



# A novel simulation model, BK\_BiogaSim for design of onsite anaerobic digesters using two-stage biochemical kinetics: Codigestion of blackwater and organic waste



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## ABSTRACT

The design of biogas reactors for blackwater treatment provides special challenges due to significant variability in blackwater characteristics, the complexity of biological systems, and the need, in many cases, to operate in an extremely hygienic environment. In this study, mathematical models were formulated based on microbial growth kinetics to analyze the anaerobic codigestion of blackwater with kitchen waste as well as compare different substrate mixing ratios. The modelling approach used has the advantage of simulating the process with very little input data and eliminates the need to quantify the viable bacteria biomass, which is usually very difficult to estimate during anaerobic digestion. The validity of models is assessed by using a new statistical coefficient ( $\alpha$ ), which cumulates the effect of four known parameters: coefficient of determination ( $R^2$ ), adjusted coefficient of determination ( $R^2_{Adj}$ ), reduced chi-square ( $\chi^2$ ) and root mean square error (RMSE). A numerical calculation interface was designed to quickly and cheaply simulate different digestion scenarios, display results to user and evaluate the effect of input variation on the system's dynamics. Three simulation cases studies were considered each with different mixing ratios of black water to kitchen waste: Case 1 (50:50), Case 2 (25:75) and Case 3 (pure kitchen waste). The, Moser and Andrew based models were most appropriate in describing biogas kinetics for case study 1 ( $\alpha$ -values of 0.2238 and 0.2596 respectively), the Monod and Moser based models most appropriate for case 2 ( $\alpha$ -values of 0.0987 and 0.1266 respectively), while the Bergter and Haldane based models were most appropriate for case 3 ( $\alpha$ -value of 0.0348 and 0.0347 respectively). The results of this study can be used to facilitate design and optimization of biogas sanitation units treating blackwater and kitchen waste.

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## Nomenclature

$A$	Maximum rate of substrate degradation by acidogenic bacteria considering non-biodegradable fraction ( $day^{-1}$ )
$a^0_{max}$	Specific affinity of acetoclastic methanogens to acidified substrate ( $L/g/day$ )
$I$	Concentration of inhibitor ( $g/L$ )
$K$	Kinetic constant of Chen and Hashimoto (–)
$K_{ha}$	Maximum rate of substrate degradation by the acidogenic bacteria ( $day^{-1}$ )
$K_i$	Substrate concentration where bacteria growth is reduced to 50% of the maximum specific growth rate due to substrate inhibition ( $g/L$ )
$K_{i,1}$	Inhibition constant for first inhibitor ( $g/L$ )
$K_{i,2}$	Inhibition constant for second inhibitor ( $g/L$ )
$K_p$	Powell's constant to describe the kinetics of growth due to enzyme activity ( $g/L$ )
$K_s$	Monod half saturation constant for the acidified substrate ( $m/L$ )
$K_u$	Maximum rate of substrate uptake by acetoclastic methanogens ( $day^{-1}$ )
$k_{1(s)}$	Rate of substrate degradation by acidogenic bacteria ( $g/g/day$ )
$L$	Parameter that describes diffusion and permeability of substrate through the cell wall ( $g/L$ )
$m$	Empirical parameter to describe on the kind of inhibition (–)
$n$	Could provide a useful measure of microbial cooperativity (–)
$n_i$	Empirical parameter to describe on the kind of inhibition (–)
$P$	Theoretical cumulative biogas yield ( $mL_{biogas}/gVS$ )
$P_{sim}$	Model-predicted biogas outputs $mL_{biogas}/gVS$
$P_{max}$	Maximum attainable biogas yield ( $mL_{biogas}/gVS$ )
$P_{exp}$	Experimental measurements of biogas produced ( $mL_{biogas}/gVS$ )
$S_a$	Concentration of acidified substrate produced by acidogenic bacteria ( $g/L$ )
$S_{nb}$	Concentration of non-biodegradable substrate ( $g/L$ )
$S_o$	Initial substrate concentration ( $gVS/L$ )
$S_u$	Concentration of substrate taken up by acetogenic/methanogenic microorganisms ( $g/L$ )
$S^*$	critical inhibitor concentration where growth stops ( $g/L$ )
$t$	Retention time ( $day$ )
$T$	Lag time included to consider deceleration during the lag phase ( $day$ )
$X$	Acidogenic bacteria concentration ( $g/L$ )
$X_{am}$	Concentration of acetogenic/methanogenic biomass ( $g/L$ )
$Y_{max}$	Maximum specific rate of biogas production by acetoclastic methanogens ( $mL_{biogas}/gVS/day$ )
$Y_{PS}$	Biogas yield coefficient ( $mL_{biogas}/gVS$ )/( $gVS_{utilized}/L$ )
$\alpha_S$	Fraction of acidified substrate taken up by the acetogenic/methanogenic biomass (–)
$\beta$	Reaction rate which represents an allosteric effect (–)
$\mu$	Specific growth rate of acetogenic/methanogenic microorganisms ( $day^{-1}$ )
$\mu_{max}$	Maximum specific growth rate of acetogenic/methanogenic microorganisms ( $day^{-1}$ )
$\mu_S$	Fraction of initial volatile substrate that is non-biodegradable (–)

## Introduction

It is now estimated that between 2.1 and 2.6 billion people in low- and middle-income countries rely on onsite sewage sanitation technologies (pit latrines, septic tanks, and other 'unimproved' sanitation facilities) for Faecal sludge (FS) and blackwater management [22]. Studies show that Pit latrines alone, which are concentrated in rural areas of developing and middle income countries, emit  $\sim 14 T_g CH_4 y^{-1}$ ,  $>4\%$  of global anthropogenic emissions [39] while the mass emission rates of greenhouse gases ( $CH_4$   $CO_2$   $N_2O$ ) from septic tanks is 11, 33.3 and 0.005  $g\ capita^{-1} day^{-1}$  [12]. These issues call for focus towards onsite energy and nutrient recovery from blackwater and faecal sludge, changing sanitation paradigms from waste-to-discharge to waste-to-resource [24,35,38]. Anaerobic digestion units, as part of an on-site blackwater treatment system are a competitive alternative to centralized treatment systems due to their operational simplicity and potential for nutrient and biogas recovery (Colón et al., 2015). However, the design of biogas reactors for blackwater treatment provides special challenges due to significant variability in blackwater characteristics, the complexity of biological systems, and the health risk associated with the use of sewage water [43,45]. One way of overcoming these challenges is via simplified mathematical models, which are required to predict gas emission kinetics, compare and select appropriate substrate mixtures as well as optimize design and operation of the system [17]. Although mathematical models to describe the anaerobic biodegradation kinetics of wastewater is well established in the literature, they are very complex and the information contained in parameter values and model structure does not translate well to simple design rules. The anaerobic digestion model no. 1 [7] and the model developed by Angelidaki et al. [4] are examples of generalized models used for studying

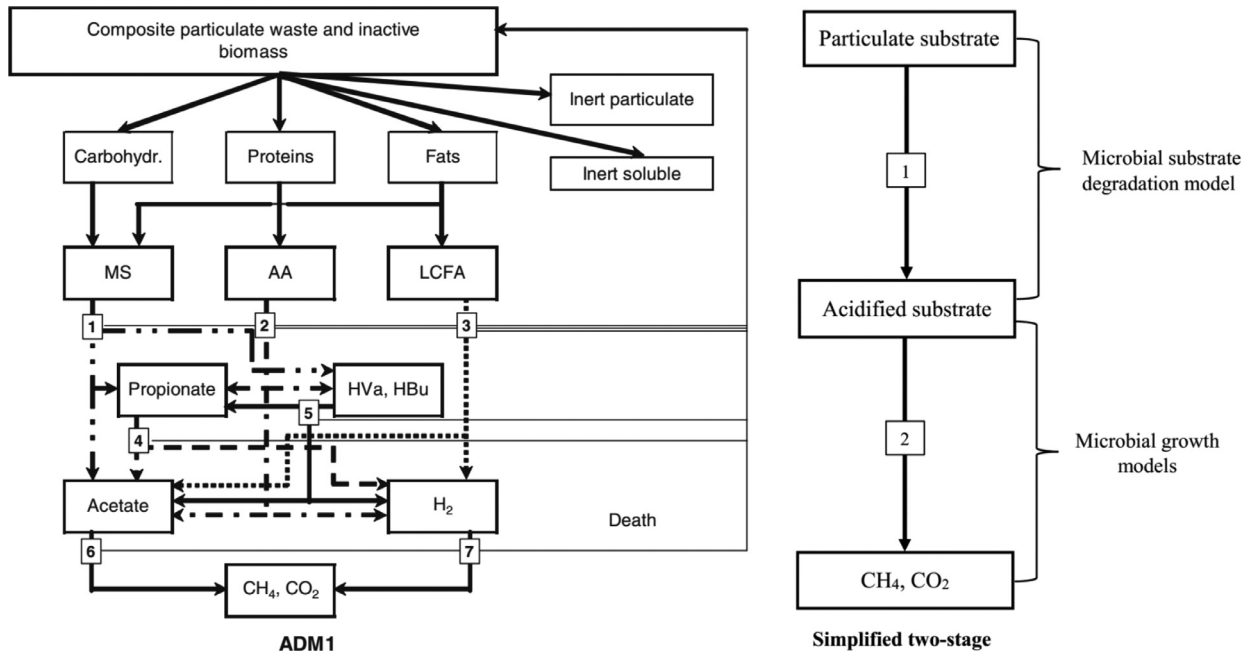


Fig. 1. Complex and simplified biochemical model structures. ADM1 contains 19 processes, and 26 state variables. Simplified 2 stage contains three processes (hydrolysis, uptake, gas production) and 3 state variables (particulate substrate, acidified substrate, and biogas) (modified from [6]).

