_N_XBOrg_mol_perC			0.2391	1.387684
1.363	3.31E-02	2.04E-03	4.51E-02	Vs_s_X_B_Inf3			0.228	1.454436
1.363	3.32E-02	2.05E-03	4.52E-02	Vs_s_X_ISS3			0.1731	1.857769
1.387	3.28E-02	2.12E-03	4.60E-02	i_O_XBInf_mol_perC			0.1731	1.857769
1.405	3.33E-02	2.13E-03	4.62E-02	Vs_s_X_U_Inf5			0.1657	1.923769
1.464	3.29E-02	2.32E-03	4.82E-02	ISS_BM			0.1603	1.974025
1.557	3.29E-02	2.64E-03	5.14E-02	i_N_SF_mol_perC			0.1435	2.143296
1.562	3.34E-02	2.71E-03	5.20E-02	X_Lim			0.1199	2.424249
							0.1187	2.439844

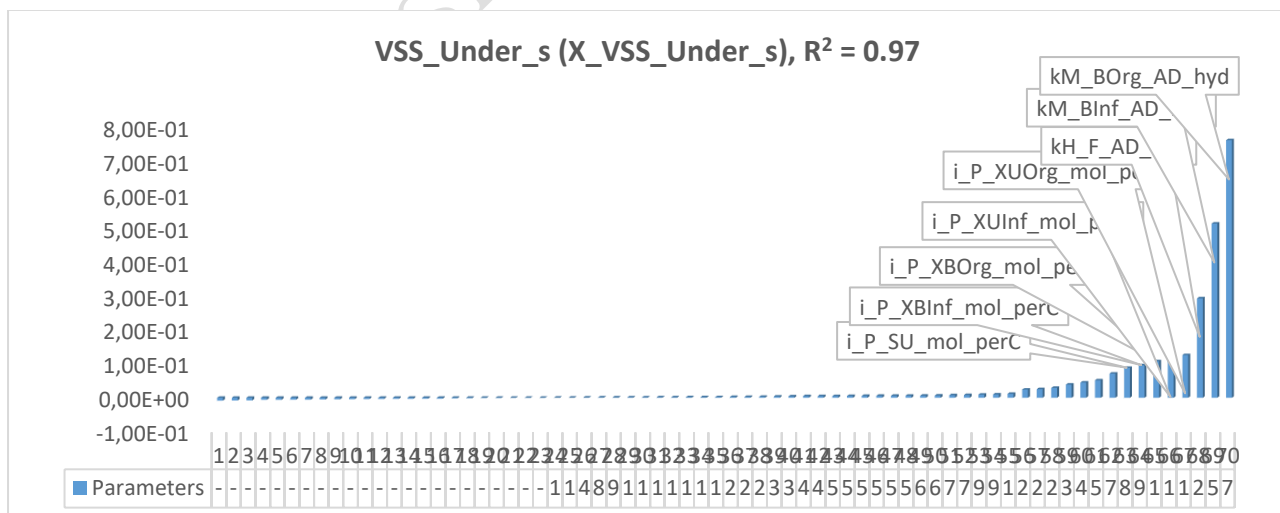
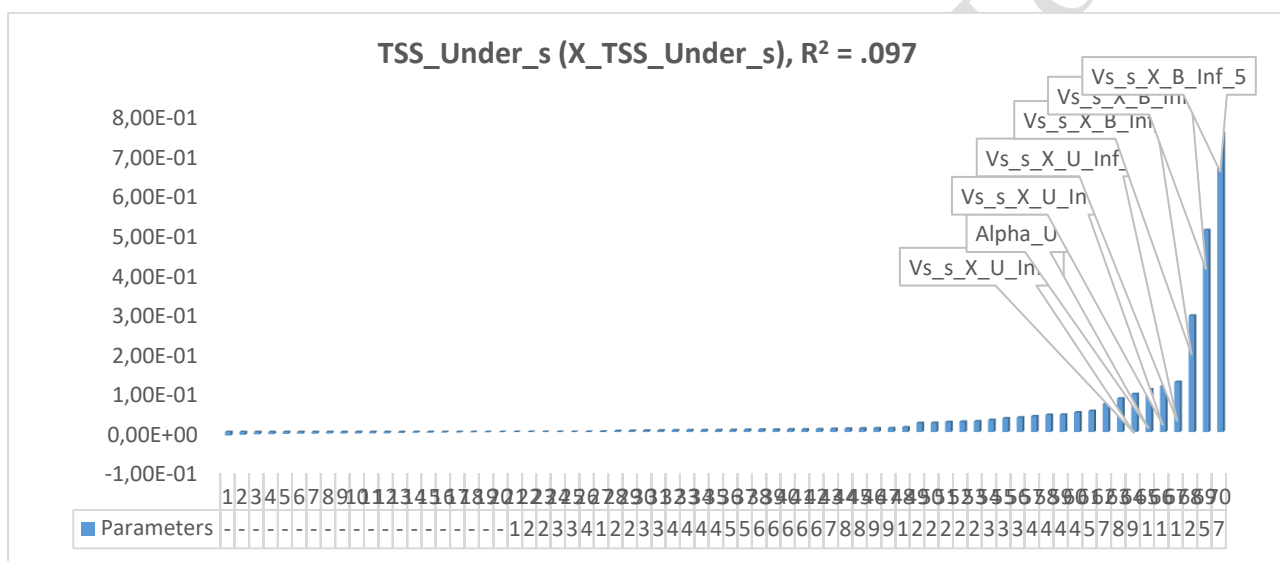
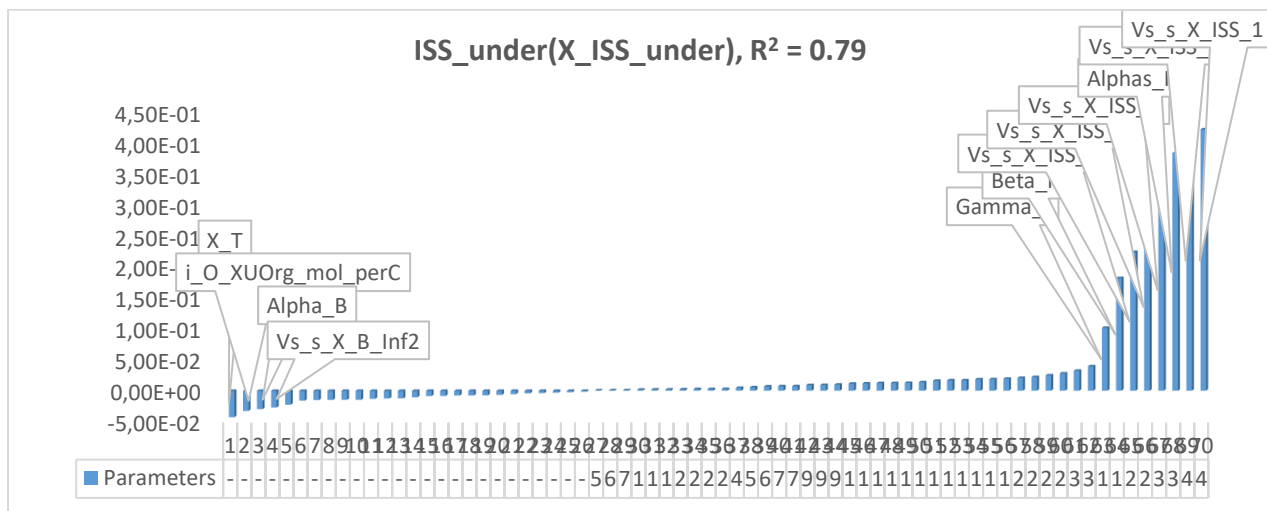
Under_X_VSS								
Multivariate regression no		Multivariate regression & intercept			Parameters			
β_0^2	SRC (β_0)	Std. Error	β^2	SRC (β)			Std. Error	β_0^2
0.094864	0.308	3.35E-02	1.07E-04	1.03E-02	Vs_s_X_B_Inf4		0.7582	0.094864
0.191844	0.438	3.30E-02	2.09E-04	1.45E-02	i_N_XUInf_mol_perC		0.6618	0.191844
0.227529	0.477	3.32E-02	2.52E-04	1.59E-02	i_N_XUOrg_mol_perC		0.6332	0.227529
0.263169	0.513	3.30E-02	2.86E-04	1.69E-02	i_H_XBInf_mol_perC		0.6077	0.263169
0.275625	0.525	3.35E-02	3.09E-04	1.76E-02	i_H_SF_mol_perC		0.5995	0.275625
0.308025	0.555	3.29E-02	3.33E-04	1.82E-02	Vs_s_X_U_Inf3		0.5791	0.308025
0.308025	0.555	3.34E-02	3.43E-04	1.85E-02	kM_BOrg_AD_hyd		0.5793	0.308025
0.357604	0.598	3.28E-02	3.85E-04	1.96E-02	Alpha_I		0.5497	0.357604
0.398161	0.631	3.29E-02	4.32E-04	2.08E-02	Vs_s_X_ISS1		0.5282	0.398161
0.405769	0.637	3.29E-02	4.40E-04	2.10E-02	KS_BInf_AD_hyd		0.524	0.405769
0.418609	0.647	3.30E-02	4.55E-04	2.13E-02	Gamma_B		0.5176	0.418609
0.442225	0.665	3.31E-02	4.83E-04	2.20E-02	i_P_XBInf_mol_perC		0.5065	0.442225
0.474721	0.689	3.31E-02	5.20E-04	2.28E-02	TempCoeff		0.4912	0.474721
0.487204	0.698	3.30E-02	5.29E-04	2.30E-02	i_H_Org_mol_perC		0.4856	0.487204
0.494209	0.703	3.35E-02	5.56E-04	2.36E-02	K_ALK		0.4821	0.494209
0.546121	0.739	3.29E-02	5.91E-04	2.43E-02	Alpha_U		0.46	0.546121
0.613089	0.783	3.30E-02	6.68E-04	2.59E-02	Lambda_B		0.4335	0.613089
0.753424	0.868	3.32E-02	8.29E-04	2.88E-02	Vs_s_X_U_Inf1		0.3857	0.753424
0.964324	0.982	3.33E-02	1.07E-03	3.27E-02	Alpha_B		0.3264	0.964324
1.028196	1.014	3.28E-02	1.10E-03	3.32E-02	Vs_s_X_ISS4		0.3109	1.028196
1.149184	1.072	3.29E-02	1.25E-03	3.53E-02	i_H_XUInf_mol_perC		0.2838	1.149184
1.153476	1.074	3.35E-02	1.30E-03	3.60E-02	Vs_s_X_U_Inf2		0.2831	1.153476
1.387684	1.178	3.30E-02	1.52E-03	3.89E-02	Vs_s_X_U_Inf4		0.2391	1.387684
1.454436	1.206	3.33E-02	1.61E-03	4.01E-02	i_N_XBOrg_mol_perC		0.228	1.454436
1.857769	1.363	3.31E-02	2.04E-03	4.51E-02	Vs_s_X_B_Inf3		0.1731	1.857769
1.857769	1.363	3.32E-02	2.05E-03	4.52E-02	Vs_s_X_ISS3		0.1731	1.857769
1.923769	1.387	3.28E-02	2.12E-03	4.60E-02	i_O_XBInf_mol_perC		0.1657	1.923769
1.974025	1.405	3.33E-02	2.13E-03	4.62E-02	Vs_s_X_U_Inf5		0.1603	1.974025
2.143296	1.464	3.29E-02	2.32E-03	4.82E-02	ISS_BM		0.1435	2.143296
2.424249	1.557	3.29E-02	2.64E-03	5.14E-02	i_N_SF_mol_perC		0.1199	2.424249
2.439844	1.562	3.34E-02	2.71E-03	5.20E-02	X_Lim		0.1187	2.439844

VSS_Under_s										
Multivariate regression no intercept			Multivariate regression & intercept				Parameters			
Std. Error	β_0^2	SRC (β_0)	Std. Error	β^2	SRC (β)					
0.4848	0.488601	0.699	5.68E-03	1.58E-05	3.97E-03	i_H_SU_mol_perC	0.7582		Std.	
0.4026	0.700569	0.837	5.58E-03	2.18E-05	4.67E-03	i_H_XBInf_mol_perC	0.6618			
0.3845	0.7569	0.87	5.66E-03	2.43E-05	4.93E-03	i_H_XBOrg_mol_perC	0.6332			
0.3708	0.801025	0.895	5.60E-03	2.51E-05	5.01E-03	i_H_XUInf_mol_perC	0.6077			
0.3422	0.9025	0.95	5.64E-03	2.88E-05	5.36E-03	i_H_XUOrg_mol_perC	0.5995			
0.3308	0.946729	0.973	5.53E-03	2.90E-05	5.38E-03	i_K_PP_mol_perP	0.5791			
0.3042	1.056784	1.028	5.62E-03	3.33E-05	5.77E-03	i_Mg_PP_mol_perP	0.5793			
0.292	1.110916	1.054	5.60E-03	3.48E-05	5.90E-03	i_N_Org_mol_perC	0.5497			
0.2826	1.155625	1.075	5.55E-03	3.56E-05	5.97E-03	i_N_SF_mol_perC	0.5282			
0.2759	1.1881	1.09	5.59E-03	3.71E-05	6.09E-03	i_N_SU_mol_perC	0.524			
0.2459	1.347921	1.161	5.56E-03	4.17E-05	6.46E-03	i_N_XBInf_mol_perC	0.5176			
0.1668	1.915456	1.384	5.55E-03	5.89E-05	7.68E-03	i_N_XBOrg_mol_perC	0.5065			
0.148	2.096704	1.448	5.51E-03	6.37E-05	7.98E-03	i_N_XUInf_mol_perC	0.4912			
0.0998	2.715904	1.648	5.61E-03	8.54E-05	9.24E-03	i_N_XUOrg_mol_perC	0.4856			
0.0813	3.045025	1.745	5.55E-03	9.37E-05	9.68E-03	i_O_Org_mol_perC	0.4821			
0.0404	4.214809	2.053	5.57E-03	1.31E-04	1.14E-02	i_O_SF_mol_perC	0.46			
1.58E-05	18.8356	4.34	5.56E-03	5.81E-04	2.41E-02	i_O_SU_mol_perC	0.4335			
5.24E-06	20.99472	4.582	5.53E-03	6.42E-04	2.53E-02	i_O_XBInf_mol_perC	0.3857			
2.20E-07	27.258841	5.221	5.60E-03	8.53E-04	2.92E-02	i_O_XBOrg_mol_perC	0.3264			
7.61E-12	48.094225	6.935	5.60E-03	1.51E-03	3.88E-02	i_O_XUInf_mol_perC	0.3109			
1.45E-15	65.966884	8.122	5.55E-03	2.03E-03	4.51E-02	i_O_XUOrg_mol_perC	0.2838			
< 2e-16	83.9056	9.16	5.61E-03	2.64E-03	5.14E-02	i_P_Org_mol_perC	0.2831			
< 2e-16	159.82016	12.642	5.64E-03	5.09E-03	7.14E-02	i_P_SF_mol_perC	0.2391			
< 2e-16	250.74722	15.835	5.57E-03	7.78E-03	8.82E-02	i_P_SU_mol_perC	0.228			
< 2e-16	296.97628	17.233	5.56E-03	9.19E-03	9.59E-02	i_P_XBInf_mol_perC	0.1731			
< 2e-16	378.45811	19.454	5.54E-03	1.16E-02	1.08E-01	i_P_XBOrg_mol_perC	0.1731			
< 2e-16	423.5364	20.58	5.59E-03	1.32E-02	1.15E-01	i_P_XUInf_mol_perC	0.1657			
< 2e-16	518.0176	22.76	5.54E-03	1.59E-02	1.26E-01	i_P_XUOrg_mol_perC	0.1603			
< 2e-16	2775.1824	52.68	5.57E-03	8.62E-02	2.94E-01	kH_F_AD_hyd	0.1435			
< 2e-16	8293.3806	91.068	5.65E-03	2.65E-01	5.14E-01	kM_BInf_AD_hyd	0.1199			
< 2e-16	18898.825	137.473	5.53E-03	5.79E-01	7.61E-01	kM_BOrg_AD_hyd	0.1187			

Variables				(Intercept)	Coefficient of Determination (R^2)	Kinetic sum (SRC^2)	Stoich. Sum (SRC^2)	Total sum (SRC^2)	Mean (SRC^2)	Std dev (SRC^2)	Most Positive (SRC)	Most negative (SRC)									
	Parameters																				
ISS_under	Multive regression &		s	1.22E-11	0.79																
				1.48E-22		0.59	0.20	0.79	0.01	0.04	0.42	-0.04									
				1.52E-02																	
	Multive regression		s	0	0.77																
				0		2378.35	817.85	3196.20	45.66	151.17	0.05	-1.87									
				1																	
				(Intercept)	Coefficient of Determination (R^2)	Kinetic sum (SRC^2)	Stoich. Sum (SRC^2)	Total sum (SRC^2)	Mean (SRC^2)	std dev (SRC^2)	Most Positive (SRC)	Most negative (SRC)									
Parameters																					
	Multive regression &		s										1.11E-11	0.05							
1.23E-22													0.02		0.03	0.06	0.00	0.00	0.05	-0.07	
3.20E-02																					
Multive regression		s	0										-0.02								
			0.00E+00	20.38	29.93	50.31	0.70	0.91	1.61	-2.12											
			1																		
				(Intercept)	Coefficient of Determination (R^2)	Kinetic sum (SRC^2)	Stoich. Sum (SRC^2)	Total sum (SRC^2)	Mean (SRC^2)	std dev (SRC^2)	Most Positive (SRC)	Most negative (SRC)									
Parameters																					
	Multive regression &		s										1.21E-11	0.05							
1.46E-22													0.03		0.02	0.05	0.00	0.00	0.05	-0.07	
3.20E-02																					
Multive regression		s	0										-0.02								
			0	27.78	20.38	48.17	0.70	0.91	1.61	-2.12											
			1																		
				(Intercept)	Coefficient of Determination (R^2)	Kinetic sum (SRC^2)	Stoich. Sum (SRC^2)	Total sum (SRC^2)	Mean (SRC^2)	std dev (SRC^2)	Most Positive (SRC)	Most negative (SRC)									
Parameters																					
	Multive regression &		s										1.21E-11	0.05							
1.46E-22													0.02		0.03	0.05	0.00	0.00	0.05	-0.07	
3.20E-02																					
Multive regression		s	0										-0.02								
			0	20.38	28.91	49.30	0.70	0.91	1.61	-2.12											
			1																		
				(Intercept)	Coefficient of Determination (R^2)	Kinetic sum (SRC^2)	Stoich. Sum (SRC^2)	Total sum (SRC^2)	Mean (SRC^2)	std dev (SRC^2)	Most Positive (SRC)	Most negative (SRC)									
Parameters																					
	Multive regression &	SRC (β)											1.31E-11	0.05							
β^2													1.71E-22		0.02	0.03	0.05	0.00	0.00	0.05	-0.07
Std. Error													3.20E-02								
Multive	SRC (β ₀)		0										-0.02								

