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Optimal design and operation of a UASB reactor for dairy cattle manure



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ABSTRACT

Optimal design and operation of a planned full-scale UASB reactor at a dairy farm are determined using optimization algorithms based on steady state simulations of a dynamic AD process model combined with models of the reactor temperature and heat exchanger temperatures based on energy balances. Available feedstock is 6 m³/d dairy manure produced by the herd. Three alternative optimization problems are solved: Maximization of produced methane gas flow, minimization of reactor volume, and maximization of power surplus. Constraints of the optimization problems are an upper limit of the VFA concentration, and an upper limit of the feed rate corresponding to a normal animal waste production at the farm. The most proper optimization problem appears to be minimization of the reactor volume, assuming that the feed rate is fixed at its upper limit and that the VFA concentration is at its upper limit. The optimal result is a power surplus of 49.8 MWh/y, a hydraulic retention time of 6.1 d, and a reactor temperature of 35.9 °C, assuming heat recovery with an heat exchanger, and perfect reactor heat transfer insulation. In general, the optimal solutions are improved if the ratio of the solids (biomass) retention time to the hydraulic retention time is increased.

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1. Introduction

The aim of this paper is to optimize the design and steady-state operation of a planned full-scale upflow anaerobic sludge blanket (UASB) reactor fed with dairy cattle waste with $6 \text{ m}^3/\text{d}$ available feedstock. The optimization is based on a mathematical model of the reactor comprising a dynamic AD process model combined with models of the reactor temperature and the heat exchanger temperatures based on energy balances. The biological parameters of the AD process model was estimated from experiments on a real pilot reactor using the same feedstock as the planned full-scale reactor.

Three sets of optimization problems are studied: Maximization of the produced methane gas flow, minimization of the reactor volume, and maximization of the power surplus. The biological product considered in the optimization problems is the produced methane gas.

Actually, the real pilot plant in Foss Biolab includes a nitrification reactor used to enhance the quality of the effluent as a biological fertilizer. The planned full-scale plant also includes a nitrification reactor. However, the present study focuses at the energy production – not fertilizer production. Therefore, the AD effluent is taken into account in the present study only through its contribution to the energy balance, and not as a fertilizer.

An early attempt to use a dynamic AD model for optimization of anaerobic digestion (AD) reactors was made by Hill (1983a). In that study, a series of simulations based on the model presented by Hill (1983b) were used to detect the optimum hydraulic retention time (HRT) that maximized the volumetric methane productivity defined as steady-state volumetric methane gas flow divided by reactor volume. The solids retention time (SRT) was assumed equal to the HRT, as in a continuous stirred tank reactor (CSTR).

In the present study, the reactor is a UASB type reactor (Lettinga et al., 1980), having SRT larger than HRT. In UASB type reactors, the dense granulated sludge bed retains the microorganisms, and prevents them from being washed out of the reactor with the effluent. The formation of the granulated sludge is due to flocculation and gravity. Since the SRT is larger than the HRT for UASB reactors, their reactor volume can be made smaller, or, alternatively, their loading (feeding) rate can be higher compared with CSTRs.

Poels et al. (1983) reported experiences from AD processing of swine waste on a farm of typical size for Belgium. They emphasized the importance of insulation and preheating the (cold) influent by the (warm) effluent.

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Bozinis et al. (1996) showed in a simulation study of a hypothetical centralized wastewater treatment plant based on co-digestion of a number of wastewater streams how optimization methods, namely nonlinear programming (NLP), can be used to identify the optimal number of CSTR AD reactors and their volumes that minimize costs. They also showed how to identify the optimal mixing of the wastewater streams that maximize the total COD (chemical oxygen demand) conversion of the plant. Simple steady-state AD process models based on Monod kinetics were assumed.

The methods of formulation and solution of optimization problems for technical systems and industrial plants presented in Edgar et al. (2001) have been useful for the present paper as they are applicable also to biological plants.

The outline of this paper is as follows. A description of the planned AD reactor and the optimization method used are described in Section 2. Optimization results are presented in Section 3. A discussion is given in Section 4, and conclusions are given in Section 5. Mathematical models are presented in Appendix A.

Unless otherwise stated, the numerical values of variables presented in this paper are steady-state values.

MATLAB (The MathWorks, Inc.) is used for numerical computations.

2. Materials and methods

2.1. The AD reactor

The AD reactor is a part of a (planned) full-scale biological plant for nutrient and energy recovery, named Foss Biolab, situated at Foss Farm, Skien, Norway. A small-scale pilot plant has been in operation for about two years. A description of the pilot plant, including its monitoring and control system, is in Haugen et al. (2013a).

The feed to the pilot reactor, which has 250 L liquid volume, is dairy waste diluted with approximately 25% water and filtered with a home-made rotary sieve with mesh-size 1.4 mm. The sieve, or separator, removes larger particles to avoid technical problems (the dry-matter from the sieve is used for vermicomposting). The wet-fraction is used as feed to the AD reactor. Feed characteristics from laboratory analysis are presented in Table 1.

The produced biogas consists of approximately 70% methane.

Fig. 1 depicts the planned full-scale reactor. The figure includes a heat exchanger (however, the pilot reactor has no heat exchanger).

2.2. Mathematical models

The mathematical model used for optimization of the planned full-scale reactor comprises the following sub-models:

 Table 1

 Characteristics of the reactor feed. (Mean ± standard deviations from laboratory analyses of totally 23 samples collected from the pilot plant approximately twice a week.)

