Use of Physical and Biological Process Models to Understand the Performance of Tubular Anaerobic Digesters

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Abstract

Tubular anaerobic digesters are used in developing countries to produce biogas from livestock waste. In this research, field measurements and physical and biological process modeling studies were used to investigate transport and transformation mechanisms for particulate and soluble organic matter in household-scale tubular digesters in the Monteverde region of Costa Rica. Greater than 75% removal of volatile solids and biochemical oxygen demand (BOD₅) were observed. The high effluent quality was attributed to the formation of a biologically active floccular sludge layer, which allowed for separation of hydraulic and mean cell residence times (HRT and MCRT). A reduced order transport model was developed and validated using field tracer study data. Key assumptions of the reduced order model were verified via computational fluid dynamics (CFD) analysis. The mean HRT predicted by the reduced order model was 23 days and was in good agreement with the tracer experiment. A simplified floccular sludge biological process model was developed and used to estimate an average MCRT of 115 days. The results showed that household-scale tubular anaerobic digesters can provide enough biogas to meet households' cooking energy needs, which was consistent with field results. This is the first study to combine mathematical modeling with field studies of tubular anaerobic digester performance.

Keywords:

Anaerobic processes; Bioreactors; Computational fluid dynamics; Modeling; Tubular anaerobic digester; Waste treatment

List of Equation Nomenclature

μ_t	Eddy viscosity	$\text{N}\cdot\text{s}/\text{m}^2$
C	Ensemble-averaged tracer concentration	$\text{g KCl}/\text{L}$
C'	Tracer fluctuation and flux	$\text{g KCl}/\text{L}$
C_d	Tracer concentration in the digester	$\text{g KCl}/\text{L}$
C_{in}	Influent tracer concentration	$\text{g KCl}/\text{L}$
C_o	Initial tracer concentration in the digester	$\text{g KCl}/\text{L}$
C_{out}	Effluent tracer concentration	$\text{g KCl}/\text{L}$
D_t	Eddy (turbulent) diffusivity	m^2/s
k	Turbulent kinetic energy	J/kg or m^2/s^2
K_d	Biomass cell decay coefficient	day^{-1}
K_m	Maximum specific substrate utilization rate	$\text{g COD utilized}/\text{g biomass COD}\cdot\text{day}$
K_S	Biomass half saturation constant	$\text{g COD}/\text{L}$
$\dot{m}$	Daily methane production rate	$\text{g COD}/\text{day}$
n	Current day	Day
p	Reynolds-averaged pressure	Pa
Q	Flow	L/day
S_b	Soluble substrate concentration	$\text{g COD}/\text{L}$
S_{CH4}	Methane content	%
Sc_t	Schmidt number	dimensionless
t	Time	day or hour
T	Flow-through period	Minute
u_i	Reynolds-averaged velocity	m/s
ν	Kinematic viscosity	m^2/s
V	Volume	L
x_i	Position	M
X_m	Active digester biomass concentration	$\text{g COD}/\text{L}$
X_{me}	Active biomass in effluent concentration	$\text{g COD}/\text{L}$
X_{mi}	Active biomass in influent concentration	$\text{g COD}/\text{L}$
Y_m	Biomass yield coefficient	$\text{g biomass COD}/\text{g COD utilized}$
ε	Turbulent kinetic energy dissipation rate	m^2/s^3
ρ	Density	kg/m^3

List of Acronyms

ADM1	Anaerobic Digestion Model 1
BOD ₅	Five day Biochemical Oxygen Demand
CFD	Computational Fluid Dynamics
CSTR	Completely Stirred Tank Reactor
HRT	Hydraulic Retention Time
FOG	Fats Oils Grease
LCFA	Long Chain Fatty Acids
MCRT	Mean Cell Retention Time
OLR	Organic Loading Rate
RANS	Reynolds-Averaged Navier-Stokes
STP	Standard Temperature Pressure
SVI	Sludge Volume Index
TAN	Total Ammonia Nitrogen
TN	Total Nitrogen
TP	Total Phosphorus
TS	Total Solids
UASB	Upflow Anaerobic Sludge Blanket
VFA	Volatile Fatty Acids
VS	Volatile Solids

1 Introduction

Anaerobic digestion of livestock waste is a waste management technology that can improve the quality of life for those in the developing world. Biogas produced from small-scale anaerobic digesters is most often used as a cooking fuel, but can also be used to heat water or buildings or generate electricity for on-site use [1]. Lack of proper livestock waste management leads to runoff of pollutants into surface waters and contamination of groundwater. Anaerobic digesters can assist in reducing water pollution by decreasing the concentration of organic matter in the waste. In addition, these systems can be a useful tool to mitigate deforestation when biogas is used as a cooking fuel rather than firewood. This also results in decreased public health concerns, especially for women and children who are disproportionately affected by indoor air pollution due to cultural and social roles [1]. The effluent from anaerobic digestion also contains primary nutrients (nitrogen, phosphorus) that can be used as a soil amendment to improve crop yields [1].

