Three-dimensional numerical simulation model of biogas production for anaerobic digesters

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Wu, B., E.L. Bibeau and K.G. Gebremedhin. 2009. **Three-dimensional numerical simulation model of biogas production for anaerobic digesters**. Canadian Biosystems Engineering/Le génie des biosystèmes au Canada. x.1–x.1. A three-dimensional numerical simulation model that predicts biogas production from a plug-flow anaerobic digester is developed. The model is based on the principles of conservation of mass, conservation of energy, and species transport. A first-order kinetic model is used to predict the forward reaction rate in the digestion process. A user-defined function for computing the source terms of the reaction rate in the species transport is developed. CFD (computational fluid dynamics) simulations are conducted using Fluent 6.1 to predict the temperature profiles and concentration distributions in the digester. Model prediction is checked against measured biogas production obtained from the literature. The predicted and measured results agree within 5%. Biogas production sensitivity to chemical reaction rates is numerically determined. This simplified first-order kinetic model is part of an overall effort to develop a three-dimensional numerical model that can link digester-process controls, fluid flow conditions and anaerobic digestion for different digester design, climatic conditions and manure compositions. **Keywords:** numerical simulation, anaerobic digester, chemical reaction, biogas production, sensitivity analysis, renewable energy.

Une simulation utilisant un modèle numérique en trois dimensions est développée pour prédire la production de biogaz d'un digesteur anaérobie. Le modèle est fondé sur les principes de la conservation de la masse, de l'énergie, et du transport des espèces. Un modèle de premier ordre cinétique est utilisé pour prédire les vitesses de réaction pour le processus de digestion. Une fonction est définie pour calculer la vitesse de réaction des l'espèce. Les simulations numériques sont effectuées avec Fluent 6.1 pour prédire les profils de température et de concentration des espèces dans le digesteur. Les résultats du modèle numérique sont vérifiés en comparant la production de biogaz obtenu à partir de donnes disponible en littérature. La comparaissions des résultants numérique avec les mesure ont une erreur the 5%. L'impact de la sensibilité des réactions chimiques à la production de biogaz est évalué. La simplification de premier ordre cinétique fait partie d'un effort visant à développer un modèles numériques en trois dimensions qui lie le processus de control dans les digesteur anaérobie avec la dynamique des fluide et les conditions de digestion anaérobie pour divers conception de digesteur, conditions climatiques, et compositions de fumier. **Motsclés:** simulation numérique, digesteur anaérobique, réaction chimique, production de biogaz, analyse de sensibilité, énergie renouvelable.

INTRODUCTION

Through anaerobic digestion, cow or swine manure can be a source of energy. At the same time, the process reduces the solid content of the material and produces less offensive odors. Microorganisms break the organic compounds into microbial biomass and other simpler compounds eventually releasing water, carbon dioxide, and methane. Biogas production using anaerobic digesters has been experimentally and theoretically studied since the early 1950s (Buswell and Mueller 1952), and modeling of the process have evolved from simple models (Chen and Hashimoto 1978; Hill 1982, 1983; Hashimoto 1983, 1984; Safley and Westerman 1994; Toprak 1995; Vartak et al. 1999) to complex ones (Masse and Droste 2000; Batstone et al. 2002; Minott 2002; Blumensaat and Keller 2005). The simple models predict biogas by solving empirical algebraic equations without considering the fundamental biochemical reactions involved in the processes. In addition, since the models are not general, they are good only for the conditions they were based on. The complex models, however, are general and include biochemical reactions and contain more inputs. The inputs include: hydraulic retention time (HRT), initial volatile solids (VS) concentration, bacterial growth rate, digester volume, flow rate of manure, and biochemical reactions. Out of the complex models known to us, the ADM1 (Batstone et al. 2002) is the most comprehensive anaerobic digestion model that includes multiple steps describing biochemical and physico-chemistry processes.

