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Optimal synthesis of anaerobic digester networks

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ABSTRACT

The objective of this paper is to develop a mathematical model for the synthesis of anaerobic digester networks based on the optimization of a superstructure that relies on a non-linear programming formulation. The proposed model contains the kinetic and hydraulic equations developed by Pontes and Pinto [Chemical Engineering Journal 122 (2006) 65–80] for two types of digesters, namely UASB (Upflow Anaerobic Sludge Blanket) and EGSB (Expanded Granular Sludge Bed) reactors. The objective function minimizes the overall sum of the reactor volumes. The optimization results show that a recycle stream is only effective in case of a reactor with short-circuit, such as the UASB reactor. Sensitivity analysis was performed in the one and two-digester network superstructures, for the following parameters: UASB reactor short-circuit fraction and the EGSB reactor maximum organic load, and the corresponding results vary considerably in terms of digester volumes. Scenarios for three and four-digester network superstructures were optimized and compared with the results from fewer digesters.

1. Introduction

In wastewater treatment, there is a variety of digesters and reactors, specifically biochemical ones, which suit the task of degrading pollutants in the effluent streams. As expected, reactors and digesters have different characteristics often making them more adequate to treat specific effluents rather than others. The optimal synthesis of a reactor (digester) network in a wastewater treatment plant may present designs that significantly reduce the costs of the plant in comparison to single reactor designs.

The objective of the current paper is to develop a strategy for the synthesis of a network of anaerobic digesters. The use of multiple types and configurations of reactors (digesters) in a network can yield better results in effluent treatment than the use of only one reactor (digester) for this purpose. It is also shown how complex a network becomes once the number of candidate digesters increases, and how an understanding of the wastewater treatment process is decisive to the success of the synthesis strategy.

The current paper focuses on the synthesis of a network of anaerobic digesters that contains in particular the UASB (Upflow Anaerobic Sludge Blanket) reactor and the EGSB (Expanded Granular Sludge Bed) reactor. Like most modern biochemical digesters, the UASB and the EGSB reactors have a much higher sludge age than the hydraulic retention time, as described in Pontes and Pinto [1]. As a consequence, the sludge behavior in the system is considerably different from that of the effluent. The detailed models that describe flow and kinetic behaviors for these digesters are also described in [1]. The UASB reactor flow model is based on the one developed by Bolle et al. [2], while the EGSB reactor flow model was developed from the experiments described in Brito and Melo [3]. The kinetic models are based on the ones developed from Kalyuzhnyi [4] and Bolle et al. [5]. Also, these digesters have intrinsic characteristics that must be taken into account in their design as well as in the synthesis of the treatment process. Kalyuzhnyi and Fedorovich [6], Narayanan and Narayan [7] and Mu et al. [8] developed axial dispersion models for the UASB reactor. These models may be more precise, but are complicated to simulate and optimize, requiring a discretization in the axial direction within the reactor.

As stated by Lakshmanan and Biegler [9], there are two major approaches for synthesis of a reactor network: superstructure optimization and attainable region targeting. The first one consists of creating a superstructure containing a pre-determined number of reactors and various streams that connect these reactors. Kokossis and Floudas [10] proposed a methodology where the superstructure is composed of CSTRs (Continuous Stirred Tank Reactor) and PFRs (Plug Flow Reactor). According to their strategy, a PFR could be approximated by a series of CSTRs, and the network would be represented by a MINLP (Mixed Integer Non-Linear Programming) model. Kravanja and Grossmann [11] also used this methodology. Marcoulaki and Kokossis [12] developed a methodology using stochastic optimization to target the performance of chemical reactors. Schweiger and Floudas [13] described a superstructure composed of CSTRs and CFRs (Cross Flow Reactor). The

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Nomenclature

Bacteria types (i)

AB	butyric acid user acetogens
AE	ethanol user acetogens
F	fermentors
I	endogenous residue
MA	acetoclastic methanogens
MH	hydrogetrophic methanogens

Substrates (j)

AA	acetic acid
B	butyric acid
CH_4	methane
CO_2	carbon dioxide
E	ethanol
G	glucose
H	hydrogen

Number of reactors in the network superstructure (k)

streams (n)

BP_r	reactor *r* by-pass
FD	fresh feed
FN	final
IN_r	reactor *r* inlet
MR_r	final mixer to reactor *r* connection
OT_r	reactor *r* outlet
RF_r	fresh feed to reactor *r*
RM_r	reactor *r* to final mixer connection
RR_r	reactor *r* recycle
$S_{r-r'}$	feed from reactor *r* to *r'*

Reactors (r)

UASB	or EGSB

Section of UASB reactor (s)

a	bed
b	blanket
c	settler

Variables

$\phi_{CH_{4,r}}$	volumetric production rate of methane in reactor *r* (m^3/h)
$\phi_{CH_{4,r,s}}$	volumetric production rate of methane in section *s* of UASB reactor *r* (m^3/h)
η_r	settler efficiency of UASB reactor *r*
$\mu_{i,r}$	growth rate for bacterium *i* in EGSB reactor *r* (h^{-1})
$\mu_{i,r,s}$	growth rate for bacterium *i* in section *s* of UASB reactor *r* (h^{-1})
A_r	cross-sectional area of reactor *r* (m^2)
COD_n	chemical oxygen demand for stream *n* (kg/m^3)
DC_r	total discharged sludge flow for reactor *r* (kg/m^3 h)
$DC_{i,r}$	discharge rate for bacterium *i* from reactor *r* (kg/m^3 h)
F_n	stream *n* flow rate (m^3/h)
h_r	overall height of reactor *r* (m)
$h_{r,s}$	height of section *s* of UASB reactor *r* (m)
OL_r	organic load for reactor *r* (kg/m^3 d)
$R_{j,r}$	reaction rate for substrate *j* in EGSB reactor *r* (kg/m^3 h)
$R_{j,r,s}$	reaction rate for substrate *j* in section *s* of UASB reactor *r* (kg/m^3 h)
RC	cost of the reactors present in the network
$S_{j,n}$	concentration of substrate *j* in stream *n* (kg/m^3)
$S_{j,r}$	concentration of substrate *j* leaving reactor *r* (kg/m^3)
$S_{j,r,s}$	concentration of substrate *j* in section *s* of UASB reactor *r* (kg/m^3)
TM_r	rate of formation of the endogenous residue in EGSB reactor *r* (kg/m^3 h)
$TM_{r,s}$	rate of formation of the endogenous residue in section *s* of UASB reactor *r* (kg/m^3 h)
V_r	overall volume of reactor *r* (m^3)
v	upflow velocity (m/h)
$X_{i,n}$	concentration of anaerobic sludge component *i* in stream *n* (kg/m^3)
$X_{i,r}$	concentration of anaerobic sludge component *i* in EGSB reactor *r* (kg/m^3)
$X_{i,r,s}$	concentration of anaerobic sludge component *i* in section *s* of UASB reactor *r* (kg/m^3)
XT_r	total anaerobic sludge concentration in EGSB reactor *r* (kg/m^3)
$XT_{r,s}$	total anaerobic sludge concentration in section *s* of UASB reactor *r* (kg/m^3)

Parameters

μ_{mi}	maximum growth rate for bacterium *i* (h^{-1})
CT	computational time (h)
K_j	half-speed constant for substrate *j* (mol/m^3)
$K_{Ii,i'}$	inhibition constant for bacterium *i* by inhibitor *i'* (mol/m^3)
MM_j	molar mass of substrate *j* (kg/mol)
NE_k	number of equations in a network superstructure of *k* reactors
NF_k	number of degrees of freedom in a network superstructure of *k* reactors
NV_k	number of variables in a network superstructure of *k* reactors
$OL_{r,max}$	maximum organic load for reactor *r* (kg/m^3 d)
R	number of reactors in the network superstructure
RC_r	cost of reactor *r*
RE	number of EGSB reactors in a network superstructure
RU	number of UASB reactors in a network superstructure
SF_r	short-circuit fraction that by-passes reactor *r*
$SF_{r,s}$	short-circuit fraction that by-passes section *s* in reactor *r*
Y_i	bacterial yield (kg/mol)

latter can be used to model PFRs, MMRs (Maximum Mixed Reactor) and SFRs (Segregated Flow Reactor). Esposito and Floudas [14] described a strategy to optimize a reactor network superstructure using a NLP (Non-Linear Programming) model that divides the network into subnetworks. The network is composed by a CSTR and either a PFR or a RR (Recycle Reactor).

The attainable region targeting approach is based on the concept developed by X. Horn, according to Glasser et al. [15] and Hildebrandt et al. [16], who described the methods for obtaining the attainable region for networks that consist of CSTRs and PFRs, but their examples covered only two dimensions, i.e. reactions involving only two compounds. Balakrishna and Biegler [17] proposed a segregated flow model to achieve a LP (Linear Programming) formulation for the network model involving isothermal reactors. Balakrishna and Biegler [18] developed a strategy for the optimal synthesis of non-isothermal reactor networks. Lakshmanan and Biegler [9] proposed a method that incorporates some of the concepts of the superstructure approach into the attainable region targeting approach and created a MINLP model for the network, which is composed of CSTRs, PFRs and DSRs (Differential Sidestream Reactor). The model can be extrapolated to systems with more than two dimensions. Kauchali et al. [19] proposed a LP model to optimize a reactor network with two dimensions. Recently, Bedenika et al. [20] proposed a method for the synthesis of reactor networks based on economical criteria instead of technological criteria.

Other works propose alternative methods. Pahor et al. [21] described a method that combines aspects of both approaches, which results in a MINLP model for the reactor network. Burri et al. [22] developed the IDEAS (Infinite Dimensional State-Space) approach, which evolved from the attainable region approach. The IDEAS approach generates a LP model for the reactor networks, and was also applied to networks with non-ideal reactors [23,24], as well as to networks with variable density fluid CSTRs and PFRs [21].

Although the targeting approach is considered to have two important advantages over the first, which are simpler MINLP formulations and optimal solution not bound to the superstructure, it cannot be readily used to optimize anaerobic digester networks. The attainable region targeting approach yields results in CSTRs, PFRs, or even DSRs, but anaerobic digesters cannot be categorized as such [1]. Therefore, the approach proposed in this paper relies on superstructure optimization. Kokossis and Floudas [10] described the basic strategy for elaborating a superstructure and its corresponding optimization model. This strategy can also be used to discretize the axial dispersion models developed by [6–8].

The paper is structured as follows. First, Section 2 presents the superstructure of a single anaerobic reactor. Section 3 shows the equations, variables and degrees of freedom that are involved in a single anaerobic digester network, which can be composed by either a UASB or a EGSB reactor. In Section 4, the network is expanded to multiple anaerobic digesters, and a degree of freedom analysis is developed as a function of the number of digesters in the network. In Section 5, results of the optimization of the anaerobic digesters network superstructures are shown and discussed. Finally, Section 6 provides the major conclusions of this work.

2. Superstructure of a single digester network

2.1. Definition of the superstructure

Naturally, the simplest reactor network superstructure is the one composed by a single reactor. Following Kokossis and Floudas [10] strategy, when there is only one reactor, besides the inlet and outlet streams, there are the recycle and the by-pass streams. Fig. 1 displays the single reactor network superstructure.

Although recycle streams are commonly used for EGSB reactors [3,25], they are not common for the UASB reactors. However, recently there have been studies of UASB reactors with recycle streams, as shown in Mahmoud [26] and Ramakrishnan and Gupta [27].

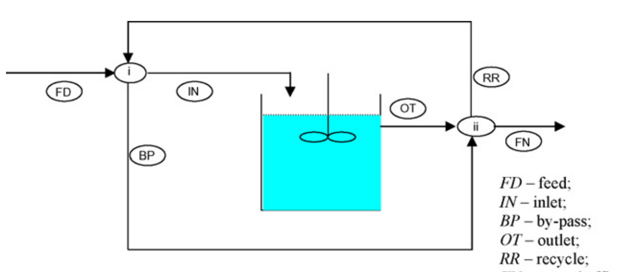


Fig. 1. Superstructure of a single reactor network.

2.2. Superstructure model

The superstructure model is composed by the kinetic and flow (or hydraulic) models of the anaerobic digester, besides the mass balances for mixers *i* and *ii* (see Fig. 1). The following assumptions are made:

A1. The substrate concentrations in stream *BP* are the same as the ones of stream *IN* ($S_{j,BPr} = S_{j,INr} \quad \forall j$);
A2. The substrate concentrations in stream *RR* are the same as the ones in stream *FN* ($S_{j,RRr} = S_{j,FN} \quad \forall j$);
A3. The effluent contaminants are in low concentration, hence there are no significant changes in the effluent flow and in the overall density once it is treated in the anaerobic digester;
A4. The concentrations of the outlet stream of reactor *r* are identical to the ones existing in the settler, in the case of an UASB reactor, or inside the reactor, in the case of an EGSB reactor ($S_{j,OTr} = S_{j,r} \quad \forall j$). To simplify the notation, the "*c*" sub-index is dropped for the concentrations in the UASB reactor settler.
A5. One of the characteristics of anaerobic digesters are that the outgoing streams can contain anaerobic sludge. To simplify the network modeling, it is considered that none of the sludge that leaves the digester is carried by the treated effluent, and also that there is no sludge present in the feed stream(s). Therefore, there is no sludge present in any stream of the superstructure ($X_{i,n} = 0, \quad \forall i, n$).
A6. The operation takes place in steady state.

