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Prediction of biogas production rate from dry anaerobic digestion of food waste: Process-based approach vs. recurrent neural network black-box model

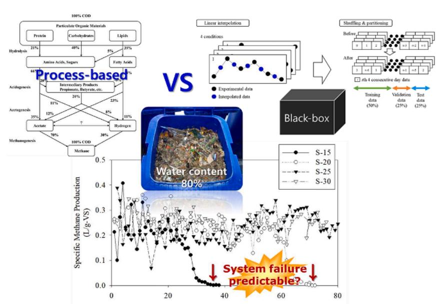
Kyu Won Seo [a,1], Jangwon Seo [b,1], Kyungil Kim [c], Seung Ji Lim [b], Jaeshik Chung [b,d,*]

[a] Institute of Environmental Technology, ISAN Corporation, Anyang-si, Gyeonggi-do 14059, Republic of Korea
[b] Water Cycle Research Center, Korea Institute of Science and Technology (KIST), Seoul 02792, Republic of Korea
[c] ECONITY Co., Ltd., Yongin-si, Gyeonggi-do 2374-41, Republic of Korea
[d] Division of Energy and Environmental Technology, KIST School, Korea University of Science and Technology (UST), Seoul 02792, Republic of Korea

HIGHLIGHTS

- The stability of dry AD of FW is highly dependent on the organic loading rate.
- SRT and water content are critical factors affecting methane production.
- The biogas production rate prediction model for dry anaerobic digestion is developed.
- The prediction model is developed via recurrent neural network black-box modeling.
- Recent three days data of HRT, SCOD, TVFA, TA, and FA are used for the prediction.

GRAPHICAL ABSTRACT



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ABSTRACT

The stability of dry anaerobic digestion (AD) of food waste (FW) as well as the resulting methane gas generation was investigated from the perspective of system dynamics. Various organic loading rates were applied to the system by modifying the water content in the FW feed and solid retention time (SRT). The excessive organic loading due to the accumulation of volatile fatty acids (VFAs) from the feed with 80% water content during the short SRT (15 and 20 d) caused system failure. In contrast, more intermediate materials, such as VFAs, was easily converted into methane at higher water contents. In addition, the biogas production rate of dry AD was effectively predicted based on SRT, soluble chemical oxygen demand, total VFA, total ammonia, and free ammonia using a recurrent neural network—the so-called “black-box” model. This implies the feasibility of applying this data-based black-box model for controlling and optimizing complex biological processes.

* Corresponding author at: Water Cycle Research Center, Korea Institute of Science and Technology (KIST), Seoul 02792, Republic of Korea (J. Chung).
E-mail address: jschung@kist.re.kr (J. Chung).
[1] These authors contributed equally to this work.

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1. Introduction

Anaerobic digestion (AD) is a sequential process in which organic materials are decomposed into organic acids by acid-producing microorganisms in the absence of dissolved oxygen; subsequently, the organic acids are decomposed into methane, which is known as renewable clean energy (Cho et al., 2013). Dry AD (also called high-solid or solid digestion) as a variation of the AD process is commonly used to treat organic matter with solid contents of 20–40% which has been observed to be particularly effective for processing organic fractions of municipal solid waste and agricultural waste (Guendouz et al., 2010). Dry AD has several advantages over wet AD as follows. It only requires a small reactor capacity and allows processing under high organic loading rate (OLR) conditions (Rocamora et al., 2020). Furthermore, because the use of smaller reactors is enabled, dry AD simplifies handling and operation, thus minimizing wastewater production and nutrient loss during the process. Despite its advantages, dry AD also has weaknesses. The decomposition time of organic matter is long. Moreover, the resulting total solid (TS) content is high and can lead to the accumulation of toxic and inhibitory compounds (e.g., volatile fatty acids (VFAs), ammonia, and heavy metals) (Jha et al., 2011). Consequently, the methane production per unit mass of volatile solid (VS) may be reduced and higher inoculation rates may be required (Chen et al., 2008; Jha et al., 2011).

For better controlling and optimization of the AD process, various modelling approaches have been proposed so far. Anaerobic Digestion Model No. 1 (ADM1) consists of various equations to describe complex biochemical and physico-chemical processes in the AD process which can be classified as a "white-box" (i.e., process-based) model (Yasui and Goel, 2010). However, it is reported that the difficulties in ADM1 calibration can be induced by an extensive substrate characterization to estimate large number of parameters (Ozkan-Yucel and Gökçay, 2010). In addition, the influent characteristics and the bacterial community of the AD reactor that affect to parameters in the white-box model can be changed over time. Subsequently, regular re-calibration or preparation of extensive data for calibration can be required. Despite of its difficulties, Ozgun (2019) calibrated and validated the ADM1 model for the full-scale anaerobic sludge digester using an extensive experimental data (Ozgun, 2019). Considering the calibration difficulties of the process-based white-box model driven by the large number of parameters, the data-driven "black-box model" can be suggested as an alternative method. Black-box model is usually developed from empirical observations. Despite the advantages that the understating of complex processes is not required, the applicability of the black-box model is limited to its experimental conditions compared to the white-box model which has relatively more general applicability. To overcome the limited applicability of the black-box model, the securing of sufficient and wide range of the experimental data needs to be preceded (Yasui and Goel, 2010).