Polyethylene tubular anaerobic digesters are commonly used in household-scale applications to recover energy from livestock waste in the developing world. These systems do not require a high level of skilled labor to install; they are easy to operate, low in cost and can operate under a range of temperature conditions. Several studies have been carried out investigating the effect of influent waste characteristics and reactor design and operation on tubular digester performance [1, 2]. However, no prior studies exist that combine mathematical modeling analyzing the physical (transport and mixing) and biochemical processes with field studies of tubular anaerobic digester performance.

Mathematical models have been used to provide insights into operating hydraulic residence time (HRT) and mean cell retention time (MCRT) in anaerobic digesters [3]. Control

of HRT and MCRT are needed to avoid wash-out of soluble substrates and slow growing microorganisms, respectively [4]. Mixing mechanisms in digesters that can affect HRT include formation of dead zones, and short-circuiting/channeling (substrate by-passing treatment) [5]. In bioreactors without solids separation and recycling, MCRT is normally considered to be equal to the HRT; however, even without solids separation or recycling, the MCRT in tubular digesters may be longer than the HRT due to solids settling and accumulation [1, 2]. Tubular digesters are fed with a high solids concentration, which favors collisions between particles to form flocs that are denser than water. Over time a floccular sludge layer forms, similar to processes occurring in anaerobic baffled and upflow anaerobic sludge blanket (UASB) reactors [6,7]. Hydrolysis of particulates into soluble substrates and formation of organic acids (intermediate substrates for methanogens) by acidogens are often considered the rate limiting steps during anaerobic digestion and are affected by the MCRT [4]. As the MCRT increases, hydrolyzing and acidogenic bacterial growth rates increase because they have adequate time to utilize solid and soluble substrates to form acetate and hydrogen (H_2), which are utilized by the methanogens [4].

Computational fluid dynamics (CFD) modeling is a useful tool that can produce residence time distribution (RTD) data for estimating the mean liquid HRT in a digester. CFD models have been successfully applied to contactors used for water and wastewater treatment [8, 31-33]. These models can also provide information on the physical mechanisms within the digester [3]. CFD models can be computationally expensive, and alternatively these models may be used to help validate or to inform simplified transport models, such as plug flow, completely mixed, tanks in series and or dispersion [9]. Several studies have been carried out using CFD to evaluate the effect of transport and mixing mechanisms on biogas production in completely

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4 mixed anaerobic digesters; however, more research is needed to understand the physical
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6 mechanisms contributing to tubular digester performance [3].
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9 While CFD modeling is useful for evaluating the physical processes and liquid HRT in
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11 anaerobic digesters, these models do not evaluate the biological processes occurring in the
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13 digesters. The anaerobic digestion model 1 (ADM1) is a steady-state bioprocess model that
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15 incorporates hydrolysis and acidogenesis with influent and effluent characteristics to estimate
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17 volatile solids (VS) removal and methane (CH_4) production [10]. The ADM1 model is complex,
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19 involving 19 process kinetics and 24 biochemical components to determine digester
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21 performance. In addition, ADM1 models the reactor as a completely stirred tank reactor
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23 (CSTR), which may not be appropriate for modeling the performance of tubular digesters with
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25 floccular sludge accumulation. To overcome this limitation, Bernard et al. [11] and Elmitwalli
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27 [12] developed simple models for anaerobic floccular sludge layer reactors. The models
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29 incorporate acidogenesis and methanogenesis and have been applied to full-scale UASB reactors
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31 [12].
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38 This study investigated the performance (biogas production and effluent quality) of a
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40 tubular digester treating livestock waste in the Monteverde region of Costa Rica through
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42 experimental studies and combined CFD and bioprocess modeling. A tracer study was performed
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44 on this digester to gain insight into transport and mixing mechanisms in the system. A reduced
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46 order model was developed following a CFD simulation of a 24 hour cycle in the digester. The
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48 CFD simulation was also used to visualize transport and mixing mechanisms in the digester.
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51 Meanwhile the reduced order transport model was used to run over several 24 hour cycles in
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53 order to estimate the operating HRT. A simplified bioprocess model, incorporating conversion of
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55 soluble substrates to CH_4 and biomass decay, was used to estimate the active biomass
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concentration in the digester. The active biomass concentration was used to estimate the operating MCRT. Results of the physical and biological process models provided a supporting framework on the relationship between the transport and transformation mechanisms and how these mechanisms affect biogas production and effluent quality in tubular digesters.

2 Materials and Methods

2.1 Site Description and Tubular Digesters

San Luis de Monteverde is a rural mountain community located on the Pacific slope of the Tilarán mountain chain in northwest region of Costa Rica with an altitude range of 600 to 1200 m (~0.85atm) above sea level. San Luis has a population of approximately 500 people. The main economic activities in San Luis are small-scale production and sale of farm products, including coffee, vegetables, fruit, beans, corn, pork, beef, chicken and eggs; rural tourism is also significant. Households in San Luis have access to potable water provided by a locally administrated aqueduct project. Domestic wastewater is normally treated using septic systems, while livestock wastewater remains largely untreated causing contamination of the watershed. To improve livestock waste management, community leaders have obtained the support of local and international collaborators, such as the University of Georgia and the Monteverde Institute, to install tubular digesters in the San Luis valley.