Measure	Value	Unit
TS	44.6 ± 2.2	g/L
VS	30.2 ± 1.0	g/L
tCOD	48.6 ± 1.5	g/L
sCOD	15.5 ± 1.0	g/L
NH4-N	0.95 ± 0.078	g/L
Alkalinity	8.6 ± 0.8	g CaCO ₃ /L
рН	7.55 ± 0.15	log[H+]

- 1. The modified Hill model of the AD processes adapted to the pilot reactor (Haugen et al., 2013a). For easy reference, the model is summarized in Appendix A.1.
- 2. A model of the reactor liquid temperature based on energy balance (Haugen et al., 2013a). The model is summarized in Appendix A.2.
- 3. A model of the temperatures of heat exchanger based on energy balances. The model is derived in Appendix A.3.

The modified Hill model is a relatively simple AD process model, however it has been successfully adapted to the real pilot reactor (Haugen et al., 2013a). The modified Hill model is selected in the present study since it is assumed sufficient for model-based optimization of the full-scale AD reactor. The most interesting alternative model is probably the comprehensive ADM1 model (Anaerobic Digestion Model No. 1) (Batstone et al., 2002), which, after adaptation to the real pilot reactor, may be used in future model-based studies.

2.3. Optimization objectives and variables

Fig. 2 shows alternative optimization variables and objective variables. In the various optimization problems discussed in Sections 3.2, 3.3 and 3.4, various subsets of these variables are used.

2.3.1. Optimization objectives

Fig. 2 defines alternative optimization objective variables (the outputs in the block diagram):

 F_{meth} , to be maximized, which is an appropriate objective if the gas is supplied (sold) to a gas grid.

V, to be minimized, which is an appropriate objective to save space and constructional and installation costs.

 P_{sur} , to be maximized, which is an appropriate objective if the gas is applied for heating within the farm. P_{sur} is calculated with Eq. (A.20), where all power terms are in units of MWh/y.

2.3.2. Optimization variables and their constraints

In the following, the optimization variables are characterized as either operational or design optimization variables. The former can be changed while the reactor is being operated, while design optimization variables can be changed in the design or constructional phase.

The various optimization variables shown in Fig. 2, and their constraints, are described in the following.

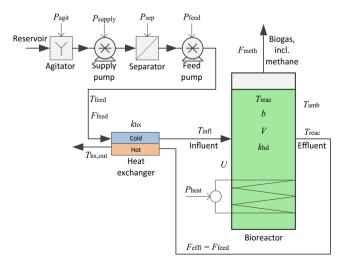


Fig. 1. Planned full-scale AD reactor. (Nomenclature is in Appendix C.)

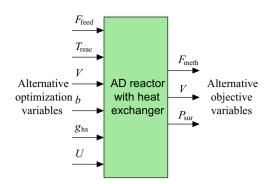


Fig. 2. Alternative optimization variables and objective variables.

 F_{feed} : The livestock of the pertinent farm counts approximately 60 cows, each producing approximately 0.1 m³ diluted raw waste per day. The wet fraction which remains after the separation, amounts to approximately 0.7 (weight base), which is fed to the reactor. Thus, feasible values of F_{feed} is

$$0 \leqslant F_{\text{feed}} \le 4.2 \text{ m}^3/\text{d} = F_{\text{feed}}^{\text{max}} \tag{1}$$

*F*_{feed} is an operational optimization variable.

 T_{reac} : According to Tchobanoglous et al. (2003), most AD reactors are operated in the mesophilic temperature range which is 30–38 °C. For the planned reactor, it is of interest to also investigate temperatures below this range mainly because of the relatively cold climate in Norway. The modified Hill model is applicable for T_{reac} in the range 20 $\leq T_{\text{reac}} \leq 60$ °C, cf. Appendix A.1. The following range of T_{reac} is considered in this paper:

$$T_{\rm reac}^{\rm min} = 20 \leqslant T_{\rm reac} \le 38 \,^{\circ}{\rm C} = T_{\rm reac}^{\rm max} \tag{2}$$

*T*_{reac} is an operational optimization variable.

V: Above, it is defined as an optimization objective, but it is also used as an optimization design variable in some of the optimization problems.

We think that it makes sense to allow *V* to become virtually unlimited in the optimization problems. However, a welldefined upper limit is necessary by computational reasons, and to this end we select 700 m³, but another very large value might have been chosen. (In one of the optimization problems, namely P_{F_3} , the optimal *V* is at this upper limit, but it is regarded as an impractical solution.)

b: In Haugen et al. (2013a), the retention times ratio is defined as

$$b = \frac{\text{SRT}}{\text{HRT}} \tag{3}$$

where SRT is the solids (biomass) retention time, and HRT is the hydraulic retention time (HRT) which is defined as (Tchobanoglous et al., 2003):

$$HRT = \frac{V}{F_{\text{feed}}} \tag{4}$$

SRT can not be less than HRT. Therefore, *b* is lower bounded to 1. It is assumed that *b* does not have a larger value than 20, i.e.

$$b_{\min} = 1 \leqslant b \le 20 = b_{\max} \tag{5}$$

This assumption is supported by simulations: Fig. 3, plot 3a, indicates that the sensitivity of F_{meth} to *b* is relatively small for *b* above 20.

