Renewable Energy 148 (2020) 1054–1064

Contents lists available at ScienceDirect

Renewable Energy

journal homepage: www.elsevier.com/locate/renene

A coupled modeling of design and investment parameters for optimal operation of methane bioreactors: Attainable region concept approach

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A R T I C L E I N F O

Article history:
Received 2 November 2018
Received in revised form
14 August 2019
Accepted 16 October 2019
Available online 23 October 2019

Keywords:
Attainable regions
Reactor economics
Modeling
Biogas plant design
Optimization

A B S T R A C T

Current practice to design methane bioreactors does not consider all degrees of freedom simultaneously, which raises question of global optimality. This study presents a model-based design framework, which simultaneously integrates process kinetics and business parameters into the design process, a key motivation for investors. Within the study, a methane bioreactor model is presented and kinetic models incorporating different economic feasibility indicators (PBP and BCR) are developed. The methane bioreactor model gives a good prediction of test data for digestion of diary manure and the natural patterns of payback period and benefit cost ratio are predicted. Stochastic stimulation is presented to include robustness in the design process and overall yield coefficients are illustrated for model dimensionality reduction. Two-dimensional attainable region is introduced as a reliable technique for defining limits of achievability as well as obtaining optimal methane bioreactor structures. Finally, a schematic model of the design process is established.

1. Introduction

In recent years, economic challenges in environmental management and organic waste sanitation has led to a change in waste management concepts from waste-to-discharge to waste-to-resource [1]. Anaerobic reactors, which can generate methane rich biogas from organic waste, have different characteristics often making them more adequate to treat specific wastes rather than others [2]. The synthesis reactor structures involving two or more single reactors may present designs that significantly reduce operational cost in comparison to single reactor designs [3]. This would however require a decision on how many reactors to consider, what reactor types, where to include bypass and recycle streams, where to include parallel reactors [4], as well as optimizing the techno-economic performance of the system by using techniques in process analysis. However, nominating specific reactor structures in an exhaustive way is not feasible as different structures can always be devised, which may have better digestion performance. Furthermore, modeling the reactions present in methane bioreactors is complex [5], and hence designing the system to maximize production of a specific byproduct is hence a challenging task.

For this reason, current practice for the design of methane bioreactors, normally involves the use of established process charts to determine the digester capacity based on operational parameters such as VS loading, temperature [2]. The design of methane digesters based on biochemical kinetics should be the ultimate goal of the bioprocess engineer, as the growth kinetics of anaerobic microorganisms will differ significantly in different waste types and characteristics [2,6]. Considerable research efforts for optimal design of methane bioreactors has focused mainly on selection of the right substrate or mixture of substrates [7,8], pretreatment of substrates and use of accelerants, as well as design of novel digesters [9,10] to improve digestion performance. In addition, capital cost of biogas plants is a key motivation for implementers but

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https://doi.org/10.1016/j.renene.2019.10.089

presented studies do not consider all degrees of freedom of the problem simultaneously as studies either focus on the process characteristics (such as the aforementioned) or on the economic analyses of methane bioreactor performance [11,12]. If the goal is to globally optimize the process performance, a methodology for design of methane bioreactors, which integrates substrate characteristics, process kinetics and business parameters into the design process, becomes indispensable for the design engineer. Thus, this work sets out with the aim of introducing an approach to simultaneously design and optimize the profitability of methane bioreactors by incorporating elements stochastic optimization, mathematical geometry and economics. The geometric technique is based on the concept of attainable regions and the motivation for this approach is that it first determines solutions to all possible optimization problems, even the ones not considered, and then we look for ways of attaining the solution [4,13–15]. In the case of methane bioreactors, we seek to obtain dynamic information of key states (methanogenic bacteria and volatile acids) for all possible digester configurations, even those that have not yet been devised. By then incorporating indicators of economic feasibility to the optimization process, we define appropriate economic performance targets than can used to make design and feasibility decisions.

2. Theoretical framework

The approach adopted to integrate process kinetics and cost effectiveness analyses in a simultaneous design and optimization procedure is that of Attainable Regions (AR). The AR technique is a systematic method to process synthesis, which integrates elements of geometry and optimization to design and improve engineering systems [13]. After specifying a set of decision variables, reaction kinetics, and initial conditions, the attainable region can be constructed, which is a geometric representation of all possible states that can be achieved by mixing and reaction only [4]. After construction of the region, the boundary can be interpreted in terms of process equipment through which the profitability of the system can be determined by defining an appropriate economic objective and overlaying onto the AR to see where intersects the boundary. Fig. 1 presents the main aspects of the model-based framework proposed in this study, clearly highlighting the position of the biokinetic model, the economic evaluation model as well as AR technique.

2.1. Dynamic model of methane bioreactor

Generally, the anaerobic process occurring in methane bioreactors leading to the production of methane-rich biogas can be simplified to a two-stage process involving waste conversion and stabilization, which is catalyzed by two main groups of bacteria. Based on this assumption, four key state variables of the process have been defined, which include: biodegradable organics, organic acids, acid-forming bacteria and methane bacteria, whereby the acid-forming bacteria converts the biodegradable organics to organic acids, which are in turn converted to methane gas by methane bacteria.

The reaction rates of the anaerobic microorganisms can be expressed by the Monod equation for cell growth, Eq. (1)

$$\mu = \mu_m \frac{S}{K_s + S} \tag{1}$$

The inhibition effect of organic acids on acid-forming and methane bacteria is modelled by respectively including a linear, Eq. (2) and an exponential inhibition term, Eq. (3) to the Monod equation. We used different factors for both bacteria groups since they differ in their physiology, growth kinetics, and response to environmental conditions [16].

$$\mu_{ac} = \mu_{m_{ac}} \frac{S_{BO}}{K_{S_{ac}} + S_{BO}} \left(1 - K_{i_{ac}} S_{OA}\right) \tag{2}$$

$$\mu_{me} = \mu_{m_{me}} \frac{S_{OA}}{K_{S_{me}} + S_{OA}} exp\left(-K_{i_{me}} S_{OA}\right) \tag{3}$$

The maximum reaction rates $\mu_{m_{ac}}$ and $\mu_{m_{ac}}$ are temperature dependent and this effect is modelled using a linear function, Eq.