Eight farmers in San Luis use Taiwanese-model tubular polypropylene bag digesters with PVC piping to treat livestock waste and produce biogas for cooking. The digesters have a 9-12 m³ working volume with a 4 m³ biogas storage bag. These household digesters typically treat swine waste from 4-10 pigs and provide fuel for approximately 4 hours of cooking per day, which meets the needs of an average family of 5 people. The operating parameters for the digester that was analyzed in this study, over a 5 week field-study are shown in Table 1.

2.2 Tracer study

A tracer study was performed to understand the digester's transport and mixing behavior. It should be noted that this is the first study to perform a tracer study on a tubular digester to understand these system's hydrodynamic mechanisms. Fertilizer grade potassium chloride (KCl) (Mezcla Distribuido, Limón Costa Rica) was used as a tracer due to its ease of use and lack of hazardous waste produced, as the effluent from the digester is used to fertilize cattle pastureland. A calibration curve was developed to allow effluent tracer conductivity measurements to be reported in terms of KCl concentration (g KCl/L). The target influent concentration was 9.42 g KCl/L. This concentration was selected to ensure that the effluent conductivity was significantly higher than the measured background conductivity and that the chloride concentration did not inhibit methanogenesis [13]. Note that biogas production in the digester remained stable during the tracer study, as will be discussed later. A mass of 4.75 kg of KCl was added to the 572 L of influent, mixed thoroughly and quickly poured into the digester through the influent pipe. Samples were collected from the outlet pipe every other day for 32 days and conductivity was measured as described below.

2.3 Analytical Methods

All laboratory analyses were carried out at the University of Georgia Costa Rica campus (San Luis, Puntarenas, Costa Rica). Influent and effluent samples were collected and analyzed weekly from the digester for 5 weeks. Standard Methods [14] were used to measure BOD₅ (5210), VS, and total solids (TS) (2540 G). Hach high range TNT test kits and a Hach DR 890 portable colorimeter (Loveland, CO) were used to measure total ammonia nitrogen (TAN) (TNT 832), total nitrogen (TN) (TNT 827) and total phosphorus (TP) (TNT 845) concentrations. pH was measured using Oakton portable waterproof pHTestr 10 (Vernon Hills, IL). COD

measurements could not be carried out during the field-study because there were no facilities to dispose the hazardous waste generated. Biogas volume in the tubular digester was measured using a wet tip gas meter (Wayne, PA). CH₄ content of the biogas was measured using RKI Eagle 72-5335RK-05 portable gas detector equipped with CH₄ and CO₂ sensors. Digester temperature was measured using a Thomas traceable digital thermometer (Philadelphia, PA). Conductivity was measured using a Fisher scientific traceable conductivity meter (Hanover Park, IL) with a conductivity detection limit of 19.99mS/m. Method detection limits (MDL) were (mg/L): TAN (2), TN (5) and TP (1.5). A sample of floccular sludge from the tubular digester was collected from the outlet pipe (Figure 1a). A 0.25 L container was securely taped to a 1.5 m tube and slowly introduced into the tubular digester from the outlet pipe. A sample volume of 5.0 L was collected and analyzed based on standard methods [14] for total suspended solids (TSS) (2540 D), volatile suspended solids (VSS) (2540 E) and sludge volume index (SVI) (2710 D).

2.4 Data Analysis

Oracle Crystal Ball (Redwood City, CA) was used for Monte Carlo simulation. A Monte Carlo uncertainty analysis was performed by running 1,000 trials with selected parameter values within the range previously reported in the literature (Table 2) to determine which model inputs affected the MCRT value predicted by the simplified bioprocess model developed. All the kinetic inputs to the bioprocess model were considered uncertain inputs with **triangular distributions**. **Triangular distributions were** used due to lack of sufficient kinetic input data to fit a uniform distribution. Crystal Ball calculates the sensitivity by ranking what inputs significantly correlate with the output while the simulation is running. If an input and output have a high **correlation percentage**, it means that the input will have a significant impact on the output. The percentage is the rank of correlations normalized to 100%. A positive contribution means that the

input will increase the output and a negative contribution means the input will decrease the output.

3 Model Development

3.1 Physical Processes Modeling

3.1.1 Computational Fluid Dynamics: Governing Equations for Flow and Tracer Transport

In this study, the unsteady Reynolds-averaged Navier-Stokes equations (RANS) simulation technique was employed for flow and tracer transport simulation in the tubular digester. In the present unsteady RANS simulation, the governing equations for flow and tracer transport were solved simultaneously at each time step. Governing equations for the flow consisted of the Reynolds-averaged continuity equation and incompressible Navier-Stokes equations:

$$\frac{\partial \langle u_i \rangle}{\partial x_i} = 0 \quad (\text{Eq. 1})$$

$$\frac{\partial \langle u_i \rangle}{\partial t} + \langle u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} + \nu \frac{\partial^2 \langle u_i \rangle}{\partial x_j^2} - \frac{1}{\rho} \frac{\partial \langle u'_i u'_j \rangle}{\partial x_j} \quad (\text{Eq. 2})$$

where a bracket denotes Reynolds-averaging, vector $\langle u_i \rangle$ is the Reynolds-averaged velocity, vector x_i is position, t is time, $\langle p \rangle$ is Reynolds-averaged pressure, ρ is density, and ν is kinematic viscosity.