		β_0^2	0		20.38	28.91	49.30	0.70	0.91	1.61	-2.12	
		Std. Error	1									
					Coefficient of Determination (R^2)	Kinetic sum (SRC^2)	Stoich. Sum (SRC^2)	Total sum (SRC^2)	Mean (SRC^2)	std dev (SRC^2)	Most Positive (SRC)	Most negative (SRC)
TSS_Under_s	Parameters			(Intercept)								
	Multive regression &	s	s	9.95E-12	0.97							
		β	β	9.89E-23		0.98	0.02	1.00	0.01	0.08	0.76	-0.01
		s	t	5.53E-03								
	Multive regression	s	s	0	0.97							
		β	β_0	0		30078.07	584.55	30662.61	438.04	2315.44	133.26	-1.51
		s	t	1								
***					Coefficient of Determination (R^2)	Kinetic sum (SRC^2)	Stoich. Sum (SRC^2)	Total sum (SRC^2)	Mean (SRC^2)	std dev (SRC^2)	Most Positive (SRC)	Most negative (SRC)
Under_X_B_Inf	Parameters			(Intercept)								
	Multive regression &	s	s	7.35E-12	0.05							
		β	β	5.40E-23		0.03	0.03	0.06	0.00	0.00	0.05	-0.07
		s	t	3.20E-02								
	Multive regression	s	s	0	-0.02							
		β	β_0	0		22.81	29.17	51.98	0.74	0.92	1.56	-2.24
		s	t	1								
					Coefficient of Determination (R^2)	Kinetic sum (SRC^2)	Stoich. Sum (SRC^2)	Total sum (SRC^2)	Mean (SRC^2)	std dev (SRC^2)	Most Positive (SRC)	Most negative (SRC)
Under_X_ISS	Parameters			(Intercept)								
	Multive regression & intercept	SRC (β)		7.35E-12	0.05							
		β^2		5.40E-23		0.03	0.03	0.06	0.00	0.00	0.05	-0.07
		Std. Error		3.20E-02								
	Multive regression no intercept	SRC (β_0)		0	-0.02							
		β_0^2		0		22.81	29.17	51.98	0.74	0.92	1.56	-2.24
		Std. Error		1								
					Coefficient of Determination (R^2)	Kinetic sum (SRC^2)	Stoich. Sum (SRC^2)	Total sum (SRC^2)	Mean (SRC^2)	std dev (SRC^2)	Most Positive (SRC)	Most negative (SRC)
Under_X_U_Inf	Parameters			(Intercept)								
	Multive regression &	s	s	6.35E-12	0.05							
		β	β	4.03E-23		0.03	0.03	0.06	0.00	0.00	0.05	-0.07
		s	t	3.20E-02								
	Multive regression	s	s	0	-0.02							
		β	β_0	0		22.81	29.17	51.98	0.74	0.92	1.56	-2.24
		s	t	1								
				(Intercept)								

Summary of Results for UCTPSU Uncertainty and Sensitivity Analysis using SRC Method												
Variables	Standard Regression Coefficient (β)				highest β2 value	R^2	Kinetic sum (SRC2)	Stoich. sum (SRC2)	Total sum (SRC2)	Mean (β2)	Std Dev. (β2)	Coeff. of Variation
	Most Positive		Most Negative									
ISS_under	Out_X_B_Inf	OutX_ISS	OutX_U_Inf	OutX_VSS	TSS_Under_s	Under_X_B_Inf	UnderX_ISS	UnderX_U_Inf	UnderX_VSS	VSS_Under_s		
Vs_s_X_ISS1	X_Lim	X_Lim	X_Lim	X_Lim	Vs_s_X_B_Inf5	X_Lim	X_Lim	X_Lim	X_Lim	kM_BOrg_AD_hyd	Vs_s_X_ISS1	
0.42	0.05	0.05	0.05	0.05	0.76	0.05	0.05	0.05	0.05	0.76	0.42	
X_T	kH_F_AD_hyd	kH_F_AD_hyd	kH_F_AD_hyd	kH_F_AD_hyd	i_P_XBOrg_mol_perC	kH_F_AD_hyd	kH_F_AD_hyd	kH_F_AD_hyd	kH_F_AD_hyd	Gamma_J	X_T	
-0.04	-0.07	-0.07	-0.07	-0.07	-0.01	-0.07	-0.07	-0.07	-0.07	-0.01	-0.04	
Vs_s_X_ISS1	X_Lim	X_Lim	X_Lim	X_Lim	Vs_s_X_B_Inf5	X_Lim	X_Lim	X_Lim	X_Lim	kM_BOrg_AD_hyd	Vs_s_X_ISS1	
0.178	0.005	0.005	0.005	0.005	0.572	0.006	0.006	0.006	0.006	0.579	0.178	
0.79	0.05	0.05	0.05	0.00	0.97	0.05	0.05	0.05	0.05	0.97	0.79	
0.59	0.02	0.03	0.02	0.02	0.98	0.03	0.03	0.03	0.03	0.93	0.59	
0.20	0.03	0.02	0.03	0.03	0.02	0.03	0.03	0.03	0.03	0.07	0.20	
0.79	0.06	0.05	0.05	0.05	1.00	0.06	0.06	0.06	0.06	1.00	0.79	
0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.01	
0.04	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.08	0.04	
0.3026	0.7764	0.7764	0.7764	0.7764	0.1903	0.8028	0.80276	0.80276	0.80276	0.80276	0.3026	



APPENDIX F: PARAMETER ESTIMATION INPUT VARIABLES

TABLE F.1.1 SHOW THE VARIABLES IN EQUIVALENT CONTROL 1 SAMPLE

#.t	.AD_1.COD_total	.AD_1.F SA	.AD_1. OP	.AD_1.VSS	.AD_1.ISS m	.AD_1.H2CO3alkalini ty	.AD_1.VFA	.AD_1. p_H_s
#h								
0	6720	155	3	3399	834	979	18	7.93
24	7135	175	4	3542	1011	1006	40	7.49
48	7240	169	4	3689	988	1070	117	7.42
72	6691	167	5	3181	927	1058	45	7.40
96	7045	157	2	3266	905	1140	83	7.37
120	6984	141	4	3166	813	1045	54	7.42
144	7194	170	5	3247	910	1098	57	7.43
168	6978	161	4	3139	780	1021	70	7.36
216	6882	199	3	2857	697	0	0	7.32
264	5927	192	2	3291	1156	1111	44	7.38
312	6012	200	4	3283	1123	1174	8	7.31
360	6076	187	2	3160	776	1169	20	7.32
408	5948	197	4	3377	1129	1200	22	7.30
480	5678	208	3	2772	758	1191	17	7.32
552	5266	189	3	3222	1039	1213	40	7.35
624	5698	205	3	3255	1111	1191	20	7.33
696	5570	223	3	2963	762	1246	33	7.33
768	5642	230	2	3097	814	1286	41	7.42
888	5618	229	3	3050	1062	1252	5	7.43
1008	5620	249	3	2799	739	1274	36	7.43
1080	5180	248	3	2601	593	1258	43	7.36
1248	0	0	0	0	0	0	0	0.00

Table F.1.2 show the variables in Equivalent Control 2 Sample

#.t	.AD_1.COD_total	.AD_1.F SA	.AD_1. OP	.AD_1.VSS	.AD_1.ISS m	.AD_1.H2CO3alkalini ty	.AD_1.VFA	.AD_1. p_H_s
#h								
0	6720	155	3	3399	834	979	18	7.89
24	6300	156	3	3503	832	883	24	7.42
48	6182	151	4	3127	732	882	21	7.42
72	4969	134	3	2776	676	890	19	7.34
96	4874	136	2	2241	576	941	22	7.34
120	5166	157	3	2974	576	941	22	7.43
144	5619	145	3	3322	741	942	28	7.33
168	6179	182	3	2648	866	951	4	7.24
216	5698	176	3	2685	695	965	25	7.19
264	5014	180	3	2774	592	992	31	7.23
312	4952	169	4	3026	655	1064	62	7.25
360	5115	158	2	2681	823	945	34	7.20

408	4790	169	4	2744	661	972	21	7.23
480	4266	179	3	2318	691	1027	56	7.23
552	4274	162	3	2376	587	1019	7	7.27
624	4674	183	3	2489	588	994	6	7.28
696	4658	184	3	2614	687	1036	24	7.22
768	3996	192	4	2021	929	966	-2	7.27
888	4056	193	2	1983	646	1016	28	7.36
1008	3730	206	2	1741	559	1061	75	7.30
1080	3868	199	2	2316	548	1020	90	7.28
1248	0	0	0	0	0	0	0	0.00

Table F.1.3 show the variables in Equivalent Control Average Sample

#.t	.AD_1.COD_total	.AD_1.F SA	.AD_1.Ortho P	.AD_1.VSS	.AD_1.ISS m	.AD_1.H2CO3alkalini ty	.AD_1.VFA	.AD_1.p_H_ s
#h								
0	6720	155	3	3399	834	979	18	7.93
24	6718	166	4	3523	922	945	32	7.49
48	6711	160	4	3408	860	976	69	7.42
72	5830	150	4	2979	802	974	32	7.40
96	5960	146	2	2754	741	1040	52	7.37
120	6075	149	3	3070	695	993	38	7.42
144	6407	157	4	3285	826	1020	42	7.43
168	6579	171	3	2894	823	986	37	7.36
216	6290	188	3	2771	696	483	13	7.32
264	5471	186	3	3033	874	1051	38	7.38
312	5482	184	4	3155	889	1119	35	7.31
360	5596	172	2	2921	800	1057	27	7.32
408	5369	183	4	3061	895	1086	21	7.30
480	4972	193	3	2545	725	1109	37	7.32
552	4770	176	3	2799	813	1116	23	7.35
624	5186	194	3	2872	850	1092	13	7.33
696	5114	203	3	2789	725	1141	28	7.33
768	4819	211	3	2559	872	1126	20	7.42
888	4837	211	2	2517	854	1134	16	7.43
1008	4675	227	2	2270	649	1167	55	7.43
1080	4524	223	3	2459	571	1139	67	7.36
1248	0	0	0	0	0	0	0	0.00

Table F.2.1 show the variables in PVC1a – C1 Sample										
Day	Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
1	0.0	10180	168	104	5	6605	5567	1038	1115	-12
2	240.0	4235	205	55	7	4168	3400	723	1262	145
3	271.0	5926	213	57	11	5035	4305	730	1173	44
4	179.5	4605	202	82	2	3480	2757	723	1243	-14
5	188.0	8253	173	100	1	7173	4972	2201	1213	20
6	-73.0	7254	166	102	2	5803	4078	1725	1376	-11
7	116.5	9062	189	96	5	6699	5949	750	1380	-31
9	233.5	9184	256	92	3	5563	4115	1448	1428	-82
11	102.0	8590	253	92	3	5784	4565	1219	0	0
13	105.0	7225	283	119	3	4815	4229	586	1479	0
15	59.0	6520	263	28	5	5420	4269	1151	1443	54
17	59.0	8348	255	73	2	5588	4438	1150	1542	35
20	47.0	6648	254	85	2	5642	4245	1397	1734	49
23	4.0	6662	253	82	2	5560	3972	1588	1618	84
26	23.0	6806	236	57	2	5001	4064	937	1612	77
29	39.0	6570	274	78	2	6158	4253	1905	1600	20
32	21.0	6602	287	65	3	6643	3929	2714	1557	41
37	6.0	5966	272	70	4	6013	3703	2310	1607	12
42	-3.0	5454	267	73	4	2858	2612	246	1633	181
45	-11.5	5528	256	50	2	3162	2165	997	1408	101
52	87.0	5876	300	50	2	3888	3115	773	1695	182
Table F.2.2 show the variables in PVC1a – C2 Sample										
Day	Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
1	0	10180	168	104	5	6605	5567	1038	1115	-12
2	274	5070	224	57	8	4341	3439	902	1385	160
3	321	6984	231	47	12	5853	4867	986	1361	140
4	220	6327	236	99	3	4136	3162	974	1411	13
5	259	10424	194	111	0	8527	5997	2530	1411	80
6	5	9072	151	108	3	6067	4270	1962	1479	21
7	186	10637	213	106	7	6668	5874	919	1536	-2
9	357	9983	235	76	3	6139	4606	1362	1497	-16
11	186	9774	276	98	3	6061	4737	1221	-965	-25
13	188	8138	295	117	2	5833	4746	1150	1597	13
15	102	7580	293	29	5	5977	4526	1619	1553	0
17	106	9309	283	90	2	6182	4917	1103	1767	21
20	76	7806	283	79	3	6713	4878	1865	1962	51
23	26	8074	282	74	3	6185	4426	1655	1782	45
26	42	7798	263	80	2	6298	4910	1389	1806	111
29	54	7594	296	90	3	7348	5019	2428	1797	33
32	39	7514	326	80	3	6825	4278	2789	1768	49

37	31	7612	310	82	3	7257	4779	2195	1927	55
42	14	7016	303	55	4	4428	3679	662	1869	157
45	7	7418	300	65	4	4411	3223	1177	1622	61
52	101	7188	349	56	3	4017	3400	818	1933	135

Table F.2.3 show the variables in PVC1b-C1 Sample

Day	Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
1	0	10180	168	64	5	6605	5567	1038	1115	-12
2	-56	7705	201	99	6	5382	4408	929	1228	140
3	82	4830	212	106	8	2259	2067	192	1268	-13
4	28	7701	177	74	-1	4868	3893	975	1288	19
5	-1	10077	178	87	2	5647	4520	1127	1280	-35
6	-12	10170	207	92	5	3669	2956	713	1337	-81
7	-44	11600	192	86	3	5043	4055	988	1252	-42
9	-23	4310	262	110	3	3453	3007	446	1619	17
11	-9	5026	255	100	1	3192	2725	467	2721	56
13	-81	4917	285	88	3	2879	2781	98	1432	61
15	-31	4408	254	64	4	2764	2619	145	1521	109
17	-31	6018	213	66	1	3516	2726	790	1519	111
20	-31	5440	233	90	3	3610	3265	345	1473	98
23	-26	5594	253	105	2	3902	2920	982	1568	223
26	-19	6978	223	53	0	4141	3592	549	1635	305
29	-19	7522	280	71	1	4046	3711	335	1628	261
32	-20	6558	300	71	3	4605	3303	1302	1634	362
37	-35	5934	258	67	2	4183	2701	1482	1648	424
42	-21	5334	254	115	1	3318	2306	1012	1500	433
45	-15	4376	267	47	0	2338	1721	617	1255	414
52	-17	4108	316	51	1	2794	1937	857	1210	413

Table F.2.4 show the variables in PVC1b-C2 Sample

Day	Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
1	0	10180	168	64	5	6605	5567	1038	1115	-12
2	-22	8540	220	101	7	5555	4447	1108	1351	155
3	132	5888	230	96	9	3077	2629	448	1456	83
4	68	9423	211	91	1	5524	4298	1226	1456	45
5	70	12248	199	98	1	7001	5545	1456	1478	26
6	66	11988	192	98	6	3933	3148	950	1440	-49
7	26	13175	216	96	5	5012	3980	1157	1408	-13
9	101	5109	241	94	3	4029	3498	360	1688	83
11	75	6210	278	106	1	3469	2897	469	1756	31
13	2	5830	297	86	2	3897	3298	662	1550	74
15	12	5468	284	65	4	3321	2876	613	1631	55
17	16	6979	241	83	1	4110	3205	743	1744	97

20	-3	6598	262	84	4	4681	3898	813	1701	100
23	-4	7006	282	97	3	4527	3374	1049	1732	184
26	-1	7970	250	76	0	5438	4438	1001	1829	339
29	-4	8546	302	83	2	5236	4477	858	1825	274
32	-2	7470	339	86	3	4787	3652	1377	1845	370
37	-10	7580	296	79	1	5427	3777	1367	1968	467
42	-4	6896	290	97	1	4888	3373	1428	1736	409
45	4	6266	311	62	2	3587	2779	797	1469	374
52	-3	5420	365	57	2	2923	2222	902	1448	366

Table F.2.5 show the variables in PVC1a-Cave Sample

Day	Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
1	0	10180	168	104	5	6605	5567	1038	1115	-12
2	257	4653	215	56	8	4255	3420	813	1324	152
3	296	6455	222	52	11	5444	4586	858	1267	92
4	200	5466	219	91	2	3808	2960	849	1327	-1
5	224	9339	183	105	0	7850	5485	2366	1312	50
6	-34	8163	158	105	2	5935	4174	1844	1427	5
7	151	9850	201	101	6	6684	5912	835	1458	-16
9	295	9584	245	84	3	5851	4361	1405	1462	-49
11	144	9182	265	95	3	5923	4651	1220	-483	-13
13	147	7682	289	118	3	5324	4488	868	1538	7
15	81	7050	278	28	5	5699	4398	1385	1498	27
17	83	8829	269	81	2	5885	4678	1127	1654	28
20	61	7227	268	82	2	6178	4562	1631	1848	50
23	15	7368	267	78	2	5873	4199	1622	1700	65
26	32	7302	250	69	2	5650	4487	1163	1709	94
29	47	7082	285	84	2	6753	4636	2167	1698	26
32	30	7058	306	72	3	6734	4104	2752	1662	45
37	19	6789	291	76	3	6635	4241	2253	1767	33
42	6	6235	285	64	4	3643	3146	454	1751	169
45	-2	6473	278	57	3	3787	2694	1087	1515	81
52	94	6532	324	53	3	3953	3258	796	1814	159

Table F.2.6 show the variables in PVC1b-Cave Sample

Day	Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
1	0	10180	168	64	5	6605	5567	1038	1115	-12
2	126	8123	211	100	7	5469	4428	1019	1290	147
3	227	5359	221	101	8	2668	2348	320	1362	35
4	144	8562	194	83	0	5196	4096	1101	1372	32
5	165	11163	188	92	1	6324	5033	1292	1379	-4
6	36	11079	199	95	5	3801	3052	832	1388	-65
7	106	12388	204	91	4	5028	4018	1073	1330	-27
9	229	4710	251	102	3	3741	3253	403	1653	50

11	131	5618	267	103	1	3331	2811	468	2239	44
13	95	5374	291	87	3	3388	3040	380	1491	68
15	57	4938	269	64	4	3043	2748	379	1576	82
17	61	6499	227	74	1	3813	2966	767	1631	104
20	37	6019	247	87	3	4146	3582	579	1587	99
23	11	6300	267	101	2	4215	3147	1016	1650	204
26	21	7474	237	65	0	4790	4015	775	1732	322
29	25	8034	291	77	1	4641	4094	597	1726	267
32	19	7014	319	78	3	4696	3478	1340	1739	366
37	11	6757	277	73	1	4805	3239	1425	1808	445
42	5	6115	272	106	1	4103	2840	1220	1618	421
45	6	5321	289	54	1	2963	2250	707	1362	394
52	49	4764	340	54	2	2859	2080	880	1329	390

Table F.2.7 show the variables in PVC1ave-Cave Sample

Day	Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
1	0	10180	168	84	5	6605	5567	1038	1115	-12
2	109	6388	213	78	7	4862	3924	916	1307	150
3	202	5907	221	76	10	4056	3467	589	1315	64
4	124	7014	206	87	1	4502	3528	975	1350	16
5	129	10251	186	99	1	7087	5259	1829	1345	23
6	-4	9621	179	100	4	4868	3613	1338	1408	-30
7	71	11119	202	96	5	5856	4965	954	1394	-22
9	167	7147	248	93	3	4796	3807	904	1558	1
11	89	7400	266	99	2	4627	3731	844	878	16
13	54	6528	290	103	3	4356	3764	624	1514	37
15	36	5994	273	46	5	4371	3573	882	1537	55
17	38	7664	248	78	2	4849	3822	947	1643	66
20	22	6623	258	84	3	5162	4072	1105	1718	74
23	0	6834	267	89	2	5044	3673	1319	1675	134
26	11	7388	243	67	1	5220	4251	969	1720	208
29	18	7558	288	81	2	5697	4365	1382	1712	147
32	10	7036	313	75	3	5715	3791	2046	1701	205
37	-2	6773	284	74	2	5720	3740	1839	1787	239
42	-4	6175	279	85	2	3873	2993	837	1685	295
45	-4	5897	283	56	2	3375	2472	897	1438	237
52	42	5648	332	53	2	3406	2669	838	1572	274

Table F.3.1 show the variables in PVC2a-C1 Sample									
Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10220	197	97	7	5879	5585	294	1177	129
263	3595	214	45	4	3834	3476	313	1197	245
328	2078	269	80	10	1471	1261	210	1191	14
280	1357	188	72	1	2454	2331	123	1242	-5
181	1253	187	70	3	1047	874	173	1279	-73
148	1462	224	82	3	1207	800	407	1394	191
122	954	203	54	8	575	471	104	1326	-35
266	1298	245	85	6	1423	1069	354	1326	-110
172	3322	253	51	4	3314	2611	703	0	0
99	3703	269	41	5	2625	2329	296	1408	16
139	4272	239	29	6	2412	2137	275	1247	4
103	8542	231	73	2	4228	3608	620	1415	26
-10	6524	220	66	3	4134	3597	537	1444	63
26	6856	210	61	6	5222	4104	1118	1498	4
11	6086	239	48	3	3883	3236	647	1479	47
9	6162	257	52	2	3980	3577	403	1496	15
-2	6254	268	44	3	4615	3873	742	1598	10
23	5654	267	49	6	4043	3335	708	1531	13
20	5698	257	71	5	3302	2918	384	1503	62
17	5844	263	47	3	4130	3261	869	1425	20
-17	6040	273	53	3	4458	3939	519	1446	20
Table F.3.2 show the variables in PVC2a-C2 Sample									
Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10220	197	97	7	5879	5585	294	294	129
297	4430	233	47	5	4007	3515	492	492	260
378	3136	287	70	11	2289	1823	466	466	110
320	3079	222	89	2	3110	2736	374	374	22
252	3424	208	81	2	2401	1899	502	502	-12
226	3280	209	88	4	1471	992	644	644	223
191	2529	227	64	10	544	396	273	273	-6
389	2097	224	69	6	1999	1560	268	268	-44
256	4506	276	57	4	3591	2783	705	705	-25
182	4616	281	39	4	3643	2846	860	860	29
182	5332	269	30	6	2969	2394	743	743	-50
150	9503	259	90	2	4822	4087	573	573	12
19	7682	249	60	4	5205	4230	1005	1005	65
48	8268	239	53	7	5847	4558	1185	1185	-35
30	7078	266	71	3	5180	4082	1099	1099	81
24	7186	279	64	3	5170	4343	926	926	28
16	7166	307	59	3	4797	4222	817	817	18