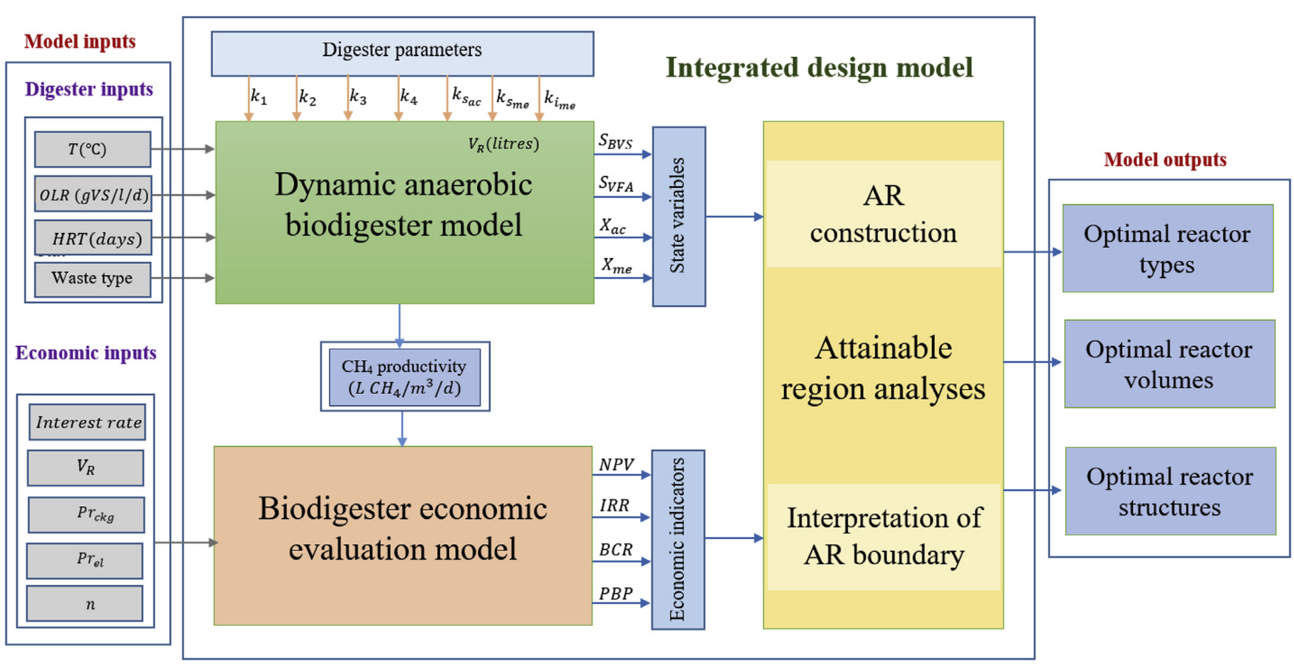

Fig. 1. Framework for coupled modeling of design and investment parameters.

(4) [17,18].

$$\mu_{m_{ac}}(T) = \mu_{m_{me}}(T) = 0.012T - 0.086 \quad (4)$$

$$10^{\circ}C < T < 60^{\circ}C$$

Assuming the specific death rate of acid-forming and methane bacteria is negligible compared to the growth rate, the material balance for the four species in the reactor can be expressed by Eqs. (5)–(8), while Eq. (9) computes the flowrate of methane gas produced

$$\frac{dS_{BO}}{dt} = r_{S_{BO}} = -k_1\mu_{ac}X_{ac} \quad (5)$$

$$\frac{dS_{OA}}{dt} = r_{S_{OA}} = k_2\mu_{ac}X_{ac} - k_3\mu_{me}X_{me} \quad (6)$$

$$\frac{dX_{ac}}{dt} = r_{X_{ac}} = \mu_{ac}X_{ac} \quad (7)$$

$$\frac{dX_{me}}{dt} = r_{Xme} = \mu_{me}X_{me} \quad (8)$$

$$Q_{CH_4} = V\mu_{me}k_4X_{me} \quad (9)$$

The raw organic substrate is fractionated into two parts; a biodegradable portion and an acid portion using the biodegradable constant (B_0) and the acidity factor (A_f) respectively as shown by Eqs. (10) and (11).

$$S_{BO_{in}} = B_0S_{O_{in}} \quad (10)$$

$$S_{OA_{in}} = A_fS_{BO_{in}} \quad (11)$$

The inoculum added to ease start-up of the digestion process is characterized using the acidogenic fraction (ϑ), as shown in Eqs. (12) and (13).

$$\frac{X_{ac_{in}}}{X_{in}} = \vartheta \quad (12)$$

$$\frac{X_{me_{in}}}{X_{in}} + \frac{X_{ac_{in}}}{X_{in}} = 1 \quad (13)$$

During design and operation of methane bioreactors, the effect of substrate characteristics as well as operating conditions such as temperature, digestion time, organic loading, etc. on the methane productivity is often of significant interest. The volumetric methane production rate is modelled by Eq. (14)

$$\gamma_{CH_4} = \gamma_s\mu_{me}X_{me}(k_3 - 1) \times 1000 \quad (14)$$

2.2. Economic evaluation model for methane bioreactor

For the purpose of this study, the economic evaluation model is based on two out of the four known economic indicators of financial viability; the benefit cost ratio (BCR) and the payback period (PBP) [19]. The BCR indicates whether an investment is cost-efficient (BCR >1) or not (BCR <1) while the decision rule for PBP is that one accepts projects that require shorter number of years to recover the investment.

The economic evaluation considers that biogas is utilized for cooking and electricity generation. The total annual income (benefit, B_t) from installing a biomethane plant is determined by Eq. (15). The benefits include the annual savings from electricity consumption, Eq. (15a) and LPG for cooking, Eq. (15b).

$$B_t = B_{ckg} + B_{el} \quad (15)$$

$$B_{el} = 0.9P_{el} \times T_{el} \times b \times Pr_{el} \times V_R \times \gamma_{CH_4} \quad (15a)$$

$$B_{ckg} = 0.9P_{ckg} \times T_{ckg} \times a \times Pr_{ckg} \times V_R \times \gamma_{CH_4} \quad (15b)$$

The total annual expenses or operating cost (cost, C_t) is computed by Eq. (16). The operating costs are assumed to be a function of two factors: the repair and maintenance costs, Eq. (16a) which is taken to by 1% of the capital cost ($0.01C_{plant}$) and the cost of H_2S removal from biogas, which is a function of the biogas volume, Eq. (16b).

$$C_t = C_m + C_{pf} \quad (16)$$

$$C_m = 0.01C_{Inv} \quad (16a)$$

$$C_{pf} = V_R \times \gamma_{CH_4} \times T_{pr} \times Pr_{pf} \quad (16b)$$

The cost of investment is computed using Eq. (17), which uses the rates of a commercial biogas company in Ghana, stating the cost of digester construction to be $300 per cubic meter [12]. This includes administrative, transport costs, consultancy fees and other logistic aspects.

$$C_{Inv} = C_{con} + C_{Gen} + C_{stv} + C_{misc} \quad (17)$$

$$C_{con} = 300V_R \quad (17a)$$

Table 1 presents of summary of the parameter sets that are used to perform the economic evaluation of designing a constructing a methane plant.

As mentioned at the beginning of section 2, the boundary of the attainable region can be interpreted in terms of reactor structures by defining an appropriate economic objective and overlaying over the AR to see where intersects the boundary. The economic objective must therefore be modelled to contain at least one of the state variables that make up the AR boundary. The volumetric methane productivity, Eq. (14), the payback period, the annual savings from electricity and LPG, Eq. (15) as well as the annual operating cost, Eq. (16) were utilized to express the payback period in the $[S_{OA}, X_{me}]$ concentration space as given by Eq. (18).

Table 1
Summary of input parameters used in the biodigester economic evaluation model.