Variables $S_{j,BPr}$, $S_{j,OTr}$ and $S_{j,RRr}$ are not, therefore, included in this model, according to Assumptions A1, A2 and A4. Moreover, due to Assumption A3:

$$F_{INr} - F_{OTr} = 0 \tag{1}$$

Hence, the mass balances for the mixers are given by

$$F_{FD} + F_{RRr} - F_{INr} - F_{BPr} = 0 \tag{2}$$

$$F_{BPr} + F_{OTr} - F_{RRr} - F_{FN} = 0 \tag{3}$$

$$F_{FD} \cdot S_{j,FD} + F_{RRr} \cdot S_{j,r} - F_{INr} \cdot S_{j,INr} - F_{BPr} \cdot S_{j,INr} = 0$$
$$j = \text{G, E, B, AA, H and } CO_2 \tag{4}$$

$$F_{BPr} \cdot S_{j,INr} + F_{OTr} \cdot S_{j,r} - F_{RRr} \cdot S_{j,FN} - F_{FN} \cdot S_{j,FN} = 0$$
$$j = \text{G, E, B, AA, H and CO2} \tag{5}$$

The chemical oxygen demand (COD) of a stream can be calculated by the following expression [28]:

$$COD_n = 1.33 \cdot S_{G,n} + 2.09 \cdot S_{E,n} + 1.82 \cdot S_{B,n} + 1.07 \cdot S_{AA,n} + 8.00 \cdot S_{H,n}$$
$$n = FD, IN_r, OT_r \text{ and } FN \tag{6}$$

Due to Assumptions A1 and A2, the COD values of streams BP_r and RR_r are identical to the ones of streams IN_r and *FN*, respectively.

3. Analysis of a single anaerobic digester network

3.1. Kinetic model for anaerobic digesters

Both flow models for the UASB and EGSB reactors incorporate the kinetic model based on the one elaborated and described by Kalyuzhnyi [4]. The integration of the flow and kinetic models is developed and described in [1], whose equations are summarized in Appendices A and B.

3.2. Flow model for an UASB reactor in steady state

The UASB reactor flow model is based on the one developed by [2] and is integrated in the model of [1]. According to Assumption A5, for an UASB reactor r, the discharge rate for component i of the anaerobic sludge ($DC_{i,r}$) is defined by

$$DC_{i,r} = \frac{X_{i,c,r}.F_{OT}}{V_{r,c}} \quad i = F, AE, AB, MA, MH \text{ and } I \tag{7}$$

And the total sludge discharge rate (DC_r) in reactor r is defined by

$$DC_r = \sum_i DC_{i,r} \tag{8}$$

The variables for a single UASB reactor network superstructure are given in Appendix B. The superstructure model of a single UASB reactor network has 112 variables. The UASB reactor model itself contributes with 84 variables (Appendix B).

The complete set of equations that describe the single UASB reactor network superstructure model is presented in Appendix B. This model contains 100 equations, which 81 are intrinsic to the UASB reactor and 19 to the network. Hence, the model has 12 degrees of freedom, which are:

- F_n $n = FD, RR$ and BP
- $S_{j,FD}$ j = G, E, B, AA, H and CO_2
- V_r
- A_r or h_r
- η_r

Generally, the feed stream would have its composition and flow rate defined in such optimization problem, so there would be only 4 degrees of freedom:

- F_n $n = RR$ and BP
- V_r
- A_r or h_r
- η_r

According to [2] and [29], the sludge concentration in the UASB reactor bed is constant. That value was made equal to 85 kg/m3, which is the experimental value used by [2] and within 5% of the one used by [29].

The short-circuit fractions for the UASB reactor, SF_a and SF_b, are a function of the height of both bed and blanket sections of the reactor. Bolle et al. [30] calculated these variables using a set of equations, however these were specific to that UASB reactor used in the experiment, as described in [1]. The short-circuit fractions values for this work were set arbitrarily and varied from 0 to 0.145 as shown in Section 5.

3.3. Flow model for an EGSB reactor in steady state

The flow model for an EGSB reactor is based on the experiments of [25] and those of [3].

The variables and equations for a single EGSB reactor network superstructure are given in Appendix B. For a single EGSB reactor, the superstructure network model has 65 variables. The EGSB reactor model itself contributes with 37 variables.

The single EGSB reactor superstructure model contains 53 equations, which 34 are intrinsic to the EGSB reactor and 19 to the network. As in the UASB reactor case, the EGSB reactor model has 12 degrees of freedom, which are:

- F_n $n = FD, RR$ and BP
- $S_{j,FD}$ j = G, E, B, AA, H and CO_2
- V_r
- A_r or h_r
- XT_r

Similarly for the UASB reactor, the feed stream would have its composition and flow rate fixed in an optimization problem, so there are only 5 degrees of freedom:

- F_n $n = RR$ and BP
- V_r
- A_r or h_r
- XT_r

3.4. Anaerobic digesters model constraints

The inequality constraints for an anaerobic digester can be categorized into 3 groups: non-negativity constraints, physical and operational constraints, and treated effluent quality constraints. Except for the reaction rates, all model variables are non-negative, so there is one constraint for each of them.

3.4.1. UASB reactor model constraints

In steady-state, all variables for the UASB and EGSB reactor models are continuous. Except for the substrate reaction rates, all other variables are non-negative.

It is necessary to constrain the reactor dimensions, so inconsistent designs are avoided in the optimization. Constraints (9) and (10) are based on the internal dimensions of the UASB reactors used by [2] and [29]. Neither [2] nor [29] establish an upper bound for the upflow velocity in the UASB reactor, but it is expected that a high value would dissolve the sludge bed, increase the short-circuit flow and cause undesirable sludge washout. Therefore, the proposed model would not be valid for a higher upflow velocity since the transfer of contaminants from the effluent to the bacteria would follow other mechanisms than the one proposed by the current model. More importantly, the settler efficiency would be certainly compromised as well as the entire process. Constraint (11) is also based in the same works, and the maximum liquid upflow velocity of 1.36 m/h is assumed 50% higher than the one found in [29].

$$\frac{A_r}{h_r} \leq 60\,\text{m} \tag{9}$$

$$\frac{h_r}{A_r} \leq 1.25\,\text{m}^{-1} \tag{10}$$

$$\frac{F_{IN}}{A_r} \leq 2.00\,\text{m/h} \tag{11}$$

Constraints (9)–(11) were linearized for their implementation in the models with the objective of improving solver performance. These constraints are re-written as

$$A_r - 60 \cdot h_r \leq 0 \tag{9a}$$

$$h_r - 1.25 \cdot A_r \leq 0 \tag{10a}$$

$$F_{IN} - 2 \cdot A_r \leq 0 \tag{11a}$$

Naturally, the optimization process must take into account that the treated effluent satisfies the environmental requirements of the body of water over which it will be discharged. Typically, anaerobic digesters are coupled with aerobic ones; hence, assuming there are aerobic digesters downstream, the maximum COD for the treated effluent is set 10 times higher than the required COD, whose maximum value is 0.005 kg/m^3 according to CONAMA [31].

$$COD_{FN} \leq 0.005\,\text{kg/m}^3 \tag{12}$$

Constraint (13) was added to avoid high sludge concentration in the treated effluent stream, whose maximum value was set at 1.175 kg/m^3. This value equals the sludge discharge concentration for the UASB reactor used by [2] with the lowest settler efficiency reported, 0.95. Interestingly, as it is shown in Section 5, this constraint was not active in the optimal solutions.

$$\sum_i X_{i,r,c} \le 1.175\,\mathrm{kg/m^3} \tag{13}$$

3.4.2. EGSB reactor model constraints

The non-negativity constraints for the EGSB reactor r are basically the same as those of the UASB reactor.

Kato et al. [25] present upper and lower bounds for velocity and organic charge for EGSB reactors, although other authors [3,32] operated this reactor outside those limits. According to [25], for upflow velocities lower than 5.5 m/h and maximum organic loads inferior to 7 kg COD/m^3 d, there is no sludge washout from the reactor. There is also a limitation for the organic load, since excess methane gas production rate could lead to the mentioned washout. The same authors recommend that the upflow velocity be no less than 2.5 m/h otherwise the sludge would settle at the bottom of the reactor. Therefore, the following constraints are valid:

$$\frac{F_{IN}}{A_r} \le 5.5\,\mathrm{m/h} \tag{14}$$

$$\frac{F_{IN}}{A_r} \ge 2.5\,\mathrm{m/h} \tag{15}$$

$$OL_r = \frac{24 \cdot COD_{IN} \cdot F_{IN}}{V_r} \le OL_{r,\max} = 7\,\mathrm{g/m^3\ d} \tag{16}$$

Similarly to the UASB reactor, a constraint was added for the ratio of reactor dimensions.

$$\frac{h_r}{A_r} \le 1000\,\mathrm{m^{-1}} \tag{17}$$

This maximum value for the height/area ratio in Constraint (17) is set to approximately twice the value of the EGSB reactor used by [25].

Moreover, the EGSB reactor constraints are also linearized to

$$F_{IN} - 5.5 \cdot A_r \le 0 \tag{14a}$$

$$2.5 \cdot A_r - F_{IN} \le 0 \tag{15a}$$

$$h_r - 1000 \cdot A_r \le 0 \tag{17a}$$

As technology advances, there are significant enhancements to the EGSB reactor and the microorganisms used in anaerobic digestion, pushing the operational limits of the EGSB reactor to new boundaries. Jeison and Chamy [33] mentioned values for the upflow velocity inside the EGSB reactor higher than the ones mentioned by [25]. Thus

$$F_{IN} - 10 \cdot A_r \le 0 \tag{14b}$$

Van Lier et al. [32] experimented on an EGSB reactor operating with organic loads of 12 kg of COD/m^3 d that corresponds to a value significantly higher than the one presented by [25] as the maximum organic load for an EGSB reactor. Hence

$$OL_{r,\max} = 12\,\mathrm{kg/m^3\ d} \tag{16a}$$

The treated effluent quality constraints (12) and (13) that were defined for the UASB reactor are also applied to the EGSB reactor model.

4. Networks of multiple anaerobic digesters

4.1. Superstructure of a two anaerobic digester network

A network of multiple reactors allows solutions that combine anaerobic digesters, even different ones, but it also makes its superstructure representation more complex. For the sake of illustration, Fig. 2 shows a two-reactor network.

Besides the recycle and by-pass streams, the superstructure contemplates other streams. For instance, if either stream S_{1-2} and/or S_{2-1} exist in the superstructure it yields a serial configuration for the network. There are also the $\mathrm{MR_r}$ streams that recycle the treated effluent streams to reactor r.

4.1.1. Mass balances for a superstructure of a two anaerobic digester network

The following assumptions are made, besides A1 through A5, for any substrate j and reactor r:

A6 The substrate concentrations in stream RF_r for all reactors are the same as those of stream FD ($S_{j,RFr} = S_{j,FD}$);
A7 The substrate concentrations in stream $S_{r-r'}$ are the same as those of stream RM_r ($S_{j,Sr-r'} = S_{j,RMr}$);
A8 The substrate concentrations in stream MR_r are the same as those of stream FN ($S_{j,MRr} = S_{j,FN}$);

The mass balances for the mixers and splitters are

$$\text{(i)}\ F_{FD} = F_{RF1} + F_{RF2} \tag{18}$$

$$\text{(ii)}\ F_{RF1} + F_{RR1} + F_{S2-1} + F_{MR1} = F_{BP1} + F_{IN1} \tag{19}$$

$$\begin{aligned} &F_{RF1} \cdot S_{j,FD} + F_{RR1} \cdot S_{j,1} + F_{S2-1} \cdot S_{j,2} + F_{MR1} \cdot S_{j,FN} \\ &\quad = (F_{IN1} + F_{BP1}) \cdot S_{j,IN1} \qquad j = \mathrm{G,\ E,\ B,\ AA,\ H\ and\ CO_2} \end{aligned} \tag{20}$$

$$\text{(iii)}\ F_{BP1} + F_{OT1} = F_{RR1} + F_{S1-2} + F_{RM1} \tag{21}$$

$$\begin{aligned} &F_{BP1} \cdot S_{j,IN1} + F_{OT1} \cdot S_{j,1} = (F_{RR1} + F_{S1-2}) \cdot S_{j,1} + F_{RM1} \cdot S_{j,RM1} \\ &j = \mathrm{G,\ E,\ B,\ AA,\ H\ and\ CO_2} \end{aligned} \tag{22}$$

$$\text{(iv)}\ F_{RF2} + F_{RR2} + F_{S1-2} + F_{MR2} = F_{BP2} + F_{IN2} \tag{23}$$

$$\begin{aligned} &F_{RF2} \cdot S_{j,FD} + F_{RR2} \cdot S_{j,2} + F_{S1-2} \cdot S_{j,1} + F_{MR2} \cdot S_{j,FN} \\ &\quad = (F_{IN2} + F_{BP2}) \cdot S_{j,IN2} \qquad j = \mathrm{G,\ E,\ B,\ AA,\ H\ and\ CO_2} \end{aligned} \tag{24}$$

$$\text{(v)}\ F_{BP2} + F_{OT2} = F_{RR2} + F_{S2-1} + F_{RM2} \tag{25}$$

$$\begin{aligned} &F_{BP2} \cdot S_{j,IN2} + F_{OT2} \cdot S_{j,2} = (F_{RR2} + F_{S2-1}) \cdot S_{j,2} + F_{RM2} \cdot S_{j,RM2} \\ &j = \mathrm{G,\ E,\ B,\ AA,\ H\ and\ CO_2} \end{aligned} \tag{26}$$

$$\text{(vi)}\ F_{RM1} + F_{RM2} = F_{FN} + F_{MR1} + F_{MR2} \tag{27}$$

$$\begin{aligned} &F_{RM1} \cdot S_{j,RM1} + F_{RM2} \cdot S_{j,RM2} = (F_{FN} + F_{MR1} + F_{MR2}) \cdot S_{j,FN} \\ &j = \mathrm{G,\ E,\ B,\ AA,\ H\ and\ CO_2} \end{aligned} \tag{28}$$

Splitter (i) and mixer (vi) are denominated henceforth in this paper as the feed splitter and the final mixer.