The Reynolds stress tensor $\langle u'_i u'_j \rangle$ (expressed in terms of velocity fluctuation u'_i) was closed using an eddy viscosity model in which

$$\langle u'_i u'_j \rangle = -\mu_t \frac{\partial \langle u_i \rangle}{\partial x_j} \quad (\text{Eq. 3})$$

and the eddy viscosity is

$$\mu_t = C_\mu \frac{k^2}{\varepsilon} \quad (\text{Eq. 4})$$

where k is the turbulent kinetic energy and ε is the turbulent kinetic energy dissipation rate.

Transport equations for k and ε were specified via the k - ε model equipped with standard wall functions [15]. Model coefficient, C_μ was taken as $C_\mu = 0.09$, its standard value.

Tracer transport was governed by the Reynolds-averaged advection-diffusion equation:

$$\frac{\partial \langle C \rangle}{\partial t} + \langle u_j \rangle \frac{\partial \langle C \rangle}{\partial x_j} = - \frac{\partial \langle u'_j C' \rangle}{\partial x_j} \quad (\text{Eq. 5})$$

where $\langle C \rangle$ is the ensemble-averaged tracer concentration, C' denotes tracer fluctuation and turbulent flux. $\langle u'_j C' \rangle$ was modeled as:

$$-\langle u'_j C' \rangle = D_t \frac{\partial \langle C \rangle}{\partial x_j} \quad (\text{Eq. 6})$$

Note that $\langle C \rangle$ is time-dependent due to transient boundary conditions, which are described below.

The eddy (turbulent) diffusivity was taken as $D_t = \frac{\mu_t}{\rho \cdot Sc_t}$ where the eddy viscosity μ_t , was computed via the k - ε model and the turbulent Schmidt number, Sc_t , was taken as 0.7 [16]. Note that in Eq. 5, molecular diffusivity has been neglected with respect to the turbulent diffusivity for reasons to be discussed further below.

It should be noted that in the present CFD simulation, the tubular digester's flexible walls, solids accumulation and biogas bubble generation were not considered. Although incorporating those features into the CFD model may make the CFD simulation more accurate and detailed, this additional complexity had no significant impacts on the primary function of the CFD model for this study, which was to validate the two assumptions that were used to develop the reduced order model (Section 3.1.3).

3.1.2 CFD Flow Set-Up

The digester is 8m long with a 1.59m-internal diameter; other digester dimensions and components are shown in Figure 1a. The computational domain is shown in Figure 1b. Based on our interviews with the farmers and participant observations [17], the normal operating procedure was that each day swine waste was mixed with water to obtain a slurry with an average TS concentration of 6.35g/L. The slurry was fed into the digester for approximately 15 minutes at a rate of approximately 2,280 L/h. The Reynolds number was estimated to be 7,964 at the inlet zone based on inlet diameter (0.1 m) and influent velocity (0.078 m/s), and 674 in the main digester based on the diameter of the digester (1.59 m) and bulk velocity (4×10^{-4} m/s). The CFD numerical digester was run to simulate the first day of the physical tracer study. During the 15 minutes of feeding (flow-through) at the beginning of the 24-hour cycle, the inlet of the digester was assigned a constant influent velocity. A pressure outlet boundary condition was applied to the outlet of the digester. The other boundaries employed no-slip wall boundary conditions. After the 15-minute flow-through period ended, the flow into the digester was shut down and thus the digester behaved as a batch-reactor for the remainder of the simulation . During this stage the boundary conditions for the inlet and outlet changed to no-slip wall boundary conditions since the system was assumed to be closed. The other boundary conditions did not change.

To understand the general flow behavior and transport within the digester, a conservative tracer with a concentration 8.3 g KCl/L was injected into the digester during the initial feeding 15-minute flow-through period of the CFD simulation. This was calculated by dividing the total tracer mass (4.75 kg) by the influent flow (572 L) during the 15 minute flow-through period.

Note that a CFD RTD could be generated based on the tracer transport but would require

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4 simulating the physical experiment for 32 days. This would increase computational cost and the
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6 projected computing period would take months. Instead, the reduced-order transport model
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8 developed in sub-section 3.1.3 was used to predict the RTD curve and a mean HRT.
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11 An unstructured grid, which was generated using Gambit (Fluent, Inc. 2004), was
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13 employed for the physical processes model simulations. The total number of grid cells was
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15 85,134. This mesh is shown over half of the domain in Figure 1b. All simulations were
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17 conducted using OpenFOAM (OpenCFD Ltd., 2012), a collection of C++ libraries for solving
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19 continuum mechanics problems using the well-known finite volume method.
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23 **3.1.3 Reduced Order Transport Model**

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25 A general mass balance equation for the system during the 15 minute flow-through
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27 period was written as
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$$30 \quad V \frac{dC_d}{dt} = QC_{in} - QC_{out} \quad (\text{Eq. 7})$$