Recently, the artificial neural network (ANN) model has drawn interest due to its distinct performance in predicting nonlinear and nonstationary time series data (Mishra and Desai, 2006). In addition, the ANN model can cope with noise and measurement errors in the data (ASCE Task Committee, 2000; Mishra and Desai, 2006). One of the methods of ANN that exhibits satisfactory performance in dealing with sequential data is a recurrent neural network (RNN) (Biancofiore et al., 2017). RNN is specialized technique for predicting sequential time-series data by memorizing previous time step data using a recurrent hidden layer. However, recurrent learning leads to gradient vanishing or exploding problems, which can degrade performance. A long short-term memory (LSTM) network was developed to resolve the vanishing gradient problem encountered in the use of traditional RNNs by selecting the data to retain or discard (Hochreiter and Schmidhuber, 1997; Sundermeyer et al., 2012). Although the LSTM method is mainly used for natural language processing (Chen et al., 2017; Wang and Jiang, 2016; Yao and Guan, 2019; Yin et al., 2017) and stock change prediction (Li et al., 2018; Qin et al., 2017), it can be applied to forecast time-series water quality data (Liu et al., 2019; Hu et al., 2019). The prediction performance of standalone LSTM can be improved by formulating a hybrid deep learning model or by implementing an attention mechanism. A hybrid convolutional neural network (CNN)–LSTM model is proposed and compared with standalone models (CNN, LSTM, support vector regression, and decision tree) by its performance, and the CNN–LSTM model generally outperformed the standalone models (Barzegar et al., 2020). The CNN–LSTM model was also employed to predict water level and water quality data collected from the real-time information (Baek et al., 2020). Another study employed LSTM to predict the performance of a brackish water desalination plant using a dual-stage attention-based LSTM (DA-LSTM), which exhibited significantly improved performance (R^2 greater than 0.99) than the LSTM method ($0.531 \le R^2 \le 0.884$) (Yoon et al., 2021).

In this study, the performance of dry AD treating FW is investigated. The resulting methane generation efficiency is evaluated under different OLRs by varying SRT and water content in the feed. Furthermore, the prediction of methane production based on RNN has been demonstrated as a so-called "black-box model" using the experimental data. Subsequently, the performance of the prediction model is evaluated to assess feasibility of the early detection of the system failure. The framework for the system control and optimization used in this study can be applied to predict the behavior of complex, non-linear systems including dry AD processes.

2. Material and methods

2.1. Feed preparation

Raw FW samples were collected from the pipeline collection system of an apartment in Seoul, South Korea. The collected FW samples were pulverized twice by machine milling, then adequately mixed for homogeneity. They were stored in a sealed container at 4 ℃ to minimize potential deterioration until use. The raw FW contains ca. 80% of water while deionized water was added to the raw FW to prepare the substrates for the operations under different water contents (85% and 90%).

2.2. FW characterization

The AD of organic solid wastes, such as FWs, is considerably influenced by the physicochemical characteristics of samples. Accordingly, this study analyzed these characteristics (i.e., TS, VS, pH, chemical oxygen demand (COD), total nitrogen (T-N), total phosphorus (T-P), and NH_3 content) once a month for more than a year using FW samples collected from the pipeline. To determine TS and VS, these samples were dried at 105 °C. Then, they were heated at 550 °C and subsequently weighed. The total COD (TCOD), T-N, and T-P were measured after diluting the FW samples 2000 times. The soluble COD (SCOD) and NH_3 content were measured after the centrifugation and filtration of FW samples diluted 500 times. The pH level was measured using a pH meter (Mettler Tolledo GmbH, USA). All samples were analyzed according to standard methods (Federation and Association, 2005).

2.3. Continuous dry AD process

For the continuous dry AD operation, the reactor (10 L) temperature was maintained at 35 °C, and the sample in the reactor was mixed at a speed of 150 rpm (see supplementary material). Dehydrated sludge collected from the sewage treatment plant in K-City (South Korea) was diluted to contain 80% water and used as inoculum source for dry AD. Diluted dehydrated sludge and FW were mixed at 4:1 (food-to-microorganism ratio, F/M = 0.25) and used as initial reactor substrates. The SRT (15, 20, 25, and 30 d) of the system and water content (80%, 85%, and 90%) of the influent were adjusted differently to change the OLR. Subsequently, the operation stability and the reduction in organic matter as well as methane production in the dry AD system were evaluated.

2.4. Analysis of operation parameters

2.4.1. VFA analysis

The VFA analysis was performed by gas chromatography (GC) (Younglin, ACME-6000) with a flame ionization detector (FID). The operating temperatures of the oven, detector, and injector were adjusted to 150, 240, and 240 °C, respectively. The oven temperature was held 40 ℃ for 2 min, then increased gradually to 150 ℃ at the rate of 10 ℃/min and held for 1 min. The column used for VFA analysis was HP-Innowax (15 m × 0.25 mm i.d, 0.25 μm thicknesses). Sample (1 μl) was injected, and helium (He) was supplied as a carrier gas at 3.0 mL/min for the system.

2.4.2. Methane production

The gas generated by continuous dry AD was collected using a Tedlar gas sampling bag, and the amount of generated gas was measured by a wet gas meter. The methane content was analyzed by GC–TCD (thermal conductivity detector) (Younglin, ACME-6000) at temperatures of 35, 120, and 120 °C for the oven, detector, and injector, respectively. The column for methane composition was CTR I (6′ 1/4′′ outer and 6′ 1/8′′ inner SS, Alltech, USA).