4.1.2. Degrees of freedom in a superstructure of a two anaerobic digester network model

The number of equations and variables involved in the model depend on the type(s) of anaerobic digester(s) used in the superstructure. As previously mentioned, the UASB reactor has 84

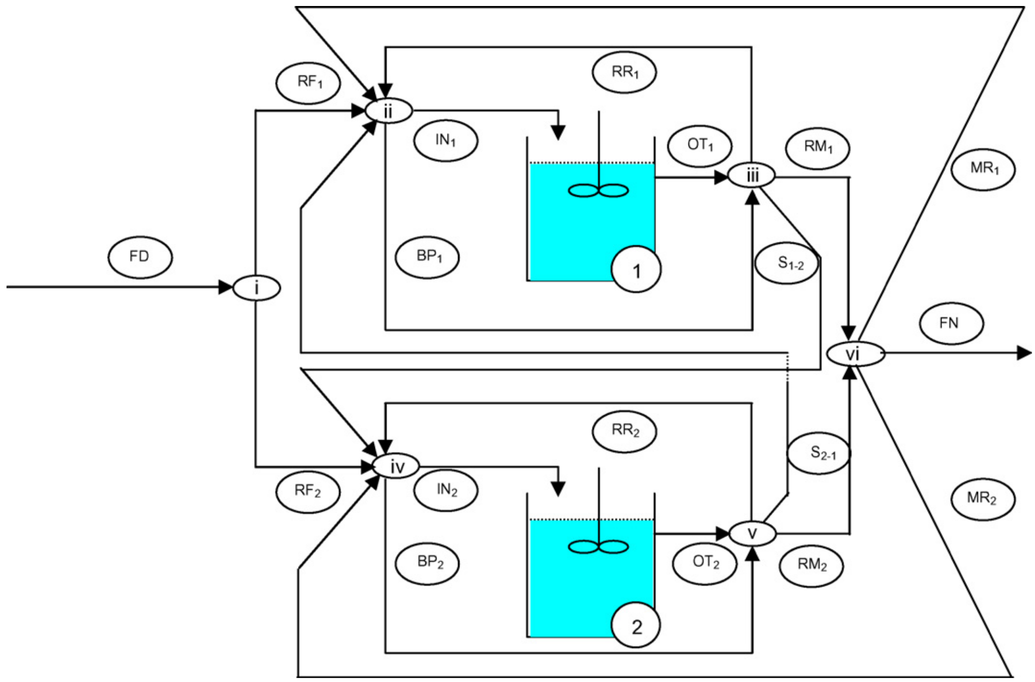


Fig. 2. Two-reactor network superstructure.

variables and 81 equations, and the EGSB reactor has 37 variables and 34 equations. Interestingly, there are 3 degrees of freedom per reactor (V_r, h_r or A_r, and η_r-UASB or XT_r-EGSB), regardless of its type.

The network itself contributes with 60 variables and 44 equations, all given in Appendix C. The network, therefore, has 16 degrees of freedom, which are

- F_n n = FD, BP_r, RR_r, $S_{r-r'}$ and MR_r; r = 1 and 2, $r \neq r'$
- F_n n = RF_r; r = 1 or 2
- $S_{j,FD}$ j = G, E, B, AA, H and CO_2

Therefore, the number of equations, NE_2, for the two anaerobic digesters network superstructure model in steady state is given by the following equation:

$$NE_2 = 44 + 81 \cdot RU + 34 \cdot RE \tag{29}$$

where

RU number of UASB reactors present in the network
RE number of EGSB reactors present in the network

$$RU + RE = 2 \tag{30}$$

The number of variables, NV_2, is given by

$$NV_2 = 60 + 84 \cdot RU + 37 \cdot RE \tag{31}$$

Therefore, the number of degrees of freedom, NF_2, is given by

$$NF_2 = 16 + 3 \cdot RU + 3 \cdot RE \tag{32}$$

Substituting (30) into (32) yields $NF_2 = 22$, which means that the number of degrees of freedom of the optimization model does not depend on the type of anaerobic digester selected for the network superstructure.

4.2. Mass balances for a superstructure of a multiple anaerobic digesters network

From Fig. 2, the necessary equations can be inferred in order to describe a network containing multiple anaerobic digesters. In a network with R reactors ($R > 1$), the following equations can be defined:

For the feed (FD) splitter:

$$F_{FD} = \sum_{r}^{R} F_{RF_r} \tag{33}$$

For the reactor r upstream mixer:

$$F_{RF_r} + F_{RR_r} + F_{MR_r} + \sum_{r' \neq r}^{R} F_{S_{r'-r}} = F_{BP_r} + F_{IN_r} \quad r = 1, \ldots, R \tag{34}$$

$$F_{RF_r} \cdot S_{j,FD} + F_{RR_r} \cdot S_{j,r} + F_{MR_r} \cdot S_{j,FN} + \sum_{r' \neq r}^{R} F_S \cdot S_{j,r'} = (F_{BP_r} + F_{IN_r}) \cdot S_{j,IN_r} \quad r = 1, \ldots, R \quad j = \text{G, E, B, AA, H and } CO_2 \tag{35}$$

For the reactor r downstream mixer:

$$F_{BP_r} + F_{OT_r} = \sum_{r' \neq r}^{R} F_{S_{r-r'}} + F_{RR_r} + F_{RM_r} \quad r = 1, \ldots, R \tag{36}$$

$$F_{BP_r} \cdot S_{j,IN_r} + F_{OT_r} \cdot S_{j,r} = \left(\sum_{r' \neq r}^{R} F_{S_{r-r'}} + F_{RR_r} \right) \cdot S_{j,r} + F_{RM_r} \cdot S_{j,RM_r} \quad r = 1, \ldots, R \quad j = \text{G, E, B, AA, H and } CO_2 \tag{37}$$

For each reactor r:

$$F_{IN_r} = F_{OT_r} \quad r = 1, \ldots, R \tag{38}$$

And for the final mixer:(39) $\sum_{r}^{R} F_{RM_r} = F_{FN} + \sum_{r}^{R} F_{MR_r}$

$$\sum_{r}^{R} F_{RM_r} \cdot S_{j,RM_r} = (F_{FN} + \sum_{r}^{R} F_{MR_r}) \cdot S_{j,FN}$$
$$j = \text{G, E, B, AA, H and } CO_2 \quad (40)$$

Besides these equations, Eq. (6) that defines the values of COD_n must also be added.

4.3. Degrees of freedom in a multiple anaerobic digester network superstructure

From item 4.1.1, in a network with R anaerobic digesters, there are $(17 \cdot R + 10)$ equations for the network itself (excluding the ones intrinsic to the digesters). The network itself has $(R^2 + 20 \cdot R + 16)$ variables, which are given in Appendix B. Hence the number of equations of the network superstructure model is given by

$$NE_R = 17 \cdot R + 81 \cdot RU + 34 \cdot RE + 10 \quad (41)$$

and the number of variables is given by

$$NV_R = R^2 + 20 \cdot R + 84 \cdot RU + 37 \cdot RE + 16 \quad (42)$$

Hence the number of degrees of freedom is given by

$$NF_R = R^2 + 3 \cdot R + 3 \cdot RU + 3 \cdot RE + 6 \quad (43)$$

And remembering that:

$$RU + RE = R \quad (44)$$

which yields:

$$NF_R = R^2 + 6 \cdot R + 6 \quad (45)$$

Again, Eq. (45) shows that the number of degrees of freedom of the network does not depend on the type of reactors selected.

The following variables can be considered as optimization variables:

- For the network:
  - F_n $n = FD, BP_r, RR_r, MR_r, S_{r-r'}$; $r = 1, \ldots, R$ $r' \neq r$
  - F_n $n = RF_r$ $r = 1, \ldots, R$ for $(k-1)$ reactors
  - $S_{j,FD}$ j = G, E, B, AA, H and CO_2
- For each UASB reactor r:
  - V_r $r = 1, \ldots, RU$
  - A_r or h_r $r = 1, \ldots, RU$
  - η_r $r = 1, \ldots, RU$
- For each EGSB reactor r:
  - V_r $r = 1, \ldots, RE$
  - A_r or h_r $r = 1, \ldots, RE$
  - X_r $r = 1, \ldots, RE$

There are only non-negativity constraints for the variables that are intrinsic to the network. Hence, these constraints are

$$F_n \geq 0 \quad \forall n \quad (46)$$

$$S_{j,n} \geq 0 \quad \forall n, j = \text{G, E, B, AA, H and } CO_2 \quad (47)$$

4.4. Objective function

The objective function of the network superstructure may target the overall cost reduction of the wastewater treatment. The optimizations performed in the current work, relied on a simple objective function which only targets the reduction of the overall volumes, ignoring other costs. Therefore, the objective function is:

$$\min \ RC = \sum_{r}^{R} RC_r \cdot V_r \quad (48)$$

Initially, RC_r was set to 1 for all kind of reactors.

An economical objective function could be used, but it would require parameters, such as detailed design and operational costs for individual reactors, which are not available in the literature and not provided by manufacturers.

Table 1
Effluent to be treated by the anaerobic digester networks.

Parameter	Value	Unit
F_{IN}	200	m^3/h
$S_{AA,IN}$	3	kg/m^3
$S_{j,IN}$ ($j \neq AA$)	0	kg/m^3
COD_{IN}	3.21	kg/m^3

5. Computational results

The resulting mathematical model for the anaerobic digester network is a NLP problem. The model was implemented and optimized in *GAMS V*2.25 [34] using the global optimization *BARON* [35] and the local optimization *CONOPT* [36] solvers, using a PC platform with Intel® Core™2 CPU, 1.86 GHz and 0.99 GB of RAM. There are no constraints for minimum values for digesters volumes and stream flowrates.

All the variables and expressions were finitely bounded, which according to Sahinidis and Tawarmalani [35] guarantees the global optimum. Regarding the optimality of the solver, in general the local solver CONOPT can be sensitive to the initial point. The global optimality of the smaller problems was guaranteed by solving them with BARON. These problems provide upper bounds and in fact their optimal solutions serve as initial points for the larger problems. This strategy was used throughout the paper and did not yield local optima. Furthermore, the solutions can be in principle degenerate. Networks with two or more reactors of the same type could present solutions with the same objective function value and different combinations of reactors. In order to avoid degeneracy, we added a small epsilon value to penalize reactors with higher indices. For instance, in the case of 4 reactors, indices 1 and 3 refer to UASB reactors; the selection of index 3 is "ε more expensive" than that of index 1.

Table 2
Optimal solutions for cases U1–U4 for one UASB reactor.

Variable	Case U1	Case U2	Case U3	Case U4	Unit
$SF_a = SF_b$	0.145	0.100	0.050	0.000	–
V_r	19665.8	8363.9	2160.5	226.5	m^3
$V_{r,a}$	2710.9	1656.0	36.7	4.3	m^3
$V_{r,b}$	13316.7	5160.6	1724.1	180.3	m^3
$V_{r,c}$	3638.2	1547.3	399.7	41.9	m^3
A_r	1086.3	708.4	360.0	116.6	m^2
h_r	18.10	11.81	6.00	1.94	m
ν	1.82	2.00	2.00	2.00	m/h
$X_{b,r}$	15.3	23.8	30.0	30.0	kg/m^3
$X_{MA,r,a}$	5.7	9.3	39.2	81.2	kg/m^3
$X_{MA,r,b}$	1.0	2.6	13.8	28.7	kg/m^3
$X_{I,r,a}$	79.3	75.7	45.8	3.7	kg/m^3
$X_{I,r,b}$	14.3	21.2	16.2	1.3	kg/m^3
η_r	0.9984	0.9999	0.9997	0.997	–
COD_{FN}	0.050	0.050	0.050	0.050	kg/m^3
F_{IN}	2172.5	1416.8	720.1	233.2	m^3/h
F_{RR}	1972.5	1216.8	520.1	33.2	m^3/h
F_{BP}	0.0	0	0	0	m^3/h

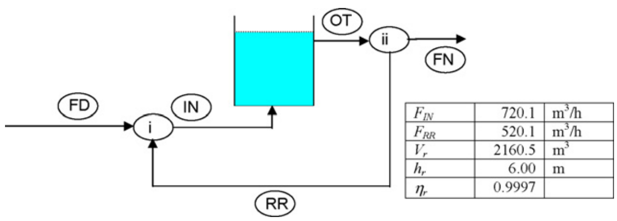


Fig. 3. Optimal solution configuration for case U3.