Biogas production is sensitive to digester temperature, pH of the liquid manure (Angelidaki and Ahring 1993; Angelidaki et al. 1999; Keshtkar et al. 2003; Yilmaz and Atalay 2003), and non-uniformity of flow of liquid manure inside the digester (Fleming 2002; Vesvikar and Al-Dahhan 2005). These parameters are time and spatially dependent. All the biogas production models mentioned previously but Minott (2002) are either algebraic or time-dependent differential equations without considering the spatial coordinates.

With the simple models, biogas or methane prediction is generally a function of manure temperature inside the digester. For example, Chen and Hashimoto (1978) predicted methane production rate as a function of volatile

solids concentration, kinetic parameter, and specific growth rate, which is dependent on manure temperature. Hill (1982) used Chen and Hashimoto's (1978) model and performed a computer analysis of microbial kinetics of methane fermentation and determined the maximum volumetric methane production. Hashimoto (1983) studied the effects of temperature (35 and 55°C), volatile solids concentration and hydraulic retention time on methane production from swine manure, and developed a mathematical formulation for calculating methane production rate as a function of a kinetic parameter (K). Later, Hashimoto (1984) experimentally determined the kinetic parameter specific for swine manure. He concluded that K increased exponentially as the volatile solids concentration (S_0) increased, and manure temperature had no significant effect on K for S_0 between 33.5 and 61.8 kg VS m^{-3}.

Safley and Westerman (1994) studied methane yield in a low-temperature digestion system. They reported a linear relationship between methane yield and temperature. In another study by Toprak (1995), however, a power-law relationship between biogas production and air temperature was reported. Vartak et al. (1999) experimentally determined biogas production based on loading rate of volatile solids at a specific low temperature (10°C). In addition to digestion temperature, pH of the liquid manure is another important variable in biogas production. Angelidaki and Ahring (1993) studied the effect of pH and temperature on the growth rate of microorganisms for thermophilic digestion of cattle manure. Later, Angelidaki et al. (1999) extended their previous work to develop a dynamic model involving co-digestion of different types of wastes. Similarly, Keshtkar et al. (2003) developed a mathematical model for anaerobic digestion that describes the dynamic behavior of non-ideal mixing of continuous flow reactors, and concluded that methane yield was strongly dependent on pH of the reactor and increased with increasing HRT. Yilmaz and Atalay (2003) addressed the effect of various factors including pH and alkalinity, temperature, nutrients, and toxins on anaerobic bacteria behavior, and pointed out that the optimum pH range for anaerobic digestion is between 6.8 and 7.5, and the optimum temperature for mesophilies appears to be around 35°C.

The complex models are more general and include more factors than the simple models. Masse and Droste (2000) conducted a comprehensive literature review on anaerobic digestion models and developed an improved mathematical model for a sequencing batch-reactor process. They expressed volumetric methane flow rate as a function of volume of 1 mole of gas, volume of liquid in the reactor, and biological activity.

Minott (2002) developed a model based on a moving coordinate system that yields total biogas prediction for a plug-flow digester. The model is a function of HRT, total volatile solids, total substrate degradation, digester volume, and operation temperature. Batstone et al. (2002) developed a general anaerobic digestion model based on biochemical processes (including acidogenesis from sugars, amino acids, long-chain fatty acids, propionate, butyrate and valerate, aceticlastic methanogenesis, and hydrogenotrophic methanogenesis). This model contains 34 differential and algebraic equations and another 32 differential equations. The differential equations are functions of time but are not functions of position. Blumensaat and Keller (2005) did several modifications to the original ADM1 model, which include: extension to a pilot-scale digestion process, calibration to a two-stage thermophilic/mesophilic process configuration, and for use with municipal sewage sludge.