In the majority of the optimization problems studied in the article, *b* is set to 2.9, the estimated value for the real pilot reactor. The upper

limit of *b* of 20 is questionable, and we do not have real data supporting this limit. However, the main purpose of setting such a specific upper limit is to allow for qualitative results, i.e. demonstrating the importance of attempting to design the reactor so that b becomes as large as possible.

b is a design optimization variable, but may be changed after the reactor has been set into operation. As shown in Section 3, it is beneficial in the optimization scenarios that *b* is as large as possible. A large *b* is obtained with a relatively large SRT. Khanal (2008) presents different techniques to increase the SRT for AD reactors, e.g. settling and filtering. For the existing real pilot reactor, granules have been added in an attempt to increase the SRT, however, the effect of adding granules has not been analyzed.

For the pilot reactor, *b* is estimated from time-series as 2.9 (Haugen et al., 2013a). It is interesting to compare this value with the parameter α estimated in Bernard et al. (2001) where a dynamical AD model which resembles the modified Hill model in important aspects, is adapted to a 0.95 m³ real fixed-bed reactor with recycling using wine distillery vinasses as substrate. α is denoted "proportion of dilution rate for bacteria". It can be shown that $b = 1/\alpha$. From real data, α was estimated as 0.5, corresponding to b = 1/0.5 = 2 which is relatively close to 2.9 which is estimated for our reactor. Although these two reactors differs in many aspects, the resemblance between *b* and α is reassuring.

- g_{hx} , the heat exchanger coefficient, is defined with Eq. (A.14) in Appendix A. g_{hx} is a design optimization variable. In the optimization problems, g_{hx} has value either ∞ (perfect heat exchange) or 0 (no heat exchange, or no heat exchanger). On a real heat exchanger, perfect heat exchange can of course not be obtained, corresponding to a limited value of g_{hx} . Still, it is decided to assume an ideal heat exchanger to avoid complicating the analysis. Also, the principal difference between applying heat exchange and not is expected to be principally the same for a real heat exchanger as for an ideal heat exchanger.
 - *U*, the specific heat transfer coefficient of the reactor, is calculated from the value of the real pilot reactor as explained in Appendix A. In optimization problems where perfect thermal insulation of the reactor walls is assumed, *U* is set to zero. *U* is a design optimization variable.

The constraints on S_{vfa} is an important optimization constraint. According to the discussion in Haugen et al. (2013b) based on the results in Hill et al. (1987), the range of S_{vfa} for safe reactor operation is

$$S_{\rm vfa} \le 0.8 g/L = S_{\rm vfa}^{\rm max} \tag{6}$$

In each of the optimization problems, both T_{amb} and T_{feed} are set to 10 °C.¹ The rationale for this is as follows. It is assumed that the reactor is indoor in a barn or similar. It is assumed that the filtered feed is stored for so long time "inhouse" that T_{amb} and T_{feed} are approximately equal. Furthermore, the value of 10 °C is a rough estimate of the average for the real pilot plant.

2.4. Optimization algorithm

The optimization problems are solved using the straightforward "brute force" (BF) method: Assume that the vector of optimization variables is $x = \{x_i\}$, with i = 1, ..., n where n is the number of optimization variables. For example, in optimization problem P_{F_1} studied below, $x_1 = F_{feed}$ and $x_2 = T_{reac}$. For each $\{x_i\}$, an array of

¹ In an online system for optimal reactor operation, online temperature measurements may be used as inputs to the optimizer.

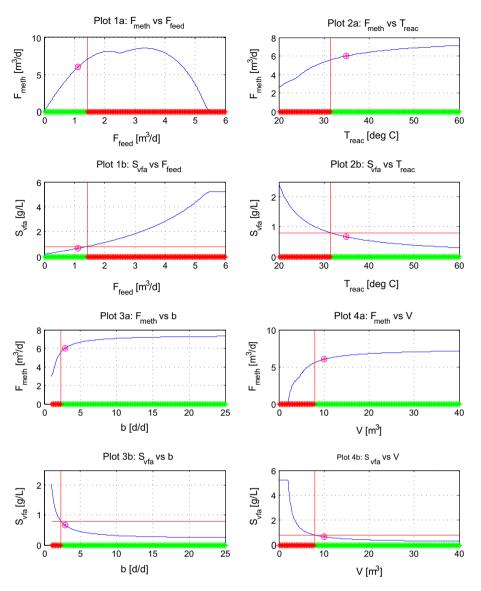


Fig. 3. F_{meth} and S_{vfa} as function of F_{feed} , T_{reac} , *b* and *V*. Along the abscissa axes, green color represents safe operation, i.e. $S_{vfa} \leq S_{vfa}^{max}$. Red color corresponds to $S_{vfa} > S_{vfa}^{max}$, i.e. unsafe operation. The red vertical lines correspond to $S_{vfa} = S_{vfa}^{max}$. In each plot, the magenta circle with star corresponds to the steady-state operating point given in Table 3. This operating point is a typical operating point of the real pilot reactor. (Comment by the publisher: For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

discrete values is generated. A reasonable range of this array is guessed, and the resolution of the array is adapted (manually), but is typically selected as $1/N_{x_i}$ where $N_{x_i} = 100$ (the number of elements in the array). By regarding each $\{x_i\}$ as a coordinate, the *n* arrays constitute a grid. The objective function, f_{obj} , is calculated at each grid point (or joint), i.e. for each possible combination of the elements in each x_i . The optimal solution, x_{opt} , is that particular value of *x* which corresponds to the optimal value of f_{obj} , i.e. either the maximum or the minimum depending on how "optimal" is defined for the given optimization problem.

In general, precise solutions are desired. To obtain more precise solutions, the following alternative approaches were tested on some of the optimizations problems: (1) Reducing the range. (2) Improving the resolution by increasing number of grid intervals. (3) Applying a local optimizer (Edgar et al., 2001) with the global optimal solution found with the BF method as the initial (guessed) optimal solution. The fmincon function in MATLAB was used as local optimizer. It was found that the differences between approach No.