anaerobic digestion of complex and co-digested biomass respectively. However, with the field of anaerobic digestion shifting from operation/technology development to application development, rigorous models involving detailed, mechanistic studies of metabolic pathways and ponderous substrate characterization become problematic, which hinders their practicality for simulation, and design [16]. For designing of on-site anaerobic systems for blackwater sanitation, simplified models are considered most appropriate [6] but published studies on simplified models for anaerobic treatment of domestic sewage are limited in number, but well directed at specific substrates. A variety of simplified models have been applied in the literature, which include the first order biogas yield model in sizing continuous stirred tank and batch reactors [25,31] and substrate specific simplified kinetic models for organic fraction of municipal solid waste [15]. Also presented is the modified Gompertz model for determining the maximum biogas production potential of substrates [44,46] and Dual pooled first order kinetic model for food waste and pig manure anaerobic co-digestion [11]. Other authors presented kinetic models for psychrophilic anaerobic sequencing batch reactor treating flushed dairy manure [27], simplified anaerobic digestion models for studying anaerobic biodegradability and kinetics of complex biomass [30], maximum biogas production potential and stability assessment (MBPPSA) model for the co-digestion of food waste and maize husk [36]. In addition, optimum performance of the anaerobic treatment process is seldom achieved because of the high degree of empiricism that still prevails in the design and operation of anaerobic digesters. This results in increased demand for efficient digester operation through model-based design and software based on kinetic models of the anaerobic digestion process has therefore gained extensive attention. There becomes a need to simultaneously study the different kinetic models and develop a simulation software for easy implementation of the models. In this study, mathematical models have been formulated and validated considering various known bacteria growth kinetic models, and a numerical calculation software is developed to easily simulate the models at different treatments scenarios with a case study of blackwater co-digested with kitchen waste.

### Mathematical modeling of anaerobic blackwater treatment

The motivations for modeling anaerobic treatment of domestic wastewater has been grouped into three key categories [6]. These include (a) acquisition of parameters and laws for system design; (b) operational analyses in terms of reactor stability and prediction by-products (COD, nutrients and gases); (c) develop new technologies to improve anaerobic treatment efficiency. In this study, the focus is on design, which is particularly important, as it determines capital cost, a key motivation for investment in the technology. Reactor hydraulics and particulate matter (biomass and substrate) are the important aspects of consideration in the development of models for the design of anaerobic wastewater treatment [6]. It becomes important to develop relatively simple but realistic kinetic model structures, which can easily be extended to include more complex hydraulic and particulate aspects. Fig. 1 compares the biochemical structure of the standard ADM1 with the simplified two-step based modelling approach of this study.

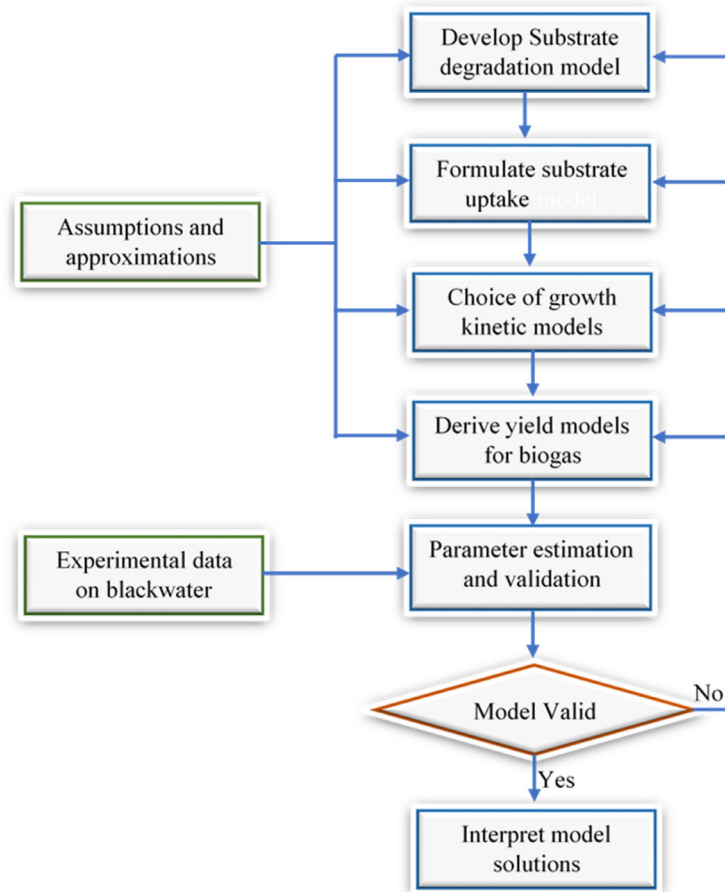


Fig. 2. Steps to develop kinetic models for prediction of biogas yield.

#### Mathematical model development process

Fig. 2 presents the algorithm used to develop and validate the simplified two-stage based modes to predict biogas yield. Four main aspects were considered in the model development procedure, which include; substrate degradation, substrate uptake, cell growth and biogas prediction. This led to a series of ordinary differential equations to assist in better understanding of biogas production from blackwater.

#### Formulation of substrate degradation

Many constituents of domestic sewage water and organic wastes behave as complex substrates (polysaccharides, proteins, fats etc.). The multicomponent substrate degradation model assumes that the different components are simultaneously removed and transported into the cells [18]. The Grau model presented in Eq. (1), which has widely been used to model multiple substrate removal kinetics [23,26,30] was therefore adopted for this study.

$$-\frac{dS}{dt} = k_{n(s)}X\left(\frac{S}{S_0}\right)^n \quad (1)$$

For optimal digester operation, blackwater is usually co-digested with other substrates and it becomes important to consider the non-biodegradable part of the complex substrate mixture. The model is then modified as shown in Eq. (2)

$$-\frac{dS}{dt} = k_{n(s)}X\left(\frac{S}{S_0}\right)^n \left(1 - \frac{S_{nb}}{S_0}\right) \quad (2)$$

where,  $S_{nb}$  represents the concentration of the non-biodegradable fraction of the complex substrate mixture. If we assume a first order substrate degradation kinetics ( $n = 1$ ) and integrate Eq. (2) we obtain Eq. (3). Similar assumption about first order degradation kinetics has been put forward in the literature [25,31,36]

$$\frac{S}{S_0} = \exp\left[-\frac{k_{1(s)}X}{S_0} \left(1 - \frac{S_{nb}}{S_0}\right)t\right] \quad (3)$$

Assuming hydrolysis and acidogenesis are catalyzed by acidogenic bacteria, whose concentration is constant, then Eq. (3) can be re-written as Eq. (4). Vavilin et al. [41], Vavilin and Angelidaki [40] and Momoh et al., [30] put forward similar assumptions where substrate hydrolysis/acidogenesis and acetogenesis/methanogenesis were included in a model as the two possible rate-limiting steps of the overall anaerobic digestion process.

$$\frac{S}{S_0} = \exp[-K_{ha} (1 - \mu_S)t] \tag{4}$$

Eq. (4) represents the substrate degradation kinetics, where  $S$  is the concentration of initial substrate left at every instant following onset of hydrolysis and  $\mu_S$  is the fraction of initial volatile substrate that is non-biodegradable (that is,  $S_{nb} = \mu_S S_0$ ). However, we are interested in the concentration of acidified substrate produced after substrate degradation by acidogenic bacteria. Thus assuming the difference between the initial substrate concentration and the remaining substrate gives the acidified substrate produced, and then the expression for acidified substrate can be expressed as follows

$$S_a = S_0[1 - \exp(-At)] \tag{5}$$

$A = K_{ha} (1 - \mu)$  represents the maximum rate of substrate degradation by acidogenic bacteria when we consider the non-biodegradable fraction of the initial particulate substrate

*Modeling of substrate uptake*

The uptake or transfer of acidified substrate into acetogenic/methanogenic microorganisms was modeled considering two theories; the collision frequency theory for nutrient uptake by microorganisms and the interfacial mass transfer theory. This considers that the rate of substrate uptake is directly proportional to the concentration gradient across the extracellular and intracellular environments, and to the concentration of the active cell biomass  $X_{am}$ . Based on this, the substrate uptake rate can be represented mathematically by Eq. (6).

$$\frac{dS_u}{dt} = a^0_{max} X_{am} (S_a - S_u) \tag{6}$$

Here,  $a^0_{max}$  represents the specific affinity of the active cell biomass to acidified substrate [9]. Assuming maximum growth rate of acetogenic/methanogenic microorganisms is attained where by biomass concentration,  $X_{am}$  becomes constant, and expressing  $S_u$  in terms of  $S_a$ , Eq. (6) can be written as follows

$$\frac{dS_u}{dt} = K_u (S_a - S_u) \tag{7}$$

The parameter  $K_u$  represents the maximum rate of substrate uptake by the acetogenic/methanogenic microorganisms ( $\text{day}^{-1}$ ). If we substitute Eq. (5) into Eq. (7) and integrate using the Matlab Symbolic Calculation Toolbox, we obtain Eq. (8), which is the expression of the substrate uptake model.

$$S_u = \frac{S_0}{A - K_u} [A(1 - e^{-K_u t}) - K_u(1 - e^{-At})] \tag{8}$$

This represents the kinetics of acidified substrate taken up by the acetoclastic methanogens at every instant following onset of anaerobic digestion.

