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Variation of ADM1 by using temperature-phased anaerobic digestion (TPAD) operation

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ABSTRACT

The objective of the study was to examine the application of the Anaerobic Digestion Model No. 1 (ADM1) developed by the IWA task group for mathematical modelling of anaerobic process. Lab-scale temperature-phased anaerobic digestion (TPAD) process were operated continuously, and were fed with co-sub-strate composed of dog food and flour. The model platform implemented in the simulation was a derivative of the ADM1. Sensitivity analysis showed that $k_{m,process}$ (maximum specific uptake rate) and $K_{S,process}$ (half saturation value) had high sensitivities to model components. Important parameters including maximum uptake rate for propionate utilisers ($k_{m,pro}$) and half saturation constant for acetate utilisers ($K_{S,ac}$) in the thermophilic digester and maximum uptake rate for acetate utilisers ($k_{m,ac}$) in the mesophilic digester were estimated using iterative methods, which optimized the parameters with experimental results. Simulation with estimated parameters showed good agreement with experimental results in the case of methane production, uptake of acetate, soluble chemical oxygen demand (SCOD) and total chemical oxygen demand (TCOD). Under these conditions, the model predicted reasonably well the dynamic behavior of the TPAD process for verifying the model.

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1. Introduction

Anaerobic digestion is one of promising and cost-effective technologies for the stabilization of food waste that is one of the most abundant and problematic organic solid wastes. The generation of food waste reached about 11,397 tons a day, which generated 32% of municipal solid wastes (Kim, 2005). Also, landfill of food waste has been banned in Korea from 2005 because it can produce other environmental problems including odours and leachate generation (Lim et al., 2008). Hence, anaerobic digestion systems have gained popularity over the past decade, which have already been applied successfully for the treatment of a number of waste streams (Poh and Chong, 2009; Zaher et al., 2008). In the last few years, different configurations of anaerobic digestion systems, such as mesophilic digestion, thermophilic digestion, and temperature-phased anaerobic digestion (TPAD), were studied (Sung and Santha, 2003). However, they showed no major differences in either the organic matter reduction or specific methane yields compared with a conventional mesophilic anaerobic digestion process (Song et al., 2004). Moreover, thermophilic operation showed several problems including a higher energy requirement, a lower quality supernatant with large quantities of dissolved solids, a higher odour potential and much poorer process stability requiring great care (Appels et al., 2008).

Many researchers have therefore proposed a solution in simulating anaerobic digestion processes. Early models were steady state model assuming a rate-limiting step, and most of the developed models were necessarily complex, partial, and unstructured types. The use of these models has been relatively low and limited in practical. Hence, a development of new models for anaerobic digestion processes is much more required. In addition, the increasing complexity of the advanced digestion technologies requires easily applicable models that can represent the impacts of changing environments on chemical and microbial species (Wayne, 2005).

Recently, International Water Association's (IWA) Task Group introduced a generic Anaerobic Digestion Model No. 1 (ADM1). It consisted of a number of processes to simulate all possible reactions occurring in anaerobic sludge including not only biological reactions, such as disintegration, hydrolysis of suspended solid, uptake (growth) and decay of microorganisms, but also physicochemical reactions including ion association/dissociation and liquid-gas transfer. In total, 19 processes, 24 components, and 56 stoichiometric and kinetic parameters were assumed for biological processes relatively, and also, additional processes and parameters were determined for physico-chemical processes. Several studies applied with the ADM1 as basic model concept were as follows; pilot-scale process for anaerobic two-stage digestion of sewage sludge (Blumensaat and Keller, 2005), anaerobic batch-type experiment with glucose (Jeong et al, 2005), and lab-scale blackwater anaerobic digestion (Feng et al., 2005). However, it has a critical





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disadvantage that it is difficult or impossible to measure many parameters (Choi, 2000; Vanrolleghem et al., 1999). Furthermore, in case of anaerobic digestion, practical application is very limited due to not only the complexity of processes and components, but also the lack of experience.