(3) – using a local optimizer – and the other two alternative approaches were negligible. The computer program implementation of the BF method is considerably simpler and more flexible (scalable) than an implementation using fmincon. Therefore, the BF method, without any local optimizer, is the selected method in this paper.

The value of f_{obj} is calculated from the steady-state of the dynamic simulations of the modified Hill model of the AD process combined with the steady-state models of the reactor temperature and the heat exchanger temperatures based on energy balances. The simulator is based on the Euler explicit numerical method implemented in for-loops. This approach to find f_{obj} is similar to that in Rivas et al. (2008) where a wastewater treatment plant is optimized. There, the GRG2² algorithm implemented in Microsoft Excel is used.

² Generalized reduced gradient.

Table 2

Results of the various optimization problems. Underlines denote values of the optimization variables. Frames denote objective variables. The first (upper) section includes optimization variables. The second section includes optimization objective variables (to be maximized or minimized), but note that also *V* in the first section is an optimization objective variable in problems P_{v_j} . The third section includes the main constraint variable. The fourth section includes auxiliary variables (6.5e4 = $6.5 \cdot 10^4$).

$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	$\frac{P_{P_5}}{\frac{1.14}{27.9}}$
$T_{\text{reac}} \underline{38} 38 38 25 25 \underline{38} \underline{38} \underline{35.9} \underline{35.9} \underline{32.1} \underline{24.9} \underline{25.5} \underline{21.5} \underline{38} \underline{38} \underline{35.9} \underline{35.9} \underline{35.9} \underline{32.1} $	27.9
V 10 10 700 10 10 25.5 25.5 28.3 28.3 5.2 137 39.5 58.5 10	
	10
b 2.9 <u>20</u> 2.9 <u>20</u> 2.9 <u>2.9</u> 2.9 <u>2.9</u> 2.9 <u>2.9</u> <u>2.9</u> <u>20</u> <u>20</u> <u>20</u> <u>20</u> <u>20</u> <u>20</u> <u>20</u> <u>20</u>	2.9
$g_{ m hx} \infty \infty \infty \infty \infty \infty \infty \infty \infty \infty $	0
U 6.5e4 6	6.5e4
$F_{\rm meth} \begin{bmatrix} 8.09 & 25.6 & 27.8 & 20.8 & 0 & 20.7 & 20.7 & 20.7 & 20.7 & 23.5 & 25.0 & 23.6 & 8.09 & 20.7$	5.61
$P_{\text{sur}} \boxed{14.0} \boxed{60.9} -7.0 57.3 -18 \boxed{14.1} 39.1 41.0 49.8 50.8 \boxed{55.4} \boxed{68.2} \boxed{56.3} \boxed{14.0} \boxed{55.4} 5$	5.7
$ \overline{S_{\rm vfa}} 0.80 0.38 0.19 0.79 5.2 0.80 0.80 0.80 0.80 0.80 0.80 0.56 0.43 0.56 0.80 $	0.80
HRT 6.1 2.4 167 2.4 2.4 6.1 6.1 6.7 6.7 1.23 32.5 9.4 13.9 6.1	8.8
SRT 17.7 48.0 484 48.0 7.0 17.7 17.7 19.4 19.4 24.6 94.3 188 278 17.7	25.5
OLR 4.9 12.7 0.18 12.7 12.7 5.0 5.0 4.5 4.5 24.4 0.93 3.2 2.2 4.9	3.4
$\gamma_{\text{meth}} \begin{vmatrix} 4.96 & 6.1 & 6.62 & 4.96 & 0 \end{vmatrix} \begin{vmatrix} 4.94 & 4.94 & 4.94 & 4.94 & 4.94 & 5.60 & 5.96 & 5.61 & 4.96 \end{vmatrix}$	4.94
$P_{\rm meth} \begin{bmatrix} 29.4 & 93.0 & 101 & 75.6 & 0 \\ 101 & 75.6 & 0 & 75.3 & 75.3 & 75.3 & 75.3 & 85.5 & 91.0 & 85.5 & 29.4 \\ 101 & 1$	20.4
$P_{\text{heat}} \begin{bmatrix} 14.5 & 29.8 & 105.6 & 15.6 & 15.6 & 58.9 & 33.9 & 32.0 & 23.2 & 22.2 & 27.8 & 20.4 & 26.9 & 14.5 \end{bmatrix}$	14.1
$P_{\text{agit}} \left 0.57 1.46 1.46 1.46 1.46 1.46 1.46 1.46 1.46 1.46 1.46 1.46 1.46 1.46 1.46 0.57 \right $	0.39
$P_{\text{supply}} _{0.057}$ 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15	0.040
$P_{\rm sep}$ 0.28 0.73 0.73 0.73 0.73 0.73 0.73 0.73 0.73	0.20
P_{feed} 0.0038 0.010 0.040 0.010 0.010 0.013 0.013 0.014 0.014 0.0078 0.014 0.015 0.018 0.00	8 0.0026
$\gamma_{\rm P} = \begin{vmatrix} 0.23 & 1.02 & -0.12 & 0.96 & -0.3 \end{vmatrix} 0.24 0.65 0.68 0.83 0.85 \begin{vmatrix} 0.92 & 1.14 & 0.94 & 0.23 \end{vmatrix}$	0.095

3. Results

3.1. Compilation of results

The results of the optimization problems presented in the subsequent sections are compiled in Table 2. Units of the table entries are defined in Appendix C. In the table, underlines denote values of the optimization variables, while frames denote objective variables.