2.5. RNN black-box modeling

2.5.1. Data preparation and preprocessing

To develop a neural network model, the preparation of a large dataset is generally desired to ensure higher accuracy. If the dataset is insufficient, the performance of a neural network model compared with traditional machine learning models is frequently less effective (Feng et al., 2019). However, preparing a large dataset is typically problematic because of the complexities involved in frequent experimental measurements. In this study, four different SRT conditions of experimental data were used to minimize algorithmic bias (Lee et al., 2019). If two other experiment conditions at SRT 25 with water content 85% and 90% involved, data with SRT 25 will be dominant compared to other SRT conditions. Similarly, the data with water content 80% condition will also become dominant compared to water content of 85% and 95% conditions; the experimental measurements were conducted every 2–3 d. To prepare an adequate dataset for model development, linear interpolation was conducted using the experimental dataset (Fig. 1(a)). No significant changes in the experimental condition were assumed to occur within three days. After implementing linear interpolation (i.e., pre-processing), a dataset based on daily information was obtained. The recent three-day SRT, SCOD, total VFA (TVFA), total ammonia (TA), and free ammonia (FA) values were employed to predict the succeeding day's specific methane production (SMP). The five parameters were chosen by the importance within the subprocess in AD combined with the data availability. Dry AD performance is affected by the variation of OLR with the solid retention time (SRT) and water content in the feed, pH, temperature (Cho et al., 2018), C–N ratio in the reactor, stabilization before process initiation (Akram and Stuckey, 2008; Cho et al., 2013a), and initial reactor seed materials (Cho et al., 2013a; Cho et al., 2013b). Among these, SRT is an independent variable that we changed, SCOD is a criteria that evaluates stable conversion of available organic components to VFAs, TVFA represents comprehensive characteristic of various VFAs while it inhibits the microbial activity when accumulated in the reactor like FA and TA. In addition, TA can be a criterion for the protein metabolism which links to successive VFA and hydrogen production in turn. In case of conducting prediction using multiple operational parameters, sensitivity analysis can be conducted to derive major operational parameters (Seo et al., 2019). Using the dataset based on daily information, data scaling was conducted to achieve 0 and 1 for mean and standard deviation, respectively. Data scaling was implemented to minimize the overestimation of the specific input value for predicting SMP.

For model training and evaluation, the dataset was partitioned into three subsets (i.e., training data (50%), validation data (25%), and test data (25%)) for model fitting, fitted model selection (based on performance evaluation), and final model performance evaluation, respectively. Prior to dataset partitioning, the subsets were randomly shuffled. The subsets were derived from the dataset with four-day consecutive data because three days of recent data were employed to predict the next-day SMP value. Subsequently, the shuffled subsets were partitioned. Subset shuffling was conducted to include the system failure phase, into the training, validation, and test data. In the case of SRT values of 15 and 20, the SMP gradually decreases over time until it finally converges to zero. If training, validation, and test data are partitioned into 0–50%, 50–75%, and 75–100%, respectively, then the system failure phase may be excluded from training data. Moreover, generally, a larger proportion of the dataset is assigned to training data. However, to derive sufficient amounts of validation and test data, 50% are arbitrarily assigned as training data in this study. Because the dataset considers four different SRT conditions, four sets of training, validation, and test data are initially prepared and subsequently merged (Fig. 1(b)).

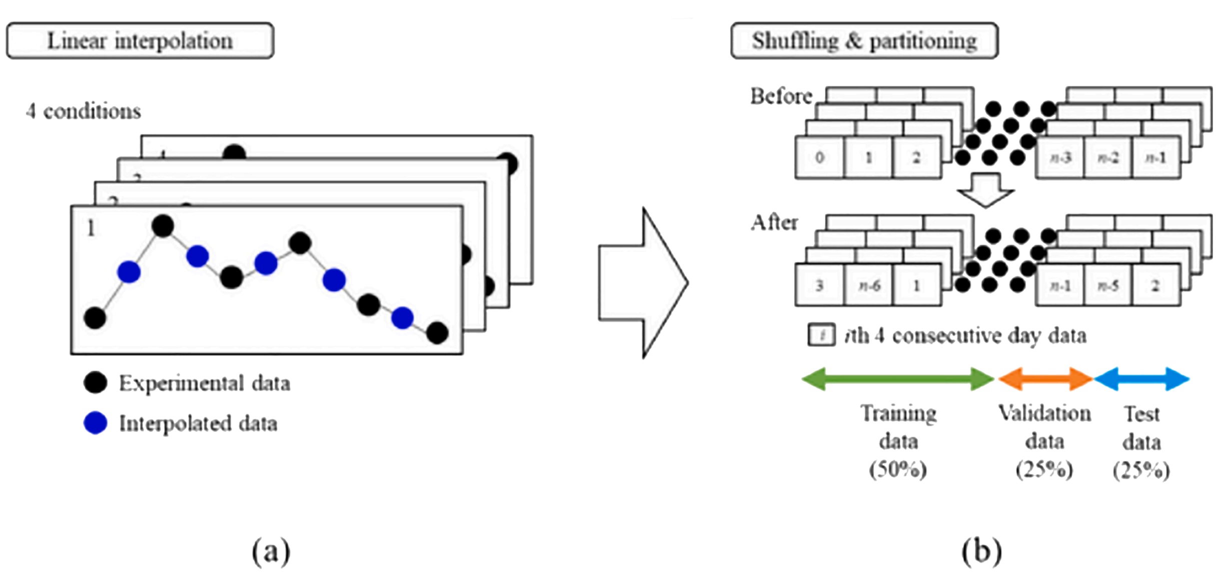

Fig. 1. Schematic diagram of data preparation and preprocessing; (a) Linear interpolation and (b) Shuffling and partitioning.