*Choice of bacteria growth models*

Though, the Monod model has been established to be more appropriate in describing the growth processes for pure culture utilizing homogenous substrates [5,26] significant amount of studies on the kinetics anaerobic digestion, which involves mixed culture and substrates are still being modelled using this Monod kinetics [1,32]. This has necessitated the consideration of a wide range of bacteria growth models as presented in Table 1.

**Table 1**  
Bacterial growth models selected to model substrate assimilation.

Author	Model equation	Eq. No.	Remark
[33]	$\mu = \frac{\mu_{max} S_u}{K_s + S_u}$	(9)	Accurate for homogenous cultures and simple substrates
[34]	$\mu = \frac{\mu_{max} S_u^n}{K_s + S_u^n}$	(10)	Integrates microbial adoption to stationary processes by mutation
[37]	$\mu = \frac{\mu_{max} (K + L + S_u)}{2L} \varphi$	(11)	Describes reaction kinetics, diffusion and substrate permeation via cell wall
[10]	$\mu = \frac{\mu_{max} S_u}{K S_u + (1 - K) S_u}$	(12)	Considers cell concentration depending on the level of substrate degradation
[8]	$\mu = \frac{\mu_{max} S_u}{K_s + S_u} [1 - \exp(-\frac{t}{T})]$	(13)	Modified Monod model to considers deceleration during the lag phase

$$\varphi = \left[ 1 - \sqrt{1 - \frac{4LS_u}{(K + L + S_u)^2}} \right] \tag{14}$$

Bacterial growth can be inhibited by certain substrate concentrations especially for mixed bacteria cultures. Increase in the substrate concentration above a certain threshold results in a high osmotic pressure of the medium or a specific

**Table 2**  
Models for bacterial growth including the effect of substrate inhibition.

Author	Model equation	Eq. No.	Remark
[19]	$\mu = \frac{\mu_{max}S_u}{(K_s+S_u)(1+S_u/K_i)}$	(15)	Derived from enzyme kinetics
[42]	$\mu = \frac{\mu_{max}S_u(1+\beta S_u/K_i)}{K_s+S_u+S_u^2/K_i}$	(16)	Integrates an allosteric effect with $\beta$ as reaction rate
[3]	$\mu = \frac{\mu_{max}S_u}{K_s+S_u+S_u^2/K_i}$	(17)	Based on Haldane for enzyme inhibition at high substrate concentrations
[2]	$\mu = \frac{\mu_{max}S_u}{K_s+S_u} \exp(-S_u/K_i)$	(18)	An empirical correlation to describe substrate inhibition
[21]	$\mu = \frac{\mu_{max}(K+L+S_u)}{K_s+S_u+S_u^2/K_{i,1}+S_u^2/K_{i,2}}$	(19)	Modified Andrew model involving a second inhibitor
[20]	$\mu = \frac{\mu_{max}S_u}{K_s(1-\frac{S_u}{S^*})^n+S_u} (1-\frac{S_u}{S^*})^{n_i}$	(20)	Includes a critical inhibitor concentration of growth stop

substrate toxicity [17]. This has necessitated the consideration of a bacteria growth models with substrate inhibition as presented in Table 2.

#### Formulation of biogas yield models

Yields can vary considerably during a fermentation process and for this reason, average yields, referred to as yield coefficients are often used when describing production efficiencies. If bacteria biomass formation and biogas formation are assumed to be directly linked to substrate utilization by yield coefficients, then the following can be written

$$\frac{dX}{dt} = -Y_{XS} \frac{dS_u}{dt} \quad (21)$$

$$\frac{dP}{dt} = -Y_{PS} \frac{dS_u}{dt} \quad (22)$$

Eq. (21) shows the relation between rate of substrate utilization and growth of acetogenic/methanogenic microorganisms while Eq. (22) represents the relation between biogas formation and substrate utilization. Additionally, the death rate of the acetogenic/methanogenic microorganisms was assumed to be negligible and the rate of change acetogenic/methanogenic microorganisms can thus be represented as shown in Eq. (23)

$$\frac{dX}{dt} = \mu X \quad (23)$$

$\mu$  is the specific growth rate of acetogenic/methanogenic microorganisms, which is modelled by the equations, presented in Tables 1 and 2. Using the Monod growth model, Eq. [9] the substrate utilization model for the acetogenic/methanogenic microorganisms can be written as follows

$$-\frac{dS_u}{dt} = \frac{1}{Y_{XS}} \frac{\mu_{max}S_u}{K_s+S_u} X \quad (24)$$

Substituting Eq. (24) into Eq. (22) the biogas yield rate can be represented as shown in Eq. (25).

$$\frac{dP}{dt} = \frac{Y_{PS}}{Y_{XS}} \frac{\mu_{max}S_u}{K_s+S_u} X \quad (25)$$

Since the study considers the growth rate of the acetogenic/methanogenic microorganisms to be very slow, the active cell concentration stays almost constant. Based on this,  $\mu_{max}X/Y_{XS}$  can be considered maximum rate of substrate assimilation, which when multiplied by  $Y_{PS}$ , gives the maximum rate of biogas production by acetoclastic methanogens  $Y_{max}$  (Eq. (26)). A similar consideration was put forward by Momoh et al., [30].

$$\frac{dP}{dt} = \frac{Y_{max}S_u}{K_s+S_u} \quad (26)$$

If we assume that as substrate is consumed, the rate of biogas production is directly correlated with the quantity of biogas produced ( $P$ ), such that the driving force for gas production is disappearing when the gas production gradually approaches its maximum then Eq. (26) can be modified as follows

$$\frac{dP}{dt} = \frac{Y_{max}S_u}{K_s+S_u} \left(1 - \frac{P}{P_{max}}\right) \quad (27)$$

Eq. (27) represents a two-stage based model to predict biogas yield during anaerobic codigestion, where the growth of acetoclastic methanogens is assumed to follow the Monod kinetics.  $S_u$ , the concentration of substrate taken up by methane producing bacteria is given by Eq. (8). Similar process was applied to develop the other biogas yield rate models by assuming that the growth process of the acetogenic/methanogenic microorganisms can be described using the bacteria growth models represented by Eqs. (10)–(20). Tables 3 and 4 presents the series of models developed for the different cell growth scenarios.

**Table 3**  
Two-stage based dynamic models to predict biogas yield.

Growth model	Derived biogas yield model	Eq. No
Monod	$\frac{dP}{dt} = \frac{Y_{max}S_u}{K_s + S_u} (1 - \frac{P}{P_{max}})$	(27)
Moser	$\frac{dP}{dt} = \frac{Y_{max}S_u^n}{K_s + S_u^n} (1 - \frac{P}{P_{max}})$	(28)
Powell	$\frac{dP}{dt} = \frac{Y_{max}(K_{p0} + L + S_u)}{2L} \varphi (1 - \frac{P}{P_{max}})$	(29)
Chen & Hashimoto	$\frac{dP}{dt} = \frac{Y_{max}S_u}{K_{S0} + (1-K)S_u} (1 - \frac{P}{P_{max}})$	(30)
Bergter	$\frac{dP}{dt} = \frac{Y_{max}S_u}{K_s + S_u} [1 - \exp(-t/T)] (1 - \frac{P}{P_{max}})$	(31)

**Table 4**  
Two-stage based models to predict biogas yield with substrate inhibited growth kinetics.

Growth model	Derived biogas yield model	Equation no
Haldane	$\frac{dP}{dt} = \frac{Y_{max}S_u}{(K_s + S_u)(1 + S_u/K_i)} (1 - \frac{P}{P_{max}})$	(32)
Webb	$\frac{dP}{dt} = \frac{Y_{max}S_u(1 + \beta S_u/K_i)}{K_s + S_u + S_u^2/K_i} (1 - \frac{P}{P_{max}})$	(33)
Andrews	$\frac{dP}{dt} = \frac{Y_{max}S_u}{K_s + S_u + S_u^2/K_i} (1 - \frac{P}{P_{max}})$	(34)
Aiba et al.	$\frac{dP}{dt} = \frac{Y_{max}S_u}{K_s + S_u} \exp(-S_u/K_i) (1 - \frac{P}{P_{max}})$	(35)
Hill & Barth,	$\frac{dP}{dt} = \frac{Y_{max}(K + L + S_u)}{K_s + S_u + S_u^2/K_{i,1} + S_u^3/K_{i,2}} (1 - \frac{P}{P_{max}})$	(36)
Han & Levenspiel	$\frac{dP}{dt} = \frac{Y_{max}S_u}{K_s(1 - \frac{S_u}{S^*}) + S_u} (1 - \frac{S_u}{S^*})^n (1 - \frac{P}{P_{max}})$	(37)

*Experimental data for model validation*

The data used for parameter estimation and validation of the series of models was obtained from the literature [29]. Kitchen organic solid waste was co-digested with blackwater under ambient temperature  $25 \pm 2$  °C using cow manure as inoculum and a retention time of 30 days. The data used was for digestion at different mixing ratios by volume of sanitary wastewater (TS = 7068 mg/L) to kitchen organic solid waste (TS = 56, 084 mg/L), 50:50 (reactor C), 25:75 (reactor B), and 0:100 (reactor A). The biogas production was measured every 5 days for the different set of experiments. A detailed description of the experimental methods and characteristics of blackwater and kitchen waste mixtures is published in Minalé and Worku [29].