The optimization problems are categorized as follows, cf. Section 2.3:

- In problems P_{F_i} , F_{meth} is maximized.³
- In problems P_{V_i} , V is minimized.
- In problems P_{P_k} , P_{sur} is maximized.

3.2. Maximization of F_{meth}

To maximize F_{meth} , the following variables are considered as optimization variable candidates in the optimization problems discussed in the following sections: F_{feed} , T_{reac} , b, and V. To provide insight into the steady-state behavior of the reactor when these variables are varied, Fig. 3 shows F_{meth} and S_{vfa} vs. each of these variables.⁴ S_{vfa} is plotted since its value determines whether the reactor is in a safe operation condition, or not, cf. Section 2.3. The simulations are based on the modified Hill model adapted to the plot reactor applied to the planned full-scale reactor. The reactor volume is set as $V = 10 \text{ m}^3$ which is assumed a possible, but not

necessarily optimal, volume of an AD reactor fed with animal waste at Norwegian farms.

Comments to the plots of Fig. 3 regarding each of the four optimization variables:

• F_{feed} : Plot 1a shows that the maximum F_{meth} is obtained with $F_{\text{feed}} = 3.34 \text{ m}^3/\text{d}$. However, this maximum is regarded as non-feasible since in Eq. (6) is violated, cf. plot 1b. As F_{feed} is increased beyond $F_{\text{feed}} = 3.34 \text{ m}^3/\text{d}$, F_{meth} decreases,

which can be explained by a "wash-out" of the methanogens. For F_{feed} beyond 5.5 m³/d, no methane gas is produced.

- T_{reac} : Plot 2a shows that F_{meth} is monotonically increasing with T_{reac} . Plot 2b shows that a reduction of T_{reac} increases S_{vfa} . If T_{reac} is too small, in Eq. (6) is violated.
- *b*: Plot 3a shows that F_{meth} is monotonically increasing with *b*. Plot 3b shows that a relatively small *b* will violate in Eq. (6). *b* is rather a design parameter than an operational parameter.

Table 3
Steady-state operating point of the AD reactor
used in simulations, as explained in the text.
Units are defined in Appendix C.

Variable	Value
V	10
T _{reac}	35
b	2.9
S _{vsin}	30.2
F _{feed}	1.13
F _{meth}	6.00
S _{bvs}	3.42
S _{vfa}	0.66
X _{acid}	2.03
X _{meth}	0.39

 $^{^3~}P_{F_5}$ is actually not an optimization problem, but is included for demonstration purposes, cf. Section 3.2.

⁴ The simulations are run over a time interval of 1000 d which is sufficient for the dynamic $F_{\text{meth}}(t)$ to get into an approximate steady state.

V: Plot 4a shows that F_{meth} is monotonically increasing with V.
 Plot 4b shows that a relatively small V will violate in Eq. (6).
 Manipulating the reactor volume during reactor operation is theoretically possible, but hardly a practical option.

3.2.1. Optimization problems (for maximization of F_{meth})

 P_{F_1} :

 $\max_{F_{\text{feed}},T_{\text{reac}}}F_{\text{meth}}$

b and *V* are fixed. Results are: The optimal F_{feed} of 1.63 m³/d is less than $F_{\text{feed}}^{\text{max}}$, which is due to the limitation by in Eq. (6). The optimal T_{reac} is 38 °C which is the maximum acceptable value. P_{F₂}:

--

 $\max_{h} F_{\text{meth}}$

 F_{feed} is fixed at $F_{\text{feed}}^{\text{max}}$. Results are: The optimal *b* is 20, its upper limit. F_{meth} is 25.6/8.09 = 3.2 times larger than in the previous case. P_{sur} is 60.9/14.0 = 4.4 times larger than in the previous case. P_{Fa} :

 $\max_{V} F_{\text{meth}} \tag{7}$

 F_{feed} is set to $F_{\text{feed}}^{\text{max}}$. Results are: The optimal *V* is 700 m³, its upper limit, corresponding to HRT = 167 d, a very large value. This optimal *V* is probably impractical to implement. Furthermore, P_{sur} is negative, due to the large heat loss, seen indirectly in the large P_{heat} .

$$P_{F_4}$$
:

 $\max_{b} F_{\text{meth}} \tag{8}$

 T_{reac} is fixed at 25 °C. This optimization problem is similar to P_{F_2} , except T_{reac} is there fixed at 38 °C. Results are: The optimal *b* is 20, its upper limit, as in P_{F_2} . Both F_{meth} and P_{sur} are comparable with the respective values for P_{F_2} . Hence, it is demonstrated that it is beneficial to have a large *b* since it allows for a lower reactor temperature.

 $P_{F_{5}}$:

This scenario is actually not an optimization problem as all parameters are fixed. Its purpose is to demonstrate the importance of parameter *b*. The conditions are as in P_{F_4} , except *b* is now set as 2.9, which is the value estimated for the real pilot reactor. Simulations show that reactor failure can be expected since $S_{vfa} = 5.2 \text{ g/L}$, which is (much) larger than the critical limit $S_{vfa}^{max} = 0.8 \text{ g/L}$. Simulations (not represented in Table 2) show that, also with T_{reac} set as 38 °C, and other parameters being the same, reactor failure can be expected. Comparing with P_{F_4} , where b = 20, these simulations demonstrate the importance of having a large *b*. This scenario also demonstrates that care must be taken when selecting *V* for a given *b* and a fixed F_{feed} , to prevent reactor failure.

