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A simplified model for simulating anaerobic digesters: Application to valorisation of bagasse and distillery spent wash

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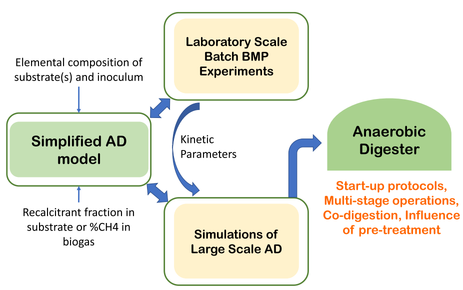
HIGHLIGHTS

- A simplified model was developed to simulate performance of anaerobic digester.
- The three model parameters can be obtained from biomethane potential data.
- The model was applied for simulating digestion of bagasse and spent wash.
- Simulated digester yield was consistent with limited available industrial data.

GRAPHICAL ABSTRACT



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ABSTRACT

Current anaerobic digestion (AD) design methods rely on crude empirical models or sophisticated anaerobic digestion models (like ADM1) requiring a large number of parameters which are difficult to obtain experimentally. A simplified model for simulating AD was developed in this work. The model requires knowledge of CH_4/CO_2 ratio in biogas or indigestible fraction in substrate and batch biomethane potential (BMP) data for estimating three kinetic parameters (maximum specific growth rate, half velocity constant and cell death rate). Reported lab scale BMP data of sugarcane bagasse and spent wash were used to first estimate the kinetics and then to simulate corresponding largescale AD. Simulated results of specific methane yield and digester performance were consistent with available largescale AD data. The potential of the model to simulate single and multi-stage AD were illustrated. The presented approach and model will be useful for effectively valorising a variety of complex biomass substrates to biogas.

1. Introduction

Anaerobic digestion (AD) is one of the mature and promising biomass valorisation platforms. The main product of AD is biogas that is predominantly a mixture of CH_4 and CO_2. Upgradation of biogas to compressed biogas (CBG) has the potential to decarbonise a variety of sectors such as transportation, domestic heating and electricity, which are currently dependant on fossil fuels (Gerres et al., 2019; Lamb, 2020; O'Shea et al., 2020). Furthermore, the by-product of AD – digestate, is rich in nutrients and has a potential to be used for recovering fertilisers

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and other valuable products. Thus, AD has a significant potential for valorising waste lignocellulosic biomass (LCB) streams. Typical waste LCB streams are composed of cellulose, hemicellulose and lignin as the major components and non-structural carbohydrates, proteins and lipids as minor components. While the valuable holocellulose (cellulose and hemicellulose) fraction in LCB is digested to produce biogas, recalcitrance posed by the interlinked polysaccharide-lignin structures limit its accessibility thus affecting gas generation and the overall digestion process. This would mean an inefficient digestion process with slow biogas generation rate requiring long residence times (~4 weeks). To improve the biogas yield, pre-treatment methods such as milling, hydrodynamic cavitation (HC) or thermal hydrolysis are used (Konde et al., 2021). There is an increasing interest in using complex LCB as a feedstock for AD using these pre-treatments. Systematic methods for designing and optimising AD systems for such complex feedstock are however not readily available. In this work, we present a simplified model suitable for design and optimisation of AD systems for treating such waste biomass streams to bridge this gap.

The design of AD for any feedstock usually starts with an estimation of theoretical maximum biomethane potential (BMP) of the feedstock. Buswell's formula is often used for calculating the theoretical BMP which is based on a reaction stoichiometry that takes into account the elemental composition of the feedstock and assumes its conversion to CH_4 and CO_2 (Buswell & Mueller, 1952). Buswell's approach considers the complete conversion of LCB to biogas. However, in reality, a part of the substrate may be indigestible (Carlsson et al., 2012). Additionally, a part of the substrate is used to fulfil microbial growth and energetic requirements. Therefore, Buswell's approach often leads to significant over-prediction of the BMP (Davidsson et al., 2007). It is therefore necessary to perform lab scale measurements to determine the realistically achievable BMP of the feedstock.

Typical laboratory scale measurement of BMP involves running small batch digesters with known quantities of inoculum and substrate and monitoring the biogas generated over time (Angelidaki et al., 2009; Holliger et al., 2016; Raposo et al., 2011; Strömberg et al., 2014). There are many studies which examine and evaluate various means of improving the BMP of LCB substrates, such as effect of pre-treatment (Nagarajan & Ranade, 2019), co-digestion (Astals et al., 2014), source of inoculum (Raposo et al., 2011), inoculum to substrate ratio (Raposo et al., 2006), etc. to name a few. Sometimes, semi-continuous and relatively larger lab scale digesters have also been investigated, focussing on parameters such as organic loading rate (Ferguson et al., 2016), digester configuration (Nizami & Murphy, 2010) and residence time (Huang et al., 2011). These lab scale investigations generate data of biogas or biomethane generation as a function of time and other key process parameters. Appropriate mathematical models are needed for interpretation and application of such lab scale data for designing of large scale AD. Several different models have been used for interpreting lab scale BMP data (Batstone et al., 2002; Bernard et al., 2001; Beuvink & Kogut, 1993; Donoso-Bravo et al., 2010; Ferraro et al., 2019; Kythreotou et al., 2014; Strömberg et al., 2015; Syaichurrozi et al., 2013; Thomsen et al., 2014). Earlier models utilised a one substrate (for example, acetate or glucose), pure microbial culture or rate limiting step based (example, hydrolysis) approach to describe BMP (Lübken et al., 2010). The models used to fit and describe kinetics of biogas generation can be broadly categorised into (i) empirical models based on lumped first order kinetics or (ii) complex comprehensive reaction engineering models such as the Anaerobic Digestion Model 1, commonly referred to as ADM 1 and their variants. The empirical models often lump the kinetic parameters to describe the gas generation with or without a lag phase and decay constants (Beuvink & Kogut, 1993; Nagarajan & Ranade, 2019; Strömberg et al., 2015). While these models are usually adequate to describe lab scale BMP data, their application in designing large scale AD has not been established. More sophisticated ADM 1 like models can be used to fit the lab scale BMP data and has potential to be used for designing large scale AD (Batstone et al., 2005; Ersahin, 2018; Hassam et al., 2015; Otuzalti & Perendeci, 2018; Zhao et al., 2019). However, the ADM 1 like models consider a complex reaction network and require significantly more information about transient profiles of large number of intermediate species beyond the lab scale BMP data for obtaining relevant parameters. More often than not, the lab scale BMP experiments are not equipped to collect such transient profiles of intermediate species that makes development and application of ADM 1 like models practically difficult. It is therefore essential to develop an intermediate modelling approach which is phenomenological and yet simpler to develop and apply than the ADM 1 like models.

In this work, we present such an intermediate model which can be used to obtain key kinetic parameters (maximum specific growth rate, death rate and half saturation constant) based on only BMP data. A lumped reaction approach was used to represent biogas production avoiding the need to consider intermediates. A Monod kinetics based approach was used to model gas generation. The simplicity of the presented model makes it novel and the subsequent sections in the manuscript will discuss this modelling approach and its implementation. For illustrating the application of the developed model, published experimental BMP data of two relevant substrates namely sugarcane bagasse (SCB) (Nagarajan & Ranade, 2019) and distillery spent wash (SW) (Nagarajan & Ranade, 2020) were considered. The best kinetic parameters obtained from the batch BMP data were used to simulate large scale AD performance with SCB and SW as feedstock. The use of two digesters in series is discussed to illustrate potential application of the developed model for design and optimisation of AD systems. The models and developed approach will be useful for effectively valorising a variety of LCB substrates to biogas.

2. Mathematical model

2.1. Physical picture and modelling approach

In this work, a well-mixed AD, processing a complex biomass substrate is considered. The schematic of a typical AD is shown in Fig. 1a. Here, S denotes carbon containing substrate, N denotes nutrient, if any, X and X_d denote live and dead cells respectively, P denotes CH_4, D denotes CO_2, W denotes water and R denotes a recalcitrant fraction of substrate. It is important to note that most of the LCB substrates contain lignin which usually does not get digested in AD. This indigestible substrate fraction along with any other inert and inaccessible fraction of the substrate is lumped into 'R' (see Reaction R(1)). Though the schematic in Fig. 1a shows input and output streams, it can also represent batch AD system by setting input ($\dot{M}_i$) and output ($\dot{M}_o$) mass flow rates (kg/h) to zero. The biogas flow rate, G (kg/h) will always be present as long as digestible substrate and living cells are present in the digester.