*Parameter estimation and model validation*

The identification of model parameters for each of the series of equations was made with Matlab (Mathworks, Natick, MA), and the Runge Kutta 4th to 5th order method, implemented by the *ode45* solver was used to simulate the differential equations. The model parameters were then estimated by minimizing the least-squares estimator, Eq. (38) between the model simulation and experimental data points, which implicitly assumed that the standard deviation of the measurement errors, is constant [13]. For this purpose, a constrained nonlinear optimization method was applied.

$$\varepsilon = \min \sum_{i=1}^N (P_{sim}(t, \theta) - P_{exp}(t))^2 \tag{38}$$

Here  $\theta$  is the vector of model parameters to be determined, as output of minimization procedure and  $N$  is the number of measurements. In order to avoid the algorithm reaching a local minimum, a multi-start strategy was employed where several different initial sets of the parameter guesses were used [14]. Once the model parameters were estimated, the goodness of fit and capability of the mathematical model to describe the anaerobic digestion process was evaluated using the coefficient of determination ( $R^2$ ), adjusted coefficient of determination ( $R^2Adj$ ), root mean square error (RMSE) and the reduced chi-square ( $\chi^2$ ). The RMSE was normalized to facilitate comparison between the different models and datasets.

The algorithm for parameter estimation can be described as follows;

**Inputs:**  $lb, ub, y_{ref}(x_{ref}), x_{ref} \in \{X_{ref0}, X_{ref1}, \dots, X_{refN}\}$

**Step 0:** Compute simulated response as a sequence of time-amplitude pairs

$$y_{sim}(x_{sim}), x_{sim} \in \{X_{sim0}, X_{sim1}, \dots, X_{simN}\}$$

**Step 1:** Formulate a new x-base,  $x_{new}$  from the union of the elements of  $x_{ref}$  and  $x_{sim}$

$$x_{new} = \{x : x_{sim} \cup x_{ref}\} \tag{39}$$

**Step 2:** Compute  $y_{sim}$  and  $y_{ref}$  at interval points in  $x_{new}$  using linear interpolation and then compute the scaled error:

$$e(x_{new}) = y_{sim}(x_{sim}) - y_{ref}(x_{ref}) \tag{40}$$

**Step 3:** Compute weighted integral square error

$$f = \int w(x)e(x)^2 \tag{41}$$

**Step 4:** Minimize weighted integral square error using optimization algorithm. The gradient descent method was used with the gradients computed using numerical perturbation as illustrated by Eqs. (42)–(47).

$$dT = \max\left(|T|, \frac{1}{10}T_{typ}\right) \sqrt[3]{e_{ps}} \tag{42}$$

$$dL = \max(T - dT, T_{min}) \tag{43}$$

$$dR = \min(T + dT, T_{max}) \tag{44}$$

$$F_L = f(dL) \tag{45}$$

$$F_R = f(dR) \tag{46}$$

$$\frac{dF}{dT} = \frac{F_L - F_R}{dL - dR} \tag{47}$$

*Development of graphical user interface*

In order to facilitate running of the models and estimation of the model parameters for each anaerobic process, an interactive numerical calculation interface was designed to quickly and cheaply simulate different digestion scenarios, display results to user. The design of the graphical user interface (GUI) and implementation of the developed models was done using the Matlab GUIDE (Graphical User Interface Development Environment). The procedure consisted of three main parts. Setting the objectives of the GUI (inputs and outputs), building the interface with objects such as push buttons, static texts, edit texts, pop-up menus, axes, etc., programming the callback functions in Matlab m-files and finally execution and testing. The Graphical User Interface and the associated Matlab programs has been compiled in a windows environment and packaged using the Matlab Compiler Runtime.

**Results and discussions**

*Model fitting and validation*

Table 5 presents the statistical validity of the different models to predict the experimental biogas yield for the three mixing ratios. The results led to the following interesting findings; for the eleven models tested, the validity and choice of model to predict the process was variable based on the ratio of blackwater to solid kitchen waste in the biogas digester. In the case of reactor A, all the models except the Powell based could accurately be utilized for prediction because each provided a high coefficient of determination ( $R^2$ ), between 0.996 and 0.997 with reduced chi-square ( $\chi^2$ ) values between 0.002 and 0.011. For reactor B, all the models except the Powell based had good values of  $R^2$ , between 0.989 and 0.991, and  $\chi^2$  between 0.021 and 0.081. For reactor C, all the models except the Powell showed good values of  $R^2$ , between 0.973

**Table 5**  
Statistical validity of the developed biogas models.

Model	Mixing ratio of blackwater of kitchen waste											
	A				B				C			
	$R^2$	Adj $R^2$	$\chi^2$	RMSE	$R^2$	Adj $R^2$	$\chi^2$	RMSE	$R^2$	Adj $R^2$	$\chi^2$	RMSE
Monod	0.997	0.996	0.003	0.0239	0.990	0.987	0.037	0.0389	0.976	0.970	0.166	0.0573
Moser	0.996	0.995	0.011	0.0258	0.991	0.988	0.067	0.0377	0.979	0.974	0.123	0.0529
Powell	0.969	0.960	0.056	0.0711	0.972	0.964	0.030	0.0649	0.939	0.921	0.552	0.0916
Chen-Hashimoto	0.996	0.996	0.003	0.0239	0.989	0.987	0.037	0.0389	0.976	0.970	0.164	0.0573
Bergter	0.997	0.996	0.002	0.0243	0.989	0.986	0.041	0.0388	0.973	0.965	0.246	0.0606
Haldane	0.997	0.996	0.005	0.0232	0.990	0.987	0.021	0.0913	0.978	0.971	0.158	0.0554
Webb	0.997	0.995	0.007	0.0234	0.991	0.987	0.065	0.0378	0.977	0.969	0.137	0.0518
Andrews	0.997	0.996	0.006	0.0235	0.990	0.987	0.057	0.0381	0.979	0.972	0.158	0.0535
Aiba	0.996	0.995	0.003	0.0242	0.990	0.987	0.037	0.0391	0.975	0.967	0.176	0.0585
Hill and Barth	0.996	0.994	0.011	0.0249	0.990	0.985	0.081	0.0381	0.981	0.970	0.150	0.0509
Hans-Levenspiel	0.996	0.994	0.007	0.0259	0.990	0.986	0.054	0.0384	0.976	0.966	0.228	0.0571



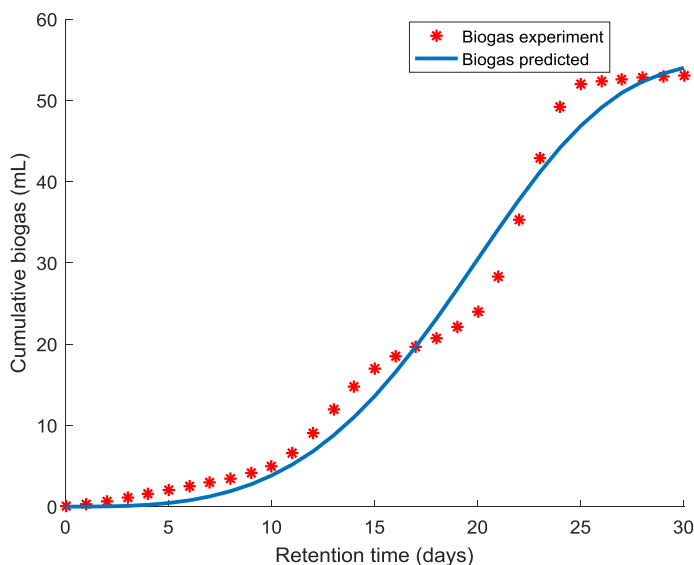


Fig. 3. Moser based model fitting using reactor C.

and 0.981, and  $\chi^2$  between 0.123 and 0.246. However, the process of selecting the most appropriate model resided in the observance of a new parameter,  $\alpha$  calculated by Eq. (48). Models with the lowest value of  $\alpha$  are considered more appropriate to describe a given data set if they share similar correlation coefficient.

$$\alpha = \chi^2 + RMSE + (1 - R^2Adj) + (1 - R^2) \quad (48)$$

The alpha parameter takes into consideration four individual statistical coefficients for its computation. These coefficients include: the reduced chi-square ( $\chi^2$ ), the root mean square error ( $RMSE$ ), the coefficient of determination ( $R^2$ ) and the adjusted coefficient of determination ( $R^2Adj$ ). Generally, for selecting models of better quality,  $\chi^2$  and  $RMSE$  should be minimized, while  $R^2$  and  $R^2Adj$  should be maximized, with a maximum possible value of 1. The role of the  $\chi^2$  and  $R^2Adj$  is to penalize models that give a good fitting due to overparameterization. The overall effect of the four statistical coefficients is cumulated in the  $\alpha$  parameter as shown in Eq. (48). The coefficients  $R^2$  and  $R^2Adj$  found in Eq. (48) have been subtracted from their maximum value of 1 and this is to simplify the problem of model discrimination into selecting models with smaller values of the  $\alpha$  parameter. Hence the  $\alpha$  parameter can be viewed as a more powerful statistical parameter formed by the combination for four commonly used statistical coefficients, whereby models with smaller values of  $\alpha$  are of better quality.