3.2.2. Conclusions (regarding maximization of F_{meth})

- In general, T_{reac} should be set to $T_{\text{reac}}^{\max} = 38 \,^{\circ}\text{C}$, and *b* should be as large as possible.
- Furthermore, *V* should be set to its maximum value. However, large *V* decreases *P*_{sur} due to increased thermal loss. Of course, increasing *V* also increases constructional and capital costs, but these factors are not discussed in this paper.
- In most cases, increasing F_{feed} gives increasing F_{meth} . However, the limitation $S_{\text{vfa}} \leq S_{\text{vfa}}^{\text{max}}$ sets an upper limit of F_{feed} . This upper limit of F_{feed} may be less than $F_{\text{feed}}^{\text{max}}$, the (normal) animal waste production.

- Assuming $F_{\text{feed}} = F_{\text{feed}}^{\text{max}}$. By selecting a sufficient large T_{reac} , V and/or b, $S_{v\text{fa}} \leq S_{v\text{fa}}^{\text{max}}$ can be maintained. However, if T_{reac} and b are fixed, the optimal V may become very large.
- Maximization of F_{meth} is a questionable optimization problem since there it may have two unfortunate results: (1) Assuming limited T_{reac} , V and/or b, the F_{feed} that maximizes F_{meth} may become less than F_{feed}^{max} implying that only a part of the bioresource volume is utilized. (2) Assuming $F_{feed} = F_{feed}^{max}$, the "optimal" V may become impractically large.
- Assuming specifically $V = 10 \text{ m}^3$ which is a plausible reactor size for Norwegian farms: Assuming $F_{\text{feed}} = F_{\text{feed}}^{\text{max}} = 4.2 \text{ m}^3/\text{d}$, and $T_{\text{reac}} = 25 \text{ °C}$, it is necessary that *b* has a large value, here 20, for the reactor to operate safely. With b = 20, the difference in F_{meth} and P_{sur} between $T_{\text{reac}} = 25 \text{ °C}$ and $T_{\text{reac}} = 38 \text{ °C}$ is not large. However, if b = 2.9 as estimated for the real pilot reactor, reactor failure may occur both with $T_{\text{reac}} = 25 \text{ °C}$ and $T_{\text{reac}} = 38 \text{ °C}$. Consequently, a large *b* is very important.

3.3. Minimization of V

Although constructional and capital costs are not included explicitly in the optimization problems discussed in this paper, it is beneficial to minimize the reactor volume, *V*. Fig. 3, plots 4a and b, show that, for a given F_{feed} , there is a lower limit of *V* while satisfying in Eq. (6). In the present section, the optimization problems aim at finding the minimum *V* under various conditions, while satisfying in Eq. (6). In each of the problems, F_{feed} is set equal to $F_{\text{feed}}^{\text{max}}$. Note that minimizing *V* assuming that F_{feed} is constant, is equivalent to minimizing HRT, cf. the definition of HRT, Eq. (4). Neither F_{meth} nor P_{sur} are included in these optimization problems, but their values are presented, cf. Table 2.

3.3.1. Optimization problems (for minimization of V) P_{V_1} :

$$\min V, \text{ without heat exchanger} \tag{9}$$

Here, heat exchanger is not used. T_{reac} is fixed at T_{reac}^{max} . Result: $P_{sur} = 14.1 \text{ MWh/y}$.

$$\min_{V} V, \text{ with heat exchanger}$$
(10)

Here, a heat exchanger is used. This problem is otherwise similar to P_{v_1} , and V is therefore the same. Result: P_{sur} becomes 39.1 MWh/y, a considerable increase comparing with P_{v_1} . This indicates that using a heat exchanger is beneficial.

$$\min_{V,T_{\text{reac}}} V, \text{ with heat exchanger}$$
(11)

 T_{reac} is now an optimization variable (in addition to *V*). The results in this problem are to be compared with P_{V_3} , see below. P_{V_4} :

 $\min_{V,T_{reac}} V, \text{ with heat exchanger and full insulation}$ (12)

This problem is similar to P_{V_3} , but with full thermal insulation of the reactor walls, i.e. U = 0, which corresponds to G = 0 in Eqs. (A.10) and (A.17). Results: The optimal V becomes 28.3 m³, the same as in P_{V_3} . The optimal T_{reac} is 35.9 °C, as in P_{V_3} . However, P_{sur} becomes larger, 49.8 vs. 41.0 MWh/y, indicating that good insulation is beneficial.

 P_{V_5} :

 P_{V_2} :

 $\min_{V,T_{\text{reac}}} V, \text{ with heat exchanger and full insulation}$ (13)

This problem is similar to P_{V_3} , but now *b* is set to $b_{max} = 20$. Results: The optimal T_{reac} is 32.1 °C. The minimum *V* is 5.2 m³, which is considerably smaller than in the other optimization problems. This indicates that it is (very) beneficial to have a large *b*.

3.3.2. Conclusions (regarding minimization of V)

Assuming b = 2.9 as for the real pilot reactor, the following conditions (P_{V4}) is recommended for design: Assuming $F_{\text{feed}} = F_{\text{feed}}^{\text{max}}$, $V = 28.3 \text{ m}^3$ is appropriate, corresponding to HRT = 6.7 d. Furthermore, the optimal T_{reac} is 35.9 °C.

The larger *b*, the smaller the minimum *V*.

3.4. Maximization of P_{sur}

The power surplus, P_{sur} , is calculated with Eq. (A.20). In optimization problems P_{P_1} , P_{P_2} and P_{P_3} , F_{feed} is set to F_{feed}^{max} .