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32 where C_d is the tracer concentration in the digester, C_{in} is the influent tracer concentration, C_{out}
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34 is the effluent tracer concentration, V is the volume of the digester, Q is flow rate and t is time.
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36 Based on the operating conditions, two assumptions were made. The first assumption was that
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38 the batch reactor period was sufficient to mix the tracer in the digester. Thus C_d was uniform
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40 everywhere in the digester at the end of the batch reactor period or at the beginning of the next
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42 flow-through period.
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$$49 \quad C_{out}^n = C_d^{(n-1)} \quad (\text{Eq. 8})$$

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51 where n indicates current day and $(n - 1)$ indicates the previous day.
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55 The second assumption was that during the 15 minute flow-through period, the impact of
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57 the inflow on the effluent concentration was negligible. That is $C_{out}^n = C_d^{(n-1)}$ was valid for all of
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the flow-through periods. The two assumptions were subsequently validated via CFD simulations. By applying the two assumptions, Equation 7 was integrated and expressed as:

$$C_d^n = C_d^{n-1} + \frac{TQ}{V} (C_{in}^n - C_d^{(n-1)}) \quad (\text{Eq. 9})$$

with conditions:

$$C_d^0 = 0 \quad (\text{Eq. 10})$$

$$C_{in}^n = \begin{cases} C_0 & n = 0 \\ 0 & n \geq 1 \end{cases} \quad (\text{Eq. 11})$$

where C_0 is the initial tracer concentration in the digester and T is the 15 minute flow-through period.

3.2 Bioprocess Model

Since floccular and granular sludge reactors, such as anaerobic baffled and UASB reactors, have been used to treat high strength swine waste [6, 7], the bioprocess model was based on a granular sludge reactor model developed by Elmitwalli [12]. Given that the active biomass concentrations inside the tubular digester (X_m) and in the effluent (X_{me}) were unknown, the bioprocess model was used to calculate these values, which were used to estimate the MCRT according to the following:

$$MCRT = \frac{VX_m}{QX_{me}} \quad (\text{Eq. 12})$$

The full bioprocess model formulation is presented in Elmitwalli [12]. Mass balances on X_m and daily methane production rate ($\dot{m}$) were sufficient to estimate the MCRT for this study, so only these equations are presented here. A steady-state mass balance on X_m in the digester yields:

$$0 = QX_{mi} - QX_{me} + Y_m \frac{K_m S_b X_m}{K_s + S_b} V - K_d X_m V \quad (\text{Eq. 13})$$

where X_{mi} is the active biomass in the influent (assumed to be negligible), S_b is the soluble biodegradable substrate concentration (assumed to be equal to the effluent BOD₅ concentration), K_S is the biomass half saturation constant and K_m is the Monod maximum substrate utilization rate. A steady-state mass balance on CH₄ in the system yields:

$$0 = -\dot{m} + (1 - Y_m) \frac{K_m S_b X_m}{K_S + S_b} V \quad (\text{Eq. 14})$$

where $\dot{m}$ is the daily methane production rate. Note that the daily methane production rate was expressed as g COD/day by adjusting the measured methane production rates (Table 2) to standard temperature and pressure (STP) and assuming 4 g COD/g CH₄. The kinetic constants that were applied to this model were obtained from studies treating swine waste at psychrophilic temperatures (Table 2). A Monte Carlo uncertainty analysis was performed as described in section 2.4 to determine how the kinetic inputs affected the MCRT value.

4 Results and Discussion

4.1 Overall Tubular Digester Performance

Average performance of the tubular digester over the 5-week field study period is shown in Table 3. The TSS and VSS concentrations retrieved from the sludge settleability analysis were 33.2 g TSS/L and 0.40 g VSS/L respectively and sludge had a SVI of 1.51 mL/g TSS. From these results, three main conclusions can be drawn.

First, the results from the settleability analysis indicate that the sludge retrieved from within the tubular digester had good settling characteristics. Sludge with a SVI below 10 mL/g TSS is considered to have good settling properties, which is characteristic of floccular sludge flocs [20]. Having biologically active floccular sludge with a low SVI has shown to improve CH₄ production in an anaerobic sequencing batch reactor treating swine waste [20]. Immobilization of methanogens and other anaerobic digestion microorganisms onto inert material and other cells to