The goal of this work was to develop a simple phenomenological model of substrate conversion to biogas in AD, which requires only BMP data, to obtain relevant model parameters. Various intermediate steps in the substrate conversion were lumped into a single reaction (R1), where live cells (X) present in the inoculum catalyse the transformation of the substrate and nutrients to produce more cells (X), biomethane (P), CO_2 (D) and water (W), leaving behind the recalcitrant fraction (R).

$$S + z_N N \xrightarrow{X} z_X X + z_P P + z_D D + z_W W + z_R R \tag{R1}$$

This main transformation reaction, R1 is supplemented by the following reaction representing death of live cells:

$$X \rightarrow X_d \tag{R2}$$

It should be noted that, the lumped reaction (R1) is based on the assumption that all the nitrogen content in the substrate and nutrients is used for forming new cells. The reaction (R1) also ignores formation of H_2S. While sulphur enters the digester primarily via the feedstock and its conversion to H_2S may interfere with the biogas quality, the decrease in yield of biogas may not be significant. For instance, when Buswell's

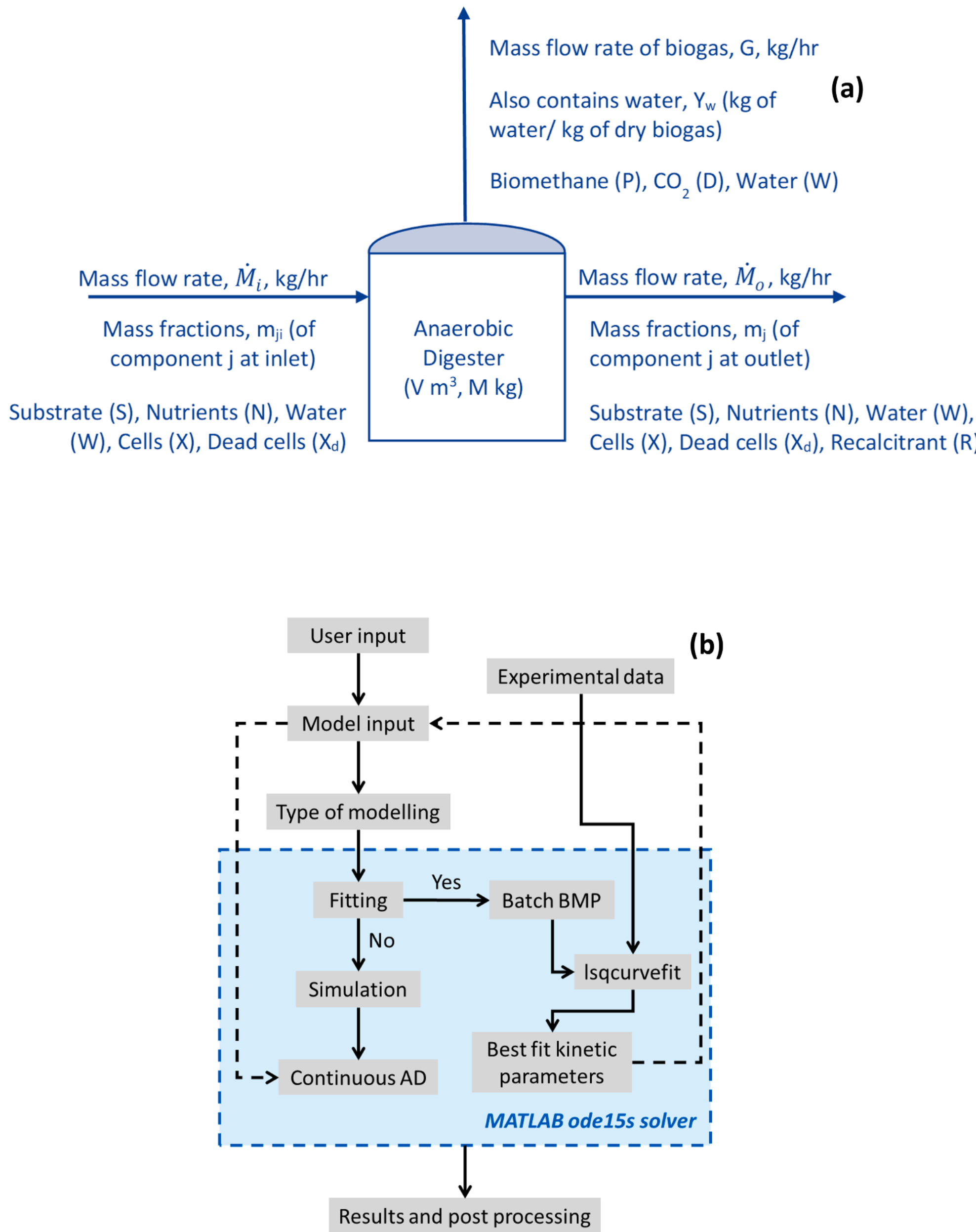


Fig. 1. (a) Schematic of an AD system (b) Solution methodology.

formula was used to calculate the ultimate BMP of the feedstock considered in this work (SCB and SW), the influence of sulphur content on methane yield was less than 2%. Therefore, the sulphur content in the biomass substrate was not considered in the present model. The overall approach however is general and may be extended to include sulphur in the biomass by appropriate modification of reaction stoichiometry.

For obtaining the relevant stoichiometric coefficients of reaction (R1), the composition of substrate (S), nutrient (N), Inoculum (which contains some substrate and living microbial cells) and cells (X) needs to be represented in terms of elements, C, H, O and N as $CH_pO_qN_r$ and values of p, q and r may be obtained from elemental analysis. For microbial cells, a generic accepted empirical formula of $CH_{1.4}N_{0.2}O_{0.4}$ may be used. Stoichiometric coefficients, z's appearing in (R1) need to be determined by balancing the reaction. Additional assumptions are needed to calculate relevant stoichiometric coefficients since there are six unknown stoichiometric coefficients and only four elemental balance equations (C, H, O and N). Even if a separate nutrient is not added, as the two illustrative examples considered in this work, there are still five unknowns and four equations. Two possible ways may be adopted to estimate required stoichiometric coefficients in such a situation:

- Assume a ratio of CH_4 to CO_2 (z_P/z_D) in generated biogas or
- Assume a known recalcitrant fraction in net substrate (denoted by Φ_C)

In the first case, the z_P/z_D ratio may be selected using the experimental or plant scale data, if available. Usually, this ratio is close to 1 for LCB substrates (Chen et al., 2014; Dell'Omo & La Froscia, 2018; Gao et al., 2013; Liu et al., 2009) and this value may be used in absence of specific data. Rest of the stoichiometric coefficients can then be calculated by balancing the reaction (by solving four linear equations simultaneously). The value of z_R obtained from this exercise indicates the indigestible fraction of the substrate. Alternatively, the fraction of indigestible substrate, Φ_C ($=M_{wR}\, z_R/M_{wNS}$), may be assumed which will allow calculation of remaining stoichiometric coefficients. In addition to the simplified reaction representing digestion process (R1), following assumptions were made to retain the simplicity of the developed model without jeopardising key abilities:

- All components of the reaction contain only four elements – C, H, N and O
- Live and dead cells have the same elemental composition
- No separate nutrient is added
- Generated biogas, G (kg/h) consists of only CH_4 (P) and CO_2 (D)
- Biogas dissolved in the liquid mass contained in AD is negligible compared to the generated biogas. The accumulation of gas (P and D) in liquid was thus neglected.
- The biogas escaping the liquid mass in AD is saturated with water vapour
- Density of the AD slurry is constant and same as that of water (1000 kg/m^3)
- In continuous mode of operation, the volume (and mass) of slurry in the AD was assumed to be constant (outflow was adjusted to maintain constant volume)

With the simplified reaction schemes (R1) and (R2) coupled with these listed assumptions, model equations can be formulated as discussed in the following.