2.5.2. Rnn

A bidirectional LSTM network was chosen to predict the biogas production rate using PyTorch (Paszke et al., 2019). The number of recurrent layers and hidden states are 1 and 20, respectively. Subsequently, the LSTM network output was used as the ANN network input to predict biogas production. The subsequent ANN network consists of 2 hidden layers with 20 and 10 hidden features. For LSTM network fitting, the ADAM optimizer with a learning rate of 0.01 was used (Kingma and Ba, 2014).

3. Results and discussion

3.1. Feed characteristics

The water content of feed samples used in this study was in the range 74.7–84.4% (w/w). The fixed solid (FS) and VS of TS were 8.3–26.3% and 70.5–88.1% (w/w), respectively. The pH range of FW was 3.86–4.61, indicating a weak acidic state. Park et al. attributed the low pH level to the acid fermentation process during FW discharge and collection (Park et al., 2001). Generally, the AD process is performed in a neutral pH range. The acidic state is maintained in the initial stage (i.e., acidogenesis); however, it finally changes to the neutral pH state when a stable state (i.e., methanogenesis) is achieved. The optimal pH-maximizing methane production is known to be 6.5–7.5. When the pH level deviates from the appropriate range (<5.0 or greater than 8.5), the methanogenesis is reported to be inhibited (Clark and Speece, 1971). Accordingly, maintaining the suitable pH level through alkali pretreatment, buffer solution addition, and/or control of operating conditions (SRT, F/M, etc.) is necessary. The TCOD and SCOD concentrations were 263,300–378,700 mg/L and 86,600–120,500 mg/L, respectively (i.e., SCOD/TCOD approximately 0.4). T-N and T-P were measured to be 2,260–3,741 and 197–516 mg/L, respectively

3.2. Dry AD performance at different SRTs

The SMP from dry AD operation at different SRTs is shown in Fig. 2; note that in all cases, the water content is 80% (i.e., raw FW). Among the four operation cases, the 15-d SRT (S-15) and 20-d SRT (S-20) were operated for approximately 30 and 60 d, respectively, because the system failed on these days. In contrast, the 25-d SRT (S-25) and 30-d SRT (S-30) were operated for more than 80 d with stable methane production. Overall, the SMP of the four reactors was observed to increase as the SRT increased. In the S-30 reactor with a longer SRT, 0.25 L/g VS of methane was generated; in the S-25 reactor with a shorter SRT, a slightly smaller amount of methane (0.24 L/g VS) was produced. As mentioned, note that S-15 and S-20 both failed. In contrast, the rate of methane production decreased with increasing SRT; in S-25 and S-30, the methane production rates were 1.738 and 1.48 L/L•d, respectively. However, in the case of S-15 and S-20, methane production was stopped after they exhibited high methane generation rates (approximately 4.6 and 3.9 L/L•d, respectively) at the beginning of operation (Fig. 2(b)).

To determine the cause of system failure in cases S-15 and S-20, the changes in VFA as well as pH were monitored. The accumulation of excessive amounts of VFA when failure occurred in the S-15 and S-20 cases were compared with the VFA amounts under normal operation (Fig. 3, (a) and (b), respectively); reductions in pH (≤5.0) were also observed. Note that the foregoing condition is unfavorable for the microbes in the AD process (Clark and Speece, 1971). Most of the VFA components were occupied by acetic acid and propionic acid, and the concentration of acetic acid and *iso*-valeric acid increased when methane generation was suppressed. In addition, the TVFA concentration increased significantly from 20,000 to more than 40,000 mg/L with the pH level significantly decreasing to approximately 5 in the cases of S-15 and S-20 (Fig. 3, (a) and (b), respectively).

In general, the accumulation of VFA during the AD process results from the imbalance between acidogenesis and methanogenesis caused by temperature variation, excessive organic loading, inflow of toxic substances, etc. (Mechichi and Sayadi, 2005). However, the failure of operation when the SRT was small (S-15 and S-20) was neither attributed to temperature change nor inflow of toxic substances (i.e., most common causes of system failure in AD) but to excessive organic loads because regular operation was maintained in S-25 and S-30 using the same substrates and temperature (35 ℃). The OLRs of the four SRT cases were 12.0, 9.0, 7.2, and 6.0 g /L•d VS, respectively.

The restriction of methane production is also indicated by the high TVFA concentration and low pH in the reactor, resulting from excessive organic loads. The TVFA concentration is capable of inhibiting methane production due to pH reduction resulting from VFA decomposition (Rehm, 1999). In particular, the activity of methanogens interferes when the VFA concentration increases from 6.7 to 9.0 mol/m^3 (400–540 mg/L as acetate) (Batstone et al., 2000). The VFA toxicity is known to be caused by the unionized form rather than the ionized form; it is converted to the latter form after the cell membrane is penetrated. This causes the pH decrease in the cells, resulting in the collapse of homeostasis (Boe et al., 2007).

When S-25, S-30, S-15, and S-20 were normally operated before system failure, the average TVFA concentration was 15,000–20,000 mg/L. The unionized VFA (UVFA) values in S-15 and S-20 were calculated using pH and pKa (Table 1).