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4 form granules is beneficial because this promotes diversity in the microbial community. This is
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6 due to metabolic interactions within the granule that promote faster substrate utilization.
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8 Formation of granules also promotes a more flexible and stable sludge that can withstand
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10 temperature and loading rate fluctuations [21]. Although the floccular sludge in the tubular
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12 digester is compared to granular sludge due to similarities in the sludge properties, low SVI and
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14 long MCRT without the presence of biofilm carriers, characteristic granules were not observed in
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16 the tubular digester contents. Since good CH₄ production was observed in the tubular digester,
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18 the low VSS concentration from the solids settleability test indicated that the microbial
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20 composition of the sludge changes diagonally within the tubular digester. This observation was
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22 in good agreement with Montteran et al. [7] who showed diagonal distinction in the microbial
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24 composition of granules from an anaerobic baffled reactor treating swine waste. Each diagonal
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26 compartment contained separate microbial groups representing each anaerobic digestion phase
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28 (fermentation, acidogenesis, acetogenesis and methanogenesis). Due to the design of the tubular
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30 digester, it was not feasible to collect samples other than from the outlet pipe. The low VSS to
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32 TSS ratio indicated that the sludge taken from the outlet pipe was mainly inert material. This was
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34 likely influenced by the MCRT. Longer MCRT allow for greater degradation of the organic
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36 matter in the influent. Results from the biological model used to estimate the MCRT are
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38 discussed later.
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48 The second main conclusion is that the digester had high VS and BOD₅ removal
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50 efficiencies (Table 3). The ability for anaerobic digestion to decrease the organic matter
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52 concentration in waste is one of its attractive benefits. The VS and BOD₅ removal efficiencies
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54 were greater than 75%. This is greater than previously reported values for complete mix
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56 digesters treating swine waste at mesophilic and thermophilic temperatures [4, 22]. These high
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organic matter removal rates provided further evidence of solids accumulation and formation of a biologically active floccular sludge layer.

The third main conclusion is that high TN and TP percent removals were observed; 83.6 and 91.6% respectively. Since there is no removal mechanism for TN and TP during anaerobic digestion, other processes were investigated to better understand TN and TP removal mechanisms. During anaerobic digestion, nitrogen, phosphorus and metal ions present in the organic matter are released as particulate organic matter is degraded. Swine waste contains high concentrations of magnesium (Mg), TN and TP, which may lead to the formation of struvite ($\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$), which can attach to solids within the reactor. Struvite precipitates can be an operational problem because they cause pumps to foul and pipe blockage [23]. Struvite precipitation during anaerobic digestion is affected by pH, rate of mixing, temperature, solids settleability and ion molar ratios [23]. To assess whether conditions in the tubular digester favored struvite precipitation, the thermodynamic solubility product of $[\text{Mg}^{2+}] [\text{NH}_4^+] [\text{PO}_4^{3-}]$ was analyzed [24]. Influent Mg concentration was assumed to be 0.21g/L based on an average value from prior studies of swine waste characteristics (see Lin [25] for review). A thermodynamic solubility product ($\log K_{\text{sp}}$) of $10^{-11.4}$ was estimated, which was within the struvite solubility product of $10^{-9.41} - 10^{-14.1}$ at 20-25°C and a pH of 6.45 – 8.97 [24].

Thermodynamic solubility products within this range indicate struvite precipitation within the digester was favored. Tubular digesters may require periodical desludging every 5-10 years due to the solids accumulation [26] and the sludge can be expected to have a high TP concentration.

4.2 CFD and Reduced Order Transport Model

Unsteady RANS simulations were conducted for the first day after releasing the tracer for the 15 minute flow-through period and the subsequent 23 hours and 45 minutes batch-reactor

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4 period. For the 15 minute flow-through period, there was flow spanning the entire digester from
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6 the inlet through the outlet. Following the coordinate system established in Figure 1b, speed
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8 contours on the middle x-z plane and three y-z planes (at x = 0, 4, and 8 m respectively) for 1, 5,
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10 10 and 15 minutes are shown in Figure 2 a-d respectively. From Figure 2, it was observed that
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12 the flow developed during the first 5 minutes and unsteady flow behavior was observed at the tail
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14 of the high-speed jet (red color) after 5 minutes (Figure 2 b, c and d). Areas within the digester
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16 with short circuiting and dead zones were also observed and are reflected in the streamline and
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18 velocity vector distribution shown in Figure 2 e and f. Tracer concentration contours on the
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20 middle x-z plane and three y-z planes (at x = 0, 4, and 8 m respectively) for 1, 5, 10 and 15
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22 minutes are shown in Figure 3 a-d respectively. From Figure 3d, it can be seen that the tracer
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24 moves quickly through the digester due to the short-circuiting pathway but does not reach the
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26 digester outlet by the end of the 15 minute flow-through period. The simulation predicted an
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28 outlet tracer concentration less than 1×10^{-30} g KCl/L at the end of the 15 minute flow-through
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30 period. This demonstrated that the influent flow had negligible effect on the effluent
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32 concentration and serves to validate the second assumption in the **reduced-order transport model**
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34 **developed in sub-section 3.1.2.**
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43 During the 23 hours and 45 minutes batch-reactor period there is no flow at the inlet or
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45 outlet. The speed contours in the middle x-z plane and three y-z planes (x=0, 4, and 8 m) at 15
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47 and 30 minutes and 1, 3, 6 and 24 hours after batch-mode initiation are shown in Figure 4a-f.
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49 From Figure 4, it was observed that although there was no flow through the inlet or outlet, flow
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51 continued within the digester. The tracer continued to move towards the outlet of the digester due
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53 to inertia, resulting in tracer transport during the first hour after the system was closed (Figure
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55 4a, b, and c). The flow gradually slowed down due to viscosity, after which the main tracer
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transport mechanism was by turbulent diffusion. The tracer concentration contour had insignificant change after one hour because transport via turbulent diffusion is slower than that by advection (Figure 4d, e, and f).