S.N	Parameter	Unit	Value
1	Percentage of methane used for cooking	%	50
2	Discount rate	%	10
3	Average cost of digester and infrastructure	$\$/m^3$ (*Base*)	300
4	House hold family stove	$	50
5	Biogas-based electricity generator (500 kW)	$/4 *PCS*	600
6	Price of LPG used for cooking	$/*kg*	0.53
7	Biodigester lifespan	*years*	20
8	Upper calorific value of methane gas	MJ/m^3	39.8
9	Density of methane	kg/m^3	0.75
10	LPG equivalent of methane	$kg\ LPG/m^3\ CH_4$	1.25
11	Electricity equivalent of methane	kWh/m^3	11.06
12	Feed-in tariff rate for biogas-based electricity	$/*kWh*	17.5

$$X_{me} = \frac{(C_n + 0.01PBP \times C_{Inv}) \times 10^{-3}}{0.5\mu_{me}(k_3 - 1) \times PBP \times A \times V_R} \tag{18}$$

where

$$A = \left(0.9P_{ckg} \times T_{ckg} \times a \times Pr_{ckg} + 0.9P_{el} \times T_{el} \times b \times Pr_{el} - T_{pr} \times Pr_{pf}\right) \tag{18a}$$

For expressing the benefit cost ratio in the AR space, Eq. (19), we utilized Eq. (14), Eq. (15) Eq. (16).

$$X_{me} = \frac{0.01C_{Inv}X_t BCR \times 10^{-3}}{0.5\mu_{me}(BV_R X_t - WX_t BCR)(k_3 - 1)} \tag{19}$$

where

$$B = 0.9P_{ckg} \times T_{ckg} \times a \times Pr_{ckg} + 0.9P_{el} \times T_{el} \times b \times Pr_{el} \tag{19a}$$

$$W = V_R \times T_{pr} \times Pr_{pf} \tag{19b}$$

$$X_t = \sum_{t=1}^{t=n} \frac{1}{(1+r)^t} \tag{19c}$$

The objective functions will be used together with the attainable regions to determine the optimal operating points as well as the digester configurations required.

2.3. Uncertainty quantification and sensitivity analyses

As presented in Fig. 1, both the attainable region technique and economic analyses require inputs predicted by the methane bioreactor model. The economic evaluation model in turn requires inputs, from which the economic indicators are computed as shown in Table 1. The objective of the sensitivity analyses is to sample and explore the design space of the methane bioreactor model in order to determine the variables that significantly affect the design decision. The reactor temperature and organic loading rate are selected as the design variables while the substrate biodegradability (B_0) and acidity (A_f) constants, and the yield coefficient values (k_1, k_2 and k_3) are specified as the uncertain variables. In order to obtain robust parameters and improve upon the reliability of the design process the uncertain input variables are propagated using the Monte Carlo procedure to estimate the output uncertainty. To understand which input parameters are responsible for the output uncertainty, three sensitivity methods (Correlation, Kendall correlation and partial correlation) were evaluated and compared. The techniques were performed using the Simulink Design Optimization Toolbox of Matlab 2018b (Mathworks Natick, NA).

3. Model identification and construction of attainable regions

3.1. Estimation of kinetic constants and range of variability

Since the structure of the methane bioreactor model has been formulated based on some considerations, the first step is to assess the model's ability to predict experimental data before proceeding with the design process. This procedure consist of determining the yield constants k_1, k_2, k_3, k_4 Monod-based constants $K_{S_{ac}}$, $K_{S_{me}}$ and inhibition constants $K_{i_{ac}}$, $K_{i_{me}}$ using experimental data and then assessing the quality of the fit using statistical techniques. Experimental data for anaerobic digestion of diary manure was utilized [20] and the criterion used to fit the model is of the form shown by Eq. (20)

$$S(k) = \sum_{i=1}^{n} [y_i - \hat{y}(t_i, k)]^T W_i [y_i - \hat{y}(t_i, k)] \tag{20}$$

Where y_i is a two-dimensional vector of experimental response values at time t_i and W_i are 3×3 weight matrices for each observation point *i*. $\hat{y}(t_i, k)$ is the predicted response value at time t_i and its relation to the bioreactor model solution is given by Eq. (21).

$$\hat{y}(t_i, k) = C.x(t_i, k) + \varepsilon \tag{21}$$

$$C = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$x(t_i, k) = [S_{BO}(t),\ S_{OA}(t),\ X_{ac}(t),\ X_{me}(t),\ Q_{CH_4}(t)]^T$ is the five-dimensional vector of the state variables that are solutions of the methane bioreactor model. C is a 2×5 observation matrix, which indicates the state variables that are measured from experiments.

The problem was solved using the Matlab optimization toolbox, where the model equations were numerically integrated using the Runge-Kutta 4–5th order method implemented by the *ode45* routine and the minimization problem solved using the interior point algorithm of the *fmincon* routine.

Once estimates were determined, the variability of the parameter estimates, or predictions were assessed using a linearization approach. The noise variance of the parameter estimates was computed using Eq. (22) and the covariance matrix is approximated using Eq. (23)

$$\sigma^2 = \frac{1}{n-p} \sum_{i=1}^{n} (y_i - \hat{y}(t_i, k))^2 \tag{22}$$

$$cov(k) = 2\hat{H}^{-1}\sigma^2 \tag{23}$$

The approximate standard error of the parameter estimates ($s_{\hat{\beta}_i}$) is given by Eq. (24). The correlation matrix is computed using Eq. (25) while the coefficients of variation was computed using Eq. (26).

$$s_{\hat{k}_i} = \sqrt{diag(cov(\hat{k}))} \tag{24}$$

$$corr(\hat{k}) = \frac{cov_{i,j}}{\sqrt{cov_{i,i}}\sqrt{cov_{i,j}}} \tag{25}$$

$$CV = \frac{\sqrt{diag(cov(\hat{k}))}}{\hat{k}_i} \tag{26}$$

3.2. Construction of attainable regions

Now that the complete set of kinetic and economic evaluation models have been defined, the next step is to define the number of dimensions for which the attainable regions will be constructed and analyzed. Since the anaerobic reactions are considered as two independent reactions respectively involving acid-forming and methane bacteria, we expect the set of points generated by the process to reside in a two-dimensional subspace [4]. Of the four state variables present in the anaerobic treatment model, two are of utmost importance for economic evaluation. The concentration of methane bacteria from where the volumetric methane productivity is calculated, and the concentration of volatile fatty acids from which process inhibitions resulting in decrease steady-state methane productivity can be assessed. It is sensible to generate the AR in $(S_{OA} - X_{me})$ space. The concept of yield coefficients was used to reduce the number of dimensions in which the AR must be constructed. By using the concept of yield coefficients, we will demonstrate that it may be possible to systematically reduce bioreactor models and still obtain same performance as that of a full state model. This is possible because the reaction rate of biodegradable organics can be expressed in terms the reaction rate of acidogenic bacteria, which can in turn be expressed as functions of production rates of organic acids and methanogenic bacteria as shown by Eqs. (27) and (28):

$$r_{S_{BO}} = -k_1 r_{X_{ac}} \tag{27}$$

$$r_{X_{ac}} = \frac{1}{k_2}\left(r_{S_{OA}} + k_3 r_{X_{me}}\right) \tag{28}$$

This implies that the concentration of biodegradable organics can be expressed in terms of concentration of acidogenic bacteria, which can in turn be expressed as a function of organic acids and methanogenic bacteria concentrations, illustrated by Eqs. (29) and (30).