2.2. AD model equations

The component mass balances may be written as:

$$Living\ \ cells: \frac{d(Mm_X)}{dt} = \dot{M}_i m_{Xi} - \dot{M}_o m_X + \mu XV - k_d XV \tag{1}$$

$$\text{where, } S = \frac{Mm_S}{V} \text{ and } X = \frac{Mm_X}{V} \text{ and } \mu = \mu_{max}\frac{S}{K_s + S} \tag{2}$$

where M is mass of slurry in AD (kg), V is volume of AD (m^3), $\dot{M}$ is the mass flow rate (kg/h) with the subscript of 'i' and 'o' indicating the mass inflow and outflow rates respectively, μ_{max} is the maximum specific growth rate of cells (1/h), K_s is the half velocity constant (kg/m^3), k_d is the cell death rate (1/h), S is substrate (kg/m^3), X is cells (kg/m^3), m_X is the mass fraction of cells (kg cells/kg AD contents), m_{Xi} is the mass fraction of cells at inlet (kg cells/kg inlet) and m_S is the mass fraction of substrate (kg substrate/kg AD contents).

$$Dead\ \ cells: \frac{d(Mm_{Xd})}{dt} = \dot{M}_i m_{Xdi} - \dot{M}_o m_{Xd} + k_d XV \tag{3}$$

where m_{Xd} is the mass fraction of dead cells (kg cells/kg AD contents) and m_{Xdi} is the mass fraction of dead cells at inlet (kg cells/kg inlet).

The substrate consumption rate, $\dot{S}$ towards cells can be written as:

$$\dot{S} = \frac{1}{Y_{XS}}(\mu X) \tag{4}$$

where Y_{XS} = kg of cells formed per kg of substrate utilized. Similarly, the nutrient consumption rate, $\dot{N}$ towards cells is:

$$\dot{N} = \frac{1}{Y_{XN}}(\mu X) \tag{5}$$

The rate of production of CH_4 ($\dot{P}$), water ($\dot{W}$), CO_2 ($\dot{D}$) and recalcitrant fraction ($\dot{R}$) are:

$$\dot{P} = \frac{1}{Y_{XP}}(\mu X) \tag{6}$$

$$\dot{W} = \frac{1}{Y_{XW}}(\mu X) \tag{7}$$

$$\dot{D} = \frac{1}{Y_{XD}}(\mu X) \tag{8}$$

$$\dot{R} = \frac{1}{Y_{XR}}(\mu X) \tag{9}$$

where Y_{XP}, Y_{XW}, Y_{XD} and Y_{XR} are yield coefficients of CH_4 (P), water (W), CO_2 (D) and recalcitrant fraction (R) with respect to cells (kg of cells formed per kg of CH_4, water, CO_2 or recalcitrant produced).

The overall substrate and nutrient consumption rates may be written as:

$$Substrate: \frac{d(Mm_S)}{dt} = \dot{M}_i m_{Si} - \dot{M}_o m_S - \dot{S}V \tag{10}$$

$$Nutrient: \frac{d(Mm_N)}{dt} = \dot{M}_i m_{Ni} - \dot{M}_o m_N - \dot{N}V \tag{11}$$

$$Recalcitrant\ \ fraction: \frac{d(Mm_R)}{dt} = \dot{M}_i m_{Ri} - \dot{M}_o m_R + \dot{R}V \tag{12}$$

where m_N and m_R are the mass fraction of nutrients and recalcitrant fraction (kg/kg AD contents), m_{Ni}, m_{Ri} and m_{Si} are the mass fraction of nutrients, recalcitrant fraction and substrates at inlet (kg components/kg inlet).

Since there is no accumulation of biogas in AD liquid, the mass balance for CH_4 and CO_2 can be written as:

$$Methane: 0 = \dot{P}V - GY_P \tag{13}$$

$$Carbondioxide: 0 = \dot{D}V - GY_D \tag{14}$$

with Y_P = kg CH_4/kg Biogas and Y_D = kg CO_2/kg Biogas

Summing over (13) and (14) with $Y_P + Y_D = 1$ we get,

$$G = (\mu XV)\left(\frac{1}{Y_{PX}} + \frac{1}{Y_{DX}}\right) \tag{15}$$

The overall mass balance of water can be written as:

$$\frac{d(Mm_W)}{dt} = \dot{M}_i m_{Wi} - \dot{M}_o m_W + \dot{W}V - GY_W \tag{16}$$

where Y_W is the water vapour in biogas (kg water/kg dry biogas).

Summing over all species, we get overall mass balance as (with setting M = constant):

$$\frac{dM}{dt} = \dot{M}_i - \dot{M}_o + (\mu XV)\left[1 + \frac{1}{Y_{PX}} + \frac{1}{Y_{DX}} + \frac{1}{Y_{WX}} + \frac{1}{Y_{RX}} - \frac{1}{Y_{SX}} - \frac{1}{Y_{NX}}\right] - G(1 + Y_W) \tag{17}$$

For continuous AD system:

Since mass in AD is maintained constant, the output flow rate may be calculated as:

$$\frac{dM}{dt} = 0 \tag{18}$$

$$\dot{M}_o = \dot{M}_i - G(1 + Y_W) \tag{19}$$

For batch AD system:

There are no solid or liquid streams that enter or exit the AD. Only generated biogas leaves the AD system. The change in mass of slurry in AD may be written as:

$$\frac{dM}{dt} = -G(1 + Y_W) \tag{20}$$

$$\dot{M}_o = \dot{M}_i = 0 \tag{21}$$

The yield coefficients, Y's appearing in the mass balance equations can be calculated using the molecular weights of components, M_{wi} and their stoichiometric coefficients, z from the reaction stoichiometry as:

$$Y_{SX} = \frac{z_X M_{wX}}{z_S M_{wS}};\quad Y_{NX} = \frac{z_X M_{wX}}{z_N M_{wN}};\quad Y_{PX} = \frac{z_X M_{wX}}{z_P M_{wP}};\quad Y_{WX} = \frac{z_X M_{wX}}{z_W M_{wW}};\quad Y_{DX} = \frac{z_X M_{wX}}{z_D M_{wD}};\quad Y_{RX} = \frac{z_X M_{wX}}{z_R M_{wR}} \tag{22}$$

The yield coefficients satisfy the following relationship from mass balance (17):

$$\left[1 + \frac{1}{Y_{PX}} + \frac{1}{Y_{DX}} + \frac{1}{Y_{WX}} + \frac{1}{Y_{RX}} - \frac{1}{Y_{SX}} - \frac{1}{Y_{NX}}\right] = 0 \tag{23}$$

The mass fraction of water in the AD contents can be calculated by subtracting sum of mass fractions of substrate, cells and recalcitrant from unity. This completes the formulation of model equations.

2.3. Solution of model equations

The model may be solved either for simulating performance of batch or continuous AD using the known values of all required parameters (kinetic parameters as well as operating conditions) or for obtaining the kinetic parameters by fitting experimental BMP data. In the present work, the model equations were solved using MATLAB R2020a. The fitting of batch data was carried out using least square fit. The non-linear AD model equations presented in Section 2.2 were solved using ODE15s solver of MATLAB (MathWorks Help Center, 2021). The overall solution methodology is shown in Fig. 1b.