In this study, in order to validate the performance of ADM1, the anaerobic model for co-substrate degradation in TPAD process was conducted based on ADM1, and the sensitivities of kinetic parameters to simulation results were analyzed. With the results of the sensitivity analysis, important parameters in the model implementation were suggested, and their values were estimated using experimental results.

2. Methods

2.1. TPAD process system

2.1.1. Substrate and inoculums

The experimental studies were carried out to determine the parameters of the model by using a lab-scale bioreactor. The loaded co-substrate consisted of flour and dog food. Dog food was crushed by an electrical blender. The substrate characteristics are summarized in Table 1. Sodium bicarbonate was added to the feed mixture to control whole system pH in a range near optimal for anaerobic treatment from 7.8 to 8.2. The seed sludge used for the thermophilic and mesophilic fermenters was obtained from a municipal wastewater treatment plant of Daejeon in Korea.

2.1.2. Reactor and operation

TPAD process consisted of two stages. In the first stage, a stepfeeding reactor was operated at the thermophilic (55 °C) condition. followed by anaerobic sequencing batch reactor (ASBR) operated at the mesophilic (35 °C) condition in the second stage. Each reactor had a working volume of 4.2 L (thermophilic condition) and 11.5 L (mesophilic condition), and a steel stirrer at 200 rpm was used for stirring. The system, which had the water batch circulator and water jacket, was operated automatically by controlling motors, peristaltic pumps and timers. They were operated on the basis of TCOD added from 15.4 to 35.7 g COD/L by stages. Each reactor had its own gas measuring unit. The thermophilic digester was fed with artificial co-substrate from a feeding tank, and the mesophilic digester was fed with the effluent from the thermophilic digester. The first step-feeding reactor was operated continuously by feeding (0.5 h) and withdrawing (0.5 h) substrate once a day (24-h cycle), while one cycle of ASBR consisted of four sequence-fill

Table 1

Characteristics of co-substrate.

Components	Unit	Total COD _{influent} (g COD/L)					
		15.4	25.2	35.7			
Total COD	g/L	15.4	25.2	35.7			
Soluble COD	g/L	2.35	3.01	5.52			
VSS	g/L	10.9	16.3	24.9			
VFA	g COD/L	0.61	1.41	1.79			
VFA composition (COD base))						
Formate	%	11.3	14.1	33.8			
Acetate	%	65.9	28.5	38.6			
Propionate	%	9.74	14.7	1.42			
Butyrate	%	9.83	22.7	18.9			
Valerate	%	3.16	20.1	7.27			
Total Kjeldahl nitrogen	g/L	0.69	1.35	1.52			
Total ammonia nitrogen	g/L	0.021	0.019	0.059			
Protein	g/L	0.69	1.05	1.29			
Carbohydrate	g/L	7.06	10.1	15.6			
рН		7.9	7.9	7.8			
Alkalinity _{added}	g/L as CaCO ₃	4	5	6			

Table 2

Operational conditions of TPAD process.

Thermophilic digester	Run1	Run2			Run3
Total COD _{inf.} (g COD/L) HRT (d) SRT (d) OLR (g COD/L/d)	15.4 4.2 4.2 3.67	25.2 4.2 4.2 6.00			35.7 4.2 4.2 8.50
Mesophilic digester	Run4	Run5	Run6	Run7	Run8
Total COD _{inf.} (g COD/L) HRT (d) SRT (d) OLR (g COD/L/d)	8.58 11.5 230 0.75	12.8 11.5 230 1.11	12.8 11.5 46 1.11	12.8 11.5 23 1.11	17.6 11.5 23 1.53

(0.5 h), react (21 h), settle (2 h), and draw (1 h). The operational conditions were shown in Table 2.