Several researchers (Fleming 2002; Vesvikar and Al-Dahhan 2005; Grebremedhin et al. 2005; Wu and Bibeau 2006; Wu and Chen 2008) studied heat transfer and fluid flow in anaerobic digesters using CFD technique. Fleming (2002) applied CFD to simulate 3-D flow patterns and heat transfer inside a covered lagoon digester. He took the simple kinetic model developed by Hill (1983), modified it by incorporating CFD formulation to calculate biological reaction rates and methane production rates. Vesvikar and Al-Dahhan (2005) performed 3-D, steady-state, CFD simulations to determine the flow patterns inside a digester and to compute hydrodynamic parameters. Grebremedhin et al. (2005) developed a CFD-based one-dimensional comprehensive heat transfer model on plug-flow anaerobic digesters. Later, Wu and Bibeau (2006) extended the 1-D model developed by Gebremedhin et al. (2005) to a 3-D heat transfer model on anaerobic digesters under cold weather applications. Wu and Chen (2008) simulated 3-D flow fields in lab-scale, scale-up, and pilot-scale anaerobic digesters by assuming liquid manure as a non-Newtonian flow, and proposed measures to reduce dead and low velocity zones. These models did not include biochemical reaction to predict biogas production.

To our knowledge, no three-dimensional numerical simulation model that predicts biogas production from anaerobic digestion systems that is based on fundamental principles of biochemical processes exists. The goal of this research is to fill that gap. The model is the first step in developing an application tool that could be used to evaluate the performance of plug-flow anaerobic digesters. Extensive validation would, however, be required before the model is used as an application tool.

Objectives

The specific objectives of the study are:

1. To develop a general 3-D model based on fundamental principles of conservation of mass, conservation of energy, and species transport that predicts biogas production from plug-flow anaerobic digesters;
2. To simulate the temperature and concentration fields in a digester by using *Fluent* CFD commercial computer software;
3. To check model prediction against measured data available in the literature; and
4. To conduct sensitivity analysis to determine the effect of reaction rate on biogas production.

MODEL DEVELOPMENT

Biogas production in an anaerobic digester is a chemical reaction process, which is governed by conservations of mass and momentum, turbulence, energy balance, species transport, and chemical reactions. Because anaerobic digestion is dependent on process flow parameters and temperatures, prediction of temperature and flow variables is critical to solve the species transport.

This model was developed based on the following assumptions:

- Heat flow and species transport through the digester are 3-D and steady.
- The model is limited to plug-flow anaerobic digesters where fluid flow velocity is very low. Thus, momentum and turbulence are considered to be negligible.
- Boundary conditions for the digester cover, walls, and floor are assumed to be adiabatic (Wu and Bibeau 2006).
- Liquid manure is considered to be Newtonian.
- Manure temperature is kept constant at 32°C before species reaction.
- PH range is between 6.8 and 7.5 (Yilmaz and Atalay 2003).
- Species reaction takes place only in one step, i.e., reactants are directly converted into final product without intermediate products.
- After reaction ($C_6H_{12}O_6$) remains at 80%.
- The model is single phase, in which phase-interaction is negligible, and thus, rise of biogas to the surface has no effect on manure transport.

Mass conservation equation

The conservation of mass or continuity equation used is expressed as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho\ u_i) = 0 \tag{1}$$

Energy equation

The energy equation used is of the form (Patankar 1980):

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(u_i(\rho E + p)) = \frac{\partial}{\partial x_i}\left(k_{eff}\frac{\partial T}{\partial x_i} - \sum_j h_j\ \vec{J}_j + u_j(\tau_{ij})_{eff}\right) + S_h \tag{2}$$

where the first three terms on the right-hand side of the equal sign represent energy transfer due to conduction, species diffusion, and viscous dissipation, respectively. S_h includes heat of chemical reaction and any other volumetric heat sources.