48	7300	305	61	5	5287	4411	593	593	56
37	7260	293	53	5	4872	3985	800	800	38
35	7734	307	62	5	5379	4319	1049	1049	-20
-3	7352	322	59	4	4587	4224	564	564	-27

Table F.3.3 show the variables in PVC2b-C1 Sample

Gas	COD mg/l	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10220	196	75	7	5479	5185	294	1177	129
17	5415	216	97	8	4364	3422	897	1243	252
86	4140	262	125	11	3509	2625	884	1088	15
55	5841	165	79	-1	3372	2633	739	1268	80
24	2491	165	95	1	2239	1692	547	1223	-43
-13	2908	202	83	3	3027	2810	217	1359	100
-26	2490	197	78	5	1355	1213	142	1321	-22
-23	2638	243	117	5	1749	1411	338	1636	49
-17	3480	246	95	2	2392	1977	415	2632	74
-9	5287	297	55	3	3119	2555	564	1572	86
-37	4976	257	87	3	3224	2647	577	1451	12
-26	5794	224	87	1	3790	2854	936	1503	79
-33	4800	246	98	4	3106	2501	605	1570	100
-29	4902	269	87	2	4734	3526	1208	1545	111
-24	4974	267	36	2	3125	2414	711	1607	244
-19	4418	282	78	1	2684	2057	627	1631	286
-20	5102	287	46	2	3067	2187	880	1692	396
-39	3934	263	51	1	1973	1245	728	1528	370
-19	3290	248	96	0	1010	890	120	1440	435
-14	3156	299	46	-1	1192	755	437	1339	414
-17	2876	320	43	0	1128	667	461	1288	17

Table F.3.4 show the variables in PVC2b-C2 Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10220	196	75	7	5479	5185	294	1177	129
51	6250	235	99	9	4537	3461	1076	1366	267
136	5198	280	115	11	4327	3187	1140	1276	111
95	7563	198	96	0	4028	3038	990	1436	106
95	4662	186	106	1	3593	2717	876	1421	18
65	4726	186	89	4	3291	3002	454	1462	132
44	4065	222	88	7	1324	1138	311	1477	8
101	3437	222	101	6	2325	1902	252	1705	115
67	4664	269	101	2	2669	2149	417	1667	49
74	6200	309	53	2	4137	3072	1128	1690	99
6	6036	288	88	3	3781	2904	1045	1561	-42
21	6755	253	104	1	4384	3333	889	1728	65
-5	5958	275	92	5	4177	3134	1073	1798	102

-7	6314	298	79	2	5359	3980	1275	1709	72
-6	5966	294	59	2	4422	3260	1163	1801	278
-4	5442	304	90	1	3874	2823	1150	1828	299
-2	6014	326	61	2	3249	2536	955	1903	404
-14	5580	301	63	0	3217	2321	613	1848	413
-2	4852	284	78	1	2580	1957	536	1676	411
5	5046	342	61	0	2441	1813	617	1553	374
-3	4188	369	49	1	1257	952	506	1526	419

Table F.3.5 show the variables in PVC2a-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10220	197	97	7	5879	5585	294	1177	129
280	4013	224	46	5	3921	3496	403	1259	252
353	2607	278	75	10	1880	1542	338	1285	62
300	2218	205	81	1	2782	2534	249	1326	9
217	2339	197	75	2	1724	1387	338	1378	-42
187	2371	216	85	3	1339	896	526	1445	207
156	1742	215	59	9	560	434	189	1404	-20
327	1698	234	77	6	1711	1315	311	1360	-77
214	3914	265	54	4	3453	2697	704	-483	-13
141	4160	275	40	5	3134	2588	578	1467	23
161	4802	254	29	6	2691	2266	509	1302	-23
127	9023	245	81	2	4525	3848	597	1527	19
4	7103	234	63	3	4670	3914	771	1558	64
37	7562	224	57	6	5535	4331	1152	1580	-16
20	6582	253	60	3	4532	3659	873	1576	64
17	6674	268	58	2	4575	3960	665	1594	21
7	6710	287	51	3	4706	4048	780	1703	14
36	6477	286	55	5	4665	3873	651	1691	34
29	6479	275	62	5	4087	3452	592	1621	50
26	6789	285	54	4	4755	3790	959	1532	0
-10	6696	297	56	4	4523	4082	542	1565	-4

Table F.3.6 show the variables in PVC2b-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10220	196	75	7	5479	5185	294	1177	129
34	5833	225	98	9	4451	3442	987	1305	259
111	4669	271	120	11	3918	2906	1012	1182	63
75	6702	181	88	-1	3700	2836	865	1352	93
60	3577	176	100	1	2916	2205	712	1322	-12
26	3817	194	86	4	3159	2906	336	1410	116
9	3278	210	83	6	1340	1176	227	1399	-7
39	3038	233	109	5	2037	1657	295	1670	82
25	4072	258	98	2	2531	2063	416	2150	62

33	5744	303	54	2	3628	2814	846	1631	93
-16	5506	272	87	3	3503	2776	811	1506	-15
-3	6275	238	95	1	4087	3094	913	1615	72
-19	5379	260	95	4	3642	2818	839	1684	101
-18	5608	283	83	2	5047	3753	1242	1627	92
-15	5470	280	48	2	3774	2837	937	1704	261
-12	4930	293	84	1	3279	2440	889	1729	292
-11	5558	307	53	2	3158	2362	918	1797	400
-27	4757	282	57	0	2595	1783	671	1688	391
-11	4071	266	87	0	1795	1424	328	1558	423
-4	4101	321	53	0	1817	1284	527	1446	394
-10	3532	345	46	0	1193	810	484	1407	443

Table F.3.7 show the variables in PVC2ave-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10220	196	86	7	5679	5385	294	1177	129
157	4923	224	72	7	4186	3469	695	1282	256
232	3638	274	97	11	2899	2224	675	1234	63
187	4460	193	84	0	3241	2685	557	1339	51
138	2958	186	88	2	2320	1796	525	1350	-27
107	3094	205	85	3	2249	1901	431	1428	162
83	2510	212	71	8	950	805	208	1402	-14
183	2368	233	93	6	1874	1486	303	1515	3
120	3993	261	76	3	2992	2380	560	834	25
87	4952	289	47	3	3381	2701	712	1549	58
73	5154	263	58	4	3097	2521	660	1404	-19
62	7649	242	88	1	4306	3471	755	1571	46
-7	6241	247	79	4	4156	3366	805	1621	82
10	6585	254	70	4	5291	4042	1197	1604	38
3	6026	266	54	3	4153	3248	905	1640	162
3	5802	280	71	2	3927	3200	777	1662	157
-2	6134	297	52	2	3932	3205	849	1750	207
5	5617	284	56	3	3630	2828	661	1689	213
9	5275	270	74	3	2941	2438	460	1590	236
11	5445	303	54	2	3286	2537	743	1489	197
-10	5114	321	51	2	2858	2446	513	1486	220

Table F.4.1 show the variables in PVC3a-C1 Sample									
Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0.0	10100	192	102	7	6007	4725	1282	1048	202
312.0	4445	217	69	12	2648	1976	627	1178	196
357.0	4156	267	66	9	2593	1997	596	1157	-84
192.5	2943	199	91	2	2546	1893	653	1241	-30
122.0	2531	174	99	4	2513	1884	629	1304	-39
117.0	3862	235	93	8	2923	2248	675	1310	-55
98.5	3838	210	94	8	2467	2051	416	1303	-29
94.5	4488	263	105	8	3725	2835	890	1740	55
35.0	4158	246	75	4	3754	3049	705	0	0
139.0	4683	263	47	3	3195	2889	306	1356	5
144.0	4176	230	44	6	2738	2437	301	1380	66
54.0	7516	227	55	5	5286	4336	950	1387	-2
7.0	6248	234	113	2	4458	3943	515	1323	-34
27.0	8134	242	109	6	6180	4524	1656	1531	33
22.0	6226	213	51	4	4851	4162	689	1549	35
7.0	6118	260	42	4	4204	3619	585	1445	-49
3.0	6078	259	49	3	4897	4061	836	1310	-163
-1.0	5966	236	77	5	5697	3915	1782	1429	10
5.0	5618	259	83	5	3974	3370	604	1281	-36
4.5	5620	256	47	3	4498	3669	829	1458	-2
-8.0	5600	284	63	2	3674	2951	723	1340	-69
Table F.4.2 show the variables in PVC3a-C2 Sample									
Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10100	192	102	7	6007	4725	1282	1048	202
346	5280	236	71	13	2821	2015	806	1301	211
407	5214	285	56	10	3411	2559	852	1345	12
233	4665	233	108	3	3202	2298	904	1409	-4
193	4702	195	110	3	3867	2909	958	1502	22
195	5680	220	99	9	3187	2440	912	1413	-23
168	5413	234	104	10	2436	1976	585	1459	1
218	5287	242	89	8	4301	3326	804	1809	121
119	5342	269	81	4	4031	3221	707	-965	-25
222	5596	275	45	2	4213	3406	870	1474	18
187	5236	260	45	6	3295	2694	769	1490	12
101	8477	255	72	5	5880	4815	903	1612	-16
36	7406	263	107	3	5529	4576	983	1551	-33
49	9546	271	101	7	6805	4978	1723	1695	-6
41	7218	240	74	4	6148	5008	1141	1743	69
22	7142	282	54	5	5394	4385	1108	1642	-35
21	6990	298	64	3	5079	4410	911	1521	-154

24	7612	274	89	4	6941	4991	1667	1749	53
22	7180	295	65	5	5544	4437	1020	1517	-59
23	7510	300	62	5	5747	4727	1009	1672	-41
6	6912	333	69	3	3803	3236	768	1578	-116

Table F.4.3 show the variables in PVC3b-C1 Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10100	192	70	7	6007	4725	1282	1048	202
68	6875	233	97	9	5882	4144	1693	1166	202
108	6112	252	102	10	4747	3685	1062	1181	-14
46	6213	158	80	0	5002	3837	1165	1314	62
-30	5347	164	100	2	4083	3206	877	1180	-36
-78	6590	227	111	3	3617	2472	1145	1484	99
-70	6418	184	86	4	4301	3309	992	1306	19
-24	7078	244	95	3	4043	3069	974	1565	13
-24	4172	243	89	2	4716	3661	1055	3040	285
-34	5749	241	99	3	3629	3011	618	1505	-83
-58	6180	242	72	4	4116	3235	881	1438	47
-41	5702	230	84	2	3602	2824	778	1502	173
-29	4572	260	105	3	2632	2171	461	1392	-34
-25	5062	289	91	3	3474	2642	832	1625	55
-20	4486	232	82	2	2723	2156	567	1463	49
-18	4982	267	65	0	3336	2579	757	1515	28
-20	5474	265	42	3	4333	3293	1040	1510	84
-32	4170	272	51	2	2527	1835	692	1516	50
-21	3702	272	96	0	2232	1860	372	1469	84
-18	4176	315	48	0	1648	1245	403	1382	88
-18	3880	363	53	-1	1910	1155	755	1434	-3

Table F.4.4 show the variables in PVC3b-C2 Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10100	192	70	7	6007	4725	1282	1048	202
102	7710	252	99	10	6055	4183	1872	1289	217
158	7170	270	92	11	5565	4247	1318	1369	82
86	7935	192	97	2	5658	4242	1416	1482	88
41	7518	185	111	1	5437	4231	1206	1378	25
0	8408	212	117	4	3881	2664	1382	1587	131
0	7993	208	96	6	4270	3234	1161	1462	49
100	7877	223	79	3	4619	3560	888	1634	79
60	5356	266	95	2	4993	3833	1057	2075	260
49	6662	253	97	2	4647	3528	1182	1623	-70
-15	7240	273	73	4	4673	3492	1349	1548	-7
6	6663	259	101	2	4196	3303	731	1727	159
-1	5730	288	99	3	3703	2804	929	1620	-33

-3	6474	318	83	3	4099	3096	899	1789	16
-2	5478	259	105	2	4020	3002	1019	1657	83
-3	6006	289	77	1	4526	3345	1280	1712	41
-2	6386	304	57	3	4515	3642	1115	1721	92
-7	5816	310	63	0	3771	2911	577	1836	93
-4	5264	308	78	0	3802	2927	788	1705	60
1	6066	359	63	1	2897	2303	583	1596	48
-4	5192	412	59	0	2039	1440	800	1672	-50

Table F.4.5 show the variables in PVC3a-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10100	192	102	7	6007	4725	1282	1048	202
190	5660	225	70	11	6055	1996	717	1240	203
233	5134	259	61	10	5565	2278	724	1251	-36
119	4578	179	100	1	5658	2096	779	1325	-17
46	3939	169	104	3	5437	2397	794	1403	-8
20	5226	231	96	5	3881	2344	794	1361	-39
15	5128	197	99	6	4270	2014	501	1381	-14
36	5783	253	97	5	4619	3081	847	1774	88
6	4165	245	78	3	4993	3135	706	-483	-13
53	5216	252	46	3	4647	3148	588	1415	12
43	5178	236	44	5	4673	2566	535	1435	39
7	6609	228	63	4	4196	4576	927	1499	-9
-11	5410	247	110	2	3703	4260	749	1437	-33
1	6598	265	105	4	4099	4751	1690	1613	14
1	5356	222	63	3	4020	4585	915	1646	52
-6	5550	263	48	2	4526	4002	847	1543	-42
-9	5776	262	56	3	4515	4236	874	1415	-158
-17	5068	254	83	3	3771	4453	1725	1589	31
-8	4660	266	74	2	3802	3904	812	1399	-47
-7	4898	286	54	1	2897	4198	919	1565	-21
-13	4740	323	66	1	2039	3094	746	1459	-93

Table F.4.6 show the variables in PVC3b-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10100	192	70	7	6007	4725	1282	1048	202
224	6495	244	98	12	5969	4164	1783	1228	206
283	6192	277	97	10	5156	3966	1190	1275	-1
160	6300	212	89	2	5330	4040	1291	1398	29
117	6110	190	105	2	4760	3719	1042	1279	-7

98	7044	216	114	6	3749	2568	1264	1535	38
84	6703	221	91	8	4286	3272	1077	1384	10
159	6582	232	87	6	4331	3315	931	1599	67
90	5349	268	92	3	4855	3747	1056	2558	130
136	6129	264	98	2	4138	3270	900	1564	-33
86	6238	266	72	5	4395	3364	1115	1493	30
54	7570	257	92	4	3899	3064	755	1614	79
18	6568	275	102	3	3168	2488	695	1506	-33
23	8010	294	87	5	3787	2869	866	1707	25
20	6348	249	94	3	3372	2579	793	1560	59
10	6574	285	71	3	3931	2962	1019	1613	-4
10	6688	301	49	3	4424	3468	1078	1615	-35
9	6714	292	57	2	3149	2373	635	1676	51
9	6222	302	87	3	3017	2394	580	1587	12
12	6788	329	55	3	2273	1774	493	1489	23
1	6052	372	56	2	1975	1298	778	1553	-60

Table F.4.7 show the variables in PVC3ave-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	10100	192	86	7	6007	4725	1282	1048	202
207	6078	235	84	11	4352	3080	1250	1234	206
258	5663	268	79	10	4079	3122	957	1263	-1
139	5439	195	94	2	4102	3068	1035	1362	29
82	5025	179	105	2	3975	3058	918	1341	-7
59	6135	223	105	6	3402	2456	1029	1448	38
49	5916	209	95	7	3369	2643	789	1383	10
97	6183	243	92	5	4172	3198	889	1687	67
48	4757	256	85	3	4374	3441	881	1038	130
94	5673	258	72	2	3921	3209	744	1489	-33
65	5708	251	58	5	3706	2965	825	1464	30
30	7090	243	78	4	4741	3820	841	1557	79
3	5989	261	106	3	4081	3374	722	1472	-33
12	7304	280	96	5	5140	3810	1278	1660	25
10	5852	236	78	3	4436	3582	854	1603	59
2	6062	274	60	2	4365	3482	933	1578	-4
1	6232	281	53	3	4706	3852	976	1515	-35
-4	5891	273	70	3	4734	3413	1180	1632	51
1	5441	284	80	2	3888	3149	696	1493	12
3	5843	307	55	2	3698	2986	706	1527	23
-6	5396	348	61	1	2857	2196	762	1506	-60

Table F.5.1 show the variables in PVC4a-C1 Sample									
Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	9420	193	85	8	6207	4869	1338	1029	212
354	6585	218	82	11	4572	3082	1445	1302	342
427	5216	269	67	11	4503	3371	1132	1337	206
317	6947	199	97	2	7126	4607	2519	1246	81
213	7143	163	88	2	6261	3904	2357	1248	-23
151	8340	236	102	5	6175	3778	2397	1375	-25
88	7184	223	84	7	5115	3903	1212	1416	46
65	7456	257	88	7	5741	4573	1168	1482	-22
18	7094	266	78	4	5804	4645	1159	0	0
108	6505	272	103	1	4375	3873	502	1372	-23
152	5980	246	93	5	4316	3499	817	1485	77
79	7570	255	62	4	5106	3952	1154	1523	56
72	6088	252	71	3	5154	4009	1145	1466	-2
35	7918	249	68	4	7396	4914	2482	1462	-9
48	7726	249	56	4	6467	3660	2807	1597	-2
21	5810	278	49	2	4458	3537	921	1566	51
16	5646	265	51	3	4849	3817	1032	1451	44
-18	5622	276	59	6	4019	3153	866	1588	232
-17	5274	272	89	5	3582	3044	538	1529	228
-3	5356	268	53	3	4792	3461	1331	1502	218
11	5864	279	63	3	5216	3837	1379	1486	277
Table F.5.2 show the variables in PVC4a-C2 Sample									
Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	9420	193	85	8	6207	4869	1338	1029	212
354	6585	218	82	11	4572	3082	1445	1425	342
427	5216	269	67	11	4503	3371	1132	1525	206
317	6947	199	97	2	7126	4607	2519	1414	81
213	7143	163	88	2	6261	3904	2357	1446	-23
151	8340	236	102	5	6175	3778	2397	1478	-25
88	7184	223	84	7	5115	3903	1212	1572	46
65	7456	257	88	7	5741	4573	1168	1551	-22
18	7094	266	78	4	5804	4645	1159	-965	0
108	6505	272	103	1	4375	3873	502	1490	-23
152	5980	246	93	5	4316	3499	817	1595	77
79	7570	255	62	4	5106	3952	1154	1748	56
72	6088	252	71	3	5154	4009	1145	1694	-2
35	7918	249	68	4	7396	4914	2482	1626	-9
48	7726	249	56	4	6467	3660	2807	1791	-2
21	5810	278	49	2	4458	3537	921	1763	51
16	5646	265	51	3	4849	3817	1032	1662	44

-18	5622	276	59	6	4019	3153	866	1908	232
-17	5274	272	89	5	3582	3044	538	1765	228
-3	5356	268	53	3	4792	3461	1331	1716	218
11	5864	279	63	3	5216	3837	1379	1724	277