It should be noted that turbulence started to decay once the system was closed and batch mode was initiated. However residual turbulence took a long time to dissipate (data not shown). For example, there was still residual motion at $t = 15$ hours and 24 hours and the turbulent viscosity in most places remained significant ($>6 \times 10^{-6} \text{ m}^2/\text{s}$), making the turbulent diffusivity (which was calculated as the turbulent viscosity divided by the turbulent Schmidt number (0.7)) to be much greater than the molecular diffusivity of the tracer (KCl), $2.47 \times 10^{-9} \text{ m}^2/\text{s}$. Therefore, it was acceptable to neglect molecular diffusivity in the simulations, as evidenced through Eq. 5. In the physical system it would be expected that the turbulent diffusivity could be even be greater than that predicted by the CFD because the mechanism of biogas generation, which occurs during the batch period and may generate turbulence, was not considered in the CFD model.

At the end of the 23 hours and 45 minutes CFD-simulated batch-reactor period, the tracer concentration was evenly distributed in the digester except for the area near the inlet. The effluent tracer concentration from the experimental data was 0.51 g KCl/L, which was 27% higher than the reduced-order model prediction (0.4 g KCl/L). In anaerobic digesters, biogas bubbles generated provide some mixing in the system. However, mixing from biogas bubbles was not considered during the unsteady RANS simulations as mentioned above. If it was considered, the tracer in the digester would be closer to completely mixed. Thus, the CFD simulation results for the tracer transport during the 23 hours and 45 minutes batch-reactor period support the first assumption of the reduced-order transport model that the system

functions as a CSTR during this period. Further corroborating of this assumption is that the experimental RTD curve (Figure 5a) is characteristic of a CSTR mixing mechanism [5].

Although considering non-Newtonian fluids may have made the simulation more accurate, this consideration may have had a minor impact on the validation of the two assumptions. First, if we were to consider non-Newtonian behavior, the second assumption that during the flow-through period, the impact of the inflow on the effluent concentration was negligible would remain valid since the non-Newtonian behavior would result in a more sluggish flow toward the outlet. Second, since our first assumption was that the batch reactor period was sufficient to mix the tracer in the digester; non-Newtonian behavior may weaken turbulent mixing. However, this could be offset by biogas generation, which was not included in the model and is known to increase mixing. Thus we believe the first assumption was still valid even though both non-Newtonian behavior and biogas generation were not considered in the CFD model.

After validating the first and second assumptions through the unsteady RANS CFD simulation, the RTD was predicted using the reduced order model. The model RTD was compared to the experimental data in Figure 5a and b. From Figure 5b the predicted RTD was in good agreement with the experimental RTD, with a coefficient of determination, denoted R^2 , of 0.874. The mean liquid HRT predicted from the reduced-order model was 22.8 days. Note that in principle the CFD simulations could have been used to obtain the mean liquid HRT, but this would require running the simulation for much longer than 24 hours, thereby making the simulation very expensive. Instead, for computational efficiency the CFD was used to validate the assumptions behind the reduced order model which is less expensive than the CFD for predicting HRT.

4.3 Bioprocess Model

Results for range of X_m , X_{me} , MCRT and CH_4 activity values are shown in Table 4. An average MCRT of 115 days was estimated with a median of 110 days, minimum of 52 days, maximum of 265 days and a standard deviation of 33.6. It should be noted that the modeled X_{me} concentration was within the range of the measured effluent VS concentrations (Table 3). A Monte Carlo sensitivity analyses (as described in Section 2.4) was carried out to determine which bioprocess kinetic inputs significantly influenced the MCRT and the probability distribution of the MCRT. The outcomes from the simulation are graphically represented in Figure 6. From these results, two main conclusions can be drawn.

First, the performance and MCRT values obtained from this study were similar to other studies using floccular sludge layer reactors to treat wastewater at psychrophilic temperatures. Lim and Fox [27] reported organic matter removal rates of approximately 90% when treating swine waste in UASB reactors at psychrophilic temperatures. Uemura and Harada [28] obtained MCRTs ranging from 110 to 117 days and CH_4 activity of 0.03-0.09 g CH_4 -COD/g VS_{added}-day while treating domestic wastewater in a UASB at 13 to 25°C. These results are similar to the results from the tubular digesters in this study (Table 4) and also in agreement with Henze et al. [29], who recommended an MCRT of 60-140 days while treating domestic wastewater at 15-25°C in a floccular sludge layer reactor. Although the recommended values are for domestic wastewater, they are a useful starting point due to limited literature on MCRT in tubular and floccular sludge layer reactors treating swine waste.