Species transport equations

The species transport equations for liquid manure can be written in a general form as (Patankar 1980):

$$\frac{\partial}{\partial t}(\rho\ Y_j) + \frac{\partial}{\partial x_i}(\rho\ u_i\ Y_i) + \frac{\partial}{\partial x_i}\vec{J}_i + R_i \tag{3}$$

For mass diffusion in laminar flow, the diffusion flux, $\vec{J}_i$, is computed as

$$\vec{J}_i = \rho D_{i,m}\frac{\partial Y_i}{\partial x_i} \tag{4}$$

Chemical reaction equations

The initial conversion of raw waste to soluble organics can be expressed as (Chang 2004)

$$C_6H_{13}NO_5 + H_2O + H^+ \rightarrow C_6H_{12}O_6 + NH_4^+ \tag{5}$$

In this study, methane production was simplified by converting ($C_6H_{12}O_6$) into CH_4 and CO_2 through chemical reaction (Buswell and Mueller 1952) as

$$C_nH_aO_b + \left(n - \frac{a}{4} - \frac{b}{2}\right)H_2O \Leftrightarrow \left(\frac{n}{2} - \frac{a}{8} + \frac{b}{4}\right)CO_2 + \left(\frac{n}{2} + \frac{a}{8} - \frac{b}{4}\right)CH_4 \tag{6}$$

where ($C_nH_aO_b$) is organic matter, and a, b, and n are dimensionless coefficients.

By substituting $n = 6$, $a = 12$ and $b = 6$ into Eq. (10), the chemical reaction of ($C_6H_{12}O_6$) results in

$$C_6H_{12}O_6 = 3CO_2 + 3CH_4 \tag{7}$$

There are three species in the mixture. One species, Y_1, representing the reactant ($C_6H_{12}O_6$) and the other two species, Y_2, and Y_3, representing the simplified biogas products, CO_2 and CH_4, respectively.

Modeling reaction rate

The reaction rate can be computed using the Arrhenius expression as

$$R_i = M_{w,i}\sum_{r=1}^{N_R}\hat{R}_{i,r} \tag{8}$$

where, $\hat{R}_{i,r}$ is molar rate of creation or destruction of species i in reaction r, which is calculated as:

$$\hat{R}_{i,r} = (v''_{i,r} - v'_{i,r})\left(k_{f,r}\prod_{j=1}^{N_r}[C_{j,r}]^{\eta'_{j,r}}\right) \tag{9}$$

Information for $k_{f,r}$ is not available in the literature. In this study, $k_{f,r}$ is calculated by using first-order BOD removal rate in an ideal plug-flow reactor (Metcalf and Eddy 2003) as:

$$\frac{C}{C_0} = \exp(-k_{f,r}\cdot\tau) \tag{10}$$

where, C/C_0 is percentage remaining of ($C_6H_{12}O_6$). The hydraulic retention time, τ, is calculated as

$$\tau = \frac{L}{v} \tag{11}$$

where, the velocity of liquid manure, v, can be calculated as

$$v = \frac{\dot{V}}{A} \tag{12}$$

Accordance to our assumption, if $C/C_0 = 80\%$, then, $k_{f,r} = 6.21 \times 10^{-8}(s^{-1})$.

CFD SIMULATION

The commercial CFD software *Fluent* 6.1 (Fluent 2005) was used to model biogas production. The mesh of the digester geometry was generated by using the *Gambit* Software (Fluent 2005). The computational domain that characterizes the liquid manure inside the digester consisted of 31,480 hexahedral grids.

The modeling procedure includes the following steps:

1. Verify the grid.
2. Solve the 3-D, steady state, implicit, and pressure-based model by activating the continuity, energy, and species transport equations. The model accounts for volumetric reactions, diffusion energy source and finite-rate/eddy-dissipation.
3. Define material properties for ($C_6H_{12}O_6$), CH_4, and CO_2.
4. Define operational conditions by activating the gravitational acceleration and keeping all other default numbers.
5. Define boundary conditions by setting heat flux to be zero at all solid walls. Also, set velocity $= 1.1 \times 10^{-5}$ m/s (by solving Eq. 12), temperature $= 305$ K, and species mass fraction ($C_6H_{12}O_6$) at the inlet $= 1.0$ (no chemical reaction takes place at the inlet). Also, assume that flow at the outlet is fully developed.
6. Anaerobic digestion reaction rate, R_i, is calculated from Eqs. (8 and 9) through user defined function in *Fluent*.