2.2. Modelling of TPAD process system

2.2.1. Model description

The model used in this study described the TPAD process experiments using composite substrate of dog food and flour, as the degradation mechanisms of the substrate could give basic information on the process and kinetic parameters. The chemical oxygen demand (COD) flow assumed in ADM1 is rather complex. The decay of microorganism and the regeneration cycle are strongly interrelated. The ADM1 model is a structured model that reflects the major processes that are involved in the conversion of complex organic substrates into methane, carbon dioxide and inert byproducts. Fig. 1 shows the COD flow in the model (Wayne, 2005), in which an overview of the substrate and conversion process that are addressed by the model is presented. As well, it can be seen that the model includes disintegration of complex solids into inert substances, carbohydrate, proteins and fats. The products of disintegration are hydrolyzed to sugars, amino acids, and long chain fatty acids (LCFA), respectively. Carbohydrates and proteins are fermented to produce volatile organic acids and molecular hydrogen.



Fig. 1. Interrelated COD flow in ADM1.

Long chain fatty acid (LCFA) is oxidized anaerobically to produce acetate (HAc) and molecular hydrogen (H₂). Propionate (HPr), butyrate (HBu) and valerate (HVa) are converted to HAc and H₂. Methane (CH₄) is produced both by HAc to CH₄ and by H₂ to CH₄. To address these mechanism, the model applies state variable to describe the behavior of soluble and particulate components. All organic species are described in terms of COD. Especially, the unit suggested from IWA ADM1 is g COD/L. The simulation results were compared with the net CH₄ production by measuring the endogenous CH₄ production and subtracting it from the total CH₄ production. The matrix form used here was presented in IWA ADM1 Science and Technical Report No. 13 (Bastone et al., 2002). It included processes, components, and stoichiometric and kinetic parameters when composite substrate was used. The processes used in this model were described by IWA (Bastone et al., 2002).

For the simple application, additional assumptions were made:

- No inhibition by pH.
- Methane was gasified as soon as it was produced.
- Hydrogen was quickly converted to methane.
- Physico-chemical process was not considered.

2.2.2. Sensitivity analysis

For the dynamic sensitivity analysis for the continuous experimental model, the average of absolute differences between simulation results with prior determined parameters values suggested by IWA (Bastone et al., 2002) and with parameters with a relative change of target parameter was used as the sensitivity index, as presented in the following equation:

Sensitivityindex =
$$\sum |C_{\text{STD}}(t) - C_{\text{SENS}}(t)|/N$$
 (1)

where *N* is the number of data (simulation time), and C_{STD} and C_{SENS} are the simulation results with suggested parameter values and the parameters with a relative change of target parameter, respectively. The sensitivity analysis of kinetic parameters for seven components was carried out by changing the value of a target parameter from -50% to 50% with respect to their suggested values (Jeong et al., 2005).

Table 3

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Schollyncy of Kinc		components i	in the	uncimopinne	ungester.
2					<u> </u>

2.2.3. Parameter estimation

This stage required that the error in model output was minimized by adjusting parameters. Proper calibration should be done using the observed data under a variety of different conditions with all parameters fixed. With the sensitivity analysis to kinetic parameters, the priority of parameters was evaluated. An iterative method was applied to estimate the parameters. Ultimately, 17 parameters were identified based on the sensitivity analysis. The 17 parameters were k_{dis} (disintegration constant), k_{dec} (decay rate for biomass death), k_{hyd} for carbohydrate, protein and lipid (hydrolysis constant), k_m for HVa, HBu, HPr and HAc (maximum uptake rate), and K_S for HVa, HBu, HPr and HAc (half saturation constant). Parameters were optimized with measured experiment data of CH₄ production, HAc concentration, SCOD concentration, and so on.

2.2.4. Model verification

To verify iterative method as a tool for estimation of model components and parameters, verification test was carried out. The simulated results were compared with the experimental results. The TPAD process was operated with variations of TCOD concentration of the influent from 35.7 to 16.4 g COD/L (loading down), and then from 16.4 to 36.6 g COD/L (loading up).