For obtaining kinetic parameters, the experimental data of biomethane generation as a function of time need to be provided as input in addition to all the required initial compositions to facilitate estimation of kinetic parameters. Once such kinetic parameters are obtained, these parameters may be used for simulating AD performance. For simulating AD performance, either batch or continuous, all initial compositions and kinetic parameters need to be specified. For continuous AD, feed flow rate and composition also need to be specified. Identification of initial conditions and establishing stoichiometric coefficients precede these solutions steps, which are not always trivial. For obtaining kinetics of digestion, batch AD experimental data is required. For illustrating the application of the developed model, our previously reported BMP data on the digestion of HC pre-treated SCB (Nagarajan & Ranade, 2019) and SW (Nagarajan & Ranade, 2020) were used. In these studies, digestate collected from an AD plant digesting grass silage and cattle manure was collected and filtered through a 1 cm sieve to remove large fibres. The resulting filtrate was degassed and used as inoculum. Although filtered, the inoculum is expected to contain some residual undigested feedstock in addition to microbial cells. Therefore, any typical inoculum would contain both substrate as well as living cells required to carry out digestion. In general, the initial mass in the AD may be written as:

$$M = M_{S1} + M_{S2} + M_I + M_N + M_W + M_R \tag{24}$$

where M_{S1} and M_{S2} are initial mass of substrate 1 and substrate 2, M_I is mass of inoculum, M_N is mass of nutrient, M_W is mass of water and M_R is the mass of recalcitrant fraction. Mapping this on to the input data required by the present model requires some pre-processing to combine all the substrates into an effective lumped substrate and estimate CHON composition of this lumped substrate based on elemental analysis of individual substrates. Similarly, mass fraction of living cells in the inoculum needs to be known for calculating initial mass fraction of living cells in the overall initial mass of AD as:

$$m_X = \frac{m_{XI} M_I}{M} \tag{25}$$

where m_{XI} is mass fraction of living cells in the inoculum (kg/kg inoculum). Once the elemental compositions of effectively lumped substrate and living cells are known, stoichiometric coefficients of (R1) and corresponding yield coefficients can be calculated either by assuming a ratio of CH_4 to CO_2 in generated biogas or recalcitrant fraction in net substrate as described earlier. Once all the initial values and other relevant input parameters are calculated, the kinetic parameters, namely maximum specific growth rate (μ_{max}, 1/h), cell death rate (k_d, 1/h) and half saturation constant (K_s, kg/m^3) may be obtained by minimising the errors between experimental and simulated BMP data using initial guess for the three parameters. Either the kinetic parameters obtained from the batch BMP data or known values of kinetic parameters may be used for simulating continuous AD system. Application of this methodology and results obtained for two illustrative examples of SCB and SW based AD systems are discussed in Section 3.

3. Results and discussion

The developed model was used to obtain relevant kinetic parameters for digestion of two substrates: SCB and SW. For both substrates, BMP measured after HC based pre-treatment as reported by Nagarajan and Ranade (Nagarajan & Ranade, 2019) (Nagarajan & Ranade, 2020) were used. In the first study (Nagarajan & Ranade, 2019), effect of number of passes (0, 9, 36 and 117) of SCB slurry through the HC device was investigated. The four data sets from this study were used for estimating kinetic parameters corresponding to four pre-treatment conditions. The obtained kinetics was then used for the simulations of large scale continuous AD for valorising SCB. In the SW case, the effect of number of passes (0, 2, 10, 20) of SW through HC device on BMP reported by Nagarajan and Ranade (2020) was used. Similar to the SCB example, all the four SW BMP data sets were used for estimating kinetic parameters. The kinetic parameters for the pre-treatment with 2 passes through the HC device were used for simulations of large scale continuous AD for valorising SW. Influence of HC pre-treatment on digestion kinetics and use of AD model for design and enhancement of large scale AD performance for valorising waste streams are discussed in the following.

3.1. Kinetics based on batch biomethane potential of bagasse and spent wash

For estimating digestion kinetics of SCB, the elemental composition (C, H and N) of the inoculum and SCB (both on a dry basis) were determined using a Series II Perkin Elmer PE2400 CHNS analyser. O was determined by difference. The empirical formula was then calculated and was found to be $CH_{1.7}N_{0.076}O_{1.1}$ for the inoculum. A range of batches of SCB were analysed for their elemental composition and the average of each element was used to represent SCB with a generic formula of $CH_{1.6}N_{0.007}O_{0.7}$. It is important to verify that all the yield coefficients calculated based on the net substrate formula are non-negative. For the SCB and inoculum considered in this example, the empirical formula for the net substrate (part coming from the inoculum and the remaining from SCB) was found to be $CH_{1.7}N_{0.047}O_{0.9}$. Using this composition and known CH_4 percentage in biogas (43%), the stoichiometric coefficients of the components in reaction (R1) and rest of the input parameters were calculated. Using the experimental BMP data, the three kinetic parameters (μ_{max}, k_d and K_s) for the digestion of SCB were obtained by least square fitting. The experimental data as reported by Nagarajan and Ranade (2019) and the corresponding simulated results obtained from the model are shown in Fig. 2a. The model was able to describe the experimental gas generation well with a correlation coefficient (R^2) of $>$ 0.99 obtained for all the analysed data sets. The enhanced BMP upon 9 passes HC treatment was captured adequately.

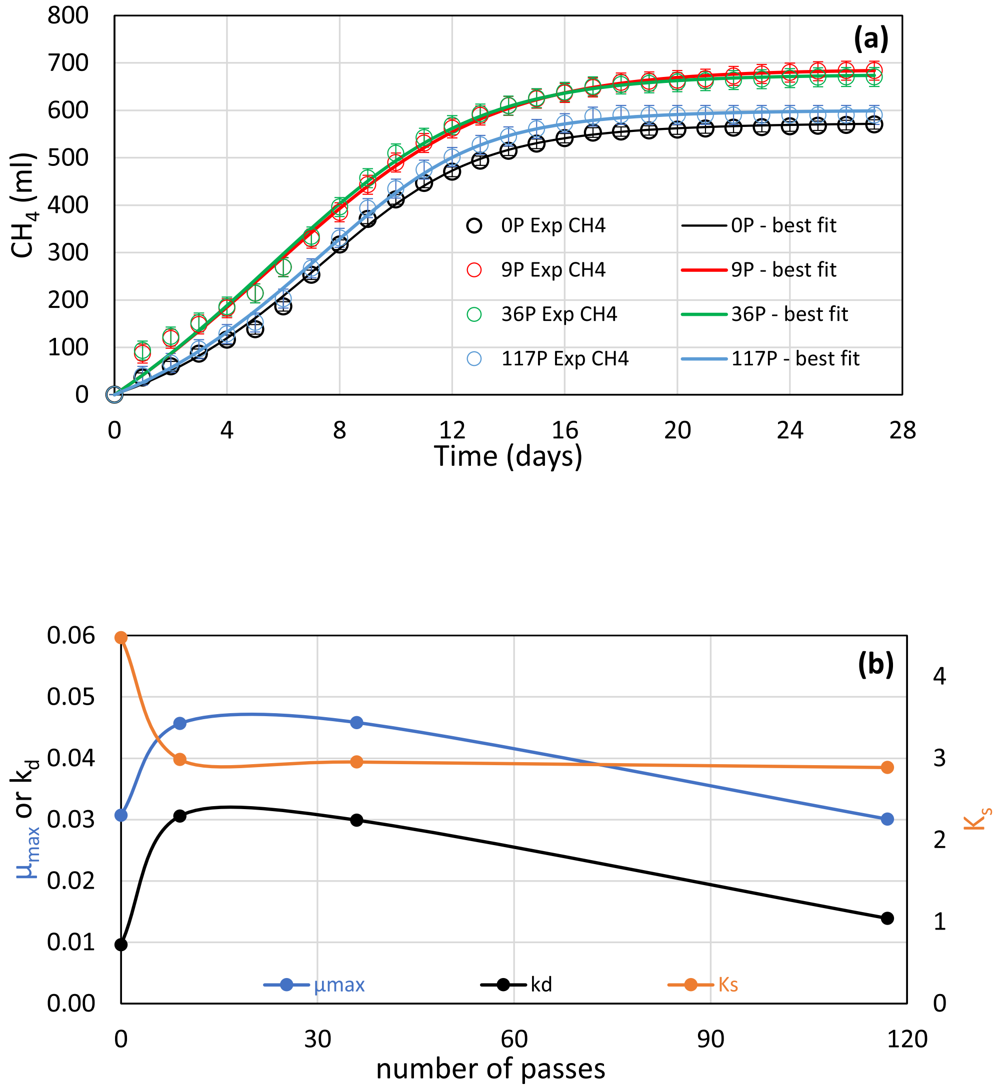
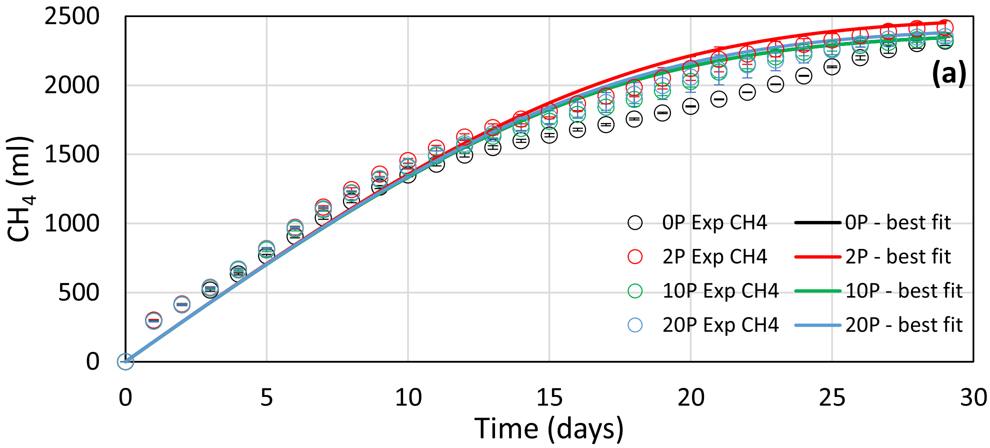