Because flow of liquid manure in plug-flow digesters is low, conservation of mass (Eq. 1), energy (Eq. 2) and the species transport (Eq. 3) are solved without flow and turbulence equations. First order upwind scheme was used to discretize the governing equations and were solved using the SIMPLE (semi-implicit method for pressure-linked equations) algorithm (Patankar 1980).

RESULTS and DISCUSSIONS

Information obtained in the literature (Gebremedhin et al. 2004) for one specific plug-flow anaerobic digester was used in the simulation to predict biogas production. The data (Table 1) included: digester dimensions, manure flow rate, hydraulic retention time and ambient temperature. Biogas is assumed to be 60% methane with a density of 0.6679 kg/m^3 (EPA 2005).

For the data given in Table 1, the model predicted 1,207 m^3/day of biogas. The measured data for the same digester (Gebremedhin et al. 2004) was 1,274 m^3/day, which is within 5% of the predicted value. This is a one-point or one data check and cannot be considered a validation. More data are necessary to establish the statistical validation between the predicted and measured results.

In the simulation, convergence occurred after 350 iterations as shown in Fig. 1. The two criteria set for convergence were: (1) residual for species is less than 1×10^{-3}, and (2) residual for energy is less than 1×10^{-5}. The trend of the simulated results was steady and without any oscillations, thus confirming convergence.

In this study, momentum and turbulence were not considered in calculating biogas predictions because velocity of liquid manure in a plug-flow digester is very low. The model is based on the principles of conservation of mass, conservation of energy, and species transport. Three convergence curves – one for energy, and two for species transport are necessary, and the results of the iterations are shown in Fig. 1. The two species are ($C_6H_{12}O_6$) and CO_2. The sum of mass fractions of all species is equal to one. For example, if there are N species in the chemical reaction, the N^{th} mass fraction is determined by $[1 - \Sigma_{i=1}^{N-1} Y_i]$. In this simulation, $N = 3$ because there are only three species. The third species is CH_4.

The range of molar concentrations for the three species ($C_6H_{12}O_6$), CH_4 and CO_2, are: $2.67 \times 10^{-5} - 3.80 \times 10^{-2}$, $8.72 \times 10^{-6} - 1.72 \times 10^{-4}$, and $1.89 \times 10^{-3} - 3.91 \times 10^{-2}$ kmol/m^3, respectively. The simulated

Table 1. Input information and comparison of measured and predicted results[1].

Digester dimension			Measured biogas production (m^3 day^{-1})	Simulated biogas production (m^3 day^{-1})	Error (%)
Length (m)	Width (m)	Depth (m)			
39.62	9.44	4.26	1274	1207	5

[1]Measured biogas production is from Gebremedhin et al. (2004)
Daily manure flow rate $= 38.336$ m^3 day^{-1}.
HRT $= 3.6 \times 10^6$ s.
Retention temperature $= 32°C$.

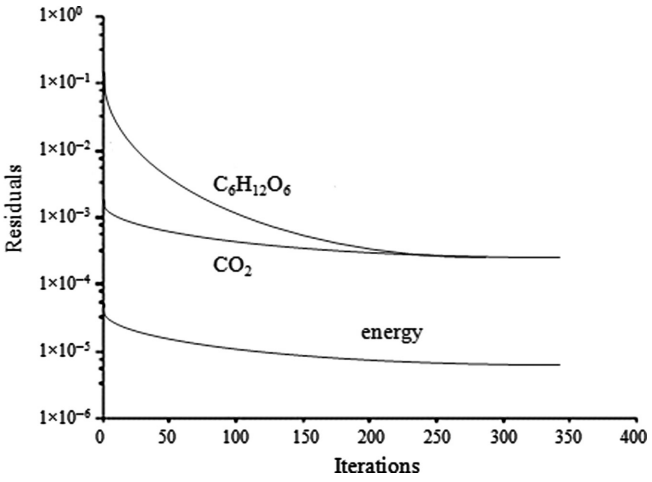

Fig. 1. Residuals versus iterations in the simulation.

contours of the molar concentrations for the three species are given in Figs. 2–4.