3.4.1. Optimization problems (for maximization of P_{sur})

 P_{P_1} :

 $\max_{V,T_{reac}} P_{sur}$

Results are: The optimal V is 137 m³, giving HRT = 32.5 d, a relatively large value. The optimal T_{reac} is 24.9 °C, a relatively small value.

 P_{P_2} :

 $\max_{b,V,T_{reac}} P_{sur}$

 F_{feed} is set to $F_{\text{feed}}^{\text{max}}$. Comparison is made with Problem P_{P_3} , see below.

 P_{P_3} :

$\max_{u,v} P_{sur}$, without heat exchanger

This problem is the same as P_{P_2} , but now without heat exchanger. Results are: Comparing P_{P_3} and P_{P_2} shows that by using an heat exchanger, P_{sur} is increased by 21% and *V* is reduced by 32%.

 P_{P_4} :

 $\max_{F_{feed}, T_{reac}} P_{sur}, \text{ with heat exchanger}$

V is fixed at 10 m³, and *b* at 2.9. Thus, P_{P_4} is the same as P_{P_1} , except in P_{P_1} , F_{meth} is to be maximized. Results are: Comparing P_{P_4} and P_{P_1} shows that when an heat exchanger is installed, maximizing P_{sur} or F_{meth} gives the same optimal solution. Only (1.63 m³/d)/(4.2 m³/d) = 39% of the available feedstock is used, which may make this solution unacceptable.

 P_{P_5} :

 $\max_{F_{\text{feed}},T_{\text{reac}}} P_{\text{sur}}, \text{ without heat exchanger}$

This problem is the same as P_{P_4} , but now without heat exchanger. Result: Comparing P_{P_5} and P_{P_4} shows that using an heat exchanger increases P_{sur} . Only $(1.14 \text{ m}^3/\text{d})/(4.2 \text{ m}^3/\text{d}) = 27\%$ of the available feedstock is used, which may be unacceptable.

3.4.2. Conclusions (regarding maximization of P_{sur})

 $P_{\rm sur}$ increases considerably if b is increased and if a heat exchanger is used.

Assuming b = 2.9 as for the present pilot reactor and F_{feed} fixed at $F_{\text{feed}}^{\text{max}}$, a maximum P_{sur} is obtained with $V = 137 \text{ m}^3$, corresponding to HRT = 32.5 d. However, this large value of V may be impractical to realize.

With *V* fixed at 10 m³, assumed a plausible reactor size, and *b* assumed 2.9, as for the pilot reactor, P_{sur} is maximized by F_{feed} equal to only 39% of F_{feed}^{max} . Hence, only a small part of biological resources is utilized.

The maximum P_{sur} is 68.2 MWh/y is obtained in P_{P_2} , corresponding to power surplus productivity $\gamma_P = 1.14$ (MWh/y)/LU. This is also the maximum over all of the optimization problems reported in Table 2.

3.5. Main results

Below are the main results of the three optimization problems discussed in Sections 3.2–3.4.

3.5.1. Maximization of F_{meth}

 T_{reac} and *b* should have values as close as possible to their assumed upper limits, 38 °C and 20, respectively.

If F_{feed} is fixed at $F_{\text{feed}}^{\text{max}}$, the maximum F_{meth} is obtained with a very large *V*, which may be impractical to implement.

In most cases, increasing F_{feed} gives increasing F_{meth} . However, the limitation $S_{\text{vfa}} \leq S_{\text{vfa}}^{\text{max}}$ sets an upper limit of F_{feed} . This upper limit of F_{feed} may be less than $F_{\text{feed}}^{\text{max}}$, the (normal) animal waste production.

The two conclusions above imply that maximization of F_{meth} is a questionable optimization problem.

Assuming specifically $V = 10 \text{ m}^3$ which is a plausible reactor size for Norwegian farms: Assuming $F_{\text{feed}} = F_{\text{feed}}^{\text{max}} = 4.2 \text{ m}^3/\text{d}$, and $T_{\text{reac}} = 25 \text{ °C}$, it is necessary that *b* has a large value, e.g. 20, for the reactor to operate safely. With b = 20, the difference in F_{meth} and P_{sur} between $T_{\text{reac}} = 25 \text{ °C}$ and $T_{\text{reac}} = 38 \text{ °C}$ is not large. However, if b = 2.9 as estimated for the real pilot reactor, reactor failure may occur both with $T_{\text{reac}} = 25 \text{ °C}$ and $T_{\text{reac}} = 38 \text{ °C}$.

3.5.2. Minimization of V

The minimization assumes the following equality constraints: $S_{vfa} = S_{vfa}^{max}$, and $F_{feed} = F_{feed}^{max}$. Assuming b = 2.9 as for the real pilot reactor, the minimum V is 28.3 m³, corresponding to HRT = 6.7 d. Furthermore, the optimal T_{reac} is 35.9 °C.

With a larger *b*, the minimum *V* is reduced.

3.5.3. Maximization of P_{sur}

*P*_{sur} increases considerably if *b* is increased and if a heat exchanger is used.

Assuming b = 2.9 as for the present pilot reactor and F_{feed} fixed at $F_{\text{feed}}^{\text{max}}$, a maximum P_{sur} is obtained with $V = 137 \text{ m}^3$, corresponding to HRT = 32.5 d. However, this large value of V may be impractical to realize.

With *V* fixed at 10 m³, assumed a plausible reactor size, and *b* assumed 2.9, as for the pilot reactor, P_{sur} is maximized with F_{feed} equal to only 39% of F_{feed}^{max} , which may be an unacceptable solution as not all of the biological resources is utilized.