For the eleven models tested, the Bergter and Haldane's based biogas yield rate models provided the lowest  $\alpha$ -value of 0.0348 and 0.0347 respectively in the case of reactor A, while for reactor B, the Monod and Moser provided the lowest  $\alpha$ -values of 0.0987 and 0.1266 respectively. In the case of reactor C, the Moser and Andrew based models provided the lowest  $\alpha$ -values of 0.2238 and 0.2596 respectively. Thus, Moser and Andrew based models are most appropriate in describing biogas kinetics from a blackwater to kitchen waste mixing ratio of 50:50, the Monod and Moser's based in the case of 25:75, and the Bergter and Haldane based in the case of pure solid kitchen waste digestion. Although, very limited study exist in literature that has applied the series of bacteria growth models in studying the kinetics of co-digesting blackwater and kitchen waste, the statistical validities as well as the numerical simulation results show good fitting with experimental data. Figs. 2–8 show experimental and simulated evolution of the cumulative biogas production during anaerobic digestion. The predicted and experimental results show reasonably close agreement, which validates the presented models. Table 6 presents the parameter estimates for the Monod, Moser, Bergter, Haldane and Andrews based models to the experimental data for reactors A and B, since the models gave better fitting in these scenarios. The parameter estimates for the other digestion scenarios can however be obtained from simulations using the interface presented in Section 3.2. For the five models shown in Table 6, the Monod half saturation constants ( $K_s$ ) were estimated to be between 0.100 g/L and 0.300 g/L respectively. The estimated parameter values agree well within the range of 0.1–0.4 g/L reported by Pavlostathis and Giraldo-Gomez (2006) for acetoclastic methanogens. The values however show slight differences from those of 0.127–0.209 g/L reported by Momoh et al. [30]. This could be attributed to the complex nature of the substrate used by Momoh et al., and the Monod's constant describes the affinity between substrate–cell pair [26]. It is interesting to note that the Moser's growth rate models, which best describe the anaerobic codigestion of blackwater and kitchen includes a very important coefficient, "n" (which is always greater than unity). Liu [26] through his thermodynamic approach to modelling microbial growth kinetics proposed that the coefficient might well describe cooperativity among microbial species and fermentation substrate. By choosing the Moser's based model for reactors A and B the coefficient 'n' was estimated to be 1.146, and 1.207 respectively, hence need for optimal mixing ratio of substrates to provide maximum cooperativity among

**Table 6**  
Parameter estimate for developed biogas yield rate models.

Parameter	Model									
	Monod		Moser		Bergter		Haldane		Andrews	
	A	B	A	B	A	B	A	B	A	B
$K_{ha}$	0.116	0.338	0.221	0.100	0.172	0.361	0.201	0.010	0.0195	0.010
$K_{li}$	0.014	0.010	0.013	0.010	0.017	0.010	0.011	0.963	0.1194	1.178
$P_{max}$	51.486	71.779	51.576	71.6788	51.546	71.829	51.483	70.696	51.4882	70.673
$Y_{max}$	0.727	0.312	0.131	0.100	0.411	0.307	0.202	0.581	0.2277	0.691
$\mu_s$	0.606	0.407	0.466	0.363	0.698	0.433	0.404	0.690	0.4599	0.700
$K_s$	0.100	0.300	0.137	0.106	0.100	0.300	0.100	0.160	0.1002	0.101
$K_i$	-	-	-	-	-	-	9.990	1.185	9.9146	1.172
$n$	-	-	1.146	1.207	-	-	-	-	-	-
$T$	-	-	-	-	3.000	1.577	-	-	-	-

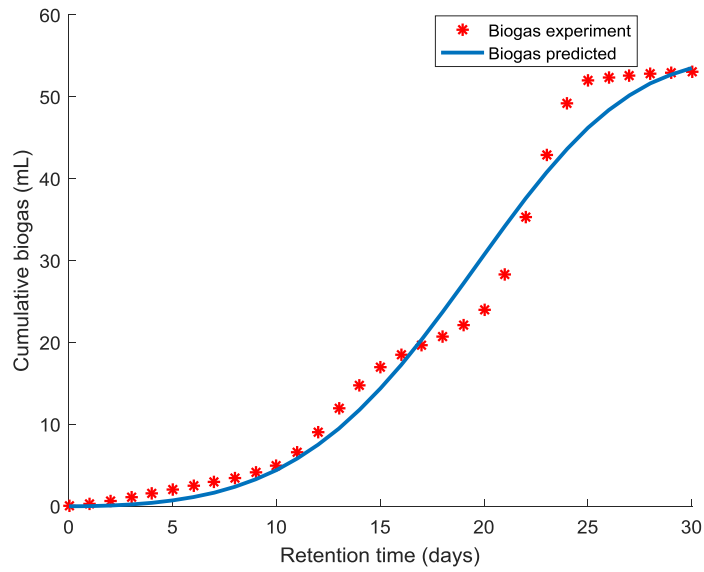


Fig. 4. Andrew based model fitting using reactor C.

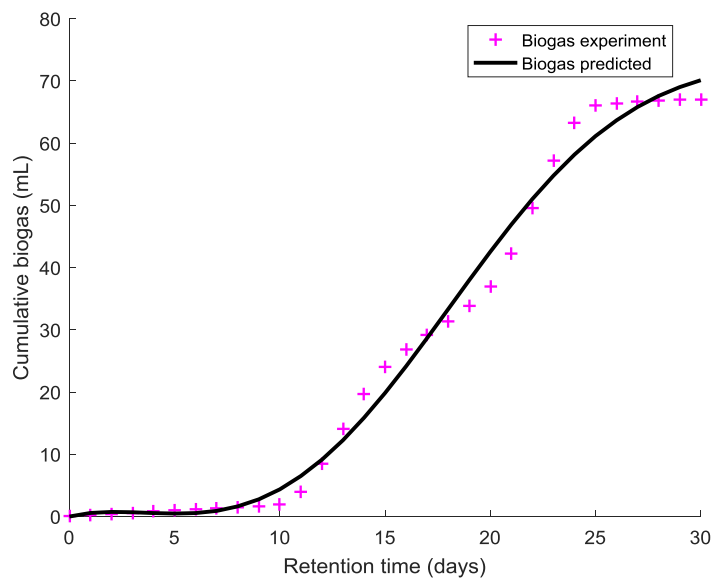


Fig. 5. Monod based model fitting using reactor B.

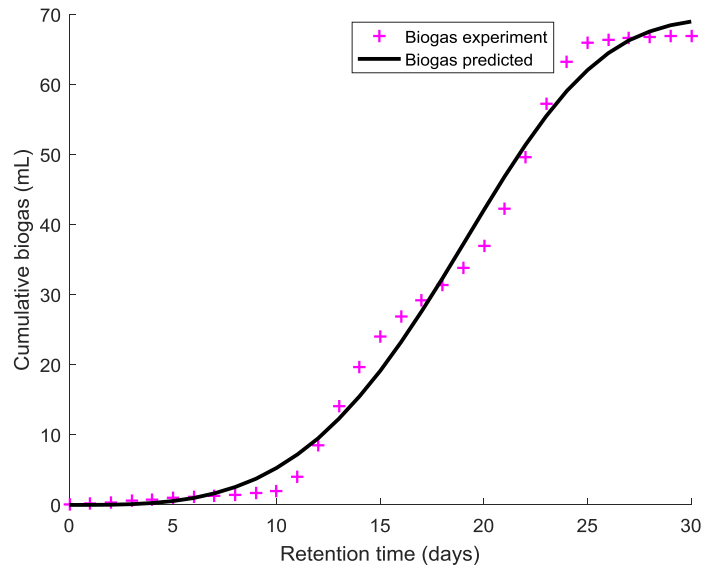


Fig. 6. Moser based model fitting using reactor B.