The reduction in pH did not significantly differ between S-15 and S-20; however, both VFA and UVFA concentrations were high. Moreover, S-15 failed (day 30) before S-20 (day 60), suggesting that the adverse effects of excessive organic loading were more severe in S-15 than in S-20. In addition, the results of S-25 and S-30 indicated that the VFA concentration and composition did not change considerably despite the increase in SRT. The VFA composition exhibited that the highest proportion of propionic acid in both SRTs; the concentration of propionic acid was stable (15,000–20,000 mg/L) without any significant

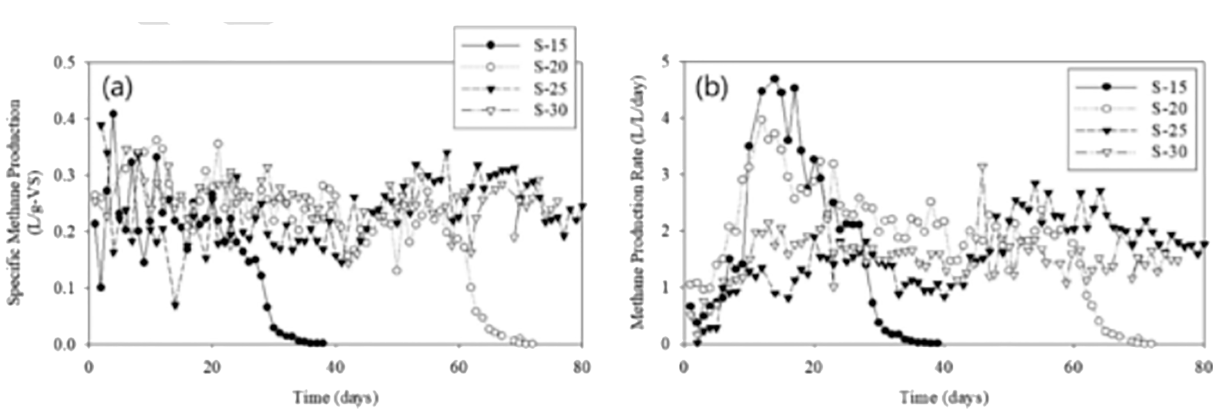

Fig. 2. Specific methane production (a) amount, and (b) rate from the dry AD system under different SRTs of 15, 20, 25, and 30 days.

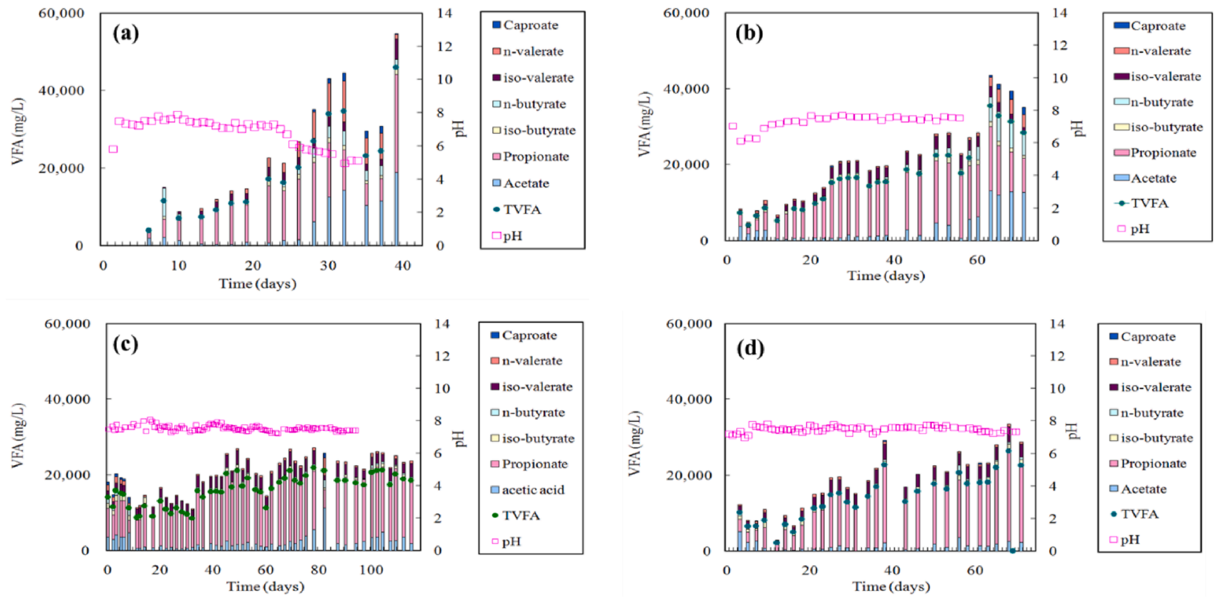

Fig. 3. The change of pH and VFA composition according to various SRT in dry AD system. (a) S-15, (b) S-20, (c) S-25, and (d) S-30.

Table 1
The values of pKa and VFAs concentration at the system failure in S-15 and S-20.

VFA content	pKa	S-15 TVFA (mg/L)	UVFA (mg/L)	S-20 TVFA (mg/L)	UVFA (mg/L)
acetic acid	4.76	18,890	11,990	13,202	8,794
propionic acid	4.88	25,334	14,406	13,916	10,186
iso-butyric acid	4.84	1,448	856	1,328	829
n-butyric acid	4.82	2,469	1,487	6,432	4,083
iso-valeric acid	4.77	5,237	3,296	2,838	1,876
n-valeric acid	3.84	1,132	1,059	2,319	2,187
caproic acid	4.88	268	153	590	355
Total acid		54,779	33,247	43,624	28,310

variations (Fig. 3(c) and 3(d)). In this study, SCOD concentrations in S-25 and S-30 remained at approximately 50,000 mg/L (see supplementary material). The concentration of SCOD was found to be proportional to TVFA concentration. Consequently, similar to VFA, SCOD did not show any substantial variations despite the increase in SRT when the system was normally operated. The TA concentration did not indicate any significant differences with changes in SRT (see supplementary material). In the cases of S-15 and S-20, which failed to operate due to organic material overloading, the TA concentration did not significantly increase compared with that in the cases of normal operation (S-25 and S-30). However, when failure occurred in S-15 and S-20, the FA concentration dropped to approximately 10 mg/L, presumably due to the concurrent decrease in pH. However, ascertaining whether this drop in FA is a direct cause of system failure is difficult. In this study, the TA concentration of 4,000–5,000 mg/L is known to hinder AD (Hobson and Shaw, 1976; Ramachandran et al., 2007). Therefore, the reactors used to treat FW with 80% water content could possibly be impeded by high TA concentrations. Consequently, a minimum SRT of 25 d (OLR: 7.2 g/L•d VS) is necessary when raw FW is dry AD-treated at mesophilic temperature without pretreatment. Moreover, significant amounts of VFA, which were not converted to methane, accumulated when the SRT was 15–30 d.