Table 1 presents the characteristics of the feed stream for all the optimization cases.

5.1. *Optimization of a single anaerobic digester network superstructure*

For a network superstructure that contemplates only a single UASB reactor, sensitivity analysis was done for the short-circuit fractions. Table 2 describes the condition of the cases studied, as well as their optimal solutions. The UASB reactor short-circuit flow has an important effect on the reactor efficiency, and the values for SF_a and SF_b were set to 0.145 (Case U1), 0.100 (Case U2), 0.05 (Case U3) and 0 (Case U4).

The upflow velocity is defined as

$$v = \frac{F_{IN}}{A_r} \tag{49}$$

The fact that the concentration of the endogenous residue is about 14 times larger than the acetoclastic methanogenic means that the volume could be smaller, if it were not for the short-circuit flow streams. If a recycle stream could not be used, there would always be a lower bound for the COD of the treated effluents due to short-circuiting. As the short-circuit fraction value is decreased, the volumes found in Optimal Solutions U2, U3 and U4 decrease, showing their strong influence in the efficiency of the UASB reactor. The volume for the UASB reactor in Optimal Solution U1 is approximately 10 times larger than the one used in the experiments described by [2], and this is due to constraints (11) and (12), which limit the upflow velocity in the reactor and the COD of the treated effluent. Anh [37] establishes the following simplified design criteria for an UASB reactor for effluents with COD inlet lower than 5 kg/m^3:

$$v = 0.5\ \text{m/h} \tag{50}$$

$$4.2\,\text{m} < h_r < 6.2\,\text{m} \tag{51}$$

$$h_{r,c} = 1.2\,\text{m} \tag{52}$$

The upflow velocity bound is 4 times smaller than the maximum value set by Constraint (11). Such constraint yields a cross-sectional area for the UASB reactor of 400 m^2. Interestingly, the reactor

Table 3
Organic load constraint variation for a network of a single EGSB reactor.

Case	Constraint		By-pass stream
E1	$OL_r \le 12\,\text{kg/m}^3\,\text{d}$	(16a)	None
E2	$OL_r \le 7\,\text{kg/m}^3\,\text{d}$	(16b)	None
E3	$OL_r \le 20\,\text{kg/m}^3\,\text{d}$	(16c)	None
E4	$OL_r \le 40\,\text{kg/m}^3\,\text{d}$	(16d)	None
E5	$OL_r \le 12\,\text{kg/m}^3\,\text{d}$	(16a)	Present
E6	$OL_r \le 7\,\text{kg/m}^3\,\text{d}$	(16b)	Present
E7	$OL_r \le 20\,\text{kg/m}^3\,\text{d}$	(16c)	Present
E8	$OL_r \le 40\,\text{kg/m}^3\,\text{d}$	(16d)	Present

Table 4
Optimal solutions for cases E1–E4 (single EGSB reactor without by-pass).

Variable	Case E1	Case E2	Case E3	Case E4	Unit
V_r	1280.4	2194.4	768.0	384.0	m^3
A_r	49.8	80.0	39.9	36.4	m^2
h_r	25.70	27.4	19.2	10.6	m
v	4.0	2.5	5.0	5.5	m/h
X_r	28.2	30.0	30.0	30.0	kg/m^3
$X_{MA,r}$	17.6	12.1	23.2	27.1	kg/m^3
$X_{I,r}$	10.6	17.9	6.8	2.9	kg/m^3
F_{IN}	200.0	200.0	200.0	200.0	m^3/h
OL_r	12	7	20	40	kg/m^3 d
COD_{FN}	0.012	0.010	0.015	0.028	kg/m^3
F_{RR}	0.0	0.0	0.0	0.0	m^3/h
F_{BP}	0.0	0.0	0.0	0.0	m^3/h

Table 5
Optimal solution for cases E5–E8 (single EGSB reactor with by-pass).

Variable	Case E5	Case E6	Case E7	Case E8	Unit
V_r	1264.6	2166.7	759.6	381.3	m^3
A_r	49.2	79.0	39.6	36.1	m^2
h_r	25.72	27.4	19.2	10.6	m
v	4.02	2.5	5.0	5.5	m/h
X_r	30.0	30.0	30.0	30.0	kg/m^3
$X_{MA,r}$	18.0	12.1	23.2	27.1	kg/m^3
$X_{I,r}$	12.0	17.9	6.8	2.9	kg/m^3
F_{IN}	197.6	197.5	197.8	198.6	m^3/h
OL_r	12	7	20	40	kg/m^3 d
COD_{FN}	0.050	0.050	0.050	0.050	kg/m^3
F_{RR}	0.0	0.0	0.0	0.0	m^3/h
F_{BP}	2.4	2.5	2.2	1.4	m^3/h

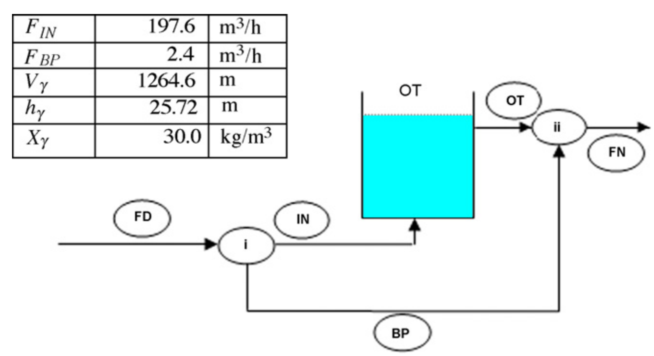


Fig. 4. Optimal solution for configuration E5.

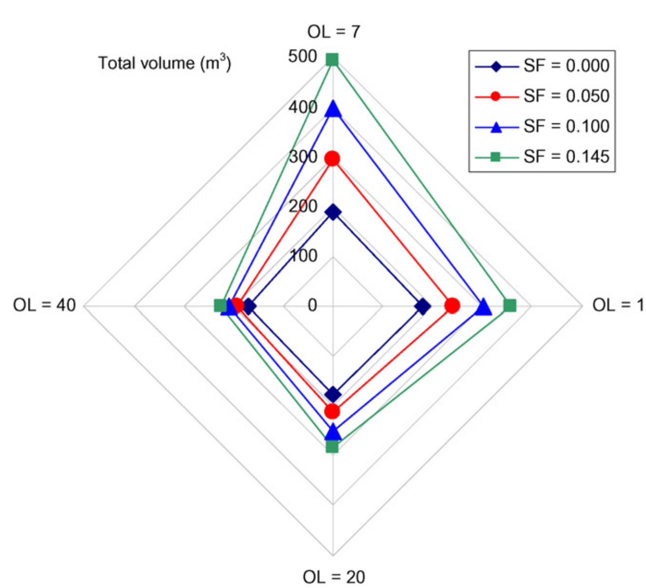


Fig. 5. Total volumes of the two-digester networks (m^3) for the 16 cases studied, values for OL in kg/m^3/d.

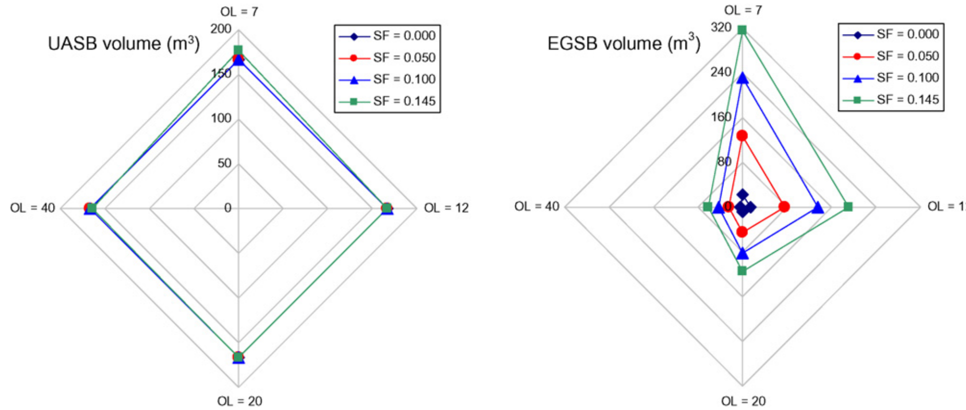


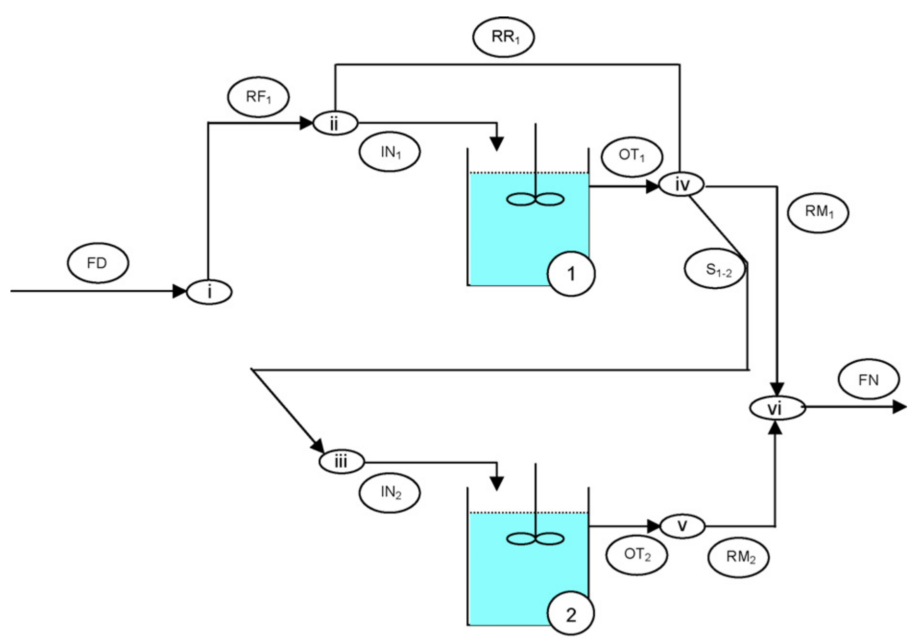
Fig. 6. UASB and EGSB reactor volumes (m^3) for the 16 two-digesters network cases studied, values for *OL* in $kg/m^3/d$.

dimensions for Case U3 are relatively close to the ones presented by Ahn's design criteria.

Fig. 3 shows the configuration of the optimal solution of Case U3.

For a network superstructure that presents a single EGSB reactor *r*, the feed stream characteristics were the same as the ones for the optimization of a single UASB reactor network. Sensitivity analysis was performed in the maximum organic load that the EGSB reactor can process, described by Constraint (16). Table 3 displays the values used for the organic load constraint. Parameter values in constraints (16a), (16c) and (16d) correspond to the limits set by [32] for EGSB reactor operation, while constraint (16b) is based on the value set by [25] as the maximum organic load for an EGSB reactor. A comparison was also done for network superstructures with and without the by-pass stream.

The optimal solutions of Table 4 indicate the sensitivity of the EGSB reactor in a network regarding the maximum organic load. As expected, as the value of the maximum organic load increases, the volume of EGSB reactor decreases. In Cases E2 and E4, the velocity constraints (14) and (15) are active, while the dimension constraint (17) is non-binding for either case.



F_{RR1}	5.7	m^3/h
F_{IN1}	205.7	m^3/h
V_1	176.3	m^3
h_1	1.67	m
η_1	0.997	
SF_1	0.145	

F_{IN2}	183.7	m^3/h
F_{RM2}	183.7	m^3/h
V_2	315.7	m^3
h_2	4.30	m
X_2	30.0	kg/m^3
OL_2	7	$kg/m^3.d$

Fig. 7. Network configuration for optimal solution T1 ($r = 1$, UASB reactor, $r = 2$, EGSB reactor).

The most surprising result from Optimal Solutions E1–E4 is the absence of a recycle stream for all cases. That would be expected for a CSTR as shown in Appendix D. The fact that the values of COD_{FN} are smaller than 0.005 kg/m^3 shows that the volume could be decreased and Constraint (12) would be respected. However, that does not happen due to the limitation of the maximum organic load for an EGSB reactor. The use of a by-pass stream solves this problem as shown in the optimal solutions E5–E8 in Table 5.