Second, the MCRT value was most sensitive to K_m , K_d and K_s and least sensitive to Y_m (Figure 6). K_m represents the maximum rate at which the active biomass can hydrolyze the particulate substrates. An increase in K_m indicates that a shorter MCRT would be needed for the

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4 observed biogas production rate. K_d is that rate at which the active biomass undergoes
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6 endogenous decay, resulting in a decrease in the active biomass in the digester. K_S is the
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8 substrate concentration at which the anaerobic processes occur at half the biomass maximum
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10 growth rate and is an indicator of the active biomass affinity for substrate [30]. A decrease in K_S
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12 indicates an increase the microbes' affinity for the substrate, thus indicating that a shorter MCRT
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14 is sufficient for hydrolysis and conversion the particulate and soluble substrates to CH_4 .
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19 In tubular digesters, the physical and biological processes are interconnected. A sufficient
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21 mean liquid HRT is needed to allow for the solubilization of complex organic matter in the
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23 influent and to provide adequate contact time between the active floccular sludge layer and the
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25 dissolved substrates for efficient biogas production. A decrease in HRT reduces the contact time
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27 between the active floccular sludge layer and the dissolved substrates resulting in decreased
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29 biogas production. From the influent and effluent characteristics, sludge settleability and CH_4
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31 production rates observed in the tubular digester, a mean liquid HRT of 23 days combined with a
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33 MCRT of 115 days indicates a robust syntrophic relationship between the physical and
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35 biological processes. This good relationship led to low organic matter in the effluent and
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37 sufficient biogas production to meet households' energy demands. Although the effluent quality
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39 in the tubular digester was good in terms of organic matter, more research is needed to determine
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41 how the physical and biological processes affect other effluent characteristics such as pathogen
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43 concentrations, and how the CFD model can be used in combination with pathogen die off
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45 models to predict pathogen removal efficiencies. This is an important public health task because
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47 effluents from tubular digesters are often used as a soil amendment on food crops to reduce cost
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49 of purchasing mineral fertilizers.
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5 Conclusions

The following is a summary of the major findings of this study:

- The low effluent organic matter concentrations were attributed to the formation of a biologically active floccular sludge layer, resulting in good biogas production to meet households' energy demands.
- CFD modeling indicated turbulent diffusion as the major transport mechanism during the batch period, with the system functioning as a CSTR. The mean liquid HRT was estimated as 22.8 days.
- The bioprocess model predicted an average MCRT of 115 days. The model can be a useful tool to design tubular anaerobic digesters but further work is needed to validate the model.

Acknowledgements

The authors acknowledge the Monteverde Institute and University of Georgia Costa Rica for their assistance with this research. The authors also acknowledge the use of the services provided by Research Computing at the University of South Florida. This research was supported by the National Science Foundation under grant number 1243510 and USF Graduate School Signature Research Fellowship. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the funding agencies.

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Table 1: Tubular digester operating parameters (n=5).

Parameter	Unit	Tubular Digester
Working volume (V)	L _d	12000
Temperature	°C	20.7 ± 0.48
Influent flow (Q)	L/day	543 ± 10.0
OLR	g VS _{added} /L _d -day	0.26 ± 0.10

Table 2: Kinetic constants applied in the bioprocess model.

Parameter	Unit	Minimum	Maximum	Reference
K_d	day ⁻¹	0.006	0.04	[18]
Y_m	g biomass COD/g COD utilized	0.23	0.25	[18]
K_m	g COD utilized/ g biomass COD-day	2.00	8.00	[19]
K_S	g/L	0.15	1.81	[18,19]

Table 3: Average tubular digester influent and effluent characteristics (n=5).

Parameter	Unit	Influent	Effluent
BOD ₅	g/L	5.09 ± 0.30	0.030 ± 0.015
TS	g TS/L	6.35 ± 2.87	0.77 ± 0.25
VS	g VS/L	5.17 ± 2.44	0.58 ± 0.24
TAN	mg NH ₄ ⁺ -N/L	140 ± 49.0	52.8 ± 4.66
TN	mg N/L	300 ± 23.6	49.3 ± 5.12
TP	mg PO ₄ /L	402 ± 126	33.9 ± 8.91
pH		7.08 ± 0.62	7.04 ± 0.14
Methane content (S _{CH₄})	%	71.0 ± 10.0	
CH ₄ production rate (ṁ)	m ³ CH ₄ /day	2.01 ± 0.87	

Table 4: Bioprocess model results and calculated CH₄ activity.

Parameter	Unit	Value
X_m	g COD/L	2.00 - 4.94
X_{me}	g COD/L	0.34 - 1.03
MCRT	day	51 - 259
CH ₄ activity	g CH ₄ -COD/g VS _{added} -day	0.056 - 0.086

Figure 1:(a) Schematic and (b) CFD domain and grid of the tubular digester

Figure 2:(a-d) Contour of speed (flow pattern) at various times on middle x-z plane and three y-z planes ($x=0, 4$, and 8 m), (e) streamline of flow in the digester and (f) velocity vector distribution on middle x-z planes

Figure 3: Contour of tracer concentration (tracer distribution) for the 15 minute flow-through period on middle x-z plane and three y-z planes ($x=0, 4,$ and 8 m)

Figure 4: Contour of tracer concentration (tracer distribution) for the batch-reactor period on middle x-z plane and three y-z planes ($x=0, 4$, and 8 m)

Figure 5: Comparison of predicted RTD from measured data (a) concentration versus time; (b) predictions versus measured data.

A

B

Figure 6: (A) MCRT variables sensitivity analysis and (B) MCRT frequency distribution from the Monte Carlo simulation.