3.3. AD performance under different water contents

Microorganisms survive by absorbing dissolved (i.e., bioavailable) forms of organic matter as nutrients. Thus, biogas production and water content in the feed are closely related. In this study, water contents of the influent were adjusted to 80% (W-80), 85% (W-85), and 90% (W-90) (w/w); all cases were operated for more than 70 d (Fig. 4). All reactors were operated with 25 d of SRT and OLRs of 7.2, 5.4, and 3.6 g/L•d VS in W-80, W-85, and W-90, respectively.

The average SMP per unit substrate of each reactor was 0.246, 0.342, and 0.369 L CH_4/g VS in W-80, W-85, and W-90 respectively, indicating a tendency to increase as the water content increased (Fig. 4(a)). Fischer et al. (1984) reports that the high water content dilutes potentially toxic substances such as propionic acid, and also facilitates the mass transfer of nutrients and dissolved substrates under variably-saturated conditions increasing the methane generation efficiency (Fischer et al., 1984). The efficiency of methane production (i.e., rate per unit volume) of each reactor is presented in Fig. 4(a). The methane production rates of W-80 and W-85 approached 1.74 and 1.82 L/L/d, respectively. However, W-90 had a lower rate (i.e., 1.37 L/L/d) because the amount of introduced organic matter decreased as the water content of the influent increased. In contrast, the values of W-80 and W-85 are similar because the methane production per unit mass of VS in the latter is significantly higher than that in the former. These results show that a complementary relationship exists between the advantages afforded by dry AD and the enhanced mass transfer of substrates with high water contents. The optimum water content (85% in this case) is used to achieve maximum methane generation under the designated SRT.

The variation in the water content of the influent was shown to considerably affect the change in the VFA concentration. As the water content increased, the VFA concentration in the reactor significantly dropped; the VFA concentrations in W-80, W-85, and W-90 were approximately 30,000, 5,000, and 200 mg/L, respectively (see supplementary material). This means that most of the VFAs produced in the reactor when the water content is relatively high are converted to methane, and the subsequent low OLR under high water content changed the VFA composition as well; in W-80, propionic acid accounted for most of TVFAs, whereas proportion of acetic acid in VFA was found to be the highest in both W-85 and W-90. This observation is consistent with the previous report in the literature that the acetic acid ratio is the largest in TVFA when the AD process is ideally operated

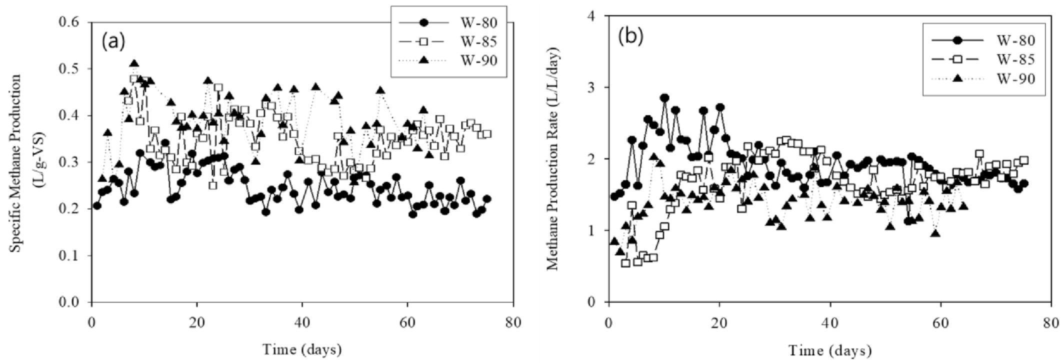

Fig. 4. Specific methane production (a) amount, and (b) rate from the dry AD system under different water contents of 80%, 85%, and 90%.

(Marchaim and Krause, 1993).

In terms of TA monitoring, W-80 was shown to have a higher TA concentration of up to 5000 mg/L, whereas that in W-85 and W-90 remained at approximately 3,000 mg/L (see supplementary material). Note that it was reported that a TA concentration exceeding 3,000 mg/L could inhibit the methanogenesis stage (Hobson and Shaw, 1976). High TA concentrations can also cause changes in the VFA composition. Methanogens can be classified into microorganisms that produce methane from acetic acid and those that produce methane using hydrogen and carbon dioxide. For both pathways, methane production could be inhibited by high concentrations of ammonia. Consequently, an excessive amount of hydrogen is not consumed, thus increasing the partial pressure exerted by hydrogen. Propionic acid has been reported to accumulate due to this high partial pressure ($\geq 10^{-5}$ bar) in the reactor, finally stopping the conversion to acetic acid (Ermler et al., 1997). The previous experiment confirmed that the high propionic acid ratio in the case of 80% water content may be attributed to the high TA concentration.