Table F.5.3 show the variables in PVC4b-C1 Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	9420	192	80	8	6207	4869	1338	1029	212
-56	4795	232	100	9	3818	3222	551	1250	329
52	5288	272	86	9	5585	4013	1572	1222	92
83	8989	161	61	-2	8272	5207	3065	1306	153
33	7261	218	100	3	8849	5912	2937	1392	84
14	7278	243	100	4	6599	4918	1681	1471	-3
7	9834	215	86	5	7187	4521	2666	1461	113
-10	7540	260	108	4	6483	3951	2532	1590	18
-38	5808	291	105	6	5388	3651	1737	0	0
-55	5305	277	80	3	4295	3179	1116	1540	75
-58	5168	260	85	5	4012	2861	1151	1534	95
-22	6462	252	98	2	3746	2822	924	1408	75
-35	5700	265	104	3	3506	2685	821	1612	232
-31	4786	278	107	4	3178	2456	722	1622	291
-23	5678	262	95	3	4087	3140	947	1655	336
-19	4618	316	51	3	2160	1743	417	1659	311
-22	4402	294	44	3	2129	1789	340	1542	217
-34	4382	298	58	3	2261	1909	352	1574	273
-21	4702	268	105	2	2144	1930	214	1645	245
-15	4744	312	52	1	3350	2415	935	1564	107
-16	4408	367	59	0	3484	2437	1047	1595	73

Table F.5.4 show the variables in PVC4b-C2 Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	9420	192	80	8	6207	4869	1338	1029	212
-22	5630	251	102	10	3991	3261	730	1373	344
102	6346	290	76	9	6403	4575	1828	1410	188
123	10711	194	78	0	8928	5612	3316	1474	179
104	9432	239	111	2	10203	6937	3266	1590	144
92	9096	228	106	5	6863	5110	1918	1574	29
76	11409	239	96	7	7156	4446	2835	1617	143
114	8339	239	92	4	7059	4442	2446	1659	84
46	6992	314	111	6	5665	3823	1739	-965	-25
28	6218	289	78	2	5313	3696	1680	1658	88
-15	6228	291	86	5	4569	3118	1619	1644	41
25	7423	281	115	2	4340	3301	877	1633	61

-7	6858	294	98	3	4577	3318	1289	1840	234
-9	6198	307	99	4	3803	2910	789	1786	252
-5	6670	289	118	3	5384	3986	1399	1849	370
-4	5642	338	63	3	3350	2509	940	1856	324
-4	5314	333	59	3	2311	2138	415	1753	225
-9	6028	336	70	2	3505	2985	237	1894	316
-4	6264	304	87	2	3714	2997	630	1881	221
4	6634	355	67	2	4599	3473	1115	1778	67
-2	5720	416	65	1	3613	2722	1092	1833	26

Table F.5.5 show the variables in PVC4a-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	9420	192	85	8	6207	4869	1338	1029	212
149	5690	225	83	10	4659	3102	1535	1364	349
240	5252	270	62	10	4912	3652	1260	1431	254
200	7968	180	106	0	7454	4810	2645	1330	94
123	7202	190	93	2	6938	4417	2522	1347	8
83	7809	240	105	4	6307	3874	2516	1426	-9
47	8509	219	89	6	5100	3866	1297	1494	61
28	7498	258	80	5	6029	4819	1125	1516	11
-10	6451	279	81	5	5943	4731	1160	-483	-13
27	5905	274	102	2	4884	4132	784	1431	-17
47	5574	253	93	5	4595	3628	1051	1540	50
29	7016	253	70	3	5403	4192	1131	1635	49
19	5894	259	68	3	5690	4326	1379	1580	-1
2	6352	263	64	4	7709	5141	2516	1544	-29
13	6702	255	68	3	7116	4083	3033	1694	15
1	5214	297	55	2	5053	3920	1183	1664	57
-3	5024	279	58	3	4940	3992	1070	1556	48
-26	5002	287	65	5	4641	3691	809	1748	253
-19	4988	270	80	3	4367	3578	746	1647	216
-9	5050	290	60	2	5417	3990	1421	1609	198
-3	5136	323	66	1	5281	3980	1402	1605	254

Table F.5.6 show the variables in PVC4b-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	9420	192	80	8	6207	4869	1338	1029	212
183	6525	244	101	11	3905	3242	641	1312	336
290	6310	288	81	10	5994	4294	1700	1316	140
240	9690	213	70	1	8600	5410	3191	1390	166
194	9373	211	105	2	9526	6425	3102	1491	114
161	9627	224	103	5	6731	5014	1800	1522	13
117	10084	243	91	8	7172	4484	2751	1539	128
151	8297	237	100	6	6771	4197	2489	1624	51

74	7635	302	108	5	5527	3737	1738	-483	-13
110	6818	286	79	1	4804	3438	1398	1599	82
90	6634	283	85	5	4291	2990	1385	1589	68
76	7977	282	106	3	4043	3062	901	1520	68
47	7052	287	101	3	4042	3002	1055	1726	233
24	7764	292	103	4	3491	2683	756	1704	272
31	7694	282	107	3	4736	3563	1173	1752	353
16	6238	319	57	3	2755	2126	679	1757	317
15	5936	318	51	3	2220	1964	378	1647	221
-1	6648	325	64	3	2883	2447	295	1734	294
-2	6550	306	96	4	2929	2464	422	1763	233
10	6940	333	59	3	3975	2944	1025	1671	87
12	6448	372	62	2	3549	2580	1070	1714	50

Table F.5.7 show the variables in PVC4ave-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	9420	298	82	8	6207	4869	1338	1029	212
166	6108	371	92	11	4282	3172	1088	1338	343
265	5781	390	71	10	5453	3973	1480	1374	197
220	8829	392	88	1	8027	5110	2918	1360	130
159	8288	294	99	2	8232	5421	2812	1419	61
122	8718	499	104	5	6519	4444	2158	1474	2
82	9297	519	90	7	6136	4175	2024	1517	94
89	7898	481	90	5	6400	4508	1807	1570	31
32	7043	474	94	5	5735	4234	1449	-483	-13
68	6362	338	91	1	4844	3785	1091	1515	33
69	6104	400	89	5	4443	3309	1218	1564	59
52	7497	330	88	3	4723	3627	1016	1578	59
33	6473	281	84	3	4866	3664	1217	1653	116
13	7058	345	83	4	5600	3912	1636	1624	122
22	7198	354	87	3	5926	3823	2103	1723	184
9	5726	342	56	3	3904	3023	931	1711	187
6	5480	284	55	3	3580	2978	724	1602	134
-14	5825	313	64	4	3762	3069	552	1741	274
-11	5769	281	88	3	3648	3021	584	1705	224
1	5995	322	60	3	4696	3467	1223	1640	142
5	5792	309	64	2	4415	3280	1236	1660	152

Table F.6.1 show the variables in PVC5a-C1 Sample									
Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	12280	10	102	8	6527	5123	1404	1082	191
16	4005	0	63	9	4840	3846	949	1189	202
107	9394	0	64	4	4617	3903	714	1110	29
293	4791	0	84	0	4184	3171	1013	1177	21
124	4215	39	83	3	4081	3090	991	998	0
57	5648	0	103	5	4035	3068	967	1213	0
51	6624	0	81	11	4603	3381	1222	1239	0
57	6002	20	76	8	4127	3091	1036	1497	50
20	5206	0	24	4	5008	3953	1055	0	0
142	4027	34	107	6	3545	3101	444	1271	14
203	4456	47	40	8	3846	3161	685	1343	44
81	7054	0	103	6	5164	4238	926	1270	3
36	6226	0	109	1	4538	3967	571	1261	0
5	6464	0	66	4	5170	5908	1065	1381	50
7	6186	0	58	4	4575	3668	907	1367	7
7	6278	0	51	2	4368	3909	459	1445	49
5	6278	0	51	4	4985	4061	924	1416	42
9	6230	0	54	9	4495	3743	752	1321	0
12	5294	0	59	7	3798	3354	444	1307	0
22	5244	0	62	5	4156	3259	897	1314	0
5	5460	0	52	4	4602	3553	1049	1345	8
Table F.6.2 show the variables in PVC5a-C2 Sample									
Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	12280	12	102	8	6527	5123	1404	1082	191
50	4840	0	65	10	5013	3885	1128	1312	217
157	10452	12	54	5	5435	4465	970	1298	125
333	6513	0	101	0	4840	3576	1264	1345	47
195	6386	60	94	2	5435	4115	1320	1196	0
135	7466	0	109	6	4299	3260	1204	1316	17
120	8199	0	91	13	4572	3306	1391	1395	0
180	6801	0	60	8	4703	3582	950	1566	116
104	6390	0	30	4	5285	4125	1057	-965	0
225	4940	46	105	5	4563	3618	1008	1389	27
246	5516	77	41	8	4403	3418	1153	1453	0
128	8015	0	120	6	5758	4717	879	1495	0
65	7384	0	103	2	5609	4600	1039	1489	0
27	7876	0	58	5	5795	6362	1132	1545	11
26	7178	0	81	4	5872	4514	1359	1561	41
22	7302	0	63	3	5558	4675	982	1642	62
23	7190	0	66	4	5167	4410	999	1627	50

34	7876	0	66	8	5739	4819	637	1641	6
29	6856	0	41	7	5368	4421	860	1543	0
40	7134	0	77	7	5405	4317	1077	1528	0
19	6772	0	58	5	4731	3838	1094	1583	0

Table F.6.3 show the variables in PVC5b-C1 Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	12280	163	67	8	6527	5123	1404	1082	191
24	7565	213	86	8	5466	4172	1249	1211	186
115	7456	237	92	7	6667	4753	1914	1401	61
-5	5131	173	84	2	6000	4395	1605	1269	32
-11	6425	169	109	1	6793	4410	2383	1245	0
-2	8036	217	88	4	6243	4448	1795	1286	7
-3	9220	181	81	7	3861	2981	880	1131	0
2	8510	211	86	3	7131	5145	1986	1459	0
-12	9694	247	109	2	8242	6127	2115	0	0
-23	7733	240	96	3	7009	5777	1232	1282	19
-29	7040	236	52	6	6042	4893	1149	1382	79
-4	5978	0	74	2	4108	3510	598	1275	0
10	6296	0	111	2	5170	3967	1203	1409	44
10	5926	0	104	2	5808	3496	2312	1624	55
8	4966	0	81	3	4139	3354	785	1528	136
17	6042	0	69	1	4284	3495	789	1463	185
10	5434	0	50	3	5213	4099	1114	1500	165
19	5406	0	58	2	4363	3355	1008	1466	183
29	4782	0	101	0	3424	2802	622	1573	326
37	4828	0	52	0	3608	2625	983	1234	131
29	3860	0	50	0	2544	1881	663	1178	105

Table F.6.4 show the variables in PVC5b-C2 Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	12280	163	67	8	6527	5123	1404	1082	191
58	8400	232	88	9	5639	4211	1428	1334	201
165	8514	255	82	8	7485	5315	2170	1589	157
36	6853	207	101	4	6656	4800	1856	1437	58
60	8596	190	120	1	8147	5435	2712	1443	7
76	9854	202	94	5	6507	4640	2032	1389	39
67	10795	206	91	9	3830	2906	1049	1287	0
125	9309	190	70	3	7707	5636	1900	1528	60
72	10878	270	115	2	8519	6299	2117	-965	0
60	8646	252	94	2	8027	6294	1796	1400	32
14	8100	267	53	6	6599	5150	1617	1492	25
43	6939	0	91	2	4702	3989	551	1500	0
39	7454	0	105	3	6241	4600	1671	1637	46

32	7338	0	96	3	6433	3950	2379	1788	16
27	5958	0	104	3	5436	4200	1237	1722	170
32	7066	0	81	1	5474	4261	1312	1660	198
28	6346	0	65	3	5395	4448	1189	1711	173
44	7052	0	70	0	5607	4431	893	1786	226
46	6344	0	83	1	4994	3869	1038	1809	302
55	6718	0	67	1	4857	3683	1163	1448	91
43	5172	0	56	1	2673	2166	708	1416	58

Table F.6.5 show the variables in PVC5a-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	12280	4	102	8	6527	5123	1404	1082	191
20	5785	55	64	8	4927	3866	1039	1251	209
111	8425	115	59	6	5026	4184	842	1204	77
144	4961	178	93	0	4512	3374	1139	1261	34
57	5320	104	88	2	4758	3603	1156	1097	-96
28	6842	106	106	4	4167	3164	1086	1264	1
24	7922	66	86	9	4588	3344	1307	1317	-99
29	7256	115	68	5	4415	3337	993	1531	83
4	7450	76	27	3	5147	4039	1056	-483	-13
60	5880	137	106	5	4054	3360	726	1330	21
87	5748	141	40	7	4125	3290	919	1398	17
39	6516	0	111	4	5461	4478	903	1382	-4
23	6261	0	106	2	5074	4284	805	1375	-2
8	6195	0	62	3	5483	6135	1099	1463	31
8	5576	0	70	3	5224	4091	1133	1464	24
12	6160	0	57	1	4963	4292	721	1543	55
8	5856	0	58	3	5076	4236	962	1521	46
14	5818	0	60	5	5117	4281	695	1481	-16
21	5038	0	50	3	4583	3888	652	1425	-21
29	5036	0	69	2	4781	3788	987	1421	-45
17	4660	0	55	2	4667	3696	1072	1464	-16

Table F.6.6 show the variables in PVC5b-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	12280	4	67	8	6527	5123	1404	1082	191
54	6620	74	87	9	5553	4192	1339	1273	193
161	9483	133	87	6	7076	5034	2042	1495	109
185	6683	211	93	2	6328	4598	1731	1353	45
128	7491	125	114	1	7470	4923	2548	1344	-23
106	8660	90	91	5	6375	4544	1914	1337	23
94	9497	90	86	11	3846	2944	965	1209	-98
153	8055	94	78	6	7419	5391	1943	1493	27
88	8634	99	112	3	8381	6213	2116	-483	-13

143	6793	149	95	4	7518	6036	1514	1341	26
130	6808	172	52	7	6321	5022	1383	1437	52
86	7477	0	82	4	4405	3750	575	1387	-222
52	7419	0	108	2	5706	4284	1437	1523	45
30	7607	0	100	4	6121	3723	2346	1706	36
26	6568	0	93	3	4788	3777	1011	1625	153
27	7184	0	75	2	4879	3878	1051	1561	191
26	6768	0	57	3	5304	4274	1152	1605	169
39	7464	0	64	4	4985	3893	951	1626	204
38	6600	0	92	4	4209	3336	830	1691	314
48	6926	0	59	4	4233	3154	1073	1341	111
31	5972	0	53	3	2609	2024	686	1297	82

Table F.6.7 show the variables in PVC5ave-Cave Sample

Gas	COD	FSA	TP	OP	TSS	VSS	ISS	H2CO3Alk	VFA
0	12280	4	84	8	6527	5123	1404	1082	191
37	6203	64	75	9	5240	4029	1189	1262	201
136	8954	124	73	6	6051	4609	1442	1350	93
164	5822	194	93	1	5420	3986	1435	1307	39
92	6406	114	101	2	6114	4263	1852	1220	-60
67	7751	98	98	5	5271	3854	1500	1301	12
59	8710	78	86	10	4217	3144	1136	1263	-99
91	7656	105	73	5	5917	4364	1468	1512	55
46	8042	87	69	3	6764	5126	1586	-483	-13
101	6337	143	101	4	5786	4698	1120	1335	23
109	6278	157	46	7	5223	4156	1151	1417	35
62	6997	0	97	4	4933	4114	739	1385	-113
37	6840	0	107	2	5390	4284	1121	1449	21
19	6901	0	81	3	5802	4929	1722	1585	33
17	6072	0	81	3	5006	3934	1072	1544	88
20	6672	0	66	2	4921	4085	886	1552	123
17	6312	0	58	3	5190	4255	1057	1563	107
27	6641	0	62	5	5051	4087	823	1553	94
29	5819	0	71	4	4396	3612	741	1558	146
38	5981	0	64	3	4507	3471	1030	1381	33
24	5316	0	54	2	3638	2860	879	1381	33

Table G.1 shows Summary of Elemental Mass Compositions in Inoculum and Test (Settleometer) Samples using WEST® by MIKE DH1

X	fSup	KS	kM	i_P_Org_mol_perC	i_N_Org_mol_g_mol_C	i_O_Org_mol_g_mol_C	i_H_Org_mol_g_mol_C	C	Parameters	
									Biomass	
									C1	C2
2.2022	0.770	21.103	8.619	0.0000	0.1143	0.400	3.178	1		
2.1876	0.575	21.103	8.619	0.0400	0.0900	0.100	3.199	1		
2.1883	0.673	4161.0	2697.	0.0000	0.0900	0.100	3.198	1		
2.8006	0.577	21.103	8.619	0.04999991	0.1000	0.649	2.499	1		
5.0000	0.403	552	234.2	0.000025	0.2	0.4	1.4	1		
2.8005	0.706	16.061	3.784	0.049999913	0.1000	0.649	2.499	1		
2.9838	0.532	21.103	8.619	1.06958E-05	0.1079	0.648	2.345	1		
2.8174	0.641	14.213	3.963	4.80066E-06	0.1012	0.649	2.484	1		
3.0806	0.467	21.103	8.619	1.16886E-05	0.2545	0.645	2.272	1		
2.8133	0.554	21.103	8.619	0.049999942	0.1003	0.648	2.488	1		
2.8710	0.590	21.103	8.619	0.000017035	0.1005	0.648	2.438	1		
4.9866	0.281	36458	6791	0.00002504	0.2003	0.395	1.403	1		
3.0634	0.719	98.298	8.744	2.09892E-05	0.1013	0.639	2.285	1		
5.0000	0.409	21.103	8.619	0.000025	0.2	0.41	1.4	1		
2.8921	0.655	49.566	6.631	1.90877E-05	0.1633	0.602	2.420	1		
5.0000	0.345	21.103	8.619	0.000025	0.2	0.41	1.4	1		
2.8111	0.500	74.96	140.8	1.34349E-06	0.1013	0.644	2.490	1		
2.8797	0.554	3582.2	644.3	2.0484E-06	0.1000	0.649	2.430	1		
5.0000	0.384	2.728	1.278	0.000025	0.2	0.4	1.4	1		
2.8213	0.684	21.103	8.619	3.4097E-06	0.1001	0.649	2.481	1		
5.0000	0.514	5.926	3.139	0.0000251	0.2	0.4	1.4	1		
2.8012	0.469	5.743	2.335	2.2812E-06	0.1027	0.649	2.498	1		
5.0000	0.599	24143.	302.3	0.000025	0.2	0.4	1.4	1		
6.0801	0.534	11.149	1.938	0.00002497	0.1116	0.618	1.151	1		
2.8265	0.622	70.116	5.965	1.47027E-05	0.1436	0.631	2.476	1		
5.0000	0.467	5.715	2.737	0.000025	0.2	0.41	1.4	1		
2.9276	0.622	16.922	2.032	0.00019562	0.1004	0.648	2.390	1		
2.8050	0.607	21.103	8.619	1.15395E-06	0.1002	0.648	2.495	1		
4.9733	0.545	6.828	1.748	0.000025075	0.1992	0.407	1.407	1		
2.8445	0.684	8.208	1.844	0.000001791	0.1000	0.649	2.460	1		
2.9362	0.614	777.6	281.5	0.00068669	0.1009	0.647	2.384	1		
13.993	0.444	21.103	8.619	1.17212E-06	0.3199	0.200	0.500	1		
3.1186	0.314	2.928	1.362	5.98143E-05	0.1001	0.648	2.244	1		
2.8274	0.551	2748	432	0.049995938	0.1000	0.649	2.475	1		
5.2634	0.421	21.103	8.619	2.85047E-05	0.2622	0.213	1.329	1		
4.1805	0.379	5.808	3.343	2.73075E-05	0.1391	0.625	1.674	1		
2.8055	0.486	21.103	8.619	0.049999929	0.1000	0.649	2.495	1		
3.0090	0.432	17.163	2.276	4.90264E-06	0.1025	0.625	2.326	1		
12.011				0.02	0.20	0.40	1.40	1.		
4										