$$S_{BO} = S_{BO_{in}} - k_1\left(X_{ac} - X_{ac_{in}}\right) \tag{29}$$

$$X_{ac} = X_{ac_{in}} + \frac{1}{k_2}\left[S_{OA} - S_{OA_{in}} + k_3\left(X_{me} - X_{me_{in}}\right)\right] \tag{30}$$

Since X_{ac} and S_{BO} has been expressed as functions of X_{me} and S_{OA}, for each X_{me} and S_{OA} in the $C = [S_{OA},\ X_{me}]$ concentration space we can compute a reaction vector, $r(C)$ that uniquely determines the trajectories of an anaerobic CSTR, Eq. (31) and PFR reactors, Eq. (32) from a given organic load, $C_f = [S_{OA_{in}},\ X_{me_{in}}]$.

$$C = C_f + \tau r(C) \tag{31}$$

$$\frac{dC}{d\tau} = r(C) \tag{32}$$

The attainable region was constructed in Matlab (Mathworks, Natick NA) using the manual procedure described in Ref. [4]. The systems of nonlinear CSTR equations were solved using 'fsolve' routine while the system differential PFR equations are solved using the 'ode45' routine. The convex hull of the entire set of geometric points was computed using 'convhull' routine, which implements the Quickhull algorithm. The modelled economic objective functions involving payback period and benefit cost ratio were plotted over the AR boundary as contours, in order to determine the intersection with the boundary, which represents the operating point for attainting a given payback period, benefit cost ratio.

4. Results and discussion

4.1. Identification and reduction of methane bioreactor model

Curve fitting and statistical analyses were used to test the ability of the model to reproduce experimental data as well as determine the variance metrics of model parameters required to perform uncertainty analyses. Fig. 2 compares the simulated and experimental values of organic acids and methane gas flowrate. It is apparent from the figure that the model gives a good reproduction of the experimental data at a 95% confidence interval. The single most striking observation to emerge from the model fitting was that even though the experimental data looked scattered, the model is still able to obtain an acceptable fitting within the data points.

The results obtained from the use of yield coefficients in model reduction are compared in Fig. 3.

The results form Fig. 3 illustrated that the yield coefficient gives an excellent approach to model reduction as comparing the states from both the reduced and full model shows no significant difference. This finding supports previous research using yield coefficients to reduce dimensions of a three-state bioreactor model in ethanol fermentation [21]. This suggests that for biological reactions in which the chemical composition of each participating species is not well known, overall yield coefficients can be used as an alternative to reaction invariants [22] for dimensionality reduction.

4.2. Attainable regions and interpretation of boundaries

Fig. 4a presents the PFR trajectory and CSTR locus obtained using the kinetic models and initial load of the methane bioreactor. The results show that using a plug flow anaerobic reactor gives a higher concentration of methanogenic bacteria (24.8 g me./L) while the CSTR only gives a maximum methanogenic concentration of 5 g me./L. By extending the results to obtain the two-dimensional candidate attainable region, Fig. 4b, it becomes interesting to

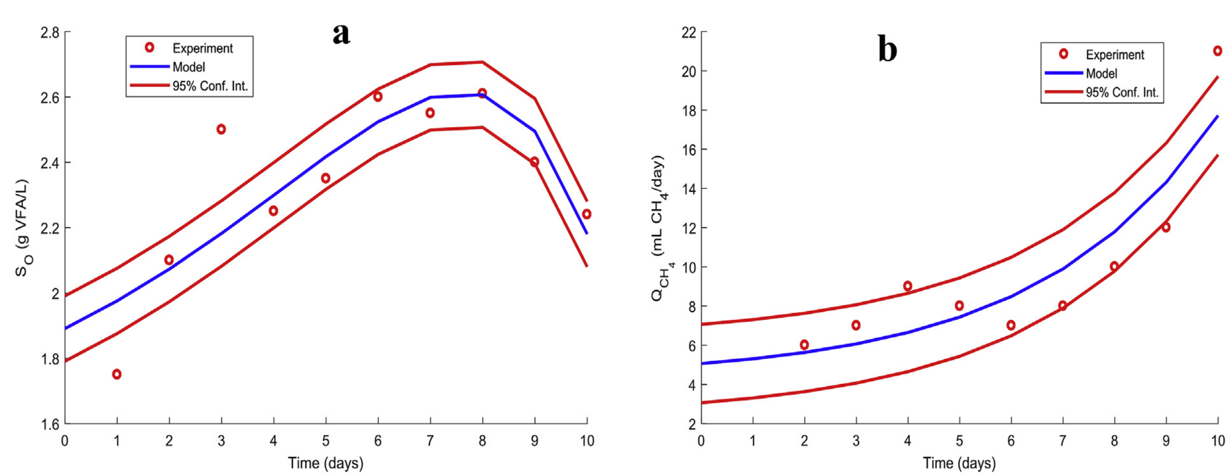

Fig. 2. Experimental and simulated concentration of volatile fatty acids (a) methane gas flowrate (b).

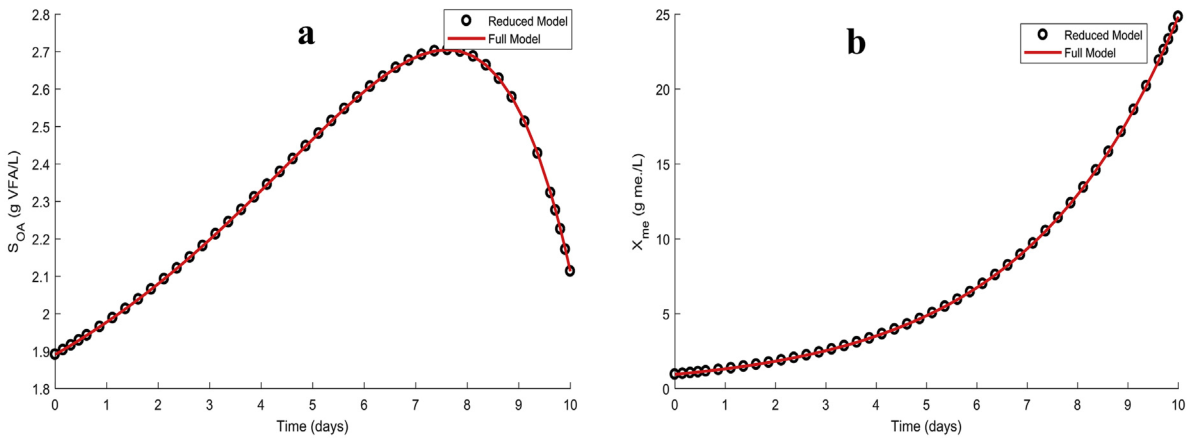

Fig. 3. Volatile acid concentration (a) and methane gas flowrate (b) predicted by reduced and full state model.