3.4. Methane production and VS reduction

One of the main purposes of AD process for FW treatment is to reduce the quantity of solid materials. Table 2 summarizes the average VS reduction and biogas production from each treatment case with various SRTs and water contents in this study. Both SRT and water content were found to considerably affect VS reduction; this tendency was also observed in methane production. The results of normally operated cases (S25-W80, S30-W80, S25-W85, and S25-W90) showed that the VS reduction efficiency increased as SRT and water content increased. Conversely, as SRT and water content decreased, the CO_2 generation/VS removal rate increased. Presumably, this was due to the suppression of methane production by the high OLR.

Table 2
Solid reduction and biogas production of dry AD system in various SRTs and water contents.

	S25-W80	S30-W80	S25-W85	S25-W90
Influent VS (kg/L)	0.182	0.182	0.132	0.09
Removed VS (kg/L)	0.105	0.106	0.085	0.056
VS removal rate (%)	57.7	58.2	64.4	62.2
Specific methane production (L/g•VS)	0.246	0.255	0.342	0.369
CO_2 production (L/g•VS)	0.217	0.211	0.213	0.198
Biogas production (L/g•VS)	0.463	0.466	0.555	0.567
Methane/VS•removed (L/g•VS)	0.426	0.437	0.531	0.593
CO_2/VS•removed (L/g•VS)	0.376	0.362	0.330	0.318

3.5. Prediction of the biogas production rate

As aforementioned, it is difficult to apply a process-based model to AD due to an extensive substrate characterization with large number of parameters (Ozkan-Yucel and Gökçay, 2010). In addition, the influent characteristics and the bacterial community of the AD reactor that affect parameters in the model changes over time, which requires extensive datasets together with a profound understanding in each sub-process for calibration (Ozgun, 2019). However, the following RNN black-box model could effectively predicted the SMP based on routine sampling of water quality parameters.

To evaluate the performance of the fitted model, experimentally measured and predicted SMP values are compared, as shown in Fig. 5. Ideally, the data points plotted in the figure must be those of an identity function, implying that a linear regression function with a slope that approaches one is desired. Accordingly, linear regression analyses were conducted to calculate this slope. The least-square method was used to derive the linear regression function. From the validation data, the calculated slope and correlation coefficient are 0.81 and 0.82, respectively (Fig. 5(a)). In contrast, from the test data, the calculated slope and correlation coefficient are 0.93 and 0.85, respectively (Fig. 5(b)). The slope derived from the validation and test data is less than one, indicating that the predicted SMP values are slightly smaller than the actual data. Moreover, the derived coefficients of determination (0.82 and 0.85) indicate strong linear relationships in the datasets; in general, coefficients exceeding 0.67 may be considered acceptable (Santhi et al., 2001; Liew et al., 2003).

To demonstrate the overall prediction performance of the model, the experimentally measured and predicted SMP values were compared, as shown in Fig. 6. Note that the training (50%), validation (25%), and test (25%) data are plotted in the same figure. The formulated SMP prediction model can describe the phases of normal biogas production and system failure (SMP converges to zero), which are observed at the end of experiments, as shown in Fig. 6, (a) and (b). Furthermore, Fig. 6, (a)–(d), indicates that the developed model effectively predicted the normal biogas production phase with different SRTs.

The developed model can be used as a new framework for the system control (e.g., early detection of the system failure) and optimization of the complex, non-linear systems including AD process. Based on the modelling method in this study, development of various prediction model can be performed that using different parameters. The model requires input values which can be measured more frequently and cost-effectively for the enhanced practical applicability. In addition, various scenarios can be evaluated such as control of operational parameters and limiting substrates by assuming the addition of chemicals. However, as described in the introduction and data preparation section, the developed model has limitations. Firstly, it is difficult to utilize the developed model to other general AD processes directly because of the nature of the black-box model. To apply this model to other AD process, training, testing and validation of the model should be conducted using

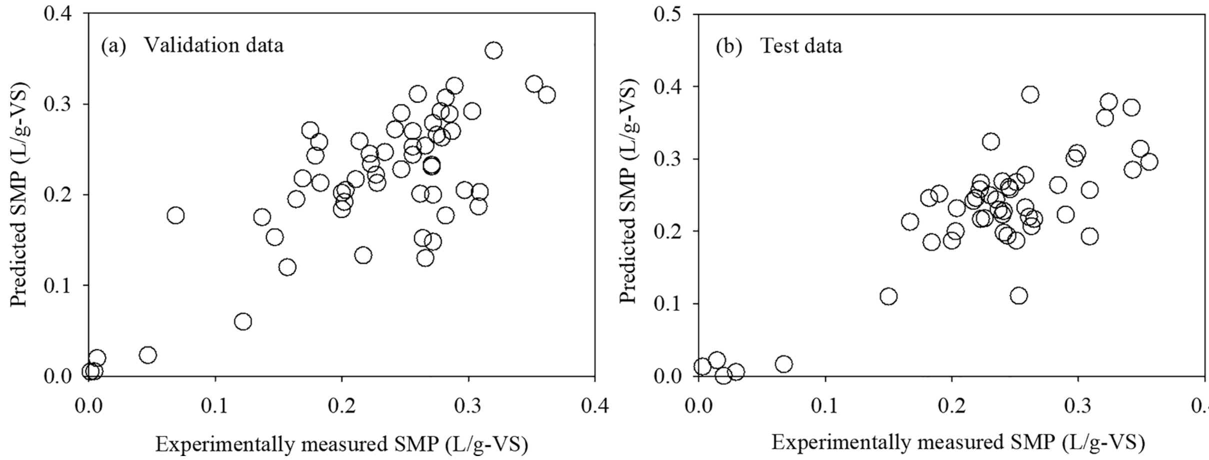

Fig. 5. Comparison of experimentally measured and predicted SMPs; (a) Validation data and (b) Test data. The measured SMPs the predicted SMPs are described on horizontal and vertical axis, respectively.