3. Results and discussion

3.1. Sensitivity analysis

The kinetic parameters were considered for sensitivity analysis, but stoichiometric parameters were negligible due to their little variations. The results of the sensitivity analysis are shown in Tables 3 and 4 for thermophilic and mesophilic digesters by using arbitrary values, respectively. The values indicated sensitivities at the maximum and minimum ranges according to their varieties. Among all kinetic parameters, $k_{m,process}$ (maximum specific uptake rate) and $K_{S,process}$ (half saturation value) were high sensitivities to almost all components; $k_{m,process}$ was much more sensitive than $K_{S,process}$. Jeong et al. (2005) mentioned that $f_{product,substrate}$ (yield of product on substrate) values showed high sensitivities to almost components. $k_{m,process}$, $Y_{substrate}$ (yield of biomass on substrate)

	Valerate		rate Butyrate Propionate Acetate			Methane			Ammonia		SCOD			
	-50%	50%	-50%	-50%	50%	50%	-50%	50%	-50%	50%	-50%	50%	-50%	50%
k _{dis}	0.12	0.20	0.07	0.17	0.09	0.06	0	0.02	0.47	0.19	0.05	0.02	1.45	0.64
k _{hydch}	0.12	0.05	0.48	0.18	0.01	0.02	0.23	0.10	0.17	0.05	0.18	0.05	0.55	0.17
k _{hydpr}	40.6	9.16	35.9	8.05	2.57	0.92	13.1	4.11	1.63	0.44	0.42	0.15	5.10	1.49
k _{hydli}	0	0	0.02	0	0	0	0.11	0.02	0.17	0.05	0.12	0.04	0.52	0.20
k _{dec}	21.1	23.8	20.5	23.1	18.5	23.1	29.2	40.3	4.79	6.12	2.58	3.09	18.9	23.2
k _{m.su}	4.95	1.93	3.52	7.69	0.02	1.93	6.17	4.50	18.4	2.41	20.9	2.40	71.8	9.26
k _{m.aa}	8.45	2.04	7.46	1.80	0.85	0.22	4.36	1.13	0.44	0.11	0.15	0.04	1.50	0.38
k _{m.fa}	0.33	0.41	0.32	0.39	0.29	0.35	0.11	0.61	4.35	4.99	2.98	3.40	16.01	18.36
$k_{m,c4}$	767	79.5	771	74.4	1.29	2.26	7.19	6.48	8.89	1.40	6.37	0.78	32.7	5.08
k _{m.pro}	0.83	0.32	0.81	0.30	190	66.1	0.46	0.28	13.7	4.78	7.75	2.69	49.5	17.2
k _{m.ac}	1.39	0.14	1.35	0.13	1.25	0.11	1166	82.2	74.9	5.28	13.5	0.95	254	17.9
K _{S.su}	1.86	1.04	7.87	1.93	1.74	0.21	4.42	1.92	2.63	2.94	2.67	3.27	10.1	11.4
K _{S.aa}	2.30	2.19	2.02	1.93	0.22	0.21	1.24	1.13	0.12	0.11	0.04	0.03	0.42	0.39
K _{S.fa}	0.35	0.25	0.34	0.24	0.31	0.22	0.33	0.01	4.35	3.31	2.97	2.26	16.0	12.1
K _{S.c4}	89.2	149	84.6	141	2.37	0.66	6.86	3.10	1.55	1.81	0.87	1.24	5.60	6.65
Ks.pro	0.26	0.24	0.25	0.24	55.2	53.8	0.22	0.04	3.99	3.88	2.25	2.19	14.3	13.9
K _{S.ac}	0.10	0.10	0.10	0.10	0.08	0.09	71.2	78.2	4.57	5.02	0.82	0.90	15.5	17.1

Note: Boldface indicates high sensitivities to all components.

 k_{dis} : disintegration constant, d⁻¹.

 k_{hydch} , k_{hydpr} , k_{hydli} : hydrolysis rate of carbohydrate, protein, and lipid, respectively, d⁻¹.

 k_{dec} : first order decay rate for biomass death, d⁻¹.

k_{msu}, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}*, *k_{maa}, <i>k_{maa}*, *k_{maa}, <i>k_{maaa*}

Table 4
Sensitivity of kinetic parameters to components in the mesophilic digester.