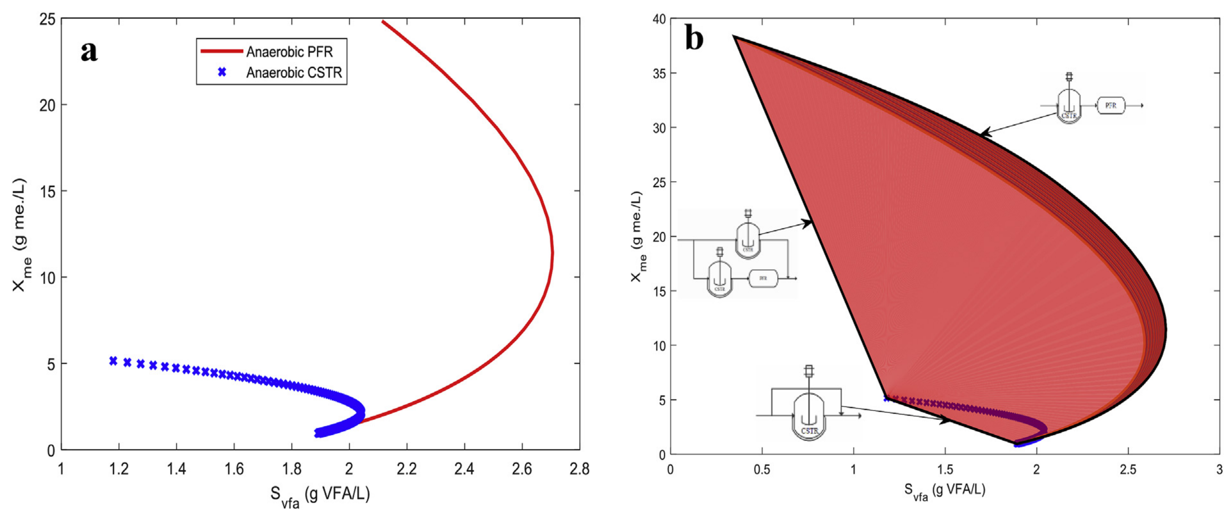

Fig. 4. CSTR locus and PFR trajectory (a) and two-dimensional candidate AR of the anaerobic treatment process (b).

observe that running a PFR from a CSTR can result in methanogenic concentrations reaching 36 g me./L. This result is explained by the fact that reaction vectors evaluated at points on a CSTR locus are collinear to the mixing vector, which makes it possible to extend the limits of achievability using a PFR trajectory [4]. From the results presented in Fig. 4b, the boundary of the AR can be interpreted into three reactor structures: An anaerobic CSTR followed by a PFR, an anaerobic CSTR with a bypass valve, as well as an anaerobic CSTR followed by a PFR run in parallel with a CSTR. What this means physically is that for the specified kinetics and organic load, all achievable points may be generated by these reactor configurations, and no other reactor structure can do better [4].

4.3. Reactor structures for meeting economic objectives

This section sets out to determine the reactor configurations require to attain the economic objectives. Fig. 5a presents contours for different payback periods overlain onto the AR boundary while Fig. 5b presents contour lines for different benefic cost ratios overlaid over the AR boundary. From Fig. 5a, we see that as the payback period decreases meanwhile the benefit cost ration increases as we move further away from the horizontal line ($X_{me} = 0$). These results are quite interesting and suggest that operating a methane bioreactor with higher methanogenic concentration produces shorter payback periods higher benefit cost ratio. An explanation for the observed patterns is that higher methanogenic concentration will result in higher methane yield and hence higher profit, which is reflected by shorter payback periods and higher benefit cost ratios as earlier mentioned in section 2.2. We therefore conclude that the approach to simultaneous design and optimization is reliable as it corroborates well with theory.

The reactor structures required to obtain each of the payback periods and benefit cost ratios presented in Fig. 5 can be read directly from Fig. 4b. Note that we have considered just two of the four economic objectives for illustrative purposes. The other two can also be overlaid onto AR boundary to determine the reactor structure required to achieve a particular target in a similar way.

4.4. Uncertainty quantification and sensitivity analysis

Several sources of uncertainties are encountered in practice when designing methane bioreactors and this section sets out to make the design robust by incorporating the variability of uncertain parameters and design parameters. The domain of variation of the uncertain parameters obtained as their 95% confidence interval during the model identification while those of other design parameters is also included based on knowledge of possible extent of variation (see Table 2). Table two also presents the statistical

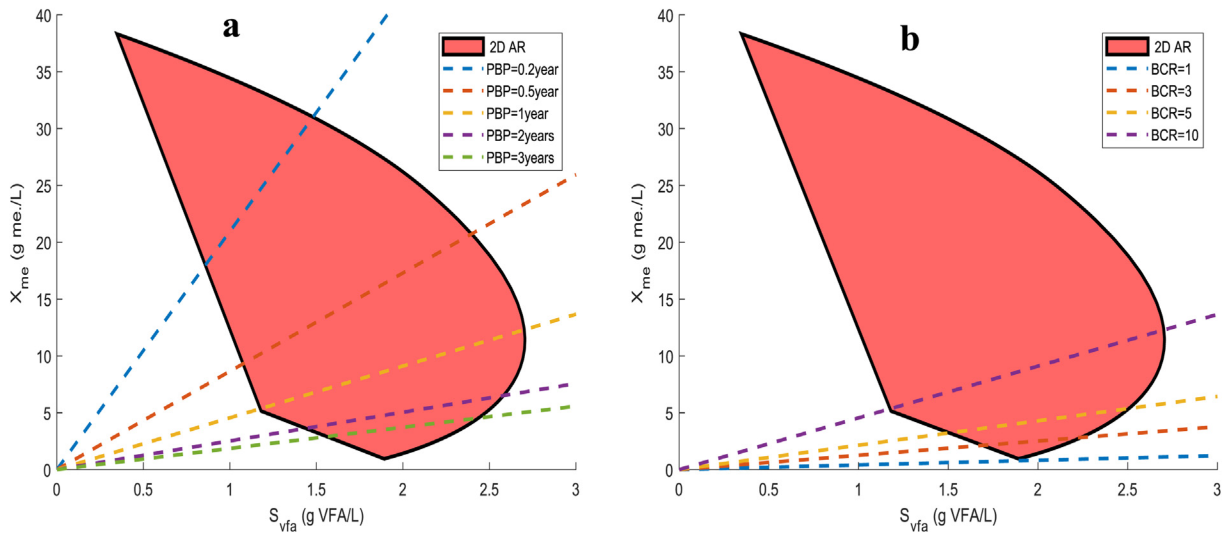

Fig. 5. Overlaid objective function of payback period (a) and benefit cost ratio (b) onto the AR.

Table 2
Probability distributions and characteristics for parameter sampling.

SN	Parameter	Sampling distribution	Characteristics	
			Minimum	Maximum
1	k_1	Uniform	0.0007	8.735
2	k_2	Uniform	0.01	13.709
3	k_3	Uniform	0.01	19.803
4	B_0	Uniform	0.80	0.95
5	A_f	Uniform	0.04	0.06
6	$VSL\ (S_{O_{in}})$	Uniform	25	45
7	T	Uniform	$25^{\circ}C$	$37^{\circ}C$

distributions and their characteristics from where the parameters have been sampled.