With the use of a by-pass stream, there is an approximately 1% decrease in the optimal volume for the EGSB reactor. The values of COD_{FN} for these optimal solutions correspond to their upper bound as in Constraint (12).

Fig. 4 shows the configuration of Optimal Solution E5.

The computational times for the optimization of one-reactor network superstructures were all under 1 min. Model dimensions are provided in Appendices A and B.

The sludge concentration in the treated effluent is lower than 0.01 kg/m^3 for all optimal solutions, showing that Constraint (13) is non-binding.

In all cases BARON used less than 10 s to find global solutions and CONOPT less than 0.1 s to find local ones.

5.2. Optimization of a two-anaerobic digester network superstructure

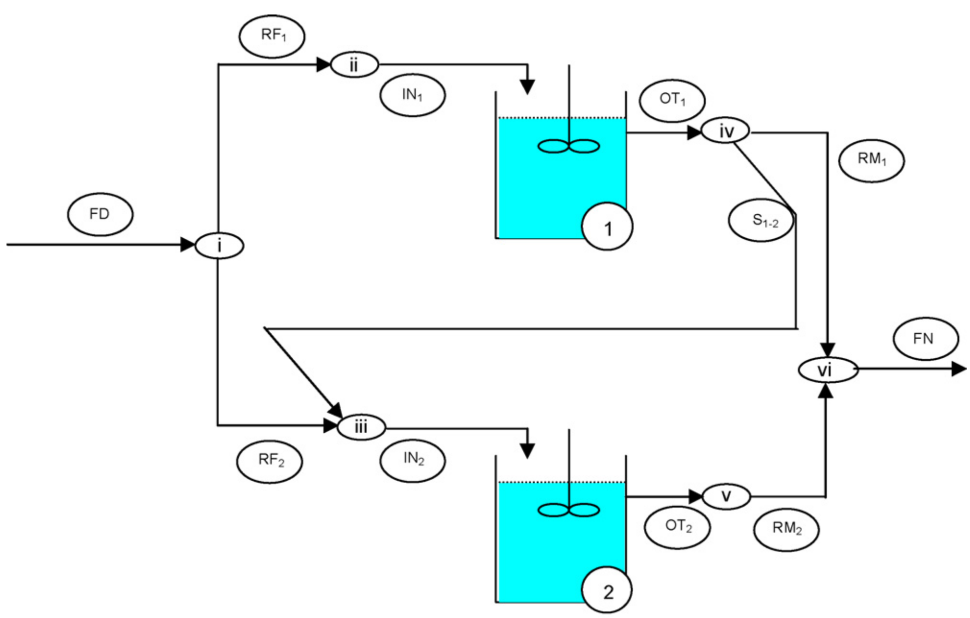
The two anaerobic digesters network superstructure considers only the configuration of a network containing one UASB and one EGSB reactor. The network could contain two UASB reactors or two EGSB reactors, but the objective is to show that with different types of digesters, the wastewater treatment process can be significantly improved.

Sixteen cases were studied, and the optimal solutions found for these cases are given in Figs. 5 and 6. The short-circuit fraction for the UASB reactor was varied from 0 to 0.145, and the maximum organic load rate for the EGSB reactor was varied from 7 to 40 kg m^3/d.

The comparison of the optimal solutions for the 16 cases shows again the strong influence of the UASB reactor short-circuit stream on the network configuration. As expected, as the fractions of the short-circuit streams increase as seen in Fig. 6, so does the EGSB reactor volume, but the UASB reactor remains the same except when the short-circuit fraction is 0.145. A larger UASB reactor volume would not reduce proportionally the COD, while a smaller one would compromise final treatment in the EGSB reactor. A recycle stream exists only for the case with the highest short-circuit fractions ($SF = 0.145$) for the UASB reactor and lowest maximum organic load for the EGSB reactor ($OL \leq 7$). As noticed previously in the one-digester network scenarios, as the maximum organic load for the EGSB reactor is increased, the EGSB reactor volume decreases.

The computational time for the global optimization of the two-digester network superstructures with BARON varied from 30 s to 16 min. CONOPT demanded less than 0.2 s in all cases to find local optima.

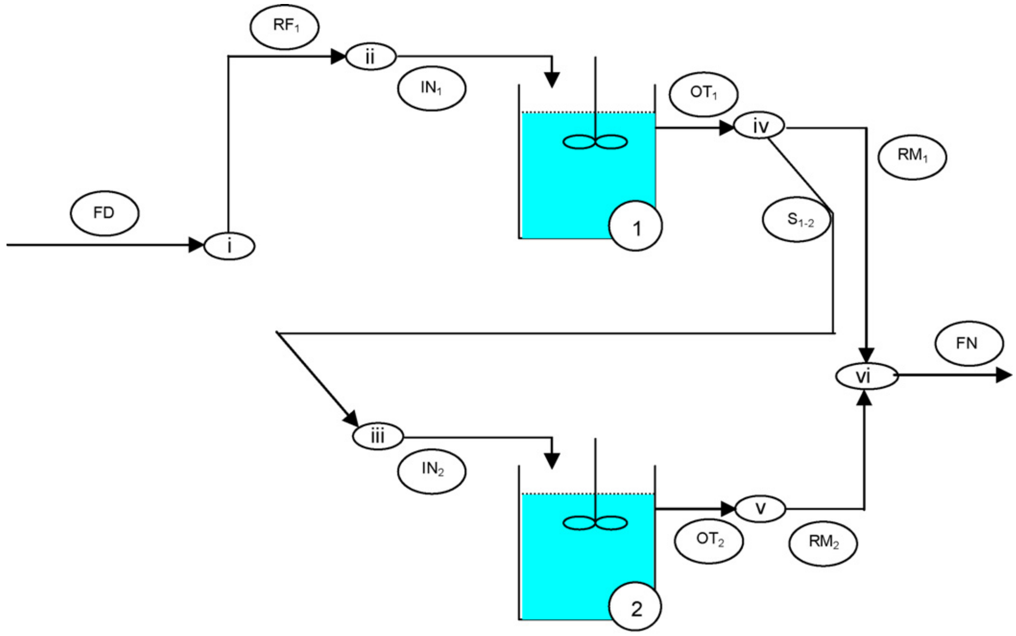
Figs. 7–9 show the optimal configurations for some of the two-digester networks. Cases, T1, T2 and T3 correspond respectively to $SF_1 = 0.145$ and $OL_{2,max} = 7$, 12 and 40 kg/m^3 d.



F_{RF1}	198.9	m^3/h
F_{IN1}	198.9	m^3/h
V_1	164.7	m^3
h_1	1.66	m
η_1	0.997	
SF_1	0.145	

F_{IN2}	190.4	m^3/h
F_{RM2}	190.4	m^3/h
V_2	115.1	m^3
h_2	1.55	m
X_2	30.0	kg/m^3
OL_2	40	kg/m^3.d

Fig. 8. Network configuration for optimal solution T2 ($r = 1$, UASB reactor, $r = 2$, EGSB reactor).



F_{RF1}	200.0	m^3/h
F_{RF2}	0.0	m^3/h
$F_{S1\text{-}2}$	184.7	m^3/h
$F_{S1\text{-}4}$	0.0	m^3/h
$F_{S2\text{-}4}$	0.0	m^3/h
F_{RM1}	15.3	m^3/h

F_{RM2}	184.7	m^3/h
V_1	166.7	m^3
V_2	190.6	m^3
V_3	0.0	m
SF_1	0.145	
$OL_{2,4}$	12	$kg/m^3.d$

Fig. 9. Network configuration for optimal solution T3 (r = 1, UASB reactor, r = 2, EGSB reactor).

Figs. 7 and 9 represent network configurations where the reactors are in series, whereas Fig. 8 represents a network where the reactors are both in series and in parallel.

All the four cases for two-digester networks consider that the costs for the UASB and EGSB reactors are the same. A sensitivity analysis was performed to study how different costs ratios (C_r) between the two reactors affect the optimal solution. The values for C_r were varied from 0.1 to 1, for which $SF_1 = 0.145$ and $OL_{2,\max} = 12\,kg/m^3\,d$. Fig. 10 shows the results for these cases. Interestingly, when C_1 is approximately the same as C_2, the value for the objective function, RC, is not changed. Only for $0.5 < C_1/C_2 < 2$, the optimal values for the digesters volumes are altered.

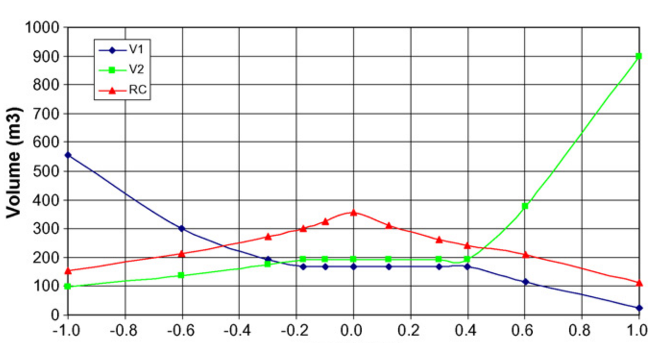


Fig. 10. Sensitivity analysis for different costs between different types of reactors in a two-digesters network (r = 1, UASB reactor, r = 2, EGSB reactor).

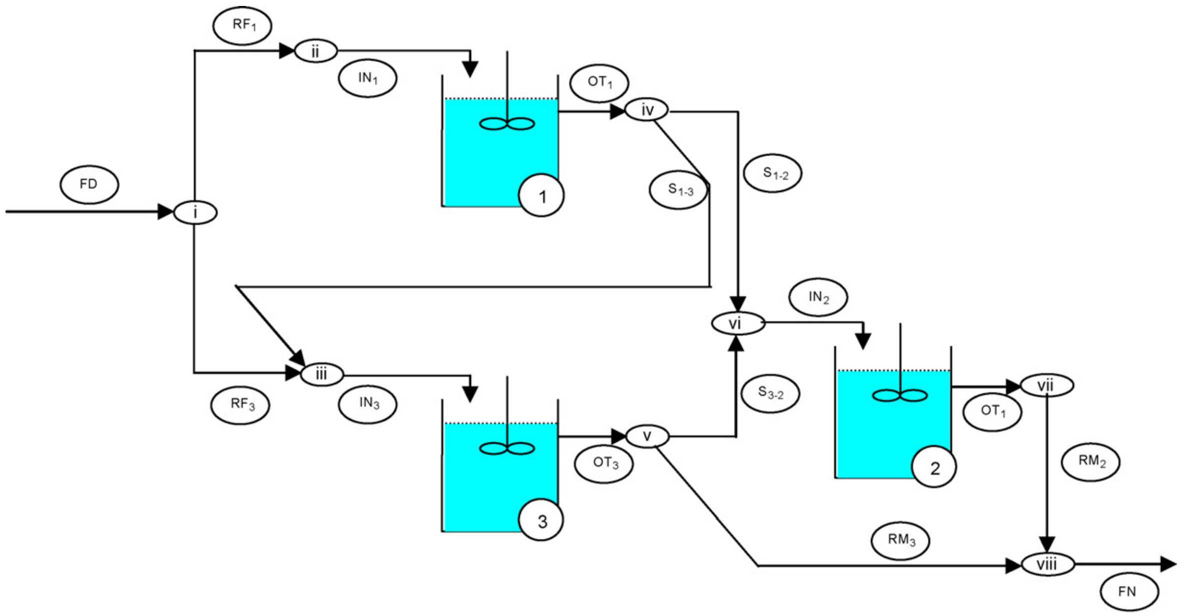
5.3. *Optimization of a three-anaerobic digester network superstructure*

The three-anaerobic digester network superstructure contains the configuration of two UASB and one EGSB reactors, as well as one UASB and two EGSB reactors. The network could in principle contain three UASB reactors or three EGSB reactors, but the objective is to show that with different types of digester, the wastewater treatment process can be significantly improved.

For the EGSB reactor(s), the value for maximum organic load, Constraint (16), was $12\,kg/m^3\,d$, while the UASB reactor(s) short-circuit fraction was 0.145.

Two cases were studied for this network superstructure; Case H1 denotes a network with 2 UASB reactors and 1 EGSB reactor, while Case H2 denotes a network with 1 UASB reactor and 2 EGSB reactors. The optimal solution for Case H1 is given in Fig. 11.