Mass Ratio	fp	fn	fo	fh	fc	fcv	MM	EDC	B	A	Z	Y
1.00	0.000	0.069	0.276	0.138	0.517	2.080	51.13	13.29	0.00000	0.251	0.880	7.00
1.00	0.064	0.065	0.083	0.167	0.621	2.866	42.31	15.16	0.08751	0.196	0.219	7.00
1.00	0.000	0.070	0.089	0.178	0.664	2.974	39.61	14.72	0.00000	0.197	0.219	7.00
1.00	0.056	0.050	0.373	0.090	0.431	1.478	78.08	14.42	0.14003	0.280	1.820	7.00
1.00	0.000	0.165	0.270	0.059	0.506	1.267	118.7	18.80	0.00005	1.400	2.000	7.00
1.00	0.056	0.050	0.373	0.090	0.431	1.478	78.08	14.42	0.14003	0.280	1.820	7.00
1.00	0.000	0.058	0.395	0.090	0.457	1.439	78.37	14.10	0.00003	0.321	1.935	7.00
1.00	0.000	0.054	0.395	0.095	0.456	1.483	74.17	13.75	0.00001	0.285	1.830	7.00
1.00	0.000	0.126	0.366	0.081	0.426	1.197	86.86	12.99	0.00004	0.784	1.988	7.00
1.00	0.056	0.050	0.372	0.090	0.431	1.477	78.33	14.46	0.14067	0.282	1.823	7.00
1.00	0.000	0.054	0.395	0.094	0.458	1.475	75.35	13.90	0.00005	0.288	1.860	7.00
1.00	0.000	0.124	0.280	0.063	0.533	1.423	112.4	20.01	0.00012	0.999	1.970	7.00
1.00	0.000	0.055	0.394	0.089	0.463	1.449	79.53	14.41	0.00006	0.310	1.958	7.00
1.00	0.000	0.123	0.288	0.062	0.527	1.398	113.9	19.90	0.00013	1.000	2.050	7.00
1.00	0.000	0.087	0.365	0.093	0.455	1.434	76.27	13.67	0.00006	0.472	1.741	7.00
1.00	0.000	0.123	0.288	0.062	0.527	1.398	113.9	19.90	0.00013	1.000	2.050	7.00
1.00	0.000	0.054	0.393	0.096	0.457	1.492	73.82	13.76	0.00000	0.284	1.812	7.00
1.00	0.000	0.053	0.396	0.093	0.457	1.472	75.62	13.91	0.00001	0.288	1.871	7.00
1.00	0.000	0.124	0.283	0.062	0.531	1.414	113.1	20.00	0.00013	1.000	2.000	7.00
1.00	0.000	0.053	0.395	0.095	0.457	1.485	74.21	13.77	0.00001	0.282	1.832	7.00
1.00	0.000	0.124	0.283	0.062	0.531	1.414	113.1	20.00	0.00013	1.000	2.000	7.00
1.00	0.000	0.055	0.394	0.096	0.456	1.485	73.84	13.70	0.00001	0.287	1.819	7.00
1.00	0.000	0.124	0.283	0.062	0.531	1.414	113.1	20.00	0.00013	1.000	2.000	7.00
1.00	0.000	0.064	0.402	0.047	0.488	1.162	149.7	21.76	0.00015	0.679	3.760	7.00
1.00	0.000	0.076	0.380	0.094	0.451	1.437	75.27	13.52	0.00004	0.406	1.786	7.00
1.00	0.000	0.123	0.288	0.062	0.527	1.398	113.9	19.90	0.00013	1.000	2.050	7.00
1.00	0.000	0.054	0.396	0.092	0.458	1.464	76.71	14.04	0.00057	0.293	1.897	7.00
1.00	0.000	0.053	0.394	0.096	0.457	1.490	73.77	13.74	0.00000	0.281	1.817	7.00
1.00	0.000	0.123	0.287	0.062	0.528	1.405	113.1	19.87	0.00012	0.990	2.026	7.00
1.00	0.000	0.053	0.395	0.094	0.457	1.479	74.78	13.83	0.00001	0.284	1.848	7.00
1.00	0.001	0.054	0.395	0.092	0.458	1.463	76.94	14.07	0.00202	0.296	1.900	7.00
1.00	0.000	0.222	0.158	0.025	0.595	1.244	282.6	43.94	0.00002	4.477	2.798	7.00
1.00	0.000	0.054	0.398	0.087	0.461	1.427	81.25	14.49	0.00019	0.312	2.022	7.00
1.00	0.056	0.050	0.373	0.090	0.431	1.472	78.75	14.49	0.14136	0.282	1.837	7.00
1.00	0.000	0.180	0.167	0.066	0.588	1.611	107.6	21.66	0.00015	1.380	1.124	7.00
1.00	0.000	0.076	0.390	0.066	0.468	1.249	107.2	16.75	0.00011	0.581	2.614	7.00
1.00	0.056	0.050	0.373	0.090	0.431	1.477	78.20	14.43	0.14028	0.280	1.823	7.00
1.00	0.000	0.056	0.388	0.091	0.466	1.479	77.62	14.35	0.00001	0.308	1.881	7.00
									30.974	14.00	15.99	1.00
									7	9	-2	79
								5	-3	-2	1	

Table G.2 Procedural Calculations for Elemental Mass Compositions of Control and Test Samples, showing Required Baseline Values and Initial Mass

Conditions applied into WEST® by MIKE DHI

AD_1.H2CO3al kalinity mgH2CO3/l as	.AD_1.ISSm mgISS/l	.AD_1.VSS mgVSS/l	.AD_1.OP mgOP/l	.AD_1.FSA mgFSA/l	.AD_1.COD_total mgCOD/l	Parameters	
						Units	
979	593	2601	3	155	5180	C1	
979	548	2316	3	155	3868	C2	
979	571	2459	3	155	4524	Cave	
1115	773	3115	5	168	5876	T1a - C1	
1115	857	1937	5	168	4108	T1b - C1	
1115	818	3400	5	168	7188	T1a - C2	
1115	902	2222	5	168	5420	T1b - C2	
1115	796	3258	5	168	6532	T1a - Cave	
1115	880	2080	5	168	4764	T1b - Cave	
1115	838	2669	5	168	5648	T1ave - Cave	
1177	519	3939	7	197	6040	T2a - C1	
1177	461	667	7	196	2876	T2b - C1	
294	564	4224	7	197	7352	T2a - C2	
1177	506	952	7	196	4188	T2b - C2	
1177	542	4082	7	197	6696	T2a - Cave	
1177	484	810	7	196	3532	T2b - Cave	
1177	513	2446	7	196	5114	T2ave - Cave	
1048	723	2951	7	192	5600	T3a - C1	
1048	755	1155	7	192	3880	T3b - C1	
1048	768	3236	7	192	6912	T3a - C2	
1048	800	1440	7	192	5192	T3b - C2	
1048	746	3094	7	192	4740	T3a - Cave	
1048	778	1298	7	192	6052	T3b - Cave	
1048	762	2196	7	192	5396	T3ave - Cave	
1029	1379	3837	8	193	5864	T4a - C1	
1029	1047	2437	8	192	4408	T4b - C1	
1029	1379	3837	8	193	5864	T4a - C2	
1029	1092	2722	8	192	5720	T4b - C2	
1029	1402	3980	8	192	5136	T4a - Cave	
1029	1070	2580	8	192	6448	T4b - Cave	
1029	1236	3280	8	298	5792	T4ave - Cave	
1082	1049	3553	8	10	5460	T5a - C1	
1082	663	1881	8	163	3860	T5b - C1	
1082	1094	3838	8	12	6772	T5a - C2	
1082	708	2166	8	163	5172	T5b - C2	
1082	1072	3696	8	4	4660	T5a - Cave	
1082	686	2024	8	4	5972	T5b - Cave	
1082	879	2860	8	4	5316	T5ave - Cave	

pKc1	pKa	T	MM_P	MM_N	MM_O	MM_H	MM_C	AD_1p_H	.AD_1.VFA
fconstan	mol/l	°C	g/mol	g/mol	g/mol	g/mol	g/mol	no unit	mgVFA/l
kinetic									
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.93	18
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.89	18
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.93	18
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	-12
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	-12
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	-12
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	-12
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	-12
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	-12
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	-12
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	129
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	129
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	129
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	129
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	129
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	129
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	129
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	129
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	202
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	202
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	202
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	202
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	202
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	202
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	202
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	202
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	202
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	212
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	212
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	212
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	212
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	212
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	212
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	191
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	191
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	191
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	191
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	191
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	191
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	191
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.13	191
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.23	191
6.31	38.64	35	30.974	14.007	15.999	1.0079	12.011	7.03	191

H_t	Conduct	Alkalinit	K	Mg	Ca	PO4	NH4	VFA
mol/l	µS/cm	mg/l	mg/	mg/L	mg/L	mgP/L	mgN/l	mg/L
2.05E-02	2000.00	979.00	0.00	0.00	0.00	3.00	154.50	18.00
2.06E-02	2000.00	979.00	0.00	0.00	0.00	3.00	154.50	18.00
2.05E-02	2000.00	979.00	0.00	0.00	0.00	3.00	154.50	18.00
3.09E-02	2000.00	1115.00	0.00	0.00	0.00	5.00	167.50	-12.00
2.91E-02	2000.00	1115.00	0.00	0.00	0.00	5.00	167.50	-12.00
2.77E-02	2000.00	1115.00	0.00	0.00	0.00	5.00	167.50	-12.00
2.60E-02	2000.00	1115.00	0.00	0.00	0.00	5.00	167.50	-12.00
2.42E-02	2000.00	1115.00	0.00	0.00	0.00	5.00	167.50	-12.00
2.96E-02	2000.00	1115.00	0.00	0.00	0.00	5.00	167.50	-12.00
2.69E-02	2000.00	1115.00	0.00	0.00	0.00	5.00	167.50	-12.00
2.60E-02	2000.00	1177.00	0.00	0.00	0.00	7.00	196.50	129.00
3.32E-02	2000.00	1177.00	0.00	0.00	0.00	6.85	196.20	129.00
7.50E-03	2000.00	294.00	0.00	0.00	0.00	7.00	196.50	129.00
2.84E-02	2000.00	1177.00	0.00	0.00	0.00	6.85	196.20	129.00
2.48E-02	2000.00	1177.00	0.00	0.00	0.00	7.00	196.50	129.00
3.26E-02	2000.00	1177.00	0.00	0.00	0.00	6.85	196.20	129.00
3.08E-02	2000.00	1177.00	0.00	0.00	0.00	6.93	196.35	129.00
2.61E-02	2000.00	1048.00	0.00	0.00	0.00	7.00	191.50	202.00
2.37E-02	2000.00	1048.00	0.00	0.00	0.00	6.70	191.80	202.00
2.53E-02	2000.00	1048.00	0.00	0.00	0.00	7.00	191.50	202.00
2.32E-02	2000.00	1048.00	0.00	0.00	0.00	6.70	191.80	202.00
2.90E-02	2000.00	1048.00	0.00	0.00	0.00	6.85	191.65	202.00
2.74E-02	2000.00	1048.00	0.00	0.00	0.00	6.85	191.65	202.00
2.78E-02	2000.00	1048.00	0.00	0.00	0.00	6.85	191.65	202.00
2.49E-02	2000.00	1029.00	0.00	0.00	0.00	8.00	192.50	212.00
2.28E-02	2000.00	1029.00	0.00	0.00	0.00	8.40	192.10	212.00
2.91E-02	2000.00	1029.00	0.00	0.00	0.00	8.00	192.50	212.00
2.60E-02	2000.00	1029.00	0.00	0.00	0.00	8.40	192.10	212.00
2.49E-02	2000.00	1029.00	0.00	0.00	0.00	8.20	192.30	212.00
2.17E-02	2000.00	1029.00	0.00	0.00	0.00	8.20	192.30	212.00
2.85E-02	2000.00	1029.00	0.00	0.00	0.00	8.20	297.50	212.00
2.83E-02	2000.00	1082.00	0.00	0.00	0.00	8.00	10.00	191.00
2.69E-02	2000.00	1082.00	0.00	0.00	0.00	8.30	162.70	191.00
2.45E-02	2000.00	1082.00	0.00	0.00	0.00	8.00	12.00	191.00
2.62E-02	2000.00	1082.00	0.00	0.00	0.00	8.30	162.70	191.00
2.39E-02	2000.00	1082.00	0.00	0.00	0.00	8.15	4.10	191.00
3.00E-02	2000.00	1082.00	0.00	0.00	0.00	8.15	4.10	191.00
2.83E-02	2000.00	1082.00	0.00	0.00	0.00	8.15	4.10	191.00

Ionic strength	Hac	H2CO3	HCO3 in	H2PO4 in	HPO4 in	f value
mol/l	mol/l	mol/l	mol/l	mol/l	mol/l	ratio
0.04	0.000305	0.0004	0.019563	4.76928E-	2.68196E-	0.150979
0.04	0.000305	0.0005	0.019563	4.76928E-	2.68196E-	0.150979
0.04	-0.000203	0.0042	0.022280	3.08255E-	2.18228E-	0.585498
0.04	-0.000203	0.0033	0.022280	2.78378E-	2.48104E-	0.528750
0.04	-0.000203	0.0026	0.022280	2.48104E-	2.78378E-	0.471249
0.04	-0.000203	0.0018	0.022280	1.97956E-	3.28526E-	0.375998
0.04	-0.000203	0.0009	0.022280	1.22116E-	4.04366E-	0.231947
0.04	-0.000203	0.0036	0.022280	2.87418E-	2.39064E-	0.545921
0.04	-0.000203	0.0022	0.022280	2.27103E-	2.99379E-	0.431358
0.04	0.002185	0.0012	0.023519	2.03036E-	5.34039E-	0.275461
0.04	0.002185	0.0048	0.023519	4.34325E-	2.86956E-	0.602158
0.04	0.002185	0.0007	0.005874	3.60053E-	3.77022E-	0.488489
0.04	0.002185	0.0024	0.023519	3.11131E-	4.1015E-	0.431358
0.04	0.002185	0.0006	0.023519	1.17968E-	6.19107E-	0.160049
0.04	0.002185	0.0044	0.023519	4.22309E-	2.98972E-	0.585498
0.04	0.002185	0.0035	0.023519	3.85553E-	3.43625E-	0.528750
0.04	0.003421	0.0025	0.020941	3.47346E-	3.89729E-	0.471249
0.04	0.003421	0.0013	0.020941	2.28365E-	4.77121E-	0.323698
0.04	0.003421	0.0021	0.020942	3.179E-05	4.191E-05	0.431358
0.04	0.003421	0.0010	0.020941	1.9433E-	5.1115E-	0.275461
0.04	0.003421	0.0039	0.020941	4.2231E-	2.9897E-	0.585498
0.04	0.003421	0.0031	0.020942	3.814E-05	3.399E-05	0.528750
0.04	0.003421	0.0033	0.020941	3.9376E-	3.2752E-	0.545921
0.04	0.003591	0.0021	0.020562	3.634E-05	4.79E-05	0.431358
0.04	0.003591	0.0010	0.020562	2.436E-05	6.408E-05	0.275461
0.04	0.003591	0.0041	0.020562	5.072E-05	3.351E-05	0.602158
0.04	0.003591	0.0026	0.020562	4.3206E-	4.5243E-	0.488489
0.04	0.003591	0.0021	0.020562	3.724E-05	4.91E-05	0.431358
0.04	0.003591	0.0005	0.020562	1.382E-05	7.252E-05	0.160049
0.04	0.003591	0.0039	0.020562	5.055E-05	3.579E-05	0.585498
0.04	0.003235	0.0032	0.021621	4.45404E-	3.96967E-	0.528750
0.04	0.003235	0.0025	0.021621	4.11853E-	4.62107E-	0.471249
0.04	0.003235	0.0013	0.021621	2.72674E-	5.69697E-	0.323698
0.04	0.003235	0.0022	0.021621	3.7699E-	4.9697E-	0.431358
0.04	0.003235	0.0011	0.021621	2.36392E-	6.21774E-	0.275461
0.04	0.003235	0.0041	0.021621	5.02455E-	3.5571E-	0.585498
0.04	0.00323	0.0032	0.021621	4.53756E-	4.0441E-	0.528750

S_M	S_C	S_K	S_N	S_H	H2O	Vol		Na_t	Ionic
							I		
gMg	gCa	gK	gNa	gH	gH2O			mol/l	mol/l
0.03	0.0	4.89	0.00	0.103	5000	0.0050	C1	-7.17E-02	0.109822
0.03	0.0	4.89	1.00	0.104	5000	0.0050	C2	-7.20E-02	0.110004
0.03	0.0	4.89	2.00	0.103	5000	0.0050	Cave	-7.17E-02	0.109822
0.03	0.0	5.57	3.00	0.155	5000	0.0050	T1a - C1	-1.08E-01	0.146517
0.03	0.0	5.57	4.00	0.146	5000	0.0050	T1b - C1	-1.03E-01	0.141274
0.03	0.0	5.57	5.00	0.139	5000	0.0050	T1a - C2	-9.90E-02	0.137110
0.03	0.0	5.57	6.00	0.130	5000	0.0050	T1b - C2	-9.38E-02	0.131899
0.03	0.0	5.57	7.00	0.121	5000	0.0050	T1a - Cave	-8.84E-02	0.126471
0.03	0.0	5.57	8.00	0.149	5000	0.0050	T1b - Cave	-1.05E-01	0.142722
0.03	0.0	5.57	9.00	0.135	5000	0.0050	T1ave - Cave	-9.66E-02	0.134715
0.03	0.0	5.88	10.0	0.131	5000	0.0050	T2a - C1	-1.01E-01	0.138671
0.03	0.0	5.88	11.0	0.167	5000	0.0050	T2b - C1	-1.22E-01	0.160237
0.03	0.0	1.47	12.0	0.037	5000	0.0050	T2a - C2	-9.65E-03	0.047766
0.03	0.0	5.88	13.0	0.143	5000	0.0050	T2b - C2	-1.08E-01	0.145853
0.03	0.0	5.88	14.0	0.125	5000	0.0050	T2a - Cave	-9.69E-02	0.135053
0.03	0.0	5.88	15.0	0.164	5000	0.0050	T2b - Cave	-1.20E-01	0.158313
0.03	0.0	5.88	16.0	0.155	5000	0.0050	T2ave - Cave	-1.15E-01	0.152795
0.03	0.0	5.24	17.0	0.131	5000	0.0050	T3a - C1	-9.65E-02	0.134625
0.03	0.0	5.24	18.0	0.119	5000	0.0050	T3b - C1	-8.95E-02	0.127604
0.03	0.0	5.24	19.0	0.127	5000	0.0050	T3a - C2	-9.43E-02	0.132374
0.03	0.0	5.24	20.0	0.116	5000	0.0050	T3b - C2	-8.78E-02	0.125933
0.03	0.0	5.24	21.0	0.146	5000	0.0050	T3a - Cave	-1.05E-01	0.143461
0.03	0.0	5.24	22.0	0.138	5000	0.0050	T3b - Cave	-1.00E-01	0.138533
0.03	0.0	5.24	23.0	0.140	5000	0.0050	T3ave - Cave	-1.02E-01	0.139894
0.03	0.0	5.14	24.0	0.125	5000	0.0050	T4a - C1	-9.25E-02	0.130577
0.03	0.0	5.14	25.0	0.114	5000	0.0050	T4b - C1	-8.62E-02	0.124287
0.03	0.0	5.14	26.0	0.146	5000	0.0050	T4a - C2	-1.05E-01	0.143156
0.03	0.0	5.14	27.0	0.131	5000	0.0050	T4b - C2	-9.58E-02	0.133872
0.03	0.0	5.14	28.0	0.125	5000	0.0050	T4a - Cave	-9.25E-02	0.130588
0.03	0.0	5.14	29.0	0.109	5000	0.0050	T4b - Cave	-8.30E-02	0.121111
0.03	0.0	5.14	30.0	0.143	5000	0.0050	T4ave - Cave	-1.09E-01	0.147316
0.03	0.0	5.41	31.0	0.142	5000	0.0050	T5a - C1	-9.43E-02	0.132418
0.03	0.0	5.41	32.0	0.135	5000	0.0050	T5b - C1	-9.88E-02	0.136873
0.03	0.0	5.41	33.0	0.123	5000	0.0050	T5a - C2	-8.31E-02	0.121252
0.03	0.0	5.41	34.0	0.131	5034	0.0050	T5b - C2	-9.64E-02	0.134548
0.03	0.0	5.41	35.0	0.120	5035	0.0050	T5a - Cave	-8.10E-02	0.119104
0.03	0.0	5.41	36.0	0.151	5036	0.0050	T5b - Cave	-9.91E-02	0.137196
0.03	0.0	5.41	37.0	0.142	5037	0.0050	T5ave - Cave	-9.40E-02	0.132107