Fig. 2. (a) Comparison of experimental and simulated batch BMP experiments of SCB (Nagarajan & Ranade, 2019). Symbols denote experimental data and lines denote simulated results (b) Kinetic parameters used for simulations shown in Fig. 2a. Symbols denote values calculated from fitting the data and lines denote the overall trend.

Sensitivity of the simulated BMP profiles with respect to the fitted parameters for the case of 9 passes HC treatment was studied.

The kinetic parameters, μ_{max}, k_d and K_s used for simulations shown in Fig. 2a are shown as a function of number of passes through the HC device in Fig. 2b. It can be seen that the specific growth rate increased upon 9 passes HC pre-treatment, coupled with a decrease in K_s. This meant that the vortex based HC pre-treatment was effective in reducing substrate complexity and increasing the affinity of the substrate to the anaerobic microbial consortia. No significant change in K_s beyond 9 passes was observed, however a decrease in μ_{max} was observed. This may be due to possible inhibitors released during pre-treatment as hypothesised earlier (Garuti et al., 2018; Langone et al., 2018). The values of fraction of net substrate utilised (m_S utilised) were examined for the four simulated cases. It was found that 9 passes through HC devices enhanced substrate conversion compared to the untreated case resulting in ~ 20% enhancement in biomethane generation. The value of μ_{max} and extent of substrate utilisation was not very sensitive to number of passes up to $n = 36$.

A similar exercise was carried out with the SW BMP data. The empirical formula of the inoculum was found to be $CH_{1.8}N_{0.076}O_{0.9}$ and that of SW was $CH_{1.9}N_{0.077}O_{0.6}$. The elemental composition of net substrate was calculated to be $CH_{1.8}N_{0.075}O_{0.8}$. The ratio of CH_4 to CO_2 was assumed to be one. The experimental data as reported by Nagarajan and Ranade (2020) and the corresponding simulated results obtained from the model are shown in Fig. 3a. The model was able to describe the overall experimental gas generation trends well with a correlation coefficient (R^2) of > 0.98. Note that diauxic digestion observed for the untreated SW was not captured by the considered model – this was expected since the model is based on a simplified single reaction. The model can be used to account for diauxic digestion, by considering each of the stages of gas generation as separate data sets to obtain two sets of kinetic parameters representing two stages. Diauxic digestion observed with untreated SW was not seen upon HC pre-treatment and the enhancement in BMP upon 2 (or more) passes HC treatment, was captured appropriately. The developed model was therefore considered as adequate for the digestion of HC treated SW. The observed variation of fitted parameters with number of passes used in the pre-treatment was not significant. The constant set of kinetic parameters was therefore used for all numbers of passes (Table 1). The sensitivity of simulated results with the model parameters for 2 passes HC treated SW was examined. HC based pre-treatment with 2 passes showed some enhancement in substrate utilisation (and therefore biogas generation) as shown in Fig. 3b. The large-scale SW AD data reported by Nagarajan and Ranade (2020) indicated that 1 pass HC pre-treatment resulted



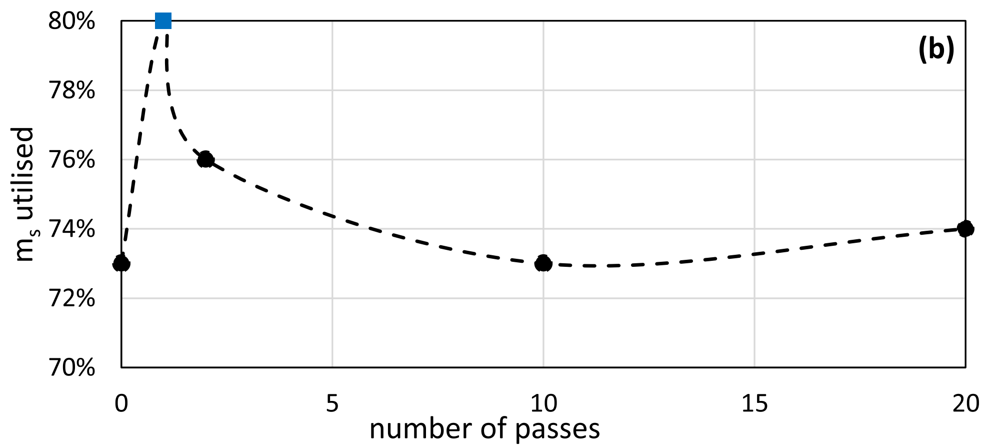


Fig. 3. (a) Comparison of experimental and simulated batch BMP experiments of SW (Nagarajan & Ranade, 2020). Symbols denote experimental data and lines denote simulated results (b) Substrate utilised as a function of number of passes through vortex based HC device for SW. The black solid circles correspond to m_s values calculated using the model from the experimental BMP data reported in (Nagarajan & Ranade, 2020), whereas the blue solid square corresponding to 1 pass is based on continuous large scale AD plant data reported in (Nagarajan & Ranade, 2020). The dotted line represents the overall trend. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1
Best fit kinetic parameters of SCB and SW BMP obtained from batch tests and corresponding inflow conditions used for continuous AD simulations.

Best fit kinetic parameters obtained from batch BMP		
Parameter (unit)\ Feedstock→	SCB	SW
Number of passes through vortex based HC device	9	2
Maximum specific growth rate, μ_{max} (h^{-1})	0.045	0.072
Cell death rate, k_d (h^{-1})	0.030	0.070
Half velocity constant, K_s (kg/m^3)	3	1
Parameters used for base case simulations of continuous AD		
Mass inflow rate, $\dot{M}_i$ (kg/h)	12,350	11,500
Hydraulic residence time, HRT (days)	6.7	29
Digester volume, V (m^3)	2000	8000
Mass fraction of substrate at inlet, m_{Si} (kg/kg inlet slurry)	0.1	0.2
Mass fraction of ash at inlet, m_{Ai} (kg/kg inlet slurry)	0.004	0.042
Mass fraction of water at inlet, m_{Wi} (kg/kg inlet slurry)	0.8960	0.7580

larger enhancement in biogas than seen for 2 pass pre-treatment. Unfortunately, BMP data was not available for corresponding pre-treatment conditions. The symbols shown in Fig. 3b indicate substrate utilisation observed in the simulations discussed here. The dotted line indicates possibly steeper maxima with respect to number of passes based on the large-scale results reported by Nagarajan and Ranade (2020).

3.2. Simulation of continuous AD systems

The model was used to simulate large scale continuous AD operation. The kinetic parameters obtained from the batch BMP of pre-treated SCB and SW (as listed in Table 1) were used. In all the simulations of continuous AD presented here, AD was considered as well mixed implying same hydraulic residence time (HRT) and solids residence or retention time (SRT) unlike some other studies which have used different HRT and SRT (Dong et al., 2016). The focus of these simulations was on examining steady state performance of SCB and SW based AD systems using the developed model. The initial conditions used to start the simulations were therefore irrelevant. The inlet conditions used for SCB and SW simulations are listed in Table 1.