Comparing Case H1 (network of 2 UASB reactors and 1 EGSB reactor) with the two-digester network (Case T3), which has the same short-circuit fraction and maximum organic load values of Case H1, the extra UASB reactor in the network yields a 19% reduction in the objective function value, RC, 288.3 m^3 Case H1 and 357.3 m^3 for Case T3. This is because the two UASB reactors in this network are basically connected in series. However, for Case H2 (network of 1 UASB reactor and 2 EGSB reactors), there is no reduction in RC from the two-digesters network solution, actually both have only one EGSB reactor in the optimal solution, therefore the solutions for Cases T3 and H2 are identical. The minimum volume for the EGSB reactor is not limited by the efficiency of the reactor to remove COD, as the UASB reactor, but by Constraint (16),



F_{RF1}	137.4	m^3/h
F_{RF3}	62.6	m^3/h
F_{S1-2}	72.5	m^3/h
F_{S1-3}	64.8	m^3/h
F_{S3-2}	101.1	m^3/h
F_{RM2}	173.6	m^3/h

F_{RM3}	26.4	m^3/h
V_1	78.6	m^3
V_2	142.0	m^3
V_3	67.7	m
$SF_{1,3}$	0.145	
OL_2	12	$kg/m^3.d$

Fig. 11. Network configuration for optimal solution H1 ($r = 1$ and 3, UASB reactors, $r = 2$, EGSB reactor).

the minimum organic load rate. Hence, there is no gain in using two EGSB reactors in series, since to satisfy Constraint (16), the first EGSB reactor volume is sufficient to remove all the required COD. The computational time of the optimization increased exponentially with the addition of the third digester to the network superstructure. For Case H1, the computational time required by BARON was about 12 h, while for Case H2 it was about 21 h. CONOPT required less than 0.2 CPU s to find an optimal solution in both cases.

Interestingly, Diamantis and Aivasidis [38] investigated a special case of the network studied in H1 and verified experimentally that the operation of a two-stage UASB reactor yielded a 50% reduction of methanization volume compared to a single-stage UASB reactor operation. There are also published works of 2-digester networks in series used for anaerobic digestion. Melidis et al. [39] made use of 2 UASB reactors, while Vankataraman et al. [40] made use 2 upflow packed-bed reactors.

5.4. Optimization of a four-anaerobic digester network superstructure

The four anaerobic digesters network superstructure contemplates the configuration of a network containing two UASB and two EGSB reactors. Case F1 was studied for this network superstructure. For the EGSB reactor(s), the value for maximum organic load, Constraint (16), was 12 kg/m^3 d, while the UASB reactor(s) short-circuit fraction was 0.145.

Solution to Case F1 was found after 80 h of optimization, although *BARON* could not converge to a global optimal, and the local optimal solution (found by *CONOPT* in 0.05 CPU s) was exactly the same as the one found in Case H1. As previously explained, due to Constraint (16) the addition of an extra EGSB reactor to the network does not reduce the value of the objective function. According to the model developed by the current work, only the addition of an extra UASB reactor, nevertheless, would in theory reduce the value of the objective function.

6. Conclusions

The present paper addresses the mathematical modeling of an anaerobic digesters network for optimal synthesis. It creates a superstructure containing UASB and EGSB reactors, as well as the streams that connect these reactors to the feed stream and to the final stream. The network superstructure contains the UASB and EGSB reactors models developed by [1], as well as network balance constraints. The proposed model also contains operational limits, non-negativity constraints and treated effluent quality constraints. The resulting model is a non-linear programming (NLP) problem that is solved to global optimality.

Networks of one up to four digesters are optimized and sensitivity analysis was done on two main process parameters, namely the short-circuit fraction in the UASB reactor and the maximum organic load rate for the EGSB reactor. It is shown that a recycle stream is only effective in case of a reactor with short-circuit, such as the UASB reactor, which is confirmed by the optimization of the one-reactor network superstructure. For the UASB reactor network, there is a recycle stream present, but not for the EGSB reactor. In the latter, a by-pass stream is present due to the maximum organic load constraint.

As the network size increases, the value for the objective function, which aims for the reduction of the overall digester volumes, decreases as expected. However, due to the maximum organic load constraint for the EGSB reactor, the inclusion of an extra EGSB reactor in the network does not improve the design of the process. It is also verified that the addition of a digestor to the network also increases drastically the computational time to solve the optimization model to global optimality.

The current paper does not aim to be a tool for designing an anaerobic digester plant, but instead it systemically investigates complex configurations for anaerobic digestion treatment based on the optimization of reactor network superstructure. It proposes multiple digester configurations that achieve COD removal efficiency that would only be achieved by extremely large single reactors or even none at all. The methodology presented here can also be adapted to optimize UASB and EGSB reactors that are described by more complex models such as the ones that present axial dispersion.

Acknowledgements

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Appendix A. Single UASB reactor *r* network superstructure model equations in steady-state

See Tables A1 and A2 and Fig. A.1.

A.1. Network equations

$$F_{IN} = F_{OT} \tag{A.1}$$

$$F_{FD} + F_{RR} = F_{IN} + F_{BP} \tag{A.2}$$

$$F_{BP} + F_{OT} = F_{RR} + F_{FN} \tag{A.3}$$

Table A2
Single UASB reactor network superstructure model equations.

Equation	Number	Quantity
Kinetic for blanket and bed	(A.7)–(A.19)	26
Flow and sludge discharge	(A.20)–(A.31)	45
General algebraic relations	(A.32)–(A.39)	10
Global mass balance in the UASB reactor	(A.1)	1
Mass balances in mixers	(A.2)–(A.5)	14
COD for streams FD, IN, OT and FN	(A.6)	4
Total		100

$$F_{FD} \cdot S_{j,FD} + F_{RR} \cdot S_{j,FN} = F_{IN} \cdot S_{j,IN} + F_{BP} \cdot S_{j,FD}$$
$$j = \text{G, E, B, AA, H and } CO_2 \tag{A.4}$$

$$F_{BP} \cdot S_{j,FD} + F_{OT} \cdot S_{j,c} = F_{RR} \cdot S_{j,FN} + F_{FN} \cdot S_{j,FN}$$
$$j = \text{G, E, B, AA, H and } CO_2 \tag{A.5}$$

$$COD_n = 1.33 \cdot S_{G,n} + 2.09 \cdot S_{E,n} + 1.82 \cdot S_{B,n} + 1.07 \cdot S_{AA,n} + 8.00 \cdot S_{H,n}$$
$$n = \text{FD, IN, OT and FN} \tag{A.6}$$

A.2. Kinetic equations (*s* = *a* and *b*)

$$\mu_{F,r,s} = \mu_{mF} \cdot \frac{S_{G,1,s}}{K_G + S_{G,1,s}} \cdot \frac{1}{1 + S_{H,1,s}/K_{IFH}} \tag{A.7}$$

$$\mu_{AE,r,s} = \mu_{mAE} \cdot \frac{S_{E,r,s}}{K_E + S_{E,r,s}} \cdot \frac{1}{1 + S_{H,r,s}/K_{IAEH}} \tag{A.8}$$

$$\mu_{AB,r,s} = \mu_{mAB} \cdot \frac{S_{B,r,s}}{K_B \cdot \left(1 + S_{AA,r,s}/K_{IABAA}\right) + S_{B,r,s}} \cdot \frac{1}{1 + S_{H,r,s}/K_{IABH}} \tag{A.9}$$

$$\mu_{MA,r,s} = \mu_{mMA} \cdot \frac{S_{AA,r,s}}{K_{AA} + S_{AA,r,s}} \cdot \frac{1}{1 + S_{E,r,s}/K_{IMAE}} \cdot \frac{1}{1 + S_{B,r,s}/K_{IMAB}} \tag{A.10}$$

Table A1
Variables for a single UASB reactor *r* network superstructure.

Variable	Definition	Quantity	
F_n	Flow rates for stream *n*	*n* = all streams	6
$S_{j,n}$	Substrate *j* concentration in stream n	*j* = G, E, B, AA, H and CO_2 *n* = FD, IN and FN	18
COD_n	Stream *n* COD	*n* = FD, IN, OT and FN	4
V_r	UASB reactor *r* volume		1
$V_{r,s}$	Volume of section *s* of the UASB reactor *r*	*s* = a, b and c	3
A_r	Cross-sectional area of UASB reactor *r*		1
h_r	UASB reactor *r* height		1
$h_{r,s}$	Height of section *s* of the UASB reactor *r*	*s* = a, b and c	3
η_r	UASB reactor *r* settler efficiency		1
$SF_{r,s}$	Short-circuit fractions that by-passes the section *s* in the UASB reactor *r*	*s* = a and b	2
$S_{j,r,s}$	Concentration of substrate *j* in section *s* of the UASB reactor *r*	*j* = G, E, B, AA, H and CO2; *s* = a, b and c	18
$X_{r,b}$	Total sludge concentration in the UASB reactor *r* blanket		1
$X_{i,r,s}$	Anaerobic sludge component *i* concentration in section *s* of the UASB reactor *r*	*i* = all 6 sludge components; *s* = a, b and c	18
DC_r	total discharged sludge flow for the UASB reactor *r*		1
$DC_{i,r}$	Discharge flow for bacterium *i* from reactor *r*	*i* = all 6 sludge components	6
$RS_{j,r,s}$	Reaction rate for substrate *j* in section *s* of the UASB reactor *r*	*j* = all 7 substrates; *s* = a and b	14
$\mu_{I,r,s}$	growth rate for bacterium *i* in section *s* of the UASB reactor *r*	*i* = F, AE, AB, MA and MH; *s* = a and b	10
$TM_{r,s}$	rate of formation of the endogenous residue in section *s* of the UASB reactor *r*	*s* = a and b	2
$\phi_{CH_{4,r,s}}$	volumetric production rate of methane in the UASB reactor *r*	*s* = a and b	2
Total			112

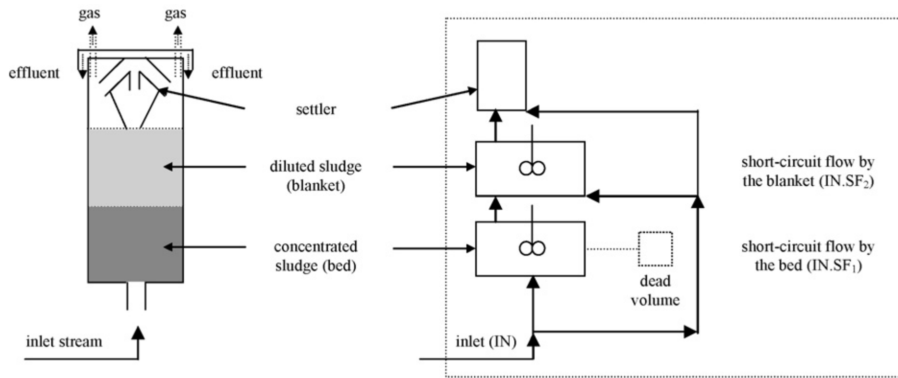

Fig. A.1. Schematic representation of the UASB reactor.

$$\mu_{MH,r,s} = \mu_{mMH} \cdot \frac{S_{H,r,s} \cdot S_{CO_2,r,s}}{(K_H + S_{H,r,s}) \cdot (K_{CO_2} + S_{CO_2,r,s})} \cdot \frac{1}{1 + S_{E,r,s}/K_{IMHE}} \cdot \frac{1}{1 + S_{B,r,s}/K_{IMHB}} \quad \text{(A.11)}$$

$$TM_{r,s} = 0.2 \sum_{i,i \neq I} b_i \cdot X_{i,r,s} \quad \text{(A.12)}$$

$$RS_{G,r,s} = -\frac{\mu_{F,r,s} \cdot X_{F,r,s}}{Y_F} \cdot MM_G \quad \text{(A.13)}$$

$$RS_{E,r,s} = \left[0.34 \cdot \left(1 - \frac{Y_F}{MM_G}\right) \cdot \frac{\mu_{F,r,s} \cdot X_{F,r,s}}{Y_F} - \frac{\mu_{AE,r,s} \cdot X_{AE,r,s}}{Y_{AE}}\right] \cdot MM_E \quad \text{(A.14)}$$

$$RS_{B,r,s} = \left[0.39 \cdot \left(1 - \frac{Y_{Fm}}{MM_G}\right) \cdot \frac{\mu_{F,r,s} \cdot X_{F,r,s}}{Y_F} - \frac{\mu_{AB,r,s} \cdot X_{AB,r,s}}{Y_{AB}}\right] \cdot MM_B \quad \text{(A.15)}$$

$$RS_{AA,r,s} = \left[1.31 \cdot \left(1 - \frac{Y_F}{MM_G}\right) \cdot \frac{\mu_{F,r,s} . X_{F,r,s}}{Y_F} + \left(1 - \frac{Y_{AE}}{MM_E}\right) \cdot \frac{\mu_{AE,r,s} \cdot X_{AE,r,s}}{Y_{AE}} + 2 \cdot \left(1 - \frac{Y_{AB}}{MM_B}\right) \cdot \frac{\mu_{AB,r,s} \cdot X_{AB,r,s}}{Y_{AB}} - \frac{\mu_{MA,r,s} \cdot X_{MA,r,s}}{Y_{MA}}\right] \cdot MM_{AA} \quad \text{(A.16)}$$

$$RS_{H,r,s} = \left[0.82 \cdot \left(1 - \frac{Y_F}{MM_G}\right) \cdot \frac{\mu_{F,r,s} \cdot X_{F,r,s}}{Y_F} + 2 \cdot \left(1 - \frac{Y_{AE}}{MM_E}\right) \cdot \frac{\mu_{AE,r,s} \cdot X_{AE,r,s}}{Y_{AE}} + 2 \cdot \left(1 - \frac{Y_{AB}}{MM_B}\right) \cdot \frac{\mu_{AB,r,s} \cdot X_{AB,r,s}}{Y_{AB}} - \frac{\mu_{MH,r,s} \cdot X_{MH,r,s}}{Y_{MH}}\right] \cdot MM_H \quad \text{(A.17)}$$

$$RS_{CO_2,r,s} = \left[1.14 \cdot \left(1 - \frac{Y_F}{MM_G}\right) \cdot \frac{\mu_{F,r,s} \cdot X_{F,r,s}}{Y_F} + \left(1 - \frac{Y_{MA}}{MM_{AA}}\right) \cdot \frac{\mu_{MA,r,s} \cdot X_{MA,r,s}}{Y_{MA}} - 0.25 \cdot \left(1 - \frac{Y_{MH}}{MM_H}\right) \cdot \frac{\mu_{MH,r,s} \cdot X_{MH,r,s}}{Y_{MH}} - 0.5 \cdot \frac{\mu_{MH,r,s} \cdot X_{MH,r,s}}{MM_H}\right] \cdot MM_{CO_2} \quad \text{(A.18)}$$

$$RS_{CH_4,r,s} = \left[\left(1 - \frac{Y_{MA}}{MM_{AA}}\right) \cdot \frac{\mu_{MA,r,s} \cdot X_{MA,r,s}}{Y_{MA}} + 0.25 \cdot \left(1 - \frac{Y_{MH}}{MM_H}\right) \cdot \frac{\mu_{MH,r,s} \cdot X_{MH,r,s}}{Y_{MH}}\right] \cdot MM_{CH_4} \quad \text{(A.19)}$$