Monte Carlo simulations where performed with the sampled parameter values and the results show that k_3 and temperature show a strong positive effect on the averaged methane productivity while the other parameters show no clear correlation. This is illustrated by the results of the sensitivity analysis, using the correlation and partial correlation method presented in Fig. 6b, which shows that k_3 and temperature contribute most to the uncertainty in the averaged methane productivity. The positive correlation obtained with temperature can be explained by the fact that an increase in temperature increases the growth rate of anaerobic microorganisms hence increasing gas production [2,16]. The parameter k_3 is a yield coefficient, which describes gram of organic acids consumed per given concentration of methanogens to produce methane and this explain the reason for the positive correlation. Even though the other parameters contribute to the methane production, they are not directly linked to the methane-producing step, reason why the correlation is not evident.

Fig. 6a presents the simulation results in the form of key performance indices plotted as histograms, which clearly shows the uncertainty by the variance of the histograms. For 100 Monte Carlo simulations, the highest occurrence of averaged methane productivity was 8128.4 $l/m^3/d$ and the values of the parameter sets that gives this methane productivity are presented in Table 3.

After identification of key performance indices and the most significant sources of uncertainty, stochastic optimization is

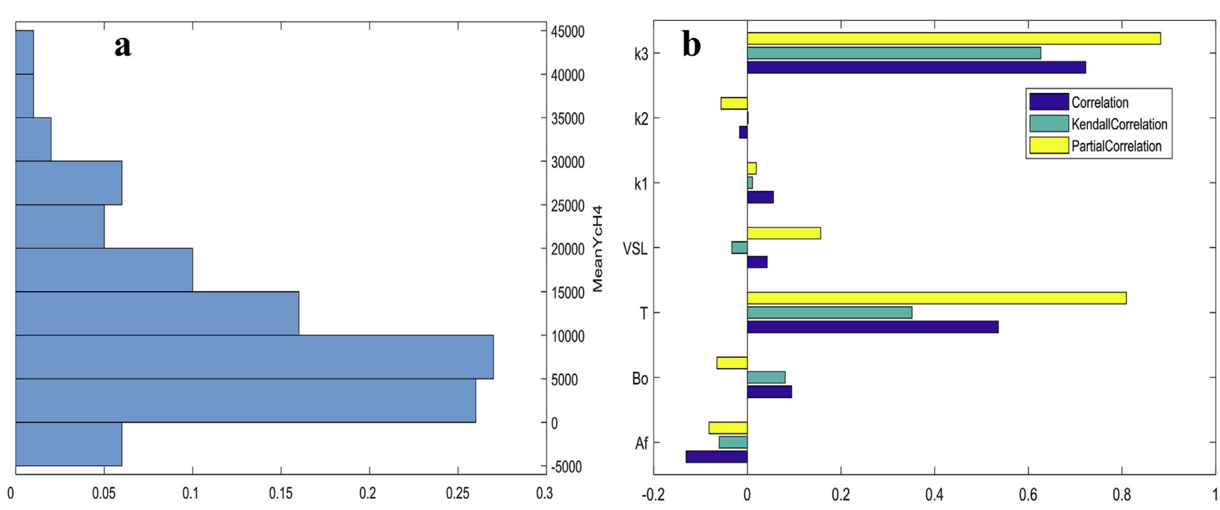

Fig. 6. Averaged volumetric methane productivity from Monte-Carlo simulations plotted as a histogram for 100 parameter samples (a) and Statistical indices showing influence of each parameter on methane productivity (b).

Table 3
Optimal design variables, model parameter values, and highest occurred methane productivity for 100 Monte-Carlo simulations.

Scenario	Uncertain parameters					Design variables		Model output
	k_1	k_2	k_3	B_o	A_f	VSL	T	Mean Y_{CH_4}
Base	0.0007	3.53	4.93	0.95	0.05	39.80	35.0	5159.2
Robust	2.47	11.33	6.64	0.92	0.05	38.57	36.0	8128.4

performed to determine the design variables (VSL and T) that maximizes averaged methane productivity under uncertain conditions (see Table 3). The robust variables are used to construct the attainable region in order to obtain optimal reactor structures that can generate all achievable points under conditions of uncertainty. Fig. 7 presents the candidate two-dimensional attainable region under uncertain conditions and Fig. 8 presents reactor structures obtained by interpreting the AR boundary.

It is important to bear in mind that some of the parameters selected in the simulations are for illustrative purposes and hence the focus of the reader should be on understanding the implementation of the methods.

The results of this study will now be compared to the findings of previous work. However, in reviewing the literature, very limited information was found on the use of attainable regions for synthesis and optimization of methane bioreactors. The only studies have been our most recent works using attainable regions to optimize volatile solids reduction and methane productivity [23] as well as operating stability of methanogenic microorganisms [24]. The results from both studies illustrated that a change in digested substrate and/or source of inoculum used to start-up the digester significantly influences the operating limits (defined by the attainable region), optimized parameter, as well as the design configuration of the optimal digester structure. However, both studies focused on the use of process objectives (volumetric methane productivity, volatile solids reduction, process stability) for synthesis of methane bioreactors. The current study expands the boundary of the previous by simultaneously considering, process kinetics and macroeconomic parameters as well as the influence of uncertainty in the use of attainable regions for the synthesis of methane bioreactors. Considering all the three studies put together, the results can be applied to design and optimize configurations of methane bioreactors considering process and economic objectives as well as uncertainty, which improves upon the reliability of decision making. It is also interesting for the readers to note that the choice of economic feasibility objective (payback

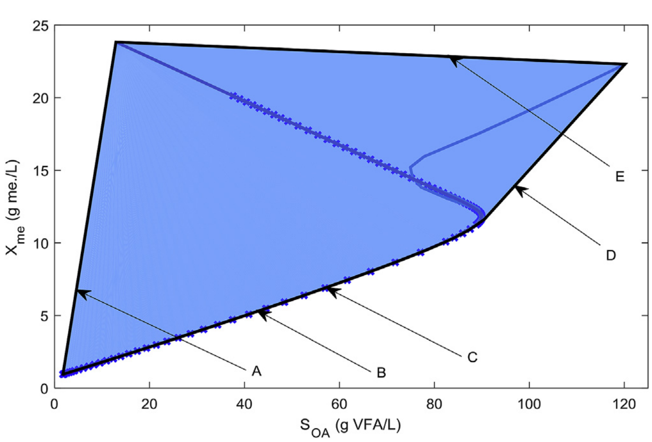

Fig. 7. Two-dimensional candidate AR for highest occurred methane productivity.

period or benefit cost ratio), as well as macroeconomic parameters (interest rate or feed-in tariff rate) influence the optimal configuration of the digester structure necessary to achieve it. What this means is that the optimal reactor configuration for a profitable investment will differ based on the economic situation of the location where the digester is to be constructed. We consider this of high significance to industrial application as it proposes as systematic model-based approach (summarized in section 4.5) that simultaneously considers process kinetics, reactor design as well as economics in order to make reliable investment decisions.

4.5. Framework for coupled modeling of design and investment parameters

Starting from a methane-bioreactor-design problem, the framework consists of seven main steps: (1) Define economic performance target. (2) Screen and identify uncertain process parameters. (3) Develop process model and determine domains of variability. (4) Stochastic simulation and uncertainty analyses. (5) Determine reactor structures that define limits of achievability. (6) Optimize reactor structure to meet economic target. (7) Validate optimal reactor configuration. Fig. 9 presents these steps, the inputs required at every step as well as the deliverables being output at every stage. The section highlighted in blue dotted lines have not been considered in this study but makes object of our next study. The following section presents a description of how each step of framework is performed.