3.2.1. Simulations of sugarcane bagasse based large scale anaerobic digester

Simulations of continuous AD with SCB as feedstock were initially performed to understand time required for attaining steady state. Later, a series of simulations were performed to understand influence of residence time on steady state substrate conversion and variety of digester performance parameters such as substrate conversion, specific methane yield (SMY, m^3 CH_4/kg VS) and digester performance (DP, m^3 CH_4/day/m^3 digester). Here, VS corresponds to the volatile solids in the net substrate.

Time required for attaining steady state was defined as the time at which the mass fraction of substrate in outflow is within 1% of mass fraction of substrate at time of 25 times HRT. Steady state is achieved at approximately 3.5 times the HRT with the given initial conditions. The model may be used to identify appropriate start-up protocol for initiating operation of a large scale AD system. For example, simulations using the presented model may be used to identify appropriate initial conditions (primarily mass fraction of live cells and substrate) so as to reduce time required to achieve steady state. By adding more substrate and inoculum (live cells) in the AD before starting the continuous feed will reduce time required for steady state. For example, in the simulated case, when the substrate mass fraction is increased by 10% and mass fraction of live cells is increased by 60% than the base case, steady state can be achieved within two times of HRT. This means that a higher initial viable cell mass is beneficial for the current simulated case for achieving earlier steady state. For large-scale continuous AD systems, achieving steady state early will mean significant economic benefits. The developed AD model can be used to optimise start-up phase to minimise time required for achieving steady state.

The transient profiles of substrate mass fraction show initial increase till strong growth of cells kicks in. The strong growth of cells causes a decrease in substrate concentration and eventually attains steady state. The steady state substrate conversion for the considered case was found to be 61%. A SMY of 0.26 m^3 CH_4/kg VS was calculated which is

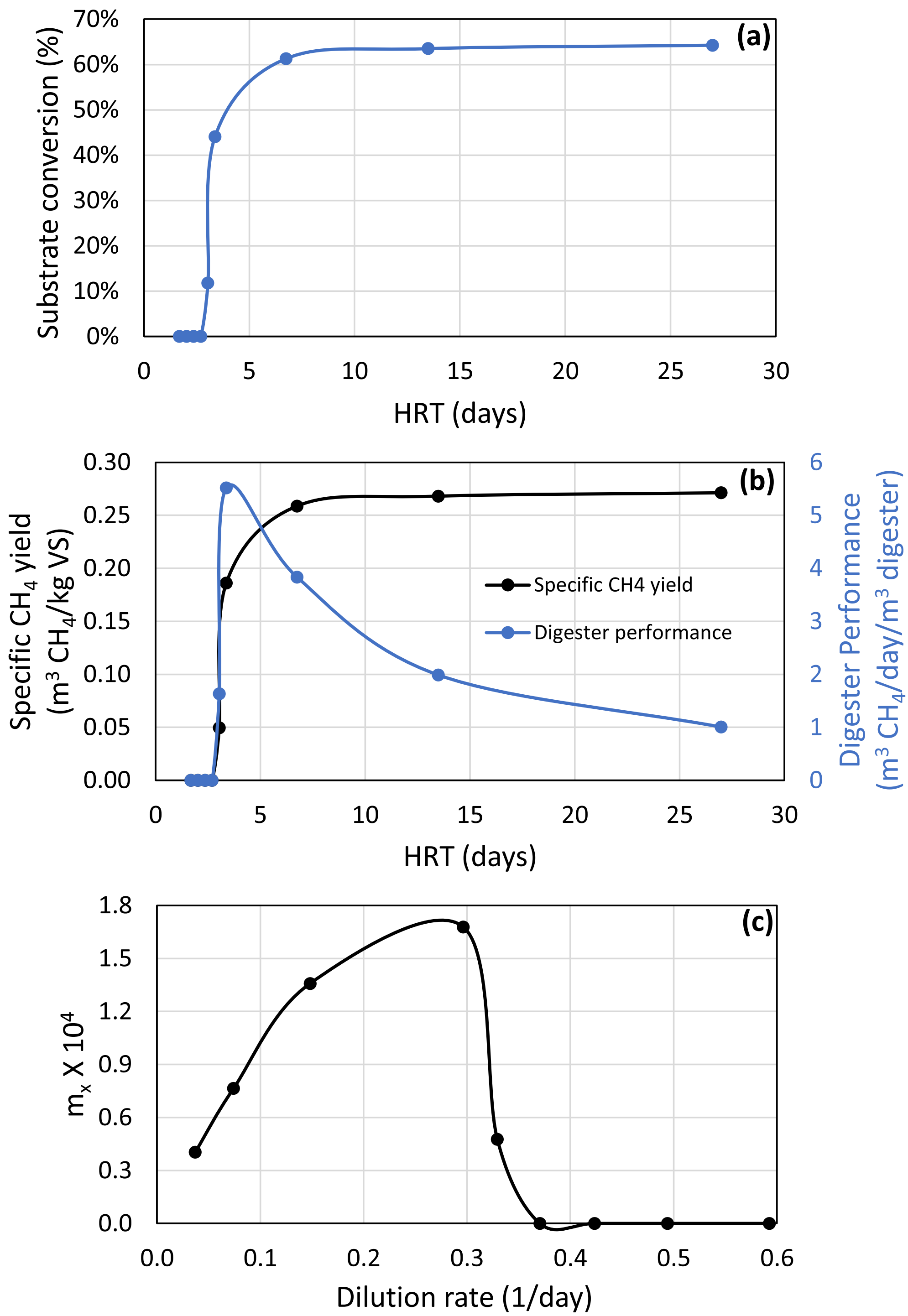


Fig. 4. Influence of HRT on (a) steady state SCB conversion to biogas and (b) SMY and digester performance; (c) influence of dilution rate on mass fraction of living cells. Symbols denote values calculated from simulation and lines denote the overall trend.

comparable to the SMY from the batch study (0.23 m^3 CH_4/kg VS) (Nagarajan & Ranade, 2019) and also in range with other published studies (0.17 – 0.31 m^3 CH_4/kg VS) (Konde et al., 2021). The simulated results for examining influence of HRT on key digester performance are shown in Fig. 4. The HRT was varied in the range of 1.7 – 27 days. As the substrate conversion as well as the SMY plateaued beyond 13.5 days, no simulations were performed beyond a HRT of 27 days. The variation in HRT can be achieved either by varying digester volume at the same feed rate or varying feed rate at the same digester volume. It was verified that, as expected, the results with respect to HRT were same for both these ways of varying HRT. It can be seen from Fig. 4 that the highest DP of 5.5 m^3 CH_4/day/m^3 digester was achieved at a lower HRT of 3.4 days. Although peak DP could be achieved at this HRT, the substrate conversion was only 44% which was lower by almost 40% than original simulated (at HRT of 6.7 days) case. Doubling the HRT to 13.5 days only improved the conversion by 4% but reduced DP by almost 50%. Further increase in HRT to 27 days (similar to batch BMP experiments) resulted in a further decrease in DP and a minimal increase in substrate conversion.