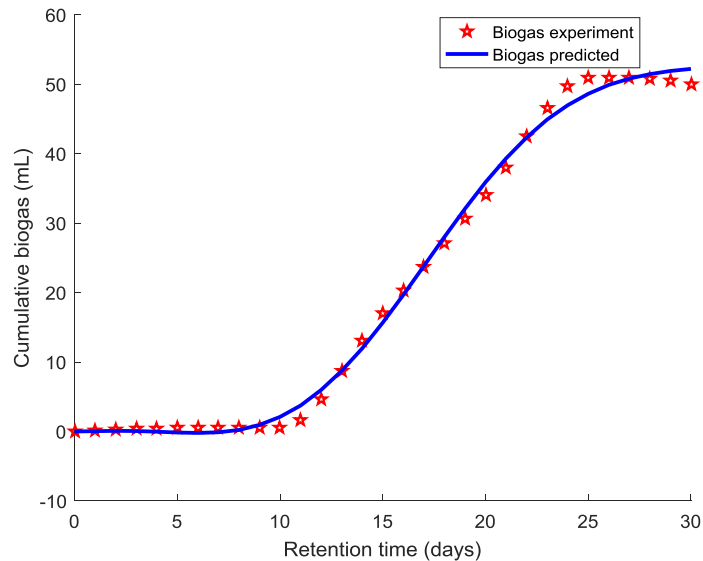


Fig. 7. Bergter based model fitting using reactor A.

microbial species substrate and hence higher biogas yield. This can explain why Minale and Worku [29] observed an increase in percentage methane yield with decrease in mixing ratio of blackwater to kitchen waste. It is important to note that the poor fitting properties observed with the Powell's based model could be because the model uniquely includes not only reaction kinetics, but also diffusion and permeation of substrate through the cell wall [37].

#### Process simulation based on estimated model parameters

Even though the modeling approach was simplified to only include kinetics of biogas production for parameter estimation, it is however possible to utilize the numeric values of the estimated parameters to simulate the kinetics of acidogenesis and uptake using Eqs. (5) and (8) respectively. Fig. 9 presents a simulated kinetics of acidogenesis and substrate uptake while Fig. 10 simulates the effects of varying the non-biodegradable fraction of initial substrate on the kinetics of acidogenesis. The results show that within the 30 days of anaerobic digestion, acidogenesis reaches a steady state faster than uptake which is in normal since acidogenesis precedes uptake as illustrate in the biochemical structure of anaerobic digestion on Fig. 1. It is also observed that increasing the fraction of non-biodegradable substrate slows down the kinetics of acidogenesis. This could be explained by a decrease in affinity of the acidogenic bacteria to substrate due to increase in the recalcitrant fraction

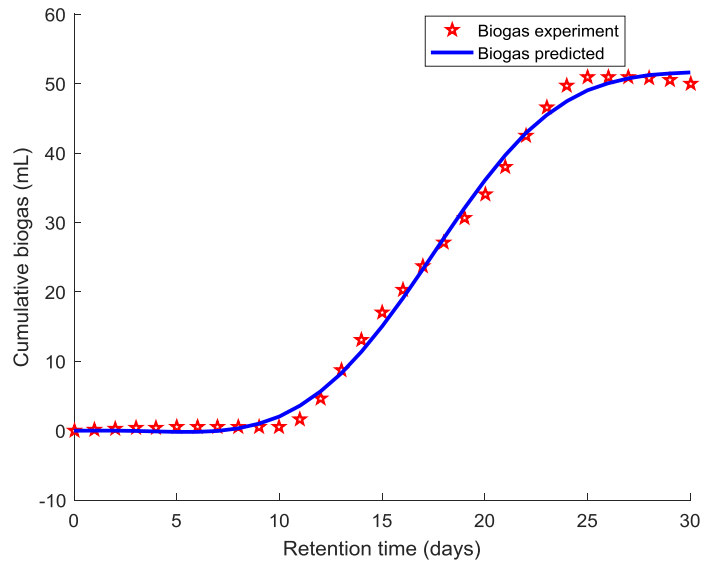


Fig. 8. Haldane based model fitting using reactor A.

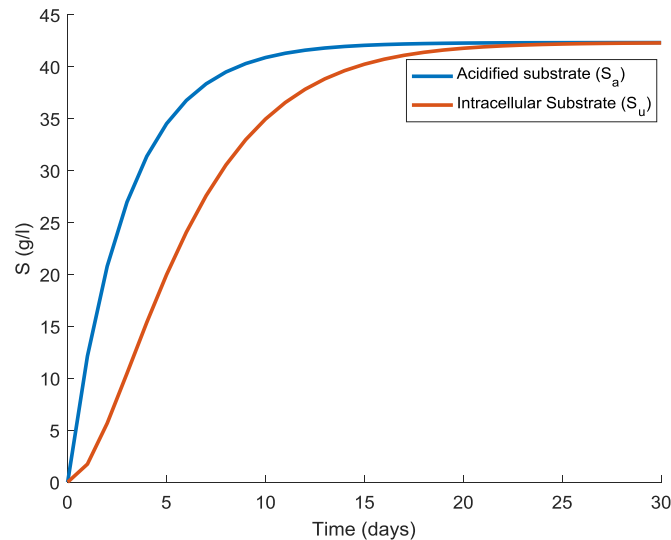


Fig. 9. Simulated kinetics of acidogenesis and uptake.

of the substrate, hence slowing down the rate at which they metabolize the particulate substrate [26,30]. In addition, the increase in the non-biodegradable fraction of a substrate mixture can render some of the biodegradable fraction unavailable for bacteria, thus reducing the rate of growth and degradation [5].

#### Numerical simulator for computational modeling

Fig. 11 presents the graphical user interface of the Blackwater and Kitchen Waste Biogas Simulation Tool (BK-BiogaSim). The interface includes sections with specific functionalities for data input, model selection, user control, simulation visualization as well as display of statistical fitting and model parameter estimates. This numerical simulator can be used to rapidly estimate anaerobic digestion parameters from the treatment of blackwater and kitchen waste, determine the most appropriate bacteria growth kinetics suited for a co-substrate as well as mixing ratio between blackwater and co-substrate.

In order to determine the capability of BK-BiogaSim in running the developed models, experimental data obtained from anaerobic digestion of kitchen waste as (consider using other data) well as the Bergter based model was utilized. The user inputs the retention time and corresponding cumulative biogas yields into the “Experimental biogas data” section of the software, selects a model, clicks on ‘Run’ from the User Controls section and the following simulation profile is obtained (Fig. 12). The values of the model parameter estimates and statistical constants are displayed on the user interface with an

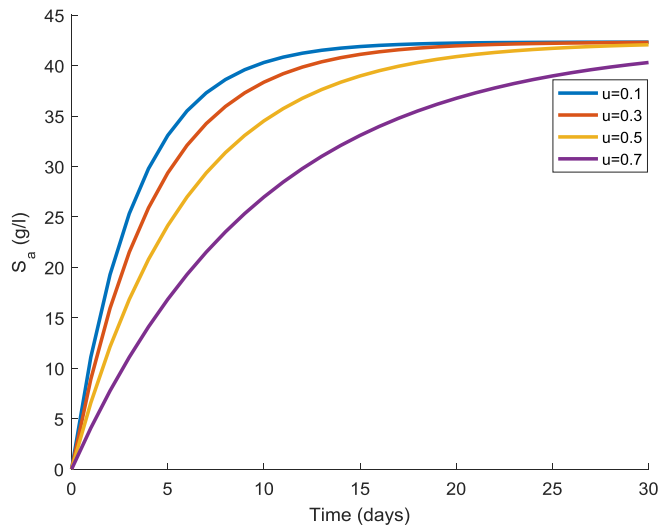


Fig. 10. Effects varying  $\mu_s$  on kinetics of acidogenesis.