The first step, definition of economic performance target involves setting an appropriate economic feasibility index that must be achieved upon investment in the project. The economic indices considered in this study are the net present value, internal rate of return, benefit cost ratio and payback period. The study has developed models for appropriate economic objectives, which integrates each of the aforementioned indices.

The second step, screen and identify uncertain process parameters involves consulting the literature to first determine all the parameters that are significant to design of methane bioreactor. This generally considers feedstock composition, kinetic parameters as well as operational parameters. Afterwards, kinetic parameters that have been well established from several previous studies are considered certain while the other kinetic parameters as well as all feedstock and operational parameters are considered uncertain. Examples of certain kinetic parameters are the Monod half saturation constants.

The third step, develop process model and determine domains of variability consist of developing a model of the process that includes all the parameters of interest. Since there exist several models to describe the anaerobic treatment process, this step might just include selection of the appropriate model to describe the process. We recommend use of the simplified five state model considered in this study, which is a compromise between models that are being highly accurate but very complex in input requirement and highly simplified but very limited in predictive ability. Once a model has been obtained to describe the process, test data from experiments is used to calibrate the model and determine the domain of variability of model parameters, which is required for uncertainty quantification. This is done by parameter estimation and statistical analyses to determine the 95% confidence interval of model parameters. The variance metrics of feedstock and operational parameters is set based on expert knowledge of the parameter.

The fourth step, uncertainty analysis and stochastic optimization explores the design space of the methane bioreactor by characterizing model parameters using probability distributions to generate random samples for Monte-Carlo evaluation of the design

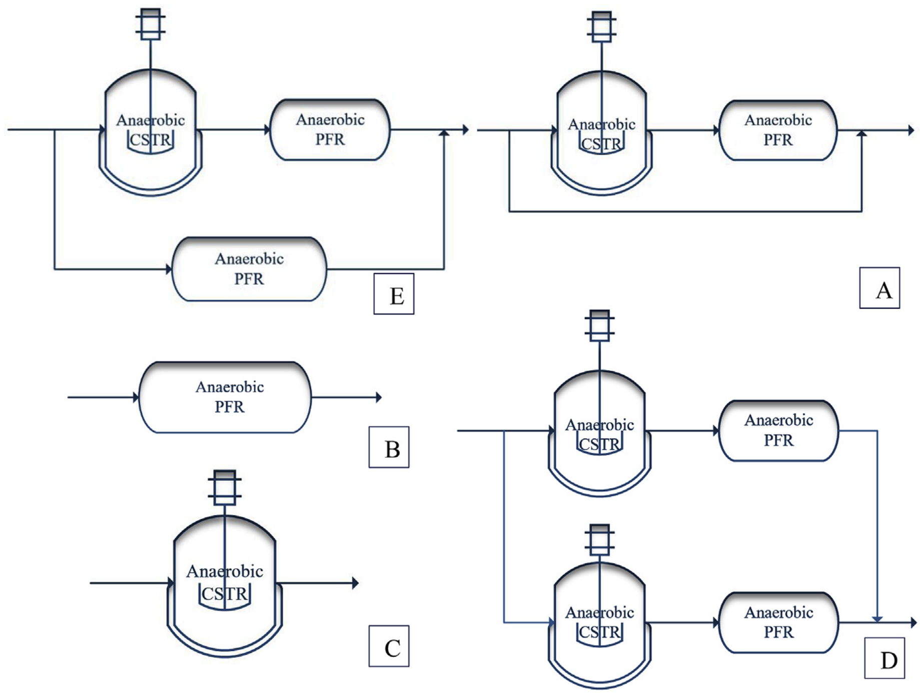

Fig. 8. Reactor structures for attaining targets in methane productivity under uncertainty.

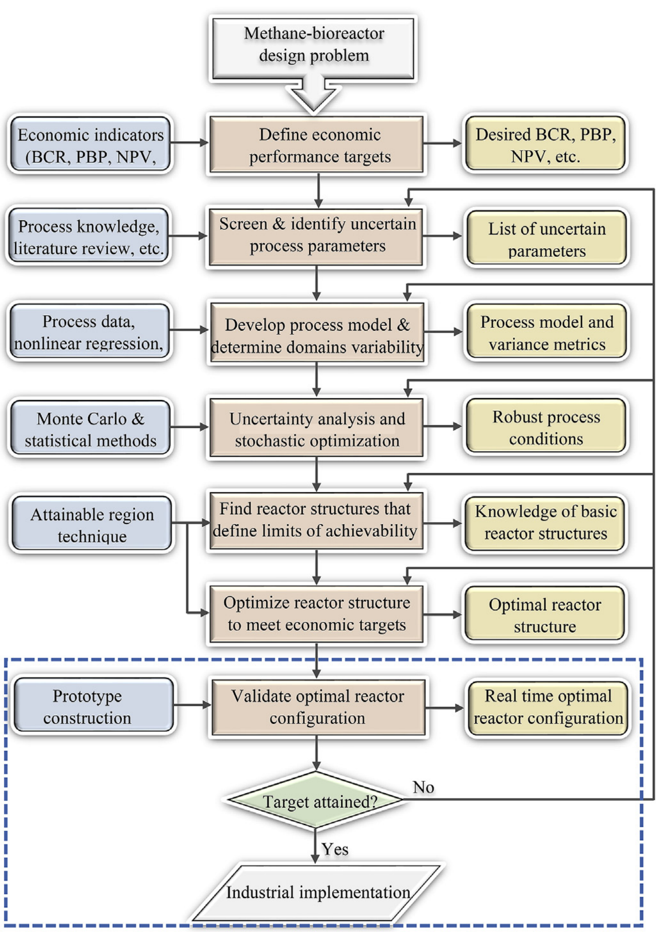

Fig. 9. Workflow of the coupled modeling methodology for methane bioreactors.

at the sample points. Sensitivity analyses is utilized to see which of the parameters significantly affect the averaged methane productivity or any other design requirement. Key performance indices plotted as histograms are used to determine which of the model parameters give the averaged methane productivity highest number of times following the number of Monte-Carlo simulations performed. Finally, stochastic optimization is performed to obtain the optimal operating conditions under conditions of uncertainty.

The firth step, determine reactor structures that define limits of achievability makes use of the decision variables, reaction kinetics and initial conditions to construct the attainable regions, using the parameters that give the averaged methane productivity the highest number of times. The boundary of the AR is then interpreted as methane bioreactor structures, which define the limits of what can be achieved in terms of methane productivity. What this means is that the methane bioreactor structures obtained at this step can be used to generate all other methane productivities that are achievable.

The sixth step, optimize reactor structure to meet economic target interprets the boundary of the AR in terms of methane bioreactor structures by overlaying the economic objective selected in step 1 onto the AR to see where intersects the boundary. The reactor structure corresponding to the point of intersection is the structure that is required to attain the defined economic objective.