A.3. Flow model equations

$$SF_{r,a} = f(h_{r,a}, h_{r,b}) \quad \text{(A.20)}$$

$$SF_{r,b} = f(h_{r,a}, h_{r,b}) \quad \text{(A.21)}$$

$$(1 - SF_{r,a}) \cdot F_{IN} \cdot (S_{j,IN} - S_{j,r,a}) + RS_{j,r,a} + V_{r,a} = 0 \quad j = \text{G, E, B, AA, H and } CO_2 \quad \text{(A.22)}$$

$$-\eta_{dr} \cdot x' \cdot \phi_{CH4r,a} \cdot X_{i,r,a} + A_r \cdot X_{i,r,b} \cdot v_s + m_{i,r,a} \cdot X_{i,r,a} \cdot V_{r,a} - b_i \cdot X_{i,r,a} \cdot V_{r,a} = 0 \quad i = \text{F, AE, AB, MA and MH} \quad \text{(A.23)}$$

$$-\eta_{dr} \cdot x' \cdot \phi_{CH_4r,a} \cdot X_{I,r,a} + A_r \cdot X_{I,r,b} \cdot v_s + TM_{r,a} \cdot V_{r,a} = 0 \quad \text{(A.24)}$$

$$(1 - SF_{r,a}) \cdot F_{IN} \cdot S_{j,r,a} - (1 - SF_{r,b}) \cdot F_{IN} \cdot S_{j,r,b} + (SF_{r,a} - SF_{r,b}) \cdot F_{IN} \cdot S_{j,IN} + RS_{j,r,b} \cdot V_{r,b} = 0 \quad j = \text{G, E, B, AA, H and } CO_2 \quad \text{(A.25)}$$

$$\eta_{dr} \cdot x' \cdot \phi_{CH_4,r,a} \cdot X_{i,r,a} - A_r \cdot X_{i,r,b} \cdot v_s - (1 - \eta) \cdot (1 - SF_{r,b}) \cdot F_{IN} \cdot X_{i,r,b} + \mu_{i,r,b} \cdot X_{i,r,b} \cdot V_{r,b} - b_i \cdot X_{i,r,b} \cdot V_{r,b} = 0 \quad i = \text{F, AE, AB, MA and MH} \quad \text{(A.26)}$$

$$\eta_{dr} \cdot x' \cdot \phi_{CH4r,a} \cdot X_{I,r,a} - A_r \cdot X_{I,r,b} \cdot v_s - (1 - \eta) \cdot (1 - SF_{r,b}) \cdot F_{IN} \cdot X_{I,r,b} + TM_{r,b} \cdot V_{r,b} = 0 \quad \text{(A.27)}$$

$$(1 - SF_{r,b}) \cdot F_{IN} \cdot S_{j,r,b} + S_{Fr,b} \cdot F_{IN} \cdot S_{j,IN} - F_{IN} \cdot S_{j,r,c} = 0 \quad j = \text{G, E, B, AA, H and } CO_2 \quad \text{(A.28)}$$

$$(1 - \eta_r) \cdot (1 - SF_{r,b}) \cdot F_{IN} \cdot X_{i,r,b} - F_{IN} \cdot X_{i,r,c} = 0 \quad i = \text{F, AE, AB, MA, MH and I} \quad \text{(A.29)}$$

$$DC_{i,r} = \frac{X_{i,r,c} \cdot F_{OT}}{V_{r,c}} \quad i = \text{F, AE, AB, MA, MH and I} \quad \text{(A.30)}$$

$$DC_r = \sum_i DC_{i,r} \quad \text{(A.31)}$$

A.4. Generic algebraic relations

$$\phi_{CH_4,r,a} = \frac{RS_{CH_4,r,a} \cdot V_{r,a}}{\rho_{CH_4}} \quad (A.32)$$

$$\phi_{CH_4,r,b} = \frac{RS_{CH_4,r,b} \cdot V_{r,b}}{\rho_{CH_4}} \quad (A.33)$$

$$h_r = h_{r,a} + h_{r,b} + h_{r,c} \quad (A.34)$$

$$V_r = V_{r,a} + V_{r,b} + V_{r,c} \quad (A.35)$$

$$V_{r,s} = A_r \cdot h_{r,s} \quad s = a, b \text{ and } c \quad (A.36)$$

$$V_{r,c} = 0.185 \cdot V_r \quad (A.37)$$

$$\sum_i X_{i,r,a} = 85 \quad (A.38)$$

$$0 = \mathrm{TM}_r - \mathrm{DC}_{I,r} \quad (A.39)$$

A.5. Model parameters

Parameter	Value	Unit	Parameter	Value	Unit
μ_{mF}	0.175	h^{-1}	b_F	0.00125	h^{-1}
μ_{mAE}	0.280	h^{-1}	b_{AE}	0.00125	h^{-1}
μ_{mAB}	0.011	h^{-1}	b_{AB}	0.00125	h^{-1}
μ_{mMA}	0.015	h^{-1}	b_{MA}	0.00083	h^{-1}
μ_{mMH}	0.058	h^{-1}	b_{MH}	0.00125	h^{-1}
K_G	0.128	mol/m^3	K_{IFH}	0.03205	mol/m^3
K_E	0.060	mol/m^3	K_{IAEH}	0.32051	mol/m^3
K_B	1.100	mol/m^3	K_{IABH}	0.00641	mol/m^3
K_{AA}	2.300	mol/m^3	K_{IABAA}	10	mol/m^3
K_H	0.008	mol/m^3	K_{IMAB}	21	mol/m^3
K_{CO2}	0.010	mol/m^3	K_{IMAE}	35	mol/m^3
Y_F	0.0220	kg/mol	K_{IMHB}	16	mol/m^3
Y_{AE}	0.0020	kg/mol	K_{IMHE}	29	mol/m^3
Y_{AB}	0.0045	kg/mol	v_s	3.5	m/h
Y_{MA}	0.0025	kg/mol	η_{dr}	0.3	
Y_{MH}	0.0004	kg/mol	x'	14.27	

Appendix B. Single EGSB reactor *r* network superstructure model equations in steady-state

See Tables B1 and B2.

B.1. Network equations

Same ones listed in A.1.

B.2. Kinetic equations

Same ones listed in A.2, but without the *s* sub-index.

B.3. Flow model equations

$$0 = \frac{F_{IN}}{V}.(S_{j,IN} - S_{j,r}) + RS_{j,r} \qquad j = \mathrm{G, E, B, AA, H\ and\ CO_2} \quad (B.1)$$

$$0 = \mu_{i,r}.X_{i,r} - b_i.X_{i,r} - DC_{i,r} \qquad i = \mathrm{F, AE, AB, MA\ and\ MH} \quad (B.2)$$

$$0 = \mathrm{TM}_r - \mathrm{DC}_{I,r} \quad (B.3)$$

$$\mathrm{DC}_r = \sum_{i,i \neq I} (\mu_{i,r}.X_{i,r} - b_i.X_{i,r}) + \mathrm{TM}_r \quad (B.4)$$

$$\mathrm{DC}_{i,r} = \frac{X_{i,r}}{X_r}.DC_r \quad i = \mathrm{F, AE, AB, MA, MH\ and\ I} \quad (B.5)$$

$$\phi_{CH_4,r} = \frac{\mathrm{RS}_{CH_4,r} \cdot V_r}{\rho_{CH_4}} \quad (B.6)$$

Table B1
Variables for a single EGSB reactor *r* network superstructure.

Variable	Definition	Quantity	
F_n	Flow rates for stream *n*	*n* = all streams	6
$S_{j,n}$	Substrate *j* concentration in stream n	*j* = G, E, B, AA, H and CO_2; *n* = FD, IN and FN	18
COD_n	Stream *n* COD	*n* = FD, IN, OT and FN	4
V_r	EGSB reactor *r* volume		1
A_r	Cross-sectional area of EGSB reactor *r*		1
h_r	EGSB reactor *r* height		1
X_r	Anaerobic sludge concentration in EGSB reactor *r*		1
$S_{j,r}$	Concentration of substrate *j* in the EGSB reactor *r*	*j* = G, E, B, AA, H and CO2	6
$X_{i,r}$	Concentration of anaerobic sludge component *i* in EGSB reactor *r*	*i* = all sludge components	6
DC_r	Total discharged sludge flow for the EGSB reactor *r*		1
$DC_{i,r}$	Discharge flow for bacterium *i* from reactor *r*	*i* = all sludge components	6
$RS_{j,r}$	Reaction rate for substrate *j* in the EGSB reactor *r*	*j* = all substrates	7
$\mu_{i,r}$	Growth rate for bacterium *i* in the EGSB reactor *r*	*i* = F, AE, AB, MA and MH	5
TM_r	Rate of formation of the endogenous residue in the EGSB reactor *r*		1
$\phi_{CH_4,r}$	Volumetric production rate of methane in the EGSB reactor *r*		1
Total			65

Table B2
EGSB reactor network superstructure model equations.

Equation	Number	Quantity
Kinetic	(A.7)–(A.19)	13
Flow and sludge discharge	(B.1)–(B.6)	20
Generic algebraic relations	(B.7)	1
Global mass balance in the EGSB reactor	(A.1)	1
Mass balances in mixers	(A.2)–(A.5)	14
COD for streams FD, IN, OT and FN	(A.6)	4
Total		53

B.4. Generic algebraic relations

$$V_r = A_r \cdot h_r \quad (B.7)$$

Appendix C

C.1. Multiple-anaerobic digester network superstructure model equations in steady-state

See Tables C1 and C2.

C.2. Multiple anaerobic digester network superstructure model equations in steady-state

See Table C3.

Table C1
Variables intrinsic to the network of two anaerobic digesters.

Variable	Definition	Quantity	
F_n	Flow rates for stream *n*	*n* = all streams	18
$S_{j,n}$	Substrate *j* concentration in stream *n*	*j* = G, E, B, AA, H and CO_2; *n* = FD, IN_r, RM_r and FN *r* = 1 and 2	36
COD_n	Stream *n* COD	*n* = FD, IN_r, RM_r and FN *r* = 1 and 2	6
Total			60

Table C2
Constraints intrinsic to the network of two anaerobic digesters.

Equation	Number	Quantity
Global mass balance in the digesters	(1)	2
Mass balance in the mixers and splitters	(18)–(28)	36
COD of 6 streams	(6)	6
Total		44

Table C3
Variables intrinsic to the network of multiple anaerobic digesters.

Variable	Definition	Quantity	
F_n	Flow rate for stream n	n = FD and FN	2
F_n	Flow rate for the n stream	$n = RF_r, IN_r, BP_r, OT_r, RR_r, RM_r, MR_r$ $r = 1,\ldots,R$	$7 \cdot R$
$F_{Sr-r'}$	Flow rate for the sidestreams	$r = 1,\ldots,R$ ($r' \neq r$)	$R \cdot (R-1)$
$S_{j,n}$	Substrate j concentration in stream n	j = G, E, B, AA, H and CO_2; n = FD and FN	12
$S_{j,n}$	Substrate j concentration in stream n	j = G, E, B, AA, H and CO_2; $n = IN_r$ and RM_r $r = 1,\ldots,R$	$12 \cdot R$
COD_n	Stream n COD	n = FD and FN	2
COD_n	Stream n COD	$n = IN_r$ and RM_r $r = 1,\ldots,R$	$2 \cdot R$
Total			$R^2 + 20 \cdot R + 16$

Appendix D

Depending on the reaction kinetics, for a CSTR, the recycle stream does not affect the conversion rate of the reactor, as shown here. Note that one of the assumptions made in a CSTR is that there is no short-circuit.