Initiation Calculations Required before Running EMC Simulation in WEST® by MIKE DHI

S_F	S_U	M(S_CH	S_H2	S_PO	S_SO	S_CO3	S_Pr	S_VFA	S_Cl	S_NH
g	g	g	gH2O	gPO4	gSO4	gCO3	gPr	gVFA	gCl	gNH
0.000	0.2197	0.00000	0.0000	0.046	0.000	6.0105	0.00	0.08	0.00	0.9948
0.000	0.2197	0.00000	0.0000	0.046	2.000	6.0105	2.00	0.08	2.00	0.9948
0.000	0.2197	0.00000	0.0000	0.076	3.000	7.9590	3.00	-0.06	3.00	1.0786
0.000	0.2197	0.00000	0.0000	0.076	4.000	7.6970	4.00	-0.06	4.00	1.0786
0.000	0.2197	0.00000	0.0000	0.076	5.000	7.4889	5.00	-0.06	5.00	1.0786
0.000	0.2197	0.00000	0.0000	0.076	6.000	7.2285	6.00	-0.06	6.00	1.0786
0.000	0.2197	0.00000	0.0000	0.076	7.000	6.9575	7.00	-0.06	7.00	1.0786
0.000	0.2197	0.00000	0.0000	0.076	8.000	7.7693	8.00	-0.06	8.00	1.0786
0.000	0.2197	0.00000	0.0000	0.076	9.000	7.3692	9.00	-0.06	9.00	1.0786
0.000	0.2197	0.00000	0.0000	0.107	10.00	7.4188	10.0	0.60	10.0	1.2653
0.000	0.2197	0.00000	0.0000	0.105	11.00	8.4977	11.0	0.60	11.0	1.2634
0.000	0.2197	0.00000	0.0000	0.107	12.00	1.9898	12.0	0.60	12.0	1.2653
0.000	0.2197	0.00000	0.0000	0.105	13.00	7.7790	13.0	0.60	13.0	1.2634
0.000	0.2197	0.00000	0.0000	0.107	14.00	7.2383	14.0	0.60	14.0	1.2653
0.000	0.2197	0.00000	0.0000	0.105	15.00	8.4015	15.0	0.60	15.0	1.2634
0.000	0.2197	0.00000	0.0000	0.106	16.00	8.1250	16.0	0.60	16.0	1.2643
0.000	0.2197	0.00000	0.0000	0.107	17.00	7.0389	17.0	0.95	17.0	1.2331
0.000	0.2197	0.00000	0.0000	0.102	18.00	6.6891	18.0	0.95	18.0	1.2350
1.25E	0.2197	1.25E-06	1.25E-	0.107	19.00	6.9264	19.0	0.95	19.0	1.2331
0.000	0.2197	0.00000	0.0000	0.102	20.00	6.6057	20.0	0.95	20.0	1.2350
0.000	0.2197	0.00000	0.0000	0.105	21.00	7.4807	21.0	0.95	21.0	1.2341
1.25E	0.2197	1.25E-06	1.25E-	0.105	22.00	7.2345	22.0	0.95	22.0	1.2341
0.000	0.2197	0.00000	0.0000	0.105	23.00	7.3025	23.0	0.95	23.0	1.2341
1.25E	0.2197	1.25E-06	1.25E-	0.122	24.00	6.8008	24.0	0.99	24.0	1.2395
1.25E	0.2197	1.25E-06	1.25E-	0.128	25.00	6.4859	25.0	0.99	25.0	1.2370
1.25E	0.2197	1.25E-06	1.25E-	0.122	26.00	7.4292	26.0	0.99	26.0	1.2395
0.000	0.2197	0.00000	0.0000	0.128	27.00	6.9643	27.0	0.99	27.0	1.2370
1.25E	0.2197	1.25E-06	1.25E-	0.125	28.00	6.8008	28.0	0.99	28.0	1.2382
1.25E	0.2197	1.25E-06	1.25E-	0.125	29.00	6.3281	29.0	0.99	29.0	1.2382
1.25E	0.2197	1.25E-06	1.25E-	0.125	30.00	7.3451	30.0	0.99	30.0	1.9156
0.000	0.2197	0.00000	0.0000	0.122	31.00	7.4692	31.0	0.90	31.0	0.0644
0.000	0.2197	0.00000	0.0000	0.127	32.00	7.2672	32.0	0.90	32.0	1.0476
0.000	0.2197	0.00000	0.0000	0.122	33.00	6.9061	33.0	0.90	33.0	0.0773
0.000	0.2197	0.00000	0.0000	0.127	34.00	7.1511	34.0	0.90	34.0	1.0476
0.000	0.2197	0.00000	0.0000	0.124	35.00	6.8200	35.0	0.90	35.0	0.0264
0.000	0.2197	0.00000	0.0000	0.124	36.00	7.7234	36.0	0.90	36.0	0.0264
0.000	0.2197	0.00000	0.0000	0.124	37.00	7.4692	37.0	0.90	37.0	0.0264

M(X_Glyc	X_PAO_St	X_PAO_P	X_B_Org	X_U_I	S_O	S_NO	S_Glu
g	g	g	g	g	g	g	g
0.000001	0.000001	0.000001	0.000000	13.00	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	11.58	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	12.29	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	15.57	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	9.685	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	17.00	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	11.11	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	16.28	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	10.39	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	13.34	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	19.69	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	3.335	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	21.12	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	4.760	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	20.40	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	4.047	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	12.22	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	14.75	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	5.775	0.000000	0.000	0.0000
1.25E-06	1.25E-06	1.25E-06	1.25E-06	16.18	1.25E-06	1.25E	1.25E-
0.000001	0.000001	0.000001	0.000000	7.200	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	15.46	0.000000	0.000	0.0000
1.25E-06	1.25E-06	1.25E-06	1.25E-06	6.487	1.25E-06	1.25E	1.25E-
0.000001	0.000001	0.000001	0.000000	10.97	0.000000	0.000	0.0000
1.25E-06	1.25E-06	1.25E-06	1.25E-06	19.18	1.25E-06	1.25E	1.25E-
1.25E-06	1.25E-06	1.25E-06	1.25E-06	12.18	1.25E-06	1.25E	1.25E-
1.25E-06	1.25E-06	1.25E-06	1.25E-06	19.18	1.25E-06	1.25E	1.25E-
0.000001	0.000001	0.000001	0.000000	13.61	0.000000	0.000	0.0000
1.25E-06	1.25E-06	1.25E-06	1.25E-06	19.89	1.25E-06	1.25E	1.25E-
1.25E-06	1.25E-06	1.25E-06	1.25E-06	12.89	1.25E-06	1.25E	1.25E-
1.25E-06	1.25E-06	1.25E-06	1.25E-06	16.39	1.25E-06	1.25E	1.25E-
0.000001	0.000001	0.000001	0.000000	17.76	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	9.405	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	19.19	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	10.83	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	18.47	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	10.11	0.000000	0.000	0.0000
0.000001	0.000001	0.000001	0.000000	14.29	0.000000	0.000	0.0000

conc.	Samples & masses	G_N2	G_CH4	G_CO2	X_ISS		X_ANO	
		g	g	g		g		g
798	C1	0.000001	0.000001	0.000001		2.9650		0.000001
1082	C2	0.000001	0.000001	0.000001		2.7400		0.000001
941	Cave	0.000001	0.000001	0.000001		2.8525		0.000001
2452	T1a - C1	0.000001	0.000001	0.000001		3.8650		0.000001
3630	T1b - C1	0.000001	0.000001	0.000001		4.2850		0.000001
2167	T1a - C2	0.000001	0.000001	0.000001		4.0900		0.000001
3345	T1b - C2	0.000001	0.000001	0.000001		4.5100		0.000001
2310	T1a - Cave	0.000001	0.000001	0.000001		3.9775		0.000001
3488	T1b - Cave	0.000001	0.000001	0.000001		4.3975		0.000001
2899	T1ave - Cave	0.000001	0.000001	0.000001		4.1875		0.000001
1646	T2a - C1	0.000001	0.000001	0.000001		2.5950		0.000001
4518	T2b - C1	0.000001	0.000001	0.000001		2.3050		0.000001
1361	T2a - C2	0.000001	0.000001	0.000001		2.8200		0.000001
4233	T2b - C2	0.000001	0.000001	0.000001		2.5300		0.000001
1504	T2a - Cave	0.000001	0.000001	0.000001		2.7075		0.000001
4376	T2b - Cave	0.000001	0.000001	0.000001		2.4175		0.000001
2940	T2ave - Cave	0.000001	0.000001	0.000001		2.5625		0.000001
1774	T3a - C1	0.000001	0.000001	0.000001		3.6150		0.000001
3570	T3b - C1	0.000001	0.000001	0.000001		3.7750		0.000001
1489	T3a - C2	1.25E-06	1.25E-06	1.25E-06		3.8400		1.25E-06
3285	T3b - C2	0.000001	0.000001	0.000001		4.0000		0.000001
1632	T3a - Cave	0.000001	0.000001	0.000001		3.7275		0.000001
3428	T3b - Cave	1.25E-06	1.25E-06	1.25E-06		3.8875		1.25E-06
2530	T3ave - Cave	0.000001	0.000001	0.000001		3.8075		0.000001
1032	T4a - C1	1.25E-06	1.25E-06	1.25E-06		6.8950		1.25E-06
2432	T4b - C1	1.25E-06	1.25E-06	1.25E-06		5.2350		1.25E-06
1032	T4a - C2	1.25E-06	1.25E-06	1.25E-06		6.8950		1.25E-06
2147	T4b - C2	0.000001	0.000001	0.000001		5.4600		0.000001
890	T4a - Cave	1.25E-06	1.25E-06	1.25E-06		7.0075		1.25E-06
2290	T4b - Cave	1.25E-06	1.25E-06	1.25E-06		5.3475		1.25E-06
1590	T4ave - Cave	1.25E-06	1.25E-06	1.25E-06		6.1775		1.25E-06
1570	T5a - C1	0.000001	0.000001	0.000001		5.2450		0.000001
3242	T5b - C1	0.000001	0.000001	0.000001		3.3150		0.000001
1285	T5a - C2	0.000001	0.000001	0.000001		5.4700		0.000001
2957	T5b - C2	0.000001	0.000001	0.000001		3.5400		0.000001
1428	T5a - Cave	0.000001	0.000001	0.000001		5.3575		0.000001
3100	T5b - Cave	0.000001	0.000001	0.000001		3.4275		0.000001
2264	T5ave - Cave	0.000001	0.000001	0.000001		4.3925		0.000001

Established Baseline Values

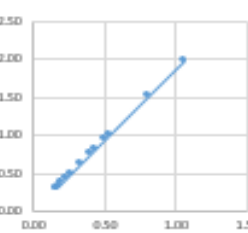
sbio	lnoc. mass	mass
-	1.995	3.99
-	2.7075	5.415
-	2.35125	4.702
12.26	-	12.26
18.15	-	18.15
10.83	-	10.83
16.72	-	16.72
11.54	-	11.54
17.43	-	17.43
14.49	-	14.49
8.23	-	8.23
22.59	-	22.59
6.805	-	6.805
21.16	-	21.16
7.517	-	7.517
21.87	-	21.87
14.69	-	14.69
8.87	-	8.87
17.85		17.85
7.445		7.445
16.42		16.42
8.157		8.157
17.13		17.13
12.64		12.64
5.16		5.16
12.16		12.16
5.16		5.16
10.73		10.73
4.447		4.447
11.44		11.44
7.947		7.947
7.85		7.85
16.21		16.21
6.425		6.425
14.78		14.78
7.137		7.137
15.49		15.49
11.31		11.31

T1a-C1										T1b-C1										T1a-C2										
ADHP_RS [A]	COD	Shpm	Shpr	ZAD	-LYZ	Shpr/ZAD AD I _q COD/ qCOD	Sprn -HYD	Sprn -HYD - pred	Sprn -HYD - pred	ADHP_RS [A]	COD	Shpm	Shpr	ZAD	-LYZ	Shpr/ZAD AD I _q COD/ qCOD	Sprn -HYD	Sprn -HYD - pred	Sprn -HYD - pred	ADHP_RS [A]	COD	Shpm	Shpr	ZAD	-LYZ	Shpr/ZAD AD I _q COD/ qCOD	Sprn -HYD	Sprn -HYD - pred	Sprn -HYD - pred	
0	10	4.00	0.91							0	10.18	4.46	3.55	0.91							0	10.18	0.11	-0.80	0.91					
2	4	0.80	1.64	3.59						2	5.34	1.57	0.37	1.20	1.63						2	5.34		-6.01	1.43	2.64	16.00	1.85	2.11	1.89
3	5	0.70	1.41	1.79						3	5.34	-1.41	-2.95	1.54	2.21						3	5.34		-3.68	1.14	1.00				
4	4	0.60	1.47	1.56						4	5.34	2.01	0.94	1.07	0.69						4	5.34		-3.02	1.03	0.59				
5	8	0.50	1.01	0.51						5	5.34	4.03	3.26	0.78	0.10	5.00	2.10	2.26	2.10		5	5.34		1.74	0.46	-0.47				
6	7	0.40	1.09	0.60						6	5.34	4.19	3.47	0.72	0.05	4.82	2.03	2.22	2.03		6	5.34		-0.07	0.63	-0.08				
7	9	0.30	0.85	0.26	2.17	0.70	0.42	0.80		7	5.34	5.41	4.88	0.53	-0.15	4.20	1.77	2.09	1.77		7	5.34		1.22	0.45	-0.25	7.10	1.30	0.94	1.16
9	5	0.20	0.73	0.16	1.98	0.64	0.38	0.74		9	5.34	-1.67	-3.02	1.35	0.77						9	5.34		-0.08	0.53	-0.04				
11	8	0.10	0.72	0.18	1.34	0.43	0.26	0.51		11	5.34	-0.86	-2.03	1.18	0.54						11	5.34		0.31	0.42	-0.06	3.70	0.68	0.49	0.71
13	7	0.00	0.70	0.19	0.83	0.27	0.16	0.32		13	5.34	-0.01	-1.00	0.99	0.39						13	5.34		-0.69	0.47	0.03				
15	6.52	0.49	-0.24	0.73	0.22					15	5.34	-0.60	-1.60	0.99	0.38						15	5.34		-1.18	0.46	0.06				
17	8.35	2.25	1.83	0.43	0.08					17	5.34	0.94	0.22	0.72	0.23						17	5.34		0.66	0.18	-0.05	3.64	0.67	0.48	0.70
20	6.65	0.68	0.16	0.52	0.16	0.32	0.10	0.06	0.13	20	5.34	0.49	-0.18	0.67	0.22						20	5.34		-0.55	0.22	0.03				
23	6.66	0.96	0.60	0.37	0.12					23	5.34	0.92	0.41	0.50	0.17	0.82	0.35	0.73	0.35		23	5.34		0.45	0.01	-0.02				
26	6.81	1.52	1.34	0.18	0.08					26	5.34	2.71	2.55	0.16	0.08						26	5.34		0.24	-0.07	0.00				
29	6.57	0.85	0.69	0.16	0.10					29	5.34	2.82	2.79	0.04	0.06						29	5.34		-0.33	-0.10	0.02	3.17	0.58	0.42	0.62
32	6.60	1.01	0.99	0.03	0.09					32	5.34	1.99	1.96	0.03	0.09	0.64	0.27	0.60	0.27		32	7.51	-0.49	-0.29	-0.21	0.02	1.39	0.25	0.18	0.30
37	5.97	0.30	0.37	-0.07	0.10					37	5.93	1.29	1.34	-0.07	0.10						37	7.61	0.27	0.76	-0.49	0.00				
42	5.45	-0.18	0.01	-0.19	0.10	0.06	0.02	0.01	0.02	42	5.33	0.72	0.89	-0.18	0.10						42	7.02	-0.29	0.20	-0.59	0.01				
45	5.53	-0.11	0.20	-0.32	0.09					45	4.38	-0.24	-0.08	-0.17	0.12	0.46	0.19	0.45	0.19		45	7.42	0.34	1.14	-0.80	-0.01	0.36	0.01	0.05	0.08
52	5.88	0.68	1.35	-0.68	0.06					52	4.11	-0.07	0.38	-0.45	0.10						52	7.19	-0.03	0.98	-1.01	0.00				
Sup_tot	5.45		51.38	265.53	1R					Sup_tot	4.11		3.80	3.438	1R						Sup_tot	7.02		96.43	7288.3	1R				
ER (ir less than)	0.70		kM	kr						ER (ir less than)	-1.07		kM	kr							ER (ir less than)	3.29		kM	kr					
Selected ER	0.02		8.615	21.103	2R					Selected ER	-1.00		234.6	952	2R						Selected ER	3.35		3.788	16.06	2R				
T2a-C1										T2b-C1										T2a-C2										
ADHP_RS [A]	COD	Shpm	Shpr	ZAD	-LYZ	Shpr/ZAD AD I _q COD/ qCOD	Sprn -HYD	Sprn -HYD - pred	Sprn -HYD - pred	ADHP_RS [A]	COD	Shpm	Shpr	ZAD	-LYZ	Shpr/ZAD AD I _q COD/ qCOD	Sprn -HYD	Sprn -HYD - pred	Sprn -HYD - pred	ADHP_RS [A]	COD	Shpm	Shpr	ZAD	-LYZ	Shpr/ZAD AD I _q COD/ qCOD	Sprn -HYD	Sprn -HYD - pred	Sprn -HYD - pred	
0	10.22	3.49	2.58	0.91						0	10.22	6.00	5.09	0.91							0	10.22	0.90	-0.01	0.91					
2	3.60	-3.55	-5.28	1.73	3.97	0.41	2.29	0.17	0.17	2	5.42	0.78	-0.72	1.50	2.94						2	4.43	-4.47	-5.99	1.52	3.03	28.00	1.90	18.34	1.94
3	2.08	-5.17	-7.07	1.90	3.26	0.31	1.71	0.12	0.12	3	5.42	0.78	-0.72	1.50	2.48	5.10	0.95	2.01	0.95		3	5.42		1.63	2.46	15.00	1.30	9.96	1.16	
4	1.36	-5.34	-7.23	1.89	2.49	0.24	1.32	0.10	0.10	4	5.42	0.78	-0.72	1.50	1.23						4	5.42		1.45	1.52					
5	1.25	-5.80	-7.71	1.91	2.10	0.20	1.10	0.08	0.08	5	5.42	0.78	-0.72	1.50	1.82						5	5.42		1.35	1.12					
6	1.46	-5.53	-7.37	1.84	1.70	0.17	0.92	0.07	0.07	6	5.42	0.78	-0.72	1.50	1.42						6	5.42		1.37	1.01					
7	0.95	-6.25	-8.14	1.89	1.57	0.15	0.83	0.06	0.06	7	5.42	0.78	-0.72	1.50	1.32						7	5.42		1.49	1.06					
9	1.30	-5.69	-7.43	1.74	1.15	0.12	0.66	0.05	0.05	9	5.42	0.78	-0.72	1.50	0.98	2.30	0.43	0.91	0.43		9	5.42		1.54	0.95	7.60	0.62	5.09	0.63	
11	3.32	-3.57	-4.97	1.40	0.72	0.09	0.52	0.04	0.04	11	5.42	0.78	-0.72	1.50	0.71						11	5.42		1.10	0.48	6.40	0.44	4.29	0.53	
13	3.70	-2.23	-3.39	1.15	0.50	0.08	0.43	0.03	0.03	13	5.42	0.78	-0.72	1.50	0.36						13	5.42		0.92	0.34					
15	4.27	-1.75	-2.77	1.02	0.39	0.07	0.39	0.03	0.03	15	5.42	0.78	-0.72	1.50	0.34						15	5.42		0.75	0.23					
17	8.54	2.46	2.05	0.41	0.07					17	5.42	0.78	-0.72	1.50	0.25	1.93	0.36	0.77	0.36		17	5.42		0.16	-0.06					
20	6.52	0.57	0.03	0.54	0.16	0.06	0.31	0.02	0.02	20	5.42	0.78	-0.72	1.50	0.26						20	5.42		0.24	0.03					
23	6.86	1.17	0.82	0.35	0.11	0.06	0.33	0.02	0.02	23	5.42	0.78	-0.72	1.50	0.21	1.89	0.35	0.75	0.35		23	5.42		-0.01	-0.02					
26	6.09	0.81	0.53	0.28	0.12					26	5.42	0.78	-0.72	1.50	0.16						26	5.42		0.03	0.03					
29	6.16	0.45	0.24	0.21	0.12					29	5.42	0.78	-0.72	1.50	0.19	1.79	0.33	0.71	0.33		29	5.42		-0.05	0.04	5.40	0.38	3.62	0.46	
32	6.25	0.67	0.60	0.08	0.10					32	5.10	2.03	1.81	0.22	0.14						32	5.10		-0.16	0.03					
37	5.65	0.00	0.03	-0.03	0.11					37	3.93	0.79	0.60	0.20	0.16						37	7.30	0.70	1.15	-0.45	0.01				
42	5.70	0.07	0.29	-0.22	0.09					42	3.29	0.17	0.08	0.09	0.16	0.94	0.18	0.38	0.18		42	7.26	0.60	1.22	-0.62	0.01				
45	5.84	0.21	0.57	-0.35	0.08					45	3.16	0.04	0.04	-0.01	0.15						45	7.73	1.40	2.24	-0.83	-0.01	0.34	0.02	0.23	0.03
52	6.04	0.85	1.54	-0.69	0.06					52	2.88	0.20	0.48	-0.29	0.13						52	7.35	0.88	1.91	-1.03	0.00		0.00	0.00	0.00
Sup_tot	5.65		8.615	21.103	1R																									