In the final step, validate optimal reactor configuration, a detailed engineering drawing of the optimal methane bioreactor configuration is performed using a CAD tool, followed by material selection, costing, construction and testing to see if the reactors design performs as predicted by the simulation. If this is the case, the design is validated and implemented for industrial production of methane; otherwise, checks are made from the second to the sixth step as shown by the backward arrows in Fig. 9.

It is encouraging to compare the methodology proposed in this study with other model-based methodologies presented in the literature for bioprocess design. This include that of [25] for model-based optimization of bioprocesses under uncertainty and that of

[3] for optimal synthesis of methane bioreactors using superstructure optimization. One common thing in both approaches is that a number of reactor configurations is first defined before optimization is performed to select the best configuration. However, an important question raised is that "Does a better reactor configuration exist? since we can always devise new reactor configurations, which perform even better. On the other hand, the power of our methodology is that the limits of achievability for all possible reactor configurations, even those that have not yet been devised, is obtained by incorporating attainable region analysis in the process [4,14,15,24]. The approach presented in this study synthesizes a reactor configuration as part of the design process and connects the evaluation process to economic parameters, which is the key interest of investors.

5. Conclusion

The present study was designed to illustrate the usefulness of attainable regions for integrating process kinetics, reactor design and economic parameters in the synthesis of optimal digester structures. The following main results have been obtained: (1) The choice of economic feasibility objective (payback period or benefit cost ratio), as well as macroeconomic parameters (interest rate or feed-in tariff rate) influence the optimal configuration of the digester structure necessary to achieve it. (2) Temperature as well as the yield coefficient, which describes gram of organic acids consumed per given concentration of methanogens to produce methane contribute most to the uncertainty in the averaged methane productivity (3) Considering the influence of uncertainty results in a change in the performance target and hence the optimal digester configurations of the anerobic treatment process. The optimal digester configurations are made up of different combinations of a plug flow and a continuous stirred tank digester. (4) A systematic model-based methodology has been developed to that simultaneously considers process kinetics, reactor design as well as economics to support optimal investment decisions in biogas plants.

The key strength of the approach is that is it is a global optimization framework: It defines the performance targets for all possible reactor configurations, for all possible economic parameters by incorporating attainable region analysis in the process. Although the current study is based on computer simulations, it provides a strong basis towards obtaining reliable computational tools to aid design and optimization of methane bioreactors. An interesting progression of the study will be to construct and test a methane bioreactor prototype, which has been designed using the proposed methodology in order to validate and/or refine the methods.

Funding

This work was supported by EnPe-NORAD under the project Upgrading Education and Research Capacity in Renewable Energy Technologies (UPERC-RET).

Acknowledgments

Our team express gratitude to the following institutions; The Brew-Hammond Energy Centre, KNUST Ghana and the Abunde Sustainable Engineering Group (AbundeSEG) for its immense technical support.

Nomenclature

A_f	Acidity factor $(g\ VFA/L)/(g\ BVS/L)$
B_0	Biodegradability constant $(g\ BVS/L)/(g\ VS/L)$
B_{ckg}	Annual savings from using LPG in cooking ($)
B_{el}	Annual savings from electricity consumption ($)
B_t	Annual income ($)
C_{Gen}	Cost of generator ($)
C_{Inv}	Cost of investment ($)
C_{con}	Cost of construction ($)
C_m	Cost of maintenance ($)
C_{misc}	Miscellaneous cost ($)
C_{pf}	Cost of biogas purification ($)
C_{stv}	Cost of biogas cooking stove ($)
C_t	Annual operating cost ($)
$K_{i_{ac}}$	Organic inhibition constant for acidogenic bacteria $(g\ OA/L)$
$K_{i_{me}}$	Organic acid inhibition constant for methanogenic bacteria $(g\ OA/L)$
$K_{s_{ac}}$	Monod half-saturation constant for acidogenic bacteria $(g\ BO/L)$
$K_{s_{me}}$	Monod half-saturation constant for acidogenic bacteria $(g\ OA/L)$
K_s	Monod half-saturation constant $(og\ /L)$
P_{ckg}	Percentage of methane utilized for cooking (%)
P_{el}	Percentage of methane utilized for electricity (%)
Pr_{pf}	Price for biogas purification $(\$/L\ CH_4)$
P_t	Net annual benefit ($)
Q_{CH_4}	Methane gas flowrate $(L\ CH_4/d)$
$S_{BO_{in}}$	Initial concentration of biodegradable organics $(g\ BO/L)$
$S_{O_{in}}$	Initial concentration of organic substrates $(g\ VS/L)$
S_{BO}	Concentration of biodegradable organics $(g\ BO/L)$
$S_{OA_{in}}$	Initial concentration of organic acids in bioreactor $(g\ OA/L)$
S_{OA}	Concentration of organic acids in bioreactor $(g\ OA/L)$
T_{ckg}	Annual time period for cooking (d)
T_{el}	Annual time period for use of electricity (d)
T_{pr}	Annual time period for biogas purification (d)
V_R	Volume of methane bioreactor (L)
$X_{ac_{in}}$	Initial concentration of acidogenic bacteria $(g\ ac./L)$
X_{ac}	Concentration of acidogenic bacteria in bioreactor $(g\ ac./L)$
X_{in}	Initial concentration of biomass in reactor (g/L)
$X_{me_{in}}$	Initial concentration of methanogenic bacteria $(g\ me./L)$
X_{me}	Concentration of methanogenic bacteria in bioreactor $(g\ me./L)$
k_1	Yield constant $(g\ BO/g\ ac./L)$
k_2	Yield constant $(g\ OA/g\ ac./L)$
k_3	Yield constant $(g\ OA/g\ me./L)$
$r_{S_{BO}}$	Reaction rate for biodegradable organics $(g\ BO/L/d)$
$r_{S_{OA}}$	Reaction rate for organic acids $(g\ OA/L/d)$
$r_{X_{ac}}$	Reaction rate for acidogenic bacteria $(g\ ac./L/d)$
$r_{X_{me}}$	Reaction rate for methanogenic bacteria $(g\ me./L/d)$
γ_{CH_4}	Volumetric methane productivity $(L\ CH_4/m^3/d)$
γ_s	Methane yield
$\mu_{m_{ac}}$	Maximum specific growth rate of acidogenic bacteria (d^{-1})
$\mu_{m_{me}}$	Maximum specific growth rate of methanogenic bacteria (d^{-1})
μ_{ac}	Specific growth rate of methanogenic bacteria (d^{-1})
μ_m	Specific growth rate of methanogenic bacteria (d^{-1})
BCR	Benefit cost ratio
IRR	Internal rate of return (%)
NPV	Net present value ($)
Pr_{ckg}	Price of LPG used for cooking $(\$/kg)$
Pr_{el}	Feed in tariff rate for biogas based electricity in Ghana $(\$/kWh)$
PBP	Payback period (d)

S	Substrate concentration $(g\ /L)$
T	Reactor temperature $(^{\circ}C)$
V_R	Volume of methane bioreactor (L)
a	LPG equivalent of methane for cooking $(kg\ LPG/\ m^3CH4)$
b	Unit conversion coefficient (kWh/m^3CH4)
r	Discount rate $(\%)$
t	Time (yr)
ϑ	Acidogenic fraction

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.renene.2019.10.089.

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