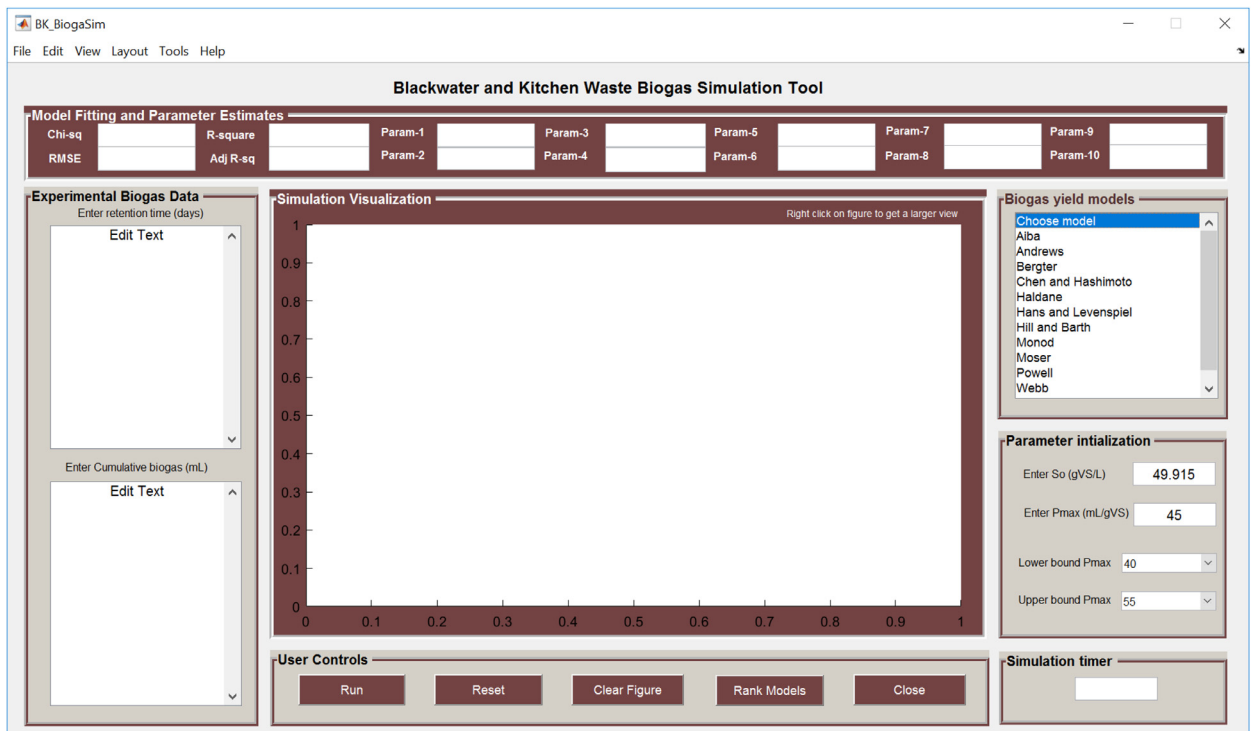


Fig. 11. Graphical user interface of the blackwater and kitchen waste biogas simulation tool.

extended description of the parameter values displayed on the command window (Fig. 13b). For simultaneous testing of all the models for a particular dataset, the user simply clicks on 'Rank Models' and the software automatically tests the fitting of all the 11 models, and arranges them in chronological all order from the best fitted to the least fitted. Fig. 14 presents a simulation scenario and the displayed model ranking. The visualization interface of BK-BiogaSim includes a context menu (Fig. 15), which provides essential functionality for extraction and documentation of simulation results in a more comprehensible and aesthetic mode, by simply right clicking on the figure window from the interface (Fig. 16). Other digestion scenarios can easily be run using the interface by simply changing the fermentation data, parameter initialization and or choice of model.

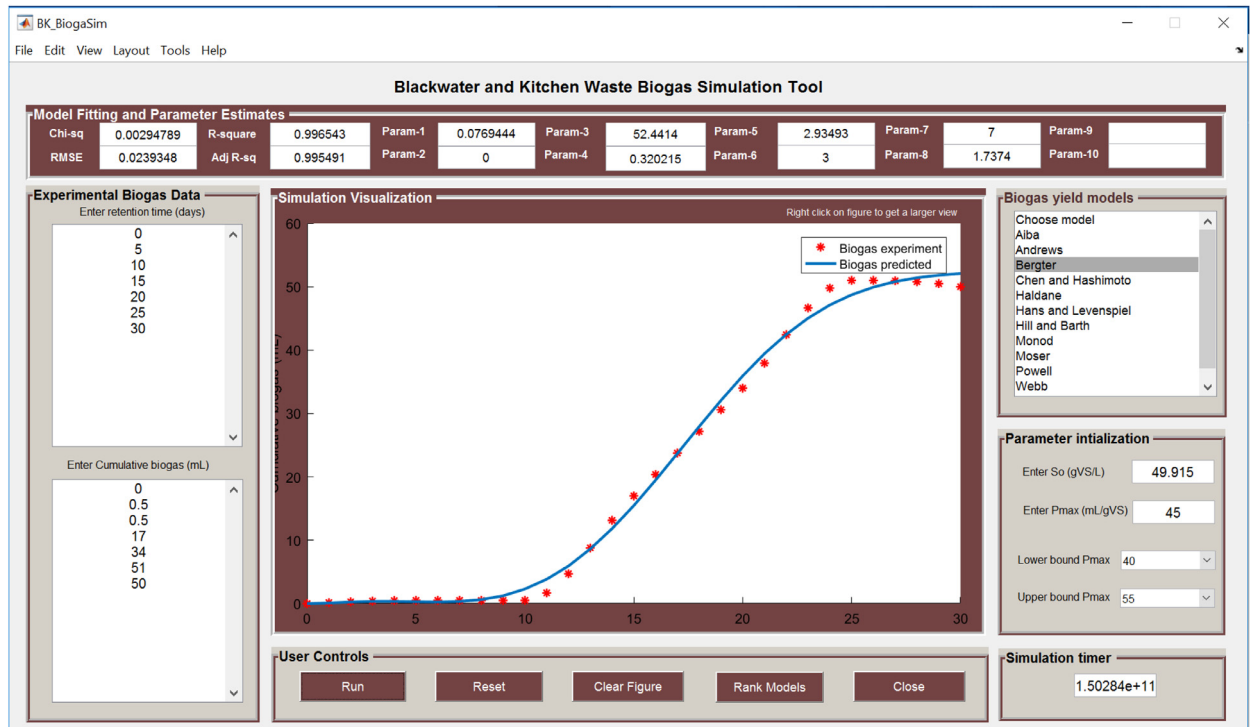


Fig. 12. Display interface of BK-BiogaSim for a simulation scenario.

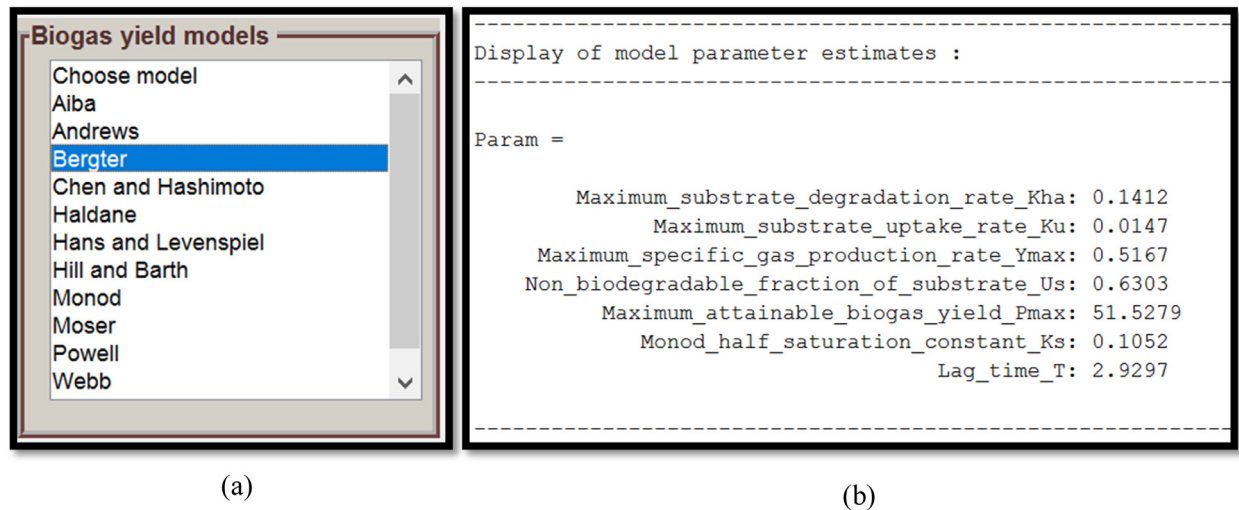


Fig. 13. A simulation case showing model selection (a) and display of parameter estimates (b).

### Practical application and relevance of the study results

#### Estimation of parameters not assessable experimentally

With the modeling approach developed in this study, it is possible to estimate process parameters such as: the maximum rate of substrate degradation, fraction of initial volatile substrate that is non-biodegradable, maximum rate of substrate, the maximum specific rate of biogas production as well as other microbial growth parameters (Table 6). These parameters are very important as they can be used to compare the anaerobic digestion efficiencies of different co-substrates and substrate mixing ratios. Although the complexity of the anaerobic treatment process is reflected in the ADM1 model, including more deterministic parameters, the identification of all these parameters in practice is virtually an impossible task. However,

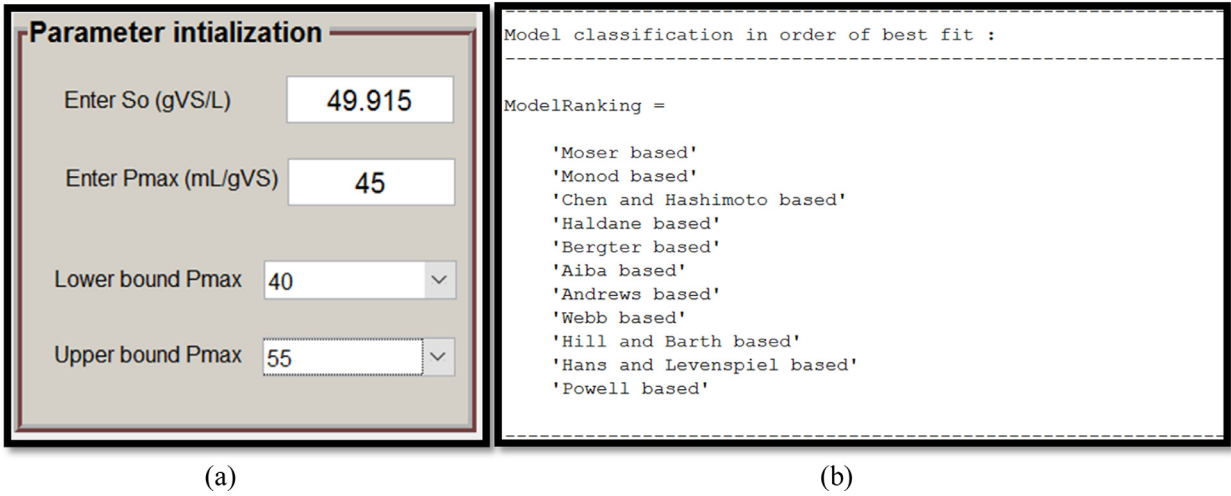


Fig. 14. A simulation case for parameter initialization (a) and display of ranked models (b).