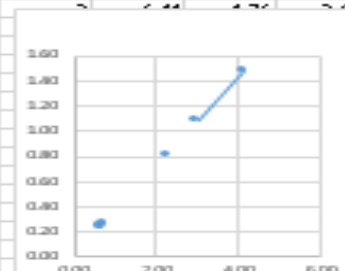
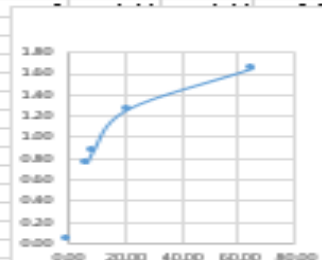
T1b-C2											T1a-Cavo											T1b-Cavo																		
ADHP_	RS [J]	COD	Shpm	Shpr	ZAD	LVZ	Shpr/ZAD	AD	I _q COD	I _q COD	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	ADHP_	RS [J]	COD	Shpm	Shpr	ZAD	LVZ	Shpr/ZAD	AD	I _q COD	I _q COD	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	
0	10.18	0.96	0.05	0.91																	0	10.18	2.06	2.06	0.91															
		3.26	-1.25	0.99	0.69																2	4.65	-3.47	-5.12	1.65	3.63	18.52	2.19	3.68	2.24										
		2.79	-4.07	1.27	1.41	3.03	1.11														3			3.04	1.39	1.74														
		1.95	1.32	0.63	-0.28																4			3.13	1.36	1.33	6.90	1.49	1.37	1.30										
		4.87	4.65	0.22	-0.88																5			1.13	0.85	0.22														
		4.32	4.07	0.26	-0.63																6			1.29	0.98	0.43	2.46	0.44	0.49	0.59										
		5.06	4.93	0.13	-0.66																7			1.28	0.77	0.15														
		3.57	-4.72	1.15	0.57	1.35	0.49														9			1.86	0.75	0.17	1.15	0.23	0.23	0.30										
		1.99	-2.86	0.87	0.30	0.95	0.35														11			1.80	0.69	0.15	1.17	0.22	0.23	0.30										
		1.68	-2.44	0.76	0.23	0.82	0.30														13			0.11	0.70	0.19														
		1.98	-2.71	0.72	0.22	0.84	0.31														15			1.54	0.71	0.21														
		3.64	-1.11	0.48	0.11	0.61	0.22														17			1.41	0.42	0.08	0.83	0.18	0.17	0.22										
		3.69	-1.07	0.37	0.09	0.68	0.25														20			1.03	0.48	0.14														
		3.24	0.10	0.14	0.04	0.67	0.25														23			1.69	0.30	0.10														
		1.20	1.29	-0.09	-0.01	0.31	0.11														26			1.96	0.17	0.08														
		1.37	1.60	-0.22	-0.02	0.20	0.07														29			1.35	0.14	0.10														
32	7.47	0.31	0.51	-0.20	0.02																32	7.06	0.54	0.52	0.03	0.09														
37	7.58	1.08	1.57	-0.48	0.00	0.02	0.01														37	6.79	0.57	0.73	-0.16	0.07														
42	6.90	0.34	0.92	-0.58	0.02																42	6.24	0.00	0.28	-0.28	0.08														
45	6.27	0.04	0.68	-0.65	0.02																45	6.47	0.40	0.84	-0.44	0.06	0.16	0.09	0.03	0.04										
52	5.42	-0.95	-0.16	-0.78	0.04																52	6.53	0.61	1.34	-0.73	0.05														
Sup _{tor}	6.27		8.619	21.103	1R																Sup _{tor}	6.24		13.61	6.826	1R														
ER (ir low)	2.54		kM	kr																	ER (ir low)	1.71		kM	kr															
Selecto	2.50		8.619	21.103	2R																Selecto	1.40		3.963	14.213	2R														

T2b-C2											T2a-Cavo											T2b-Cavo																		
ADHP_	RS [J]	COD	Shpm	Shpr	ZAD	LVZ	Shpr/ZAD	AD	I _q COD	I _q COD	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	ADHP_	RS [J]	COD	Shpm	Shpr	ZAD	LVZ	Shpr/ZAD	AD	I _q COD	I _q COD	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	Sprn	
0	10.22	2.50	1.59	0.91																	0	10.22	4.20	3.29	0.91															
2	6.25	-1.05	-2.33	1.28	2.00	10.00	1.56	9.48	2.77												2																			
3	5.70	-1.40	-2.76	1.37	1.69	8.20	1.23	7.79	2.41												3																			
4				0.87	0.26																4																			
5				1.19	0.84																5																			
6				1.18	0.74																6																			
7				1.29	0.81																7																			
9				1.37	0.78																9																			
11				1.07	0.46																11																			
13				0.72	0.20																13																			
15				0.66	0.18																15																			
17				0.51	0.12																17																			
20				0.46	0.13																20																			
23				0.24	0.07	3.43	0.43	3.27	1.20												23																			
26				0.17	0.08	3.06	0.31	2.92	1.09												26																			
29				0.18	0.11																29																			
32				-0.01	0.08																32																			
37	5.58	0.58	0.81	-0.22	0.06																37	6.48	-0.14	0.09	-0.24	0.06														
42	4.85	-0.20	0.11	-0.31	0.07	0.83	0.29	0.79	0.32												42	6.48	-0.16	0.26	-0.42	0.05														
45	5.05	0.37	0.80	-0.49	0.05	0.25	0.24	0.24	0.10												45	6.79	0.31	0.91	-0.59	0.03														
52	4.19	-0.68	-0.06	-0.62	0.07	0.10	0.09	0.09	0.04												52	6.70	0.37	1.23	-0.86	0.03														
Sup _{tor}	4.85		10.63	1110	1R																Sup _{tor}	6.48		8.619	21.103	1R														
ER (ir low)	1.12		kM	kr																	ER (ir low)	1.96		kM	kr															
Selecto	1.00		8.619	21.103	2R																Selecto	1.80		6.631	49.568	2R														

T1ave - Cave										1R	2R
ADHP_	COD	Shpm	Shpr	ZAD	-LYA	Skpr/2	AD	Skpr	Skpr	Skpr	Skpr
RS [d]						I ₀ COD	I ₀ COD	-MYD	-MYD	-MYD	-MYD
						I ₀ COD	I ₀ COD	good	good	good	good
0	10.18	2.16	1.25	0.91							
2	6.39	-1.63	-2.95	1.32	2.14	5.55	1.62	1.80	1.80		
3	5.91	-2.10	-3.44	1.34	1.60	4.09	1.20	1.40	1.40		
			-1.16	1.05	0.64						
			2.38	0.62	-0.19						
			1.57	0.67	-0.02						
			2.92	0.49	-0.20						
			1.67	0.94	0.36	1.32	0.38	0.51	0.51		
			0.99	0.80	0.24	1.03	0.30	0.40	0.40		
			0.97	0.73	0.21	0.98	0.29	0.38	0.38		
			-1.51	0.72	0.22						
			0.32	0.45	0.09	0.70	0.20	0.28	0.28		
			0.49	0.44	0.12	0.96	0.28	0.37	0.37		
			0.31	0.26	0.08	1.05	0.31	0.41	0.41		
			1.27	0.05	0.04						
			1.10	-0.03	0.04						
			0.71	-0.09	0.05						
37	6.77	0.65	0.93	-0.28	0.05						
42	6.18	0.04	0.42	-0.38	0.06						
45	5.90	-0.08	0.40	-0.48	0.06						
52	5.65	-0.18	0.55	-0.73	0.05						
Sup_ter	5.90		8.61%	21.10%	1R						
ER (ir la)	1.37		kM	kr							
Selecto	1.30		8.61%	21.10%	2R						

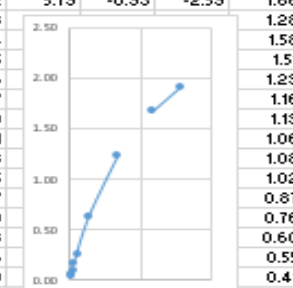
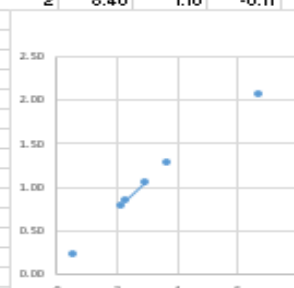


T3ave - Cave										1R	2R
ADHP_	COD	Shpm	Shpr	ZAD	-LYA	Skpr/2	AD	Skpr	Skpr	Skpr	Skpr
RS [d]						I ₀ COD	I ₀ COD	-MYD	-MYD	-MYD	-MYD
						I ₀ COD	I ₀ COD	good	good	good	good
0	10.10	2.58	1.67	0.91							
			1.35	2.27	64.63	1.68	37.45	1.65			
			1.36	1.66	21.00	1.22	13.83	1.27			
			1.24	1.06	9.00	0.86	6.16	0.87			
			1.27	0.97	7.27	0.77	5.00	0.76			
			1.11	0.62							
			1.14	0.62							
			1.05	0.47							
			1.12	0.50							
			0.83	0.28							
			0.75	0.24							
			0.52	0.13							
			0.52	0.16							
			0.19	0.05							
			0.23	0.10	0.21	0.43	0.15	0.04			
			0.15	0.10							
32	6.23	0.32	0.31	0.00	0.08						
37	5.89	0.27	0.45	-0.18	0.07						
42	5.44	-0.20	0.11	-0.30	0.07						
45	5.84	0.37	0.85	-0.49	0.06						
52	5.40	0.07	0.78	-0.71	0.05						
Sup_ter	5.44		210.8	298.8	1R						
ER (ir la)	0.87		kM	kr							
Selecto	0.80		1.93%	11.14%	2R						

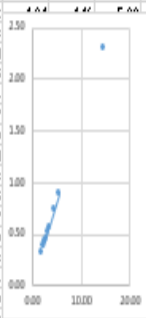
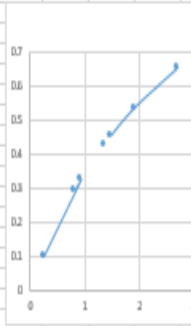
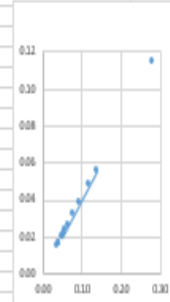


T3a-C1										T3b-C1										T3a-C2										
ADHP_RS [J]	COD	Skpm	Slpr	ZAD	-LTA	Skpm/2 AD I ₀ COD/ qCOD	Spm -HYD	Spm -HYD - pred	Spm -HYD - pred	ADHP_RS [J]	COD	Skpm	Slpr	ZAD	-LTA	Skpm/2 AD I ₀ COD/ qCOD	Spm -HYD	Spm -HYD - pred	Spm -HYD - pred	ADHP_RS [J]	COD	Skpm	Slpr	ZAD	-LTA	Skpm/2 AD I ₀ COD/ qCOD	Spm -HYD	Spm -HYD - pred	Spm -HYD - pred	
0	10.10	3.18	2.27	0.91						0	10.10	5.48	4.57	0.91							0	10.10	-0.02	-0.93	0.91					
2	4.45	-2.89	-4.50	1.61	3.42	11.87	2.13	2.13	2.13	2				1.30	2.05															
3	4.16	-3.28	-4.90	1.62	2.43	8.36	1.50	1.50	1.50	3				1.37	1.69	1.70	0.52	0.37	0.49											
4		-3.95	-5.62	1.67	2.01	6.72	1.20	1.21	1.21	4				1.25	1.09															
5		-4.71	-6.44	1.73	1.78	5.74	1.03	1.03	1.03	5				1.37	1.14															
6		-3.32	-4.84	1.51	1.22	4.50	0.81	0.81	0.81	6				1.16	0.71															
7		-3.56	-5.06	1.51	1.08	4.02	0.72	0.72	0.72	7				1.18	0.67															
9		-2.69	-4.01	1.32	0.74	3.10	0.56	0.56	0.56	9				0.99	0.41	1.22	0.37	0.27	0.40											
11		-2.92	-4.20	1.28	0.63	2.73	0.49	0.49	0.49	11				1.27	0.62															
13		-1.44	-2.46	1.01	0.40	2.21	0.40	0.40	0.40	13				0.88	0.31	1.19	0.36	0.26	0.39											
15		-2.04	-3.05	1.01	0.39	2.15	0.39	0.39	0.39	15				0.76	0.24															
17		1.24	0.72	0.52	0.13	1.37	0.25	0.25	0.25	17				0.75	0.25	1.09	0.33	0.24	0.36											
20		0.10	-0.46	0.56	0.17					20				0.77	0.27															
23		2.26	2.09	0.17	0.05	1.49	0.27	0.27	0.27	23				0.56	0.20	0.65	0.35	0.14	0.25											
26		0.76	0.51	0.25	0.10					26				0.47	0.18															
29		0.22	0.01	0.21	0.12					29				0.35	0.16															
32		0.31	0.23	0.08	0.10					32				5.47	2.00	1.84	0.16	0.12												
37		0.12	0.20	-0.08	0.09					37				4.17	0.63	0.48	0.15	0.15	0.21	0.02	0.05	0.09								
42		-0.20	0.03	-0.23	0.09					42				3.70	0.18	0.16	0.02	0.14												
45		-0.20	0.14	-0.34	0.08					45				4.18	0.66	0.81	-0.15	0.12												
52		5.60	0.22	0.87	-0.65	0.06				52				3.88	0.80	1.23	-0.43	0.10												
Sup_tort	5.62	644.3	3582.2	IR						Sup_tort	3.70	25.91	116.15	IR							Sup_tort	7.18	8.67	21.103	IR					
ER (ir less than)	0.44	kM	kr							ER (ir less than)	-1.48	kM	kr								ER (ir less than)	3.45	kM	kr						
Selected ER	0.20	644.3	3582.2	2R						Selected ER	-2.10	1.278	2.723	2R							Selected ER	3.40	8.67	21.103	2R					
T4a-C1										T4b-C1										T4a-C2										
ADHP_RS [J]	COD	Skpm	Slpr	ZAD	-LTA	Skpm/2 AD I ₀ COD/ qCOD	Spm -HYD	Spm -HYD - pred	Spm -HYD - pred	ADHP_RS [J]	COD	Skpm	Slpr	ZAD	-LTA	Skpm/2 AD I ₀ COD/ qCOD	Spm -HYD	Spm -HYD - pred	Spm -HYD - pred	ADHP_RS [J]	COD	Skpm	Slpr	ZAD	-LTA	Skpm/2 AD I ₀ COD/ qCOD	Spm -HYD	Spm -HYD - pred	Spm -HYD - pred	
0	9.42	2.60	1.69	0.91						0	9.42	3.50	2.59	0.91							0	9.42	-0.60	-1.51	0.91					
2	6.59	-0.65	-1.90	1.25	1.83					2				1.48	2.84	13	1.92	3.07	1.90											
3	5.22	-2.12	-3.52	1.40	1.78					3				1.39	1.75	4.96	1.26	1.26	1.27											
4	6.95	0.16	-0.92	1.07	0.69					4				0.81	0.11	2.8189	0.84	0.73	0.90											
5	7.14	0.00	-1.06	1.06	0.59					5				1.04	0.56															
6	8.34	1.26	0.40	0.86	0.25	3.60	0.29	1.26	0.29	6				0.99	0.45	0.1028	0.46	0.03	0.05											
7	7.18	-0.11	-1.10	0.99	0.44					7				0.66	0.01															
9	7.46	0.38	-0.48	0.86	0.28					9				0.85	0.27	0.6099	0.32	0.16	0.26											
11	7.09	0.11	-0.71	0.82	0.25					11				0.98	0.39															
13	6.51	0.48	-0.22	0.70	0.18					13				0.85	0.29															
15	5.98	-0.13	-0.83	0.70	0.21					15				0.80	0.27															
17	7.57	1.39	0.96	0.43	0.08	2.24	0.19	0.83	0.19	17				0.57	0.15															
20	6.09	0.04	-0.45	0.49	0.14					20				0.54	0.17	0.0237	0.31	0.01	0.01											
23	7.92	2.14	2.03	0.11	0.02	1.84	0.15	0.69	0.15	23				0.51	0.18															
26	7.73	2.26	2.39	-0.03	0.01					26				0.23	0.10															
29	5.81	0.01	-0.15	0.16	0.10	1.44	0.12	0.55	0.12	29				0.31	0.15															
32	5.65	-0.02	-0.07	0.05	0.09					32				4.40	-0.27	-0.98	0.21	0.14												
37	5.62	-0.12	0.00	-0.12	0.08					37				4.38	-0.46	-0.49	0.03	0.12												
42	5.27	-0.44	-0.17	-0.27	0.08	0.64	0.05	0.26	0.05	42				4.70	-0.12	0.08	-0.20	0.10												
45	5.36	-0.26	0.03	-0.39	0.07					45				4.74	-0.08	0.24	-0.31	0.09												
52	5.88	1.26	-0.77	0.04						52				4.41	0.03	0.61	-0.59	0.08												
Sup_tort	5.36	8.67	21.103	IR						Sup_tort	4.70	28.23	106.54	IR							Sup_tort	7.18	8.67	21.103	IR					
ER (ir less than)	0.18	kM	kr							ER (ir less than)	-0.48	kM	kr								ER (ir less than)	3.45	kM	kr						
Selected ER	0.10	5.969	70.118	2R						Selected ER	-0.80	2.737	5.715	2R							Selected ER	3.30	2.035	16.922	2R					