The concentration of organic material ($C_6H_{12}O_6$) is high close to the inlet and low far from the inlet (Fig. 2). The concentration remained unchanged after about one-sixth of the length from the inlet. This gradient is due to the fact that influent to the grids near the inlet has higher organic concentration. The distributions for CO_2 and CH_4 are similar (Figs. 3 and 4). The actual values of CH_4 is, however, higher than that of CO_2 because CH_4 is the main product of the chemical reaction. Both concentrations increased gradually from the inlet up to a point and then remained unchanged thereafter.

The temperature profile in the digester is given in Fig. 5. The inlet temperature is 305 K (32°C), which is the assumed boundary-condition temperature, and the outlet temperature is 311 K (38°C). A temperature gradient exists because of the chemical reaction taking place when the reactants (organic material and water) are mixing. A temperature difference of 5°C exists between the inlet and outlet. This could be because we made an assumption that species reaction takes place only in one step and adiabatic boundary conditions are assumed at the digester walls. The assumption that species reaction is taking place only in one step needs to be studied further.

Sensitivity analyses were conducted to determine the effect of reaction rate (R_i and $\hat{R}_{i,r}$ in Eqs. 8 and 9, respectively) on biogas production. The change in biogas

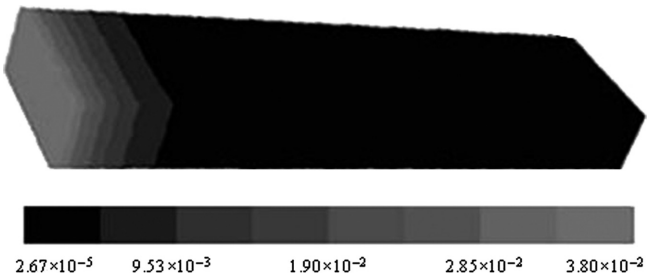

Fig. 2. Contours of simulated molar concentration of $C_6H_{12}O_6$ (kmol m^{-3}).

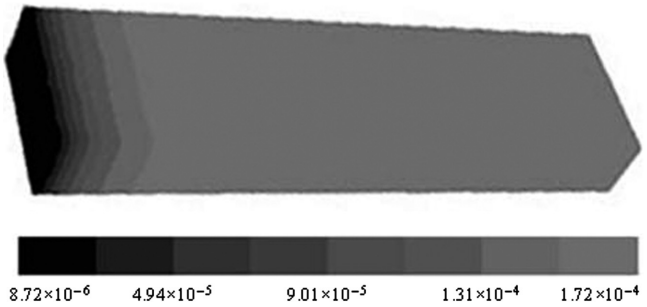

Fig. 3. Contours of simulated molar concentration of CO_2 (kmol m^{-3}).

production is defined by the change in C/C_0 (Eq. 10), which is the percentage remaining of ($C_6H_{12}O_6$). An increase in C/C_0 means that less of ($C_6H_{12}O_6$) is reacting, and consequently, less CH_4 is produced.

The forward rate constant ($k_{f,,r}$ in Eq. 10) was calculated for a given hydraulic retention time (τ). For $\tau = 3.6 \times 10_6\ s$ and $C/C_0 = 85\%$, the resulting $k_{f,r} = 4.52 \times 10^{-8}\ s^{-1}$. An increase in C/C_0 results in a decrease of the forward reaction constant, which results in a decrease of the reaction rate (R_i and $\hat{R}_{i,r}$), and consequently, less biogas is produced. For example, a 5% increase in C/C_0 (from 80 to 85%) resulted in 43% decrease in biogas production (from 1,207 to 689 m^3/day). It is apparent, therefore, that the percentage of organic matter remaining (e.g., $C_6H_{12}O_6$) is critical for the volume of biogas production. It should be noted that $C/C_0 = 80\%$ is an assumed quantity that need to be validated experimentally.