These results may also be interpreted using the conventionally used term in the AD literature – the organic loading rate (OLR, kg VS/m^3/day). Higher substrate conversion was observed with a lower OLR and below a threshold it plateaued. The importance of OLR on DP and SMY with SCB and other LCB have been previously established where a

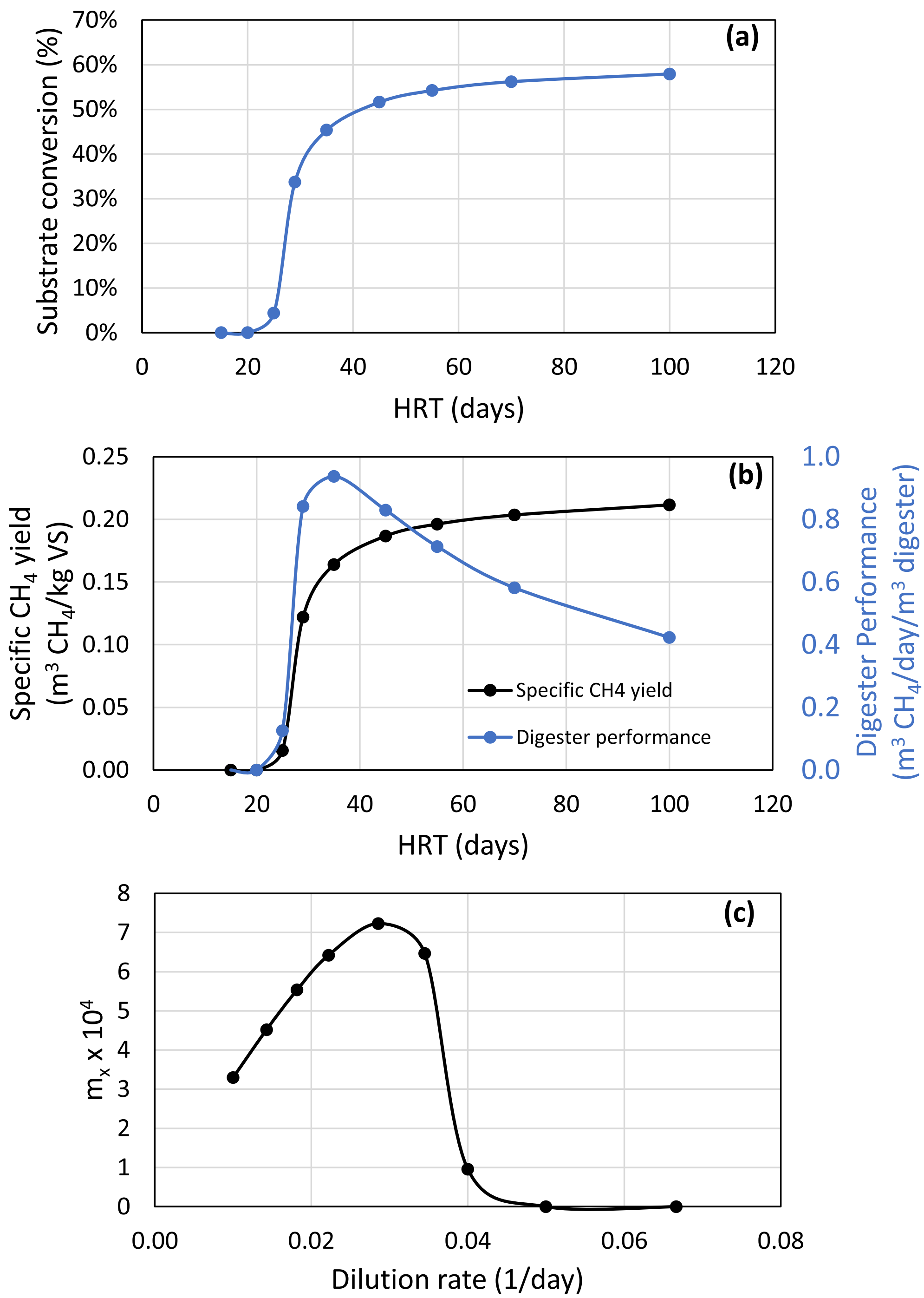


Fig. 5. (a) Influence of HRT on steady state SW conversion, (b) SMY and digester performance and (c) influence of dilution rate on mass fraction of live cells. Symbols denote values calculated from simulation and lines denote the overall trend.

number of researchers reached a similar conclusion (Leite et al., 2015; Li et al., 2015; Zealand et al., 2017). To further understand the influence of HRT on the process performance, the steady state mass fraction of live cells was plotted as a function of dilution rate (Fig. 4c). Dilution rate (day^{-1}) is the inverse of HRT (day) and is a useful indicator in determining wash out characteristics of a bioreactor. If the mass flow rate is high (corresponding to a low HRT), wash out of digester contents occur as seen in Fig. 4c. This directly influences the biogas production. At any HRT below 3 days, wash out occurs leading to a lower steady state mass fraction of live cells in the digester. A balance between mass flow rates and substrate conversion is therefore necessary to achieve optimum digester performance and is consistent with literature (Leite et al., 2015). The capital cost of digester will be inversely proportional to the digester performance (DP, m^3 CH_4/day/m^3 digester) for a given capacity of biomethane production. The cost of raw material will be inversely proportional to the specific methane yield (SMY, m^3 CH_4/kg substrate). The optimum value of HRT may be obtained using the costs of raw material (SCB in this case), required capital costs – annualised contribution and price of biogas. The developed model can be used to arrive at an optimum configuration and operating conditions of continuous AD system. Based on the simulated results presented here, it appears that the optimum HRT will be less than 27 days and likely to be in the range of 7–14 days for SCB.

3.2.2. Simulations of spent wash based large scale anaerobic digester

SW continuous AD simulations similar to SCB simulations were performed initially to obtain the time required for achieving steady state. Unlike the SCB, SW continuous AD required>15 HRTs to achieve steady state with the given set of initial conditions. This was mainly because of higher death rate observed in the case SW. However, by doubling the inlet mass fractions of live cells and increasing the inlet mass fraction of substrate by 60% reduced the time required to achieve steady state to 4 HRTs. Thus, the model can be used to identify start-up protocol for minimising the time required to achieve steady state by varying the initial conditions. The influence of HRT on performance was investigated over the range of HRT as 15 – 100 days. The simulated results are shown in Fig. 5. The highest DP of 0.94 m^3 CH_4/day/m^3 digester was achieved at a HRT of 35 days. The substrate conversion in this case was 45%. Increasing the HRT to 45 days resulted in a conversion of 52% with a SMY of 0.187 m^3 CH_4/kg VS (0.191 m^3 CH_4/kg COD) which was still lower than the SMY obtained from the batch BMP experiments (0.231 m^3 CH_4/kg VS). Similar to the observations with SCB simulations, an increase in HRT beyond a certain value resulted in a plateaued substrate conversion. The influence of HRT on substrate conversion is shown in Fig. 5a and the influence of HRT on DP as well as the SMY is shown in Fig. 5b. Again, similar to the SCB simulations, a wash out of live cells happens at higher mass inflow rates (corresponding to HRT lower than 20 days) as shown in Fig. 5c. Based on the simulations, HRT of about 30 days appears to be optimum with digester performance close to ~ 1 m^3 CH_4/day/m^3 AD. This is consistent with the limited large scale SW digester data available in literature (Nagarajan & Ranade, 2020).

3.3. Enhancing performance of large scale anaerobic digester

It was shown in Section 3.1 that the model can be successfully used for obtaining relevant kinetic parameters from the batch BMP experiments. Furthermore, Section 3.2 elaborated on the use of the model for simulating large scale continuous AD and predicting its performance based on the kinetic parameters obtained from the batch BMP data. This section illustrates use of the developed AD model for evaluating different scenarios – a case of two-stage AD (two digesters in series) is discussed here.

The base case of a single stage SCB based AD with a total volume of 8000 m^3 at a mass inflow rate of 12350 kg/h was considered. Substrate conversion as a function of HRT was first determined for this base case SCB digester. Next, for the same total volume, four cases of two digesters in series were simulated (Fig. 6a): case 1 - (4000 + 4000) m^3, case 2 - (2000 + 6000) m^3, case 3 - (1000 + 7000) m^3 and case 4 - (500 + 7500) m^3. In all the cases, the mass inflow to the first digester was fixed to 12350 kg/h. The focus was on evaluating steady state performance of the two stage digesters in comparison with the base case. The kinetic parameters of SCB digestion and inlet composition listed in Table 1 were used as the input parameters for the simulation of all these cases. In the first three cases, the net substrate conversion and DP was higher than that of the single stage digester whereas with the last case, due to the wash out of live cells at steady state in the 500 m^3 digester, the subsequent conversion achieved in the 7500 m^3 digester was comparable to that of the single stage digester.