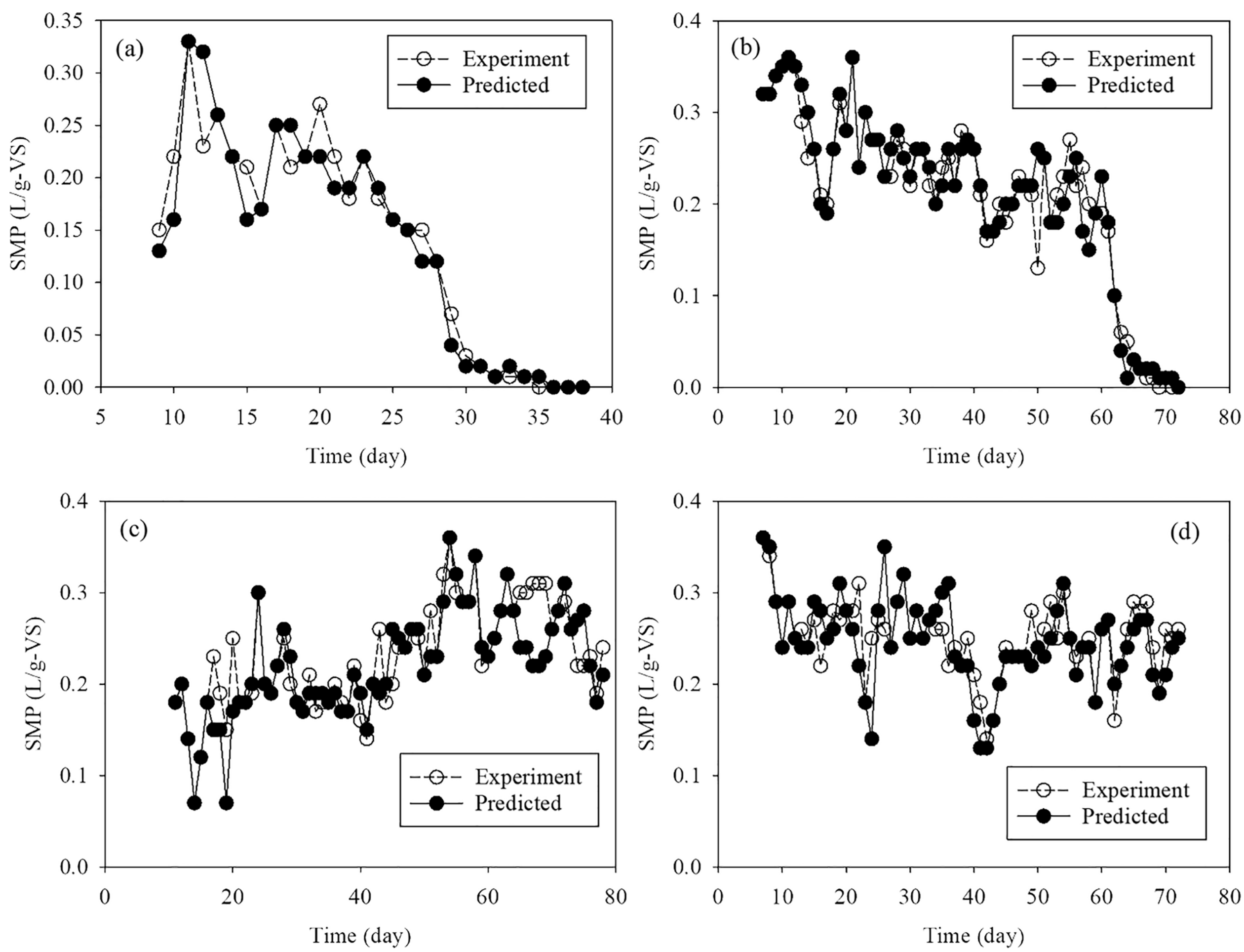

Fig. 6. Comparison of experimentally measured and predicted SMPs for entire dataset; (a) SRT of 15, (b) SRT of 20, (c) SRT of 25, and (d) SRT of 30. The measured SMPs the predicted SMPs are described on horizontal and vertical axis, respectively.

the data from the target process, the performance of which largely depends on the feed composition. However, the methodology is still valid, and if sufficiently large data from various AD process is available, generality of the model can be assessed as well. Secondly, SMP with respect to various water contents was not predicted because of potential algorithmic bias from the insufficient data. In short, with the collection of wide range of sufficient data overtime, the prediction accuracy and the generality of the model can be enhanced.

4. Conclusions

The stability of dry AD of FW was found to be considerably dependent on the OLR introduced into the system and resulting VAF production. These factors can be controlled by modifying the SRT and water content in the feed, requiring at least 25 d of SRT and 80% water content to avoid system failure. Moreover, the RNN black-box model compared with the comprehensive process-based approach could effectively predict the biogas production rate. This study provides an opportunity to apply the data-based black-box model for controlling and optimizing complex biological processes.

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CRediT authorship contribution statement

Kyu Won Seo: Methodology, Writing - original draft. **Jangwon Seo:** Conceptualization, Writing - original draft. **Kyungil Kim:** Methodology, Investigation. **Seung Ji Lim:** Writing - review & editing. **Jaeshik Chung:** Supervision, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.biortech.2021.125829.

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