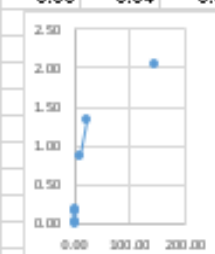
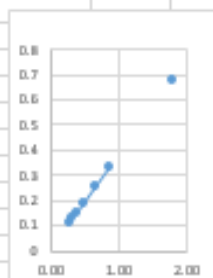
T5b - C2										T5a - Cove									
ABMP _RS (4)	COD	Sbpm	Slp _{pe}	ZAD	rLTd	ZAD (qCOD /qCOD)	Spec rHTD	Spec rHTD - pred	Spec rHTD - pred	ABMP _RS (4)	COD	Sbpm	Slp _{pe}	ZAD	rLTd	ZAD (qCOD /qCOD)	Spec rHTD	Spec rHTD - pred	Spec rHTD - pred
0	12.28	4.56	3.66	0.90						0	12.28	5.56	4.66	0.90					
2	8.40	1.10	-0.17		1.27	1.95	6.678	1.54	2.07	2	5.79	-0.93	-2.59	1.66	3.66	7.815	2.21	2.61	1.92
					1.20	1.21				3				1.28	1.45	5.808	1.30	1.99	1.67
					1.22	1.04				4				1.58	1.81				
					0.95	0.41				5				1.51	1.40	3.4	1.23	1.20	1.23
					0.79	0.16	3.655	0.60	1.27	6				1.29	0.90	1.357	0.51	0.49	0.63
					1.69	0.06				7				1.16	0.65	0.306	0.43	0.11	0.17
					1.88	0.30				8				1.19	0.61				
					0.54	0.04				11				1.06	0.45				
					0.67	0.17	2.943	0.33	1.05	13				1.08	0.45	0.476	0.41	0.17	0.25
					1.66	0.18	2.279	0.28	0.84	15				1.02	0.40				
					0.75	0.25				17				0.87	0.31				
					0.53	0.16	2.13	0.31	0.79	20				0.76	0.26	0.178	0.39	0.06	0.10
					0.37	0.12				23				0.60	0.21				
					1.43	0.17	0.575	0.25	0.23	26				0.55	0.21	0.097	0.35	0.04	0.06
					1.23	0.12				29				0.41	0.18				
					0.21	0.14				32				0.33	0.17				
37	7.05	2.06	2.20	-0.15	0.08					37	5.82	1.00	0.89	-0.11	0.14	0.064	0.26	0.02	0.04
42	6.34	1.29	1.52	-0.24	0.09					42	5.04	0.20	0.17	0.03	0.14				
45	6.72	1.99	2.42	-0.44	0.06					45	5.04	0.36	0.46	-0.10	0.13				
52	5.17	0.30	0.78	-0.48	0.09					52	4.66	0.14	0.47	-0.33	0.12				
Sup_tes	4.78		8.613	21.1	1R					Sup_tes	5.46		30.37	82.98	1R				
ER (is le	1.44		kM	ks						ER (is le	0.14		kM	ks					
Selected	1.00		8.613	21.1	2R					Selected	0.00		3.343	5.808	2R				



TSa-C1										TSb-C1										TSa-C2									
ADHP_RS [d]	COD	Shpm	Shpr	ZAD	LVZ	Shpr/Z AD 1/COD	Sprn -HYD	Sprn -HYD - pred	Sprn -HYD - pred	ADHP_RS [d]	COD	Shpm	Shpr	ZAD	LVZ	Shpr/Z AD 1/COD	Sprn -HYD	Sprn -HYD - pred	Sprn -HYD - pred	ADHP_RS [d]	COD	Shpm	Shpr	ZAD	LVZ	Shpr/Z AD 1/COD	Sprn -HYD	Sprn -HYD - pred	Sprn -HYD - pred
0	12.28	5.46	4.56	0.90						0	12.28	6.71	5.81	0.90							0	12.28	2.86	1.96	0.90				
2	4.01	-3.23	-5.17	1.94	4.90	0.28	2.53	0.11	0.11	2	7.57	1.58	0.10	1.48	2.89						2	7.57	1.58	0.10	1.48	2.89			
3	9.39	2.05	0.83	1.23	1.28					3	7.46	1.37	-0.11	1.47	2.01						3	7.46	1.37	-0.11	1.47	2.01			
4	4.79	-2.00	-3.71	1.71	2.10	0.14	1.23	0.06	0.06	4			0.07	1.66	2.01						4								
5	4.22	-2.93	-4.72	1.79	1.89	0.12	1.06	0.05	0.05	5			0.98	1.51	1.39						5								
6	5.65	-1.44	-3.00	1.56	1.30	0.09	0.83	0.04	0.04	6			0.95	1.26	0.85	2.7	0.67	0.98	0.65		6								
7	6.62	-0.67	-2.10	1.43	0.99	0.08	0.69	0.03	0.03	7			0.08	1.09	0.57	1.9022	0.52	0.71	0.54		7								
9	6.00	-1.08	-2.48	1.40	0.82	0.07	0.58	0.03	0.03	9			0.60	1.08	0.50	1.476	0.47	0.56	0.46		9								
11	5.21	-1.78	-3.19	1.42	0.74	0.06	0.52	0.02	0.02	11			0.12	0.85	0.28		0.33	0.00	0.00		11								
13	4.03	-2.00	-3.37	1.37	0.65	0.05	0.47	0.02	0.02	13			0.06	0.90	0.33		0.36	0.00	0.00		13								
15	4.46	-1.66	-2.91	1.25	0.53	0.05	0.43	0.02	0.02	15			0.25	0.93	0.34	1.3541	0.37	0.52	0.43		15								
17	7.05	0.88	0.02	0.86	0.30					17			0.06	0.99	0.38		0.38	0.00	0.00		17								
20	6.23	0.18	-0.66	0.84	0.30	0.04	0.36	0.02	0.02	20			0.67	0.83	0.29	0.8122	0.32	0.32	0.30		20								
23	6.46	0.69	0.03	0.66	0.23	0.04	0.35	0.02	0.02	23			0.67	0.73	0.26	0.9197	0.36	0.36	0.33		23								
26	6.19	0.82	0.29	0.53	0.20					26			0.16	0.69	0.25	0.2374	0.09	0.10	0.10		26								
29	6.28	0.48	0.02	0.46	0.19	0.03573	0.42	0.01	0.01	29			0.00	0.49	0.20						29								
32	6.28	0.61	0.27	0.34	0.17					32			0.57	0.44	0.20						32								
37	6.23	0.49	0.32	0.17	0.15					37			0.64	0.27	0.18						37								
42	5.29	-0.42	-0.52	0.10	0.16					42			0.15	0.16	0.17						42								
45	5.24	-0.48	-0.47	-0.01	0.15					45	4.83	0.36	0.31	0.05	0.16						45	7.13	0.70	1.19	-0.49	0.05			
52	5.46	0.18	0.53	-0.35	0.11					52	3.86	-0.17	-0.02	-0.15	0.15	0.1628					52	6.77	0.20	0.89	-0.69	0.06			
Sup_tot	5.46		8.61%	21.103	1R					Sup_tot	4.78		8.61%	21.103	1R						Sup_tot	5.46		51.65%	478.46	1R			
ER (ir less than)	0.28		kM	kr						ER (ir less than)	-0.40		kM	kr							ER (ir less than)	3.04		kM	kr				
Selected ER	0.10		8.61%	21.103	2R					Selected ER	-1.15		1.362	2.928	2R						Selected ER	2.70		43%	2748	2R			



T5b - Cave										T5ave - Cave									
ABMP _RS (4)	COD	Sbpm	Sbpa	ZAD	rkT4	Sbpa/ZAD (qCOD/qCOD)	Spec rHTD	Spec rHTD - prod	Spec rHTD - prod	ABMP _RS (4)	COD	Sbpm	Sbpa	ZAD	rkT4	ZAD (qCOD/qCOD)	Spec rHTD	Spec rHTD - prod	Spec rHTD - prod
0	12.28	4.41	3.51	0.90						0	12.28	5.01	4.11	0.90					
2	6.62	-1.25	-2.80	1.55	3.19					2	6.20	-1.07	-2.67	1.60	3.42	143.44	2.14	14.43	2.03
3	9.48	1.62	0.47	1.15	1.05	1.80	2.057	1.32	0.68	3	8.95	1.69	0.48	1.22	1.25				
4	6.68	-0.30	-1.65	1.35	1.33					4	5.82	-0.56	-2.02	1.47	1.57	24.00	1.07	9.11	1.33
5	7.49	0.38	-0.85	1.23	0.91	0.86	0.979	0.65	0.34	5	6.41	-0.10	-1.47	1.37	1.15	10.40	0.84	5.77	0.86
6	8.66	1.44	0.37	1.06	0.56	0.65	0.738	0.49	0.26	6	7.75	1.13	-0.05	1.18	0.73				
7	9.50	1.94	0.98	0.96	0.40	0.46	0.527	0.35	0.18	7	8.71	1.75	0.69	1.06	0.52				
9	8.06	0.33	-0.76	1.09	0.51	0.36	0.415	0.28	0.15	9	7.66	0.53	-0.61	1.14	0.56				
11	8.63	1.19	0.29	0.91	0.33					11	8.04	1.20	0.22	0.98	0.39	1.69	0.62	1.33	0.20
13	6.79	0.17	-0.79	0.96	0.37	0.32	0.364	0.25	0.13	13	6.34	0.32	-0.70	1.02	0.41	1.37	0.40	1.10	0.17
15	6.81	0.18	-0.71	0.89	0.32					15	6.28	0.25	-0.71	0.95	0.36				
17	7.48	0.73	-0.01	0.74	0.24					17	7.00	0.85	0.05	0.80	0.28				
20	7.42	0.90	0.29	0.61	0.20					20	6.84	0.92	0.24	0.68	0.23	0.35	0.34	0.29	0.05
23	7.61	1.49	1.06	0.42	0.14	0.28	0.324	0.22	0.11	23	6.90	1.38	0.86	0.51	0.18				
26	6.57	0.65	0.23	0.42	0.16					26	6.07	0.75	0.27	0.48	0.18				
29	7.18	0.85	0.56	0.28	0.14					29	6.67	0.94	0.59	0.35	0.16	0.06	0.34	0.05	0.01
32	6.77	0.50	0.29	0.22	0.14					32	6.31	0.65	0.37	0.27	0.15				
37	7.46	1.50	1.59	-0.10	0.09					37	6.64	1.27	1.26	0.01	0.11				
42	6.60	0.61	0.78	-0.17	0.10					42	5.82	0.43	0.50	-0.07	0.12				
45	6.93	1.10	1.44	-0.34	0.08					45	5.98	0.76	0.98	-0.22	0.11				
52	5.97	0.30	0.80	-0.50	0.09					52	5.32	0.24	0.66	-0.42	0.10				
Sup_tes	4.78		20.89	26.68	1R					Sup_tes	13.26		16.34	19.03	1R				
ER (is le	1.45		kM	ks						ER (is le	0.79		kM	ks					
Selected	1.15		8.619	21.1	2R					Selected	0.55		2.276	17.16	2R				



APPENDIX I: UCTPSU MODEL VERIFICATION

Table I.1 Composition Matrix - Balance Check									
	COD	C	H	O	N	P	Charge	Mass	
H ₂ O	0	0	0.113	0.888	0	0	0	1	
S _H	0	0	1	0	0	0	0.9921	1	
S _{Na}	0	0	0	0	0	0	0.087	1	
S _K	0	0	0	0	0	0	0.026	1	
S _{Ca}	0	0	0	0	0	0	0.050	1	
S _{Mg}	0	0	0	0	0	0	0.082	1	
S _{NHx}	0	0	0.223	0	0.777	0	0.055	1	
S _{Cl}	0	0	0	0	0	0	-0.056	1	
S _{VFA}	1.084	0.407	0.0514	0.542	0	0	-0.017	1	
S _{Pr}	1.533	0.4933	0.069	0.438	0	0	-0.014	1	
S _{CO3}	0	0.200	0	0.800	0	0	-0.033	1	
S _{SO4}	0	0	0	0	0	0	-0.021	1	
S _{PO4}	0	0	0	0.674	0	0.326	-0.032	1	
S _{H2}	7.937	0	1	0	0	0	0	1	
S _{CH4}	3.99	0.749	0.2519	0	0	0	0	1	
S _U	1.420	0.487	0.067	0.385	0.035	0.025	0	1	
S _F	1.418	0.470	0.079	0.371	0.065	0.015	0	1	
S _{Glu}	1.066	0.400	0.067	0.533	0	0	0	1	
S _O	0.031	0	0	1	0	0	0	1	
S _{NOx}	0	0	0	0.774	0.226	0	-0.016	1	
S _{N2}	0	0	0	0	0.966	0	0	1	
X _{U_Inf}	1.478	0.515	0.064	0.324	0.068	0.029	0	1	
X _{Glycogen}	1.152	0.432	0.064	0.504	0	0	0	1	
X _{B_Org}	1.447	0.515	0.063	0.243	0.137	0.041	0	1	
X _{PAO_PP}	0	0	0	0.480	0	0.310	0	1	
X _{PAO_Stor}	1.673	0.558	0.070	0.372	0	0	0	1	
X _{Str_NH4}	0	0	0.066	0.652	0.057	0.126	0	1	
X _{ACP}	0	0	0	0.41	0	0.200	0	1	
X _{Str_K}	0	0	0.045	0.600	0	0.116	0	1	
X _{Cal}	0	0.120	0	0.480	0	0	0	1	
X _{Mag}	0	0.142	0	0.5693	0	0	0	1	
X _{Newb}	0	0	0.040	0.642	0	0.178	0	1	
X _{OHO}	1.447	0.515	0.063	0.243	0.137	0.041	0	1	
X _{PAO}	1.447	0.515	0.063	0.243	0.137	0.041	0	1	

X_AD	1.447	0.515	0.063	0.243	0.137	0.041	0	1
X_AC	1.447	0.515	0.063	0.243	0.137	0.041	0	1
X_AM	1.447	0.515	0.063	0.243	0.137	0.041	0	1
X_HM	1.447	0.515	0.063	0.243	0.137	0.041	0	1
X_U_Org	1.478	0.515	0.064	0.324	0.068	0.029	0	1
X_B_Inf	1.466	0.464	0.085	0.404	0.035	0.012	0	1
X_ISS	0	0	0	0	0	0	0	1
X_ANO	1.447	0.515	0.062	0.243	0.137	0.041	0	1
G_CO2	0	0.273	0	0.727	0	0	0	1
G_CH4	3.990	0.749	0.251	0	0	0	0	1

Table I.2 Component values per unit mol									
Molecular weight		COD		C	H	O	N	P	Charge
MW_[H2O]	18.0148	COD_per_mol[H2O]	0	0	2.0158	15.999	0	0	0
MW_[S_H]	1.0079	COD_per_mol[S_H]	0	0	1.0079		0	0	1
MW_[S_Na]	22.99	COD_per_mol[S_Na]	0	0			0	0	2
MW_[S_K]	39.098	COD_per_mol[S_K]	0	0			0	0	1
MW_[S_Ca]	40.078	COD_per_mol[S_Ca]	0	0			0	0	2
MW_[S_Mg]	24.305	COD_per_mol[S_Mg]	0	0			0	0	2
MW_[S_NHx]	18.0386	COD_per_mol[S_NHx]	0	0	4.0316		14.007	0	1
MW_[S_Cl]	35.453	COD_per_mol[S_Cl]	0	0			0	0	-2
MW_[S_VFA]	59.0437	COD_per_mol[S_VFA]	63.996	24.022	3.0237	31.998	0	0	-1
MW_[S_Pr]	73.0705	COD_per_mol[S_Pr]	111.993	36.033	5.0395	31.998	0	0	-1
MW_[S_CO3]	60.008	COD_per_mol[S_CO3]	0	12.011		47.997	0	0	-2
MW_[S_SO4]	96.062	COD_per_mol[S_SO4]	0				0	0	-2
MW_[S_PO4]	94.97	COD_per_mol[S_PO4]	0			63.996	0	30.974	-3
MW_[S_H2]	2.0158	COD_per_mol[S_H2]	15.999		2.0158		0	0	0
MW_[S_CH4]	16.0426	COD_per_mol[S_CH4]	63.996	12.011	4.0316		0	0	0
MW_[S_U]	24.64532	COD_per_mol[S_U]	34.98981	12.011	1.659003	9.487407	0.868434	0.61948	0
MW_[S_F]	25.54681	COD_per_mol[S_F]	36.22974	12.011	2.025879	9.471408	1.666833	0.371688	0
MW_[S_Glu]	180.1548	COD_per_mol[S_Glu]	191.988	72.066	12.0948	95.994	0	0	0
MW_[S_O]	31.998	COD_per_mol[S_O]	1			31.998	0	0	0
MW_[S_NOx]	62.004	COD_per_mol[S_NOx]	0			47.997	14.007	0	-1
MW_[S_N2]	29.014	COD_per_mol[S_N2]	0				28.014	0	0
MW_[X_U_Inf]	23.32045	COD_per_mol[X_U_Inf]	34.46985	12.011	1.493708	7.551528	1.582791	0.681428	0
MW_[X_Glycogen]	111.0958	COD_per_mol[X_Glycogen]	127.992	48.044	7.0553	55.9965	0	0	0
MW_[X_B_Org]	23.333	COD_per_mol[X_B_Org]	33.76589	12.011	1.474558	5.679645	3.207603	0.960194	0
MW_[X_PAO_PP]	100.0196	COD_per_mol[X_PAO_PP]	0			47.997	0	30.974	0
MW_[X_PAO_Stor]	86.0894	COD_per_mol[X_PAO_Stor]	143.991	48.044	6.0474	31.998	0	0	0
MW_[X_Str_NH4]	245.4024	COD_per_mol[X_Str_NH4]	0		16.1264	159.99	14.007	30.974	0

MW_[X_ACP]	310.174	COD_per_mol[X_ACP]	0			127.992	0	61.948	0
MW_[X_Str_K]	266.4618	COD_per_mol[X_Str_K]	0		12.0948	159.99	0	30.974	0
MW_[X_Cal]	100.086	COD_per_mol[X_Cal]	0	12.011		47.997	0	0	0
MW_[X_Mag]	84.313	COD_per_mol[X_Mag]	0	12.011		47.997	0	0	0
MW_[X_Newb]	174.3273	COD_per_mol[X_Newb]	0		7.0553	111.993	0	30.974	0
MW_[X_OHO]	23.333	COD_per_mol[X_OHO]	33.76589	12.011	1.474558	5.679645	3.207603	0.960194	0
MW_[X_PAO]	23.333	COD_per_mol[X_PAO]	33.76589	12.011	1.474558	5.679645	3.207603	0.960194	0
MW_[X_AD]	23.333	COD_per_mol[X_AD]	33.76589	12.011	1.474558	5.679645	3.207603	0.960194	0
MW_[X_AC]	23.333	COD_per_mol[X_AC]	33.76589	12.011	1.474558	5.679645	3.207603	0.960194	0
MW_[X_AM]	23.333	COD_per_mol[X_AM]	33.76589	12.011	1.474558	5.679645	3.207603	0.960194	0
MW_[X_HM]	23.333	COD_per_mol[X_HM]	33.76589	12.011	1.474558	5.679645	3.207603	0.960194	0
MW_[X_U_Org]	23.32045	COD_per_mol[X_U_Org]	34.46985	12.011	1.493708	7.551528	1.582791	0.681428	0
MW_[X_B_Inf]	25.86675	COD_per_mol[X_B_Inf]	37.91443	12.011	2.207301	10.44735	0.90065	0.300448	0
MW_[X_ISS]	100	COD_per_mol[X_ISS]	0				0	0	0
MW_[X_ANO]	23.333	COD_per_mol[X_ANO]	33.76589	12.011	1.474558	5.679645	3.207603	0.960194	0
MW_[G_CO2]	44.009	COD_per_mol[G_CO2]	0	12.011		31.998	0	0	0
MW_[G_CH4]	16.0426	COD_per_mol[G_CH4]	63.996	12.011	4.0316		0	0	0

13	12	11	10	7	1	Component
Acetogenesis	Xad	Acidogenesis (biobatch)	Acidogenesis (low salt)	Hydrolysis of PDO_PS	Hydrolysis of FSC	
-51.44815363	-0.297496299	-8.835894495	-57.07592593	-0.2882368	-3.4498342	H2O
1.92663	-0.00396	3.750323	5.549626	-0.4082	-0.35025	S_H
						S_Na
						S_K
						S_Ca
						S_Mg
-0.38089	0.170728	-2.52254	-2.52254	1.159882	2.146593	S_NHx
						S_Cl
57.40229		52.70241	105.4048			S_VFA
-73.0705		65.22273				S_Pr
57.81137	0.09804	55.58775	109.1509	-11.0955	-7.93606	S_CO3
						S_SO4
-0.27145985	0.071791942	-1.79782867	-1.79782867	0.921209	1.13964	S_PO4
5.879282		1.799303	7.197212			S_H2
						S_CH4
						S_U
					-25.5468	S_F
		-180.155	-180.155	35.57757	33.99671	S_Glu
						S_O
						S_NOx
						S_N2
						X_U_Inf
						X_Glycogen
	21.46636					X_B_Org
						X_PAO_PP
						X_PAO_Stor
						X_Str_NH4
						X_ACP
						X_Str_K
						X_Cal
						X_Mag
						X_Newb
						X_OHO
						X_PAO
	-23.333	14.24855	14.24855			X_AD
2.151434						X_AC
						X_AM
						X_HM
	1.827536					X_U_Org
				-25.8667		X_B_Inf
						X_ISS
						X_ANO
						G_CO2
						G_CH4

Hauduc Proposed Method to Validate Model using mass-balance relationship								
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
Total	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00