	Valerate		alerate Butyrate		Propion	Propionate Acetate		ate Methane		Ammonia		SCOD		
	-50%	50%	-50%	-50%	50%	50%	-50%	50%	-50%	50%	-50%	50%	-50%	50%
k _{dis}	16.2	6.31	16.3	6.34	4.03	1.55	2.84	1.03	0.22	0.09	0.07	0.02	0.99	0.39
k _{hydch}	0.27	0.05	0.76	0.14	0.92	0.24	0.57	0.15	0	0	0	0	0.03	0
k _{hydpr}	12.8	0.66	11.1	0.56	5.46	1.18	5.34	1.15	0.06	0	0.09	0.01	0.33	0.07
k _{hydli}	0	0	0.02	0	0.04	0.01	1.17	0.43	0.03	0	0.02	0	0.24	0.08
k _{dec}	5.36	5.38	5.28	5.24	24.2	30.6	26.4	39.9	0.14	0.05	0.01	0	6.45	6.55
k _{m.su}	1.08	0.05	1.29	0.10	58.7	7.70	60.1	5.48	0.22	0.02	0.30	0.03	3.56	0.40
k _{m.aa}	0.02	0	0.03	0	1.01	0.25	1.09	0.27	0	0	0	0	0.06	0.01
k _{m.fa}	0.18	0.19	0.18	0.19	0.30	0.36	39.5	39.1	0.35	0.32	0.29	0.27	7.94	7.34
$k_{m.c4}$	4.27	0.28	4.83	0.40	34.0	5.11	29.5	3.78	0.21	0.02	1.21	0.11	1.37	0.20
k _{m.pro}	0.01	0.04	0.01	0.04	144	44.7	64.4	16.2	0.15	0.04	0.06	0.01	3.25	0.91
$k_{m.ac}$	0.88	0.03	0.88	0.03	1.31	0.10	4297	8.52	5.72	0.01	1.51	0	124	0.31
K _{S.su}	0.05	0.09	0.10	0.14	8.35	9.28	5.94	7.25	0.03	0.03	0.04	0.04	0.43	0.48
K _{S.aa}	0	0	0	0	0.27	0.25	0.29	0.27	0	0	0	0	0.01	0.01
K _{S.fa}	0.17	0.13	0.17	0.13	0.31	0.23	34.5	29.5	0.28	0.26	0.24	0.22	6.50	5.88
K _{S.c4}	0.25	0.36	0.39	0.54	5.66	6.93	4.18	5.34	0.02	0.04	0.12	0.20	0.22	0.26
K _{S.pro}	0.04	0.02	0.04	0.02	37.9	39.1	13.8	15.4	0.03	0.03	0.01	0.01	0.76	0.82
K _{S.ac}	0.02	0.02	0.02	0.02	0.07	0.08	7.67	11.9	0.01	0.01	0	0	0.27	0.40

Note: Boldface indicates high sensitivities to all components.

 k_{dis} : disintegration constant, d⁻¹.

 k_{hydch} , k_{hydpr} , k_{hydli} : hydrolysis rate of carbohydrate, protein, and lipid, respectively, d⁻¹.

 k_{dec} : first order decay rate for biomass death, d^{-1} .

k_{msu}, *k_{maa}*, *k_{m,fa}*, *k_{m,ca}*, *k_{m,ro}*, *k_{m,ac}*: maximum uptake rate for sucrose, amino acid, long chain fatty acid, butyrate, propionate, and acetate, respectively, kg COD/kg COD d. *K*_{S,su}, *K*_{S,aa}, *K_{S,fa}*, *K_{S,ca}*, *K_{S,fa}, <i>K_{S,ca}*, *K_{S,fa}*, *K_{S,ca}*, *K_{S,ca}, <i>K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}, <i>K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}, <i>K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}, <i>K_{S,ca}*, *K_{S,ca}*, *K_{S,ca}, <i>K_{S,ca}*, *K_{S,ca}, <i>K_{S,c*}