The mass balance for substrate j in reactor r is the following, using Assumption A4:

$$F_{INr} \cdot S_{j,INr} - F_{OTr} \cdot S_{j,r} - V_r \cdot R_{j,r} = 0 \tag{D.1}$$

If the reaction rate for substrate j is only a function of its concentration, then it can be expressed by

$$R_{j,r} = f(S_{j,r}) \tag{D.2}$$

Substituting (2), (4) and (D.2) into (D.1), and making $F_{BP} = 0$:

$$F_{FD} \cdot (S_{j,FD} - S_{j,r}) - f(S_{j,r}) \cdot V_r = 0 \tag{D.3}$$

Although the value of $S_{j,r}$ can only be calculated implicitly by (D.3), the value of F_{RR} does not influence it.

Supposing that the only substrate present in the feed stream is acetic acid (AA), it is shown in Appendix A that Eqs. (A.10) and (A.16) can be simplified to:

$$\mu_{MA,r} = \mu_{mMA} \cdot \frac{S_{AA,r}}{K_{AA} + S_{AA,r}} \tag{D.4}$$

$$R_{AA,r} = -\frac{\mu_{MA,r} \cdot X_{MA,r}}{Y_{MA}} \cdot MM_{AA} \tag{D.5}$$

Defining

$$\alpha = \frac{\mu_{mMA} \cdot X_{MA,r}}{Y_{MA}} \cdot MM_{AA} \tag{D.6}$$

Substituting (D.4) and (D.6) into (D.5):

$$R_{AA,r} = -\alpha \cdot \frac{S_{AA,r}}{K_{AA} + S_{AA,r}} \tag{D.7}$$

Substituting (2), (4) and (D.7) into (D.1), and again making $F_{BP} = 0$:

$$S_{j,r} = \frac{-\beta + \sqrt{\beta^2 + 4 \cdot S_{j,FD} \cdot K_{AA}}}{2} \tag{D.8}$$

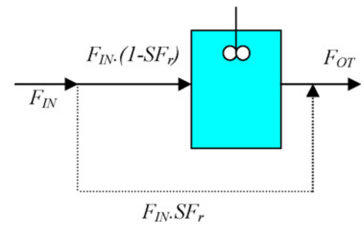

Fig. D.1. Continuous reactor with short-circuit flow.

where

$$\beta = K_{AA} + \frac{\alpha \cdot V_r}{F_{FD}} - S_{j,FD} \tag{D.9}$$

Again, the concentration of substrate j in the reactor r, $S_{j,r}$, does not depend on the recycle stream (F_{RR}).

Now, assume that the CSTR is no longer ideal and that this non-ideality can be modeled as a short-circuit stream. Hence, Assumption A4 is no longer valid ($S_{j,OT} \neq S_{j,r}$). Fig. D.1 shows a continuous reactor where there is a short-circuit flow.

In Fig. D.1, the parameter SF_r represents a fraction of the incoming stream that short-circuits the reactor.

$$F_{IN} \cdot (1 - SF_r) + F_{IN} \cdot SF_r = F_{OT} \tag{D.10}$$

Now, the mass balances for substrate j in reactor r are the following:

$$F_{IN} \cdot (1 - SF_r) \cdot S_{j,IN} - F_{IN} \cdot (1 - SF_r) \cdot S_{j,r} - V_r \cdot R_{j,r} = 0 \tag{D.11}$$

$$F_{IN} \cdot (1 - SF_r) \cdot S_{j,r} + F_{IN} \cdot SF_r \cdot S_{j,IN} = F_{OT} \cdot S_{j,OT} \tag{D.12}$$

Substituting (1), (2), (D.7), (D.11) and (D.12) into (4) and solving for $S_{j,r}$, and again making $F_{BP} = 0$:

$$S_{j,r} = \frac{-\gamma + \sqrt{\gamma^2 + 4 \cdot (1 - SF_r)^2 \cdot S_{j,FD} \cdot K_{AA}}}{2.(1 - SF_r)} \tag{D.13}$$

where

$$\gamma = K_{AA} \cdot (1 - SF_r) + \frac{F_{FD} \cdot SF_r \cdot S_{j,FD}}{F_{FD} + F_{RR}} + \frac{\alpha \cdot V_r \cdot (F_{FD} + F_{RR} \cdot (1 - SF_r))}{F_{FD}(F_{FD} + F_{RR}) \cdot (1 - SF_r)} - \frac{(F_{FD} + F_{RR} \cdot (1 - SF_r)) \cdot S_{j,FD}}{(F_{FD} + F_{RR})} \tag{D.14}$$

If $SF_r = 0$, then equation (D.13) becomes (D.8).

Note that if there is short-circuit then $S_{j,r}$ will also be a function of F_{RR}.

References

[1] R.F.F. Pontes, J.M. Pinto, Analysis of integrated kinetic and flow models for anaerobic digesters, Chemical Engineering Journal 122 (1–2) (2006) 65–80.
[2] W.L. Bolle, J. van Breugel, G.C. van Eybergen, N.W.F. Kossen, W. van Gils, An integral dynamic model for the UASB reactor, Biotechnology and Bioengineering 28 (1986) 1621–1635.
[3] A.G. Brito, L.F. Melo, A simplified analysis of reaction and mass transfer in UASB and EGSB reactors, Environmental Technology 18 (1997) 35–44.
[4] S.V. Kalyuzhnyi, Batch anaerobic digestion of glucose and its mathematical modeling. II. Description verification and application of model, Bioresource Technology 59 (1997) 249–258.
[5] W.L. Bolle, J. van Breugel, G.C. van Eybergen, N.W.F. Kossen, W. van Gils, Kinetics of anaerobic purification of industrial wastewater, Biotechnology and Bioengineering 28 (1986) 542–548.
[6] S.V. Kalyuzhnyi, V.V. Fedorovich, Dispersed plug flow model for upflow anaerobic sludge bed reactors with focus on granular sludge dynamics, Journal of Industrial Microbiology & Biotechnology 33 (2006) 221–237.
[7] C.M. Narayanan, V. Narayan, Multiparameter models for performance analysis of UASB reactors, Journal of Chemical Technology and Biotechnology 83 (2008) 1170–1176.
[8] S.J. Mu, Y. Zeng, P. Wu, S.J. Lou, B. Tartakovsky, Anaerobic digestion model No 1-based distributed parameter model of an anaerobic reactor: I. Model development, Bioresource Technology 99 (2008) 3665–3675.

[9] A. Lakshmanan, L.T. Biegler, Synthesis of optimal chemical reactor networks, Industrial and Engineering Chemistry Research 35 (1996) 1344–1353.
[10] A.C. Kokossis, C.A. Floudas, Optimization of complex reactor networks: I. Isothermal operation, Chemical Engineering Science 45 (3) (1990) 595.
[11] Z. Kravanja, I.E. Grossmann, Multilevel-hierarchical MINLP synthesis of process flowsheets, Computers and Chemical Engineering 24 (1997) 1403–1408.
[12] E.C. Marcoulaki, A.C. Kokossis, Scoping and screening complex reaction networks using stochastic optimization, AIChE Journal 45 (9) (1999) 1977–1991.
[13] C.A. Schweiger, C.A. Floudas, Optimization framework for the synthesis of chemical reactor networks, Industrial and Engineering Chemistry Research 38 (1999) 744–766.
[14] W.R. Esposito, C.A. Floudas, Deterministic global optimization in isothermal reactor network synthesis, Journal of Global Optimization 22 (2002) 59–95.
[15] D. Glasser, D. Hildebrandt, C.M. Crowe, A geometric approach to steady flow reactors: the attainable region and optimization in concentration space, Industrial and Engineering Chemistry Research 26 (1987) 1803–1810.
[16] D. Hildebrandt, D. Glasser, C.M. Crowe, Geometry of the attainable region generated by reaction and mixing: with and without constraints, Industrial and Engineering Chemistry Research 29 (1990) 49–58.
[17] S. Balakrishna, L.T. Biegler, Constructive targeting approaches for the synthesis of chemical reactor networks, Industrial and Engineering Chemistry Research 31 (1992) 300–312.
[18] S. Balakrishna, L.T. Biegler, Targeting strategies for the synthesis and energy integration of nonisothermal reactor networks, Industrial and Engineering Chemistry Research 31 (1992) 2152–2164.
[19] S. Kauchali, W.C. Rooney, L.T. Biegler, D. Glasser, D. Hildebrandt, Linear programming formulations for attainable region analysis, Chemical Engineering Science 57 (2002) 2015–2028.
[20] N.I. Bedenika, M. Ropotara, Z. Kravanja, MINLP synthesis of reactor networks in overall process schemes based on a concept of time-dependent economic regions, Computers & Chemical Engineering 31 (5–6) (2007) 657–676.
[21] B. Pahor, N. Irsic, Z. Kravanja, MINLP synthesis and modified attainable region analysis of reactor networks in overall process schemes using more compact reactor superstructure, Computers and Chemical Engineering 24 (2000) 1403–1408.
[22] J.F. Burri, S.D. Wilson, V.I. Manousiouthakis, Infinite dimensional state-space approach to reactor network synthesis: application to attainable region construction, Computers and Chemical Engineering 26 (2002) 849–862.
[23] W. Zhou, V.I. Manousiouthakis, Non-ideal reactor network synthesis through IDEAS: attainable region construction, Chemical Engineering Science 61 (21) (2006) 6936–6945.
[24] W. Zhou, V.I. Manousiouthakis, Variable density fluid reactor network synthesis—construction of the attainable region through the IDEAS approach, Chemical Engineering Journal 129 (1–3) (2007) 91–103.
[25] M.T. Kato, J.A. Field, P. Versteeg, G. Lettinga, Feasibility of expanded granular sludge bed reactors for the anaerobic treatment of low-strength soluble wastewaters, Biotechnology and Bioengineering 44 (1994) 469–479.
[26] N. Mahmoud, High strength sewage treatment in a UASB reactor and an integrated UASB-digester system, Bioresource Technology 99 (2008) 7531–7538.
[27] A. Ramakrishnan, S.K. Gupta, Effect of effluent recycling and shcok loading on the biodegradation of complex phenolic mixture in hybrid UASB reactors, Bioresource Technology 99 (2008) 3745–3753.
[28] A. Van Haandel, G.R. Marais, O Comportamento do Sistema de Lodo Ativado, Teoria e Aplicações para Projetos e Operação, Epgraf; Campina Grande, PB Brazil, 1999.
[29] S.K. Narnoli, I. Mehrotra, Sludge blanket of UASB reactor: mathematical simulation, Water Research 31 (4) (1997) 715–726.
[30] W.L. Bolle, J. van Breugel, G.C. van Eybergen, N.W.F. Kossen, R.J. Zoetemeyer, Modeling the liquid flow in up-flow anaerobic sludge blanket reactors, Biotechnology and Bioengineering 28 (1986) 1615–1620.
[31] CONAMA, Conselho Nacional do Meio Ambiente Resolution No. 357, March 17, 2005, São Paulo, Brazil.
[32] J.B. Van Lier, F.P. Van der Zee, N.C.G. Tan, S. Rebac, R. Kleerebezem, Advances in high-rate anaerobic treatment: staging of reactor systems (2001), Water Science and Technology 44 (8) (2001) 15–25.
[33] D. Jeison, R. Chamy, Comparison of the behaviour of expanded granular sludge bed (EGSB) and upflow anaerobic sludge blanket (UASB) reactors in dilute and concentrated wastewater treatment, Water Science and Technology 40 (8) (1999) 91–97.
[34] A. Brooke, D. Kendrick, A. Meeraus, R. Raman, GAMS A User's Guide, GAMS Development Corporation, Washington, DC, USA, 1998.
[35] N.V. Sahinidis, M. Tawarmalani, Accelerating branch-and-bound through a modeling language construct for relaxation-specific constraints, Journal of Global Optimization 32 (2005) 259–280.
[36] A. Drud, CONOPT: a GRG code for large sparse dynamic nonlinear optimization problems, Mathematical Programming 31 (1985) 153–191.
[37] N.T. Anh, Methods for UASB reactor design, water and wastewater.com, 2004, http://www.waterandwastewater.com/www_services/ask_tom_archive/methods_for_uasb_reactor_design.htm.
[38] V.I. Diamantis, A. Aivasidis, Comparison of single- and two-stage UASB reactors used for anaerobic treatment of synthetic fruit wastewater, Enzyme and Microbial Technology 42 (2007) 6–10.
[39] P. Melidis, D. Georgiou, A. Aivasidis, Scale-up and design optimization of anaerobic immobilized cell reactors for wastewater treatment, Chemical Engineering and Processing 42 (2003) 897–908.
[40] J. Venkataraman, S.N. Kaul, S. Satyanarayan, Determination of kinetic constants for a two-stage anaerobic upflow packed-bed reactor for dairy wastewater, Bioresource Technology 40 (1992) 253–261.