CONCLUSIONS

The following conclusions can be drawn from the study:

1. A three-dimensional numerical simulation model that predicts biogas production from plug-flow anaerobic digestion systems is developed. The model is based on the principles of conservation of mass, conservation of energy, species transport, and chemical reactions.
2. The model prediction is checked against one measured data point available in the literature, and the comparison is within 5%. More data are necessary to

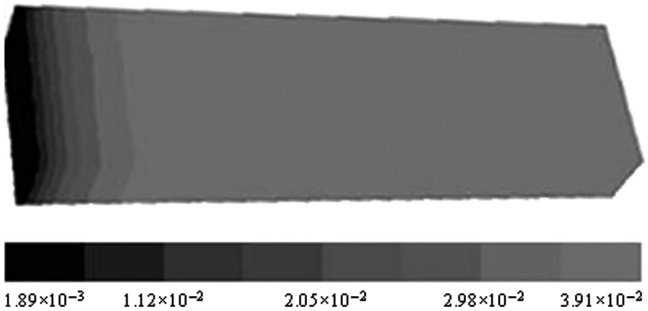

Fig. 4. Contours of simulated molar concentration of CH_4 (kmol m^{-3}).

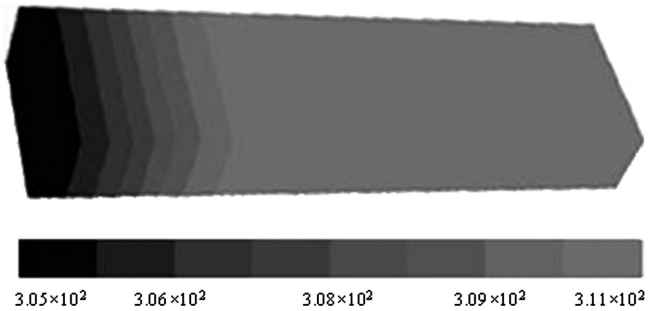

Fig. 5. Contours of simulated static temperature inside the digester (K).

establish statistical validation of the model predictions.

3. Prediction of biogas production is very sensitive to changes in chemical reaction rates. A 5% increase in C/C_0 resulted in 43% decrease in biogas production. Chemical reaction rate is calculated from the percentage remaining of organic materials and hydraulic retention time.

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LIST of SYMBOLS

A	influent area, m^2
ADM1	anaerobic digestion model 1
BOD	biological oxygen demand
BVS	biodegradable volatile solides
C	concentration, mass/volume
	methane, kmol m^{-3}
$C_nH_aO_b$	organic matter, kmol m^{-3}
CO_2	carbon dioxide, kmol m^{-3}
D	diffusivity, $m^2\ s^{-1}$
E	total energy, kJ
h	species enthalpy, kJ
H_2O	water, kmol m^{-3}
HRT	hydraulic retention time, day
J	diffusion flux, kg $m^{-2}\ s^{-1}$
K	kinetic parameter, dimensionless
K_{eff}	effective heat conductivity, W $m^{-1}\ °C^{-1}$
$k_{f,r}$	forward reaction rate constant, s^{-1}
L	digester length, m
M	molecular weight, kg $kgmol^{-1}$
N	species
p	pressure, Pa
R	reaction rate, kg $m^{-3}\ s^{-1}$
S_h	source term, kg kJ $m^{-3}\ s^{-1}$
t	time, s
T	temperature, °C
u, v	velocity magnitude, m s^{-1}
u_i, u_j	velocity in tense form
$\dot{V}$	volumetric flow rate, $m^3\ s^{-1}$
VS	volatile solides
Y	mass fraction, dimensionless
x, y, z	Cartesian coordinates
	Greek symbols
ρ	density, kg m^{-3}
τ	hydraulic retention time, s
τ	shear stress, Pa
$v'_{i,r}$, $v''_{i,r}$	stoichiometric coefficient, dimensionless
$\eta'_{j,r}$	forward rate exponent, dimensionless
	Subscripts
i	tense form
j	species
m	mixture