and $K_{S,process}$ were parameters that are not so important in their study. As shown in Table 3, the results indicated that the sensitivity of each component was most dependent on the number of processes related to them. For example, HAc concentration was mainly controlled by the "uptake of acetate" process. This meant that HAc concentration was dependent on parameters used by the "uptake of acetate" ($k_{m.ac}$ and $K_{S.ac}$) (Jeong et al., 2005). As well, k_{dec} and k_{hydpr} were highly sensitive parameters to all acids against methane and ammonia concentration. HVa and HBu were related to the $K_{s.c4}$ and $k_{m.c4}$, respectively. HPr was connected to $K_{s.pro}$ and $k_{m.pro}$, too. As shown in Table 4, they show the different tendencies compared with the thermophilic digester in case of methane, ammonia and SCOD concentration. They, in the majority of the cases, were sensitive in the whole process of the thermophilic condition, and among them, SCOD was the most sensitive component to all parameters. SCOD had interlinked to whole concentration, hence almost every parameter showed a sensitive tendency to SCOD concentration. Meanwhile, these kinds of components in the mesophilic condition were showed as less sensitive components. HAc was sensitive to all parameters. $k_{m.ac}$ was the most important parameter. $k_{m.su}$ and $k_{m.fa}$ showed higher sensitivities than the other parameters. In case of half saturation values, $K_{s.fa}$ was the important parameter, but methane showed relatively low sensitivities.

Table 5

Initial and estimated parameter values optimized.

System type	Parameter	Name	Initial values		Estimated value	Unit	
			Bastone et al. (2000)	Siegrist et al. (2002)	Blumensaat and Keller (2005)	This study	
Thermophilic digester (55 °C)	<i>k</i> _{dis}	Disintegration constant					d^{-1}
			1.0		0.5	0.9	
	k _{dec}	Decay rate for biomass death	0.04			0.02	d^{-1}
	Ka	Half saturation constant for sugar utilisers	0.04			0.03	kg COD/m ³
	NS.su	han saturation constant for sugar utilisers	1	200		1.5	kg cob/m
	K _{S.aa}	Half saturation constant for amino acid utilisers					kg COD/m ³
			0.3	200		0.6	
	K _{m.pro}	Maximum uptake rate for propionate utilisers	20		16	45	COD/COD/d
	K _{S.pro}	Half saturation constant for propionate	0.3 150		10	40	kg COD/m ³
		utilisers		150	0.4	3	
	k _{m.ac}	Maximum uptake rate for acetate utilisers					COD/COD/d
	K _{S.ac}		16		25	14	In COD/m3
		Half saturation constant for acetate	03	300	0.4	0.6	kg COD/m-
Maaanhilia dimaatan	1.	Disintegration constant	0.5	500	0.1	0.0	4 -1
(35 °C)	K _{dis}	Disintegration constant	0.5		10	0.4	u ·
(33 C)	$k_{m,pro}$	Maximum uptake rate for propionate utilisers	0.5		1.0	0.1	COD/COD/d
			13		9	12.5	
	K _{S.pro}	Half saturation constant for propionate utilisers					kg COD/m ³
	1.	Maximum untaka rato for acotato	0.1	20	0.2	0.3	con/con/d
	к _{m.ac}	utilisers	8		9	6.5	cob/cob/u
			-		-		

3.2. Parameter estimation for model calibration

The references and optimized values of selected parameters are given in Table 5. Among 17 parameters, some parameters such as maximum uptake rate for propionate utilisers ($k_{m,pro}$), half saturation constant for propionate utilisers ($K_{S,pro}$), maximum uptake rate for acetate utilisers ($k_{m.ac}$), and half saturation constant for acetate utilisers $(K_{S,ac})$ were considered as having the greatest impact on the model output, and were estimated in comparison with experimental data. In the thermophilic digester, the variations of $K_{S,pro}$, *k*_{*m.pro*}, *K*_{*S.ac*}, *K*_{*S.aa*}, and *k*_{*m.ac*} were 90%, 55%, 50%, 50%, and 13%, while only both $K_{S,pro}$ (67%) and $k_{m,ac}$ (19%) were found to be most sensitive in the mesophilic digester. However, Bastone et al. (2000) suggested that most of the kinetic parameters were considered fixed since they were generally known to have limited variability in anaerobic systems. Values with a low sensitivity and initial parameters were preferably taken from the values recommended by ADM1. This stage requires that the error in model output was minimized by adjusting parameters. Proper calibration should be done using data collected under a variety of different conditions without altering parameters. The result of methane production modelling in comparison with experimental data is shown in Fig. 2. The methane production was converted as COD value, and it was directly proportional to TCOD concentration added. The simulation results with optimised parameters showed a good agreement with the experimental data. The model predicts the increment of the methane production as a response of the load increase. However, the accuracy of the model prediction in the mesophilic digester decreased. There are two reasons to support; one was that a problem of separation between solid and liquid was occurred, the other was that mesophilic digestion sludge was washed out while controlling SRT.