The next set of simulations were performed for two equal volume digesters in series and compared against the single stage 8000 m^3 digester on the basis of substrate conversion (Fig. 6b) and on the basis of DP and SMY (Fig. 6c). Three cases were investigated in this set: case 1 – two 4000 m^3 digesters in series, case 5 – two 2000 m^3 digesters in series and case 6 – two 1000 m^3 digesters in series. In all the three cases, substrate conversion was found to be higher than that of the single stage digester (Fig. 6b). As seen in Fig. 6c, while the SMY was similar, the DP for the digester in series for all the three cases were found to be higher than the base case. Especially, the DP for case 5 and case 6 were significantly higher than the base case. Please note that the SMY is a function of S and μ_{max}. The μ_{max} used for all the simulations were based on the determined best case 9P HC treated SCB batch BMP scenario and hence the SMY remained almost unchanged. On the other hand, DP is a function of the digester volume, residence time and conversion. It is expected that for completely mixed reactors, reactor operating at lower conversion levels will have higher rate and therefore higher productivity. In terms of the viable cell fraction, typically it was found that the live cell mass fraction is lower in the second digester when compared to the first digester. For digesters operating in series, the second digester will have a considerably lower mass fraction of the substrate entering the digester compared to the first digester. A lower substrate availability affects the viable cell mass fraction and hence the second digester has a lower live cell mass fraction compared to the first digester when operating in series. Collectively, these results imply that two stage digesters will perform better than a single larger digester, which is expected considering the well-mixed behaviour of these digesters. It should however be noted that for a case of multiple AD in series, reduction in volume of individual digester restricts the operating range because of inherent constraints on maximum dilution rate (Bensmann et al., 2013). These constraints will limit how many stages in series will be feasible even disregarding the implications of multi-stage system on capital investment. It should be noted that while the presented example demonstrated the capability of the model to simulate digesters in series, it is not same as stage separated digestion (acid/acetogenesis and methanogenesis). It is however possible to extend the presented approach to simulate stage separated operation with acid/acetogenesis and methanogenesis stages in series. It will however require experimental BMP data corresponding to these two stages. The model can then be used to estimate kinetics of these two stages followed by large scale simulations of digesters in series.

It has been demonstrated that the developed model can be used to identify operating conditions for enhancing performance of AD. Furthermore, beyond single feedstock digestion, the model may also be used to simulate co-digestion of multiple substrates. The cumulative elemental composition of the mixture of substrates to be co-digested may be obtained using the elemental compositions of individual substrates and their mass fractions in the mixture. The stoichiometric coefficients appearing in reaction R(1) can then be obtained using the cumulative elemental composition of mixture of substrates. Once the stoichiometry is established with the net substrate, the model implementation is the same as what has been presented. Similarly, the effect of different type of nutrients and their dosage on AD productivity can be

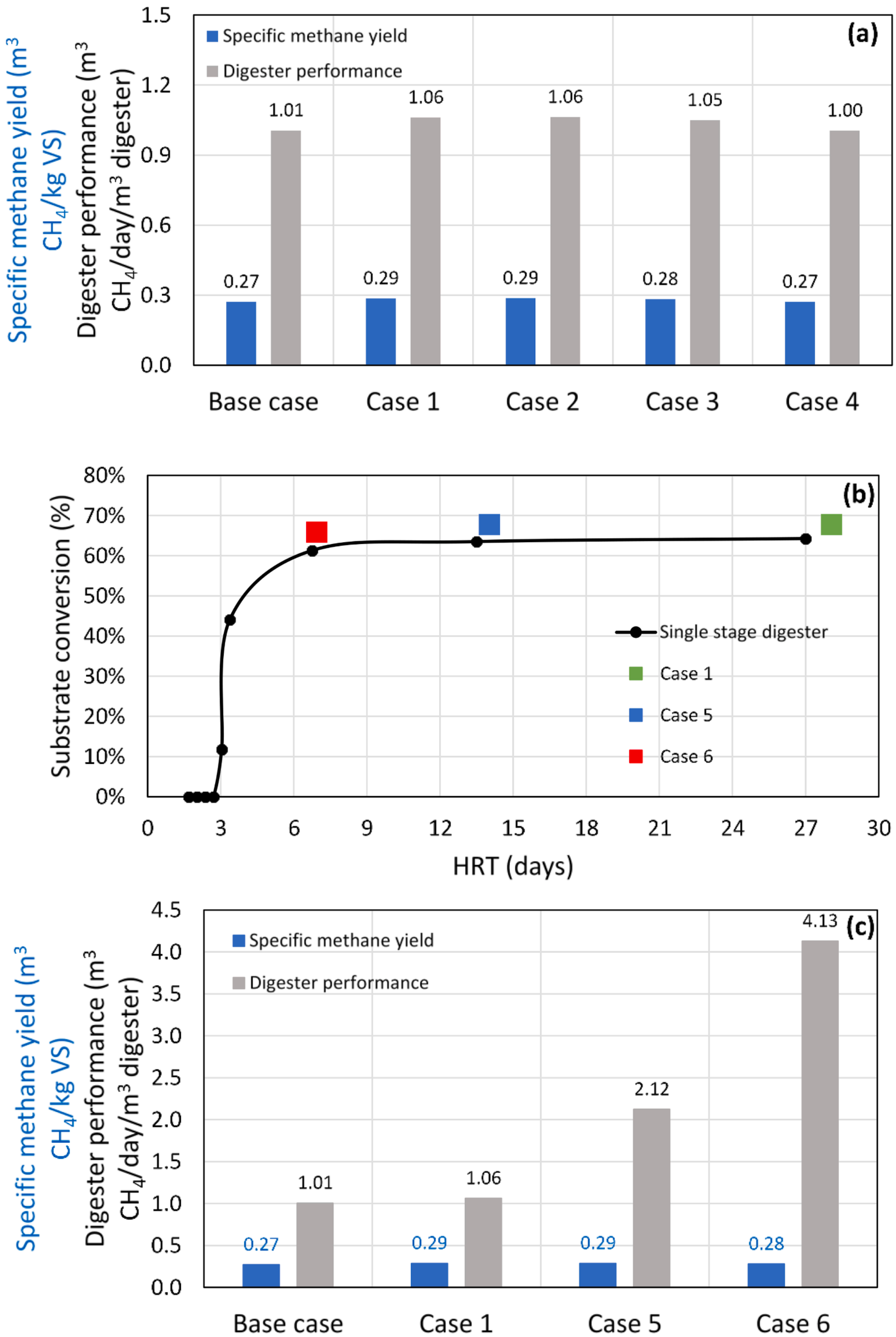


Fig. 6. (a) Digester performance and net SMY in 2 unequal volume digesters in series, (b) net substrate (SCB) conversion in 2 equal volume digesters in series at a constant inflow rate of 12350 kg/h to the first digester, Symbols denote values calculated from simulation and lines denote the overall trend, (c) digester performance and net SMY in 2 equal volume digesters in series. Substrate: SCB, pre-treated with 9 passes. Base case: single 8000 m^3 digester, case 1 - (4000 + 4000) m^3 digesters, case 2 - (2000 + 6000) m^3 digesters, case 3 - (1000 + 7000) m^3 digesters, case 4 - (500 + 7500) m^3 digesters, case 5 - (2000 + 2000) m^3 digesters and case 6 - (1000 + 1000) m^3 digesters.

simulated. The developed model, though quite simple, can be used for realistic simulations and enhancing the performance of large-scale industrial AD systems.

4. Conclusions

A simple model for simulating batch and continuous AD of complex biomasses was developed. The model requires batch BMP data and knowledge of biogas quality or recalcitrant fraction in substrate for estimating three kinetic parameters. The model was used to simulate AD of SCB and SW using the published BMP data. The simulated specific methane yield and digester performance were found to be consistent with the limited largescale data. The application of model for design, simulation and performance enhancement of single/multi-stage AD was illustrated. The developed model offers an attractive platform for design and optimisation of large scale AD.

CRediT authorship contribution statement

Sanjay Nagarajan: Investigation, Data curation, Validation. **Varaha**

Prasad Sarvothaman: Data curation, Validation. **Martin Knörich:** Investigation, Data curation. **Vivek V. Ranade:** Conceptualization, Funding acquisition, Supervision.

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.2021.125395.

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