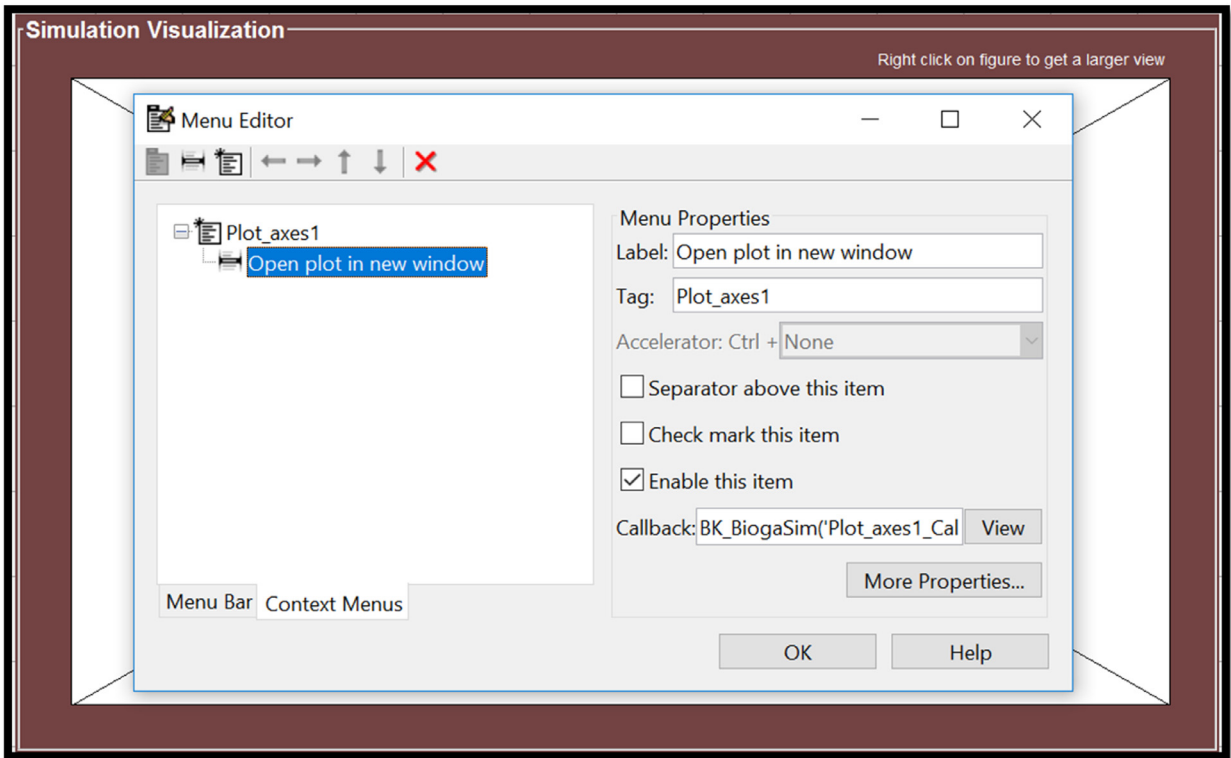


Fig. 15. GUIDE menu editor showing the context menu for extracting fitted results.

with the modeling approach developed in this study, certain parameters can be easily estimated from process data, thus, contributing to the design and optimization of anaerobic process.

*Rapid and easy simulation of different digestion scenarios*

BK-BiogaSim can be used to model and simulate anaerobic co-digestion of blackwater with eleven different kinetic models and displays results on a single click after introducing experimental data. BK-BiogaSim can also estimate process parameters based on experimental data, simulate the kinetics of acidogenesis and uptake, as well as test all the different models and rank them in order of best fit. During simulations, it is possible to determine the substrate concentration corresponding to maximum biogas yield for a particular co-substrate and mixing ratio, as well as display numerical data for possible utilization on other software programs. The interface can be used to perform sensitivity analyses by varying

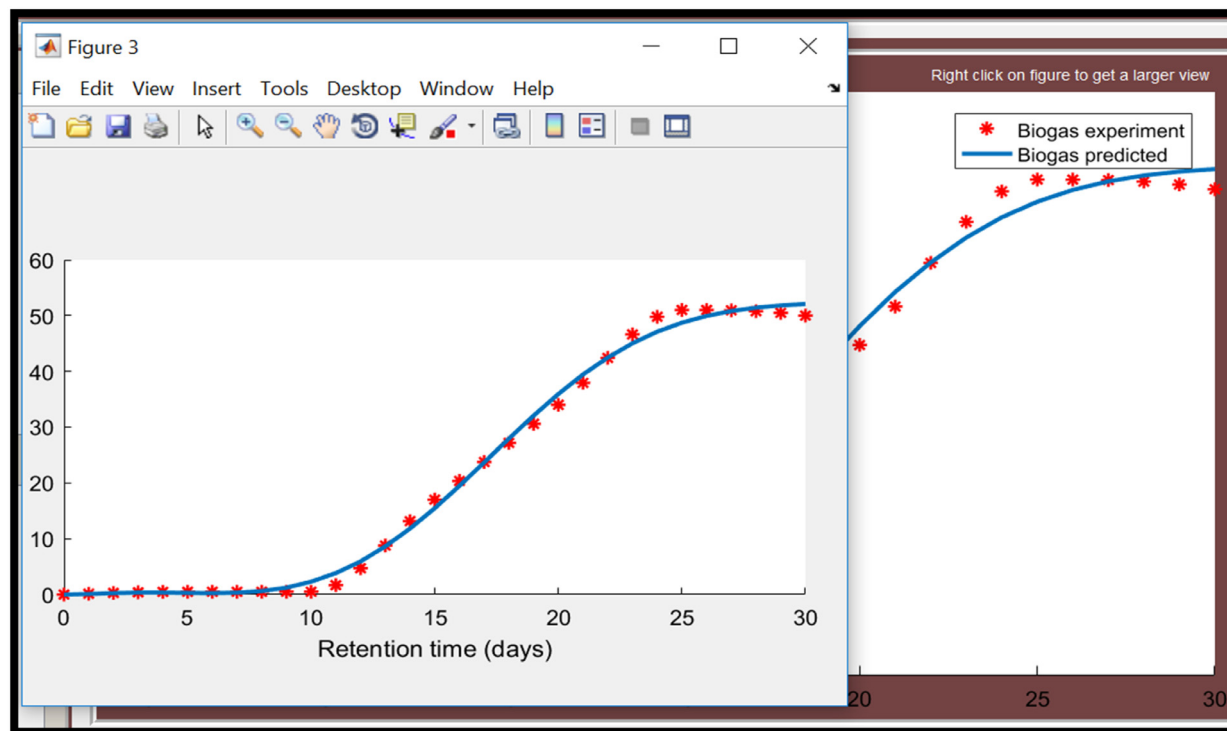


Fig. 16. Extracted view of modeling results from the user interface.

the parameter values and observing the effects on the gas output. BK-BiogaSim thus allows easy interactive design and simulation of operating conditions in an anaerobic unit treating blackwater and kitchen waste.

#### Synthesis of anaerobic digester networks

Studies have confirmed that when the reaction mechanism of a process is complex, the best performance is often achieved using a reactor network. Since the anaerobic treatment process involves a complex degradation mechanism, the use of single digesters as opposed to digester networks may limit performance as a result. Our next study seeks to use the kinetic models to develop new hydrodynamic configurations for operating anaerobic digesters based on the concept of attainable regions [28]. This is a technique for process synthesis and optimization that incorporates elements of geometry to understand how networks of chemical reactors can be designed and improved.

#### Conclusion

In this study, a series of models has been developed to describe biogas production from anaerobic codigestion of blackwater and kitchen waste. The models were formulated based on different bacteria growth kinetic models. This modeling approach has the advantage of simulating the process with very little input data and eliminates the need to quantify the viable bacteria biomass, which is usually very difficult to estimate during anaerobic digestion. A numerical interface has been designed to facilitate running of the models, making it possible to simulate, quickly and cheaply, different digestion scenarios and perform sensitivity analyses on input variations. The interface also provides functionality, which allows the user to simultaneously run, and chronologically rank all models on single click after input of experimental data. The results presented in this study can be used to facilitate design and optimization of biogas sanitation units treating blackwater and kitchen waste. An interesting progression of this study will be to apply the biogas yield models for the synthesis of anaerobic digester networks using the attainable region approach.

#### 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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