Fig. 3 shows the performance of the TCOD and SCOD. In every experimental run, the systems were considered to be in steady state, which was less than 6% variation in TCOD concentration. To ascertain that a steady state condition had been established, the reactor was operated at all period for 212 days. In the whole performance of the SCOD concentration in TPAD process, sequential utilization of the SCOD by the bacteria such as the acid producing bacteria and the methane producing bacteria, kept the SCOD concentration at a low level. It indicated that many of inert particulate matters were included in the substrate. Totally, the simulation results with optimised parameters showed a good agreement with



Fig. 2. Methane production modelling in comparison with experimental data.



Fig. 3. The performance of the COD in comparison with the model value: (a) TCOD in the thermophilic digester; (b) SCOD in the whole systems.



Fig. 4. The performance of HAc in comparison with the model value.

the experimental data in both the TCOD and the SCOD. However, in case of the model about the SCOD concentration, model values



Fig. 5. Model verification results with the data of experiments in the whole systems: (a) methane production; (b) TCOD.

were increasing sharply at the turning point of each step. It could be explained as the driving force phenomenon in the biochemical reactions. That is, the microorganism reaction was directly proportional to the biomass concentration in model simulation, while it had something to do with the substrate concentration in real reaction. It was because microorganism population was not enough to uptake the substrate, when organic loading rate loaded up. The performance of the HAc in comparison with model value is given in Fig. 4. Among the VFAs, in case of the performance of the HAc concentration, the simulated results with the estimated parameters showed a good agreement with experimental ones except for the beginning part of each step. The phenomenon was complicated to further optimise the parameter set, and a complete match of simulated and observed results for all loading conditions could not be obtained. Therefore, the ADM1 should be modified for each instance in order to get the optimum model, even though the models became either simplification or complication.

3.3. Model verification

The model outputs in comparison with experimental results for the methane production and the TCOD in the TPAD process are given in Fig. 5. To verify the model's accuracy under dynamic conditions, the TPAD process operating at HRT of 4.2 days for step feed and 11.5 days for ASBR was subjected to various TCOD concentration added. The TPAD process was operated about 80 days. Steady state conditions were reached after a start-up phase with rather unstable operation. In the model output of both the methane production and the TCOD, the simulation results showed a good agreement with the experimental data, but a model output was not a good agreement at the turning points, because model was not sensitive to these points. As mentioned previously, it could be explained as driving force phenomenon; otherwise, the differences could be explained with the non-optimisation of several parameters.

4. Conclusions

This study was to examine the application of the Anaerobic Digestion Model No. 1 (ADM1) developed by the IWA task group for mathematical modelling of anaerobic process. Lab-scale temperature-phased anaerobic digestion (TPAD) process were operated continuously, and were fed with co-substrate composed of dog food and flour. Sensitivity analysis showed that among all kinetic parameters, $k_{m.process}$ and $K_{S.process}$ were high sensitivities to almost all components. Important parameters including maximum uptake rate for propionate utilisers $(k_{m,pro})$ and half saturation value for acetate utilisers $(K_{S,ac})$ in the thermophilic digester and maximum uptake rate for acetate utilisers $(k_{m.ac})$ in the mesophilic digester were estimated using iterative methods, which optimized the parameters with experimental results. In the model output of both the methane production and the TCOD, the simulation results showed a good agreement with the experimental data. The model predicted reasonably well the dynamic behavior of the TPAD process for verifying the model.

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