3.6. Implementation of optimal solutions

Due to inevitable disturbances, it may be necessary to retain the optimal solutions using feedback control. Control of the pilot reactor, which is the basis of the planned full-scale reactor, is studied in Haugen et al. (2013b) and Haugen et al. (2014).

The implementation of feedback control may not be trivial. For example, in the optimization problems $P_{V_1} - P_{V_5}$, S_{vfa} is assumed being retained at $S_{vfa}^{max} = 0.8 \text{ g/L}$, its setpoint. Since S_{vfa} is not measured online, the feedback control can not be based on a measurement. Instead, feedback can be made from an estimate of S_{vfa} calculated by a state estimator in the form of a Kalman filter (Haugen et al., 2014).

Table 4

Comparison of one optimization results of the present article with design parameters of real UASB reactors fed with cattle manure.

Reactor	Reference	T_{reac} (°C)	HRT (d)
Theoretical UASB based on real pilot reactor	Optim. problem P_{V_1} in present article	38	6.1
Laboratory UASB, filtered and pasteurized feed	Maranon et al. (2006)	37	14
Laboratory UASB, filtered feed	Maranon et al. (2001)	<37	5.3-22.5

4. Discussion

The optimization results in this paper are based on three mathematical models – the AD process model, the model of the reactor temperature, and model of the heat exchanger temperatures. The first two models have been adapted quite successfully to the real pilot reactor (Haugen et al., 2013a). The latter has not been adapted to a physical heat exchanger, and therefore its accuracy can not be stated. However, the underlying modeling principles are assumed reasonable. It is important to recognize that possible limited reliability of the models limits the practical use of the models for the full-scale dimensioning. This limitation applies to model-based design in general.

The modified Hill model, presented in Appendix A.1, is a relatively simple AD process model. In this model, S_{vfa} is the only variable which can be used to define the conditions for safe reactor operation, and $S_{vfa}^{max} = 0.8 \text{ g/L}$ has been used as a constraint in the optimization problems discussed in this paper. In other applications, e.g. AD reactors fed with swine waste, it may be important to take other constraints taken into account, e.g. maximum ammonia concentration, minimum pH, maximum propionic to acetic acid ratio, and maximum ratio of intermediate alkalinity over total alkalinity. To these ends, more comprehensive AD models are needed. Overviews of various AD models are given by e.g. (Gavala et al., 2003; Lyberatos and Skiadas, 1999; and Strömberg, 2010). Of particular interest is the comprehensive ADM1 model (Anaerobic Digestion Model No. 1) (Batstone et al., 2002), which we may use in future studies. A short discussion of AD models regarded as candidate models for the AD reactor at Foss Biolab. including the ADM1 model, are also given by Haugen et al. (2013a). Although the modified Hill model used in the present paper is relatively simple, we think that the approach to optimization used, is applicable to alternative AD models.

The Brute Force optimization method used in this article is simplistic. However, for the optimization problems studied in this article, this method is sufficiently effective and reliable. For more comprehensive problems with a larger number of optimization variables or a more comprehensive model, alternative global optimization methods may be required (Edgar et al., 2001).

The present study does not address economical optimization, which, in general, involves constructional, capital, and operational cost. The models and results of the present paper may, however, constitute a part of the total model used in economical optimization.

As already stated in Section 1, (Hill, 1983a) seems to be one of the first attempts to optimization of operation of AD reactors. However, optimal design was not covered, and the optimization objective was limited to maximizing the volumetric methane productivity. Our literature search has actually not lead to more recent comparable approaches to model-based optimization of AD reactor operation and design.

It is of interest to compare optimization results of the present article with design parameters of real UASB reactors fed with cattle manure, although these real reactors may not be optimally designed. The HRT is here assumed the most interesting parameter. Table 4 gives a comparison of a few cases. In Maranon et al. (2006), the HRT of 14 d was used merely because it worked well in previous similar experiments. In Maranon et al. (2001), a number of different HRT are used, and no reports of reactor failure is reported at HRT = 5.3 d (the lowest HRT applied). Furthermore, in Maranon et al. (2001), the reactor temperature is not presented, but the feed enters the reactor with temperature of 37 °C. The comparison indicates that the theoretical optimization result of HRT = 6.1 d of the present article is a realistic value. Literature on HRT of other UASB reactors fed with cattle manure has not been found.

5. Conclusions

Optimal design and operation of a planned full-scale UASB reactor at a dairy farm have been determined using optimization algorithms based on steady state simulations of a dynamic AD process model combined with models of the reactor temperature and the heat exchanger temperatures based on energy balances. Available feedstock is 6 m^3/d dairy waste.

The optimization solutions have been found using the straightforward "brute force" (BF) method which is based on a scan for the global optimal solution over a grid of the optimization variables. The grid resolution is typically selected as 1/100 of the range of the pertinent variable, giving a sufficient precision of the optimal solution.

For the given AD reactor and its mathematical model, alternative optimization objectives are maximizing F_{meth} , minimizing V, and maximizing P_{sur} . Optimization variables candidates are F_{feed} , T_{reac} , b, V, g_{hx} , and U. The optimization algorithm takes into account the following constraints: $S_{vfa} \leq S_{vfa}^{max}$, and $F_{feed} \leq F_{feed}^{max}$.

The results indicate that any optimal solution is improved, for example, the maximum P_{sur} is increased, if *b* is increased, if energy is recovered with a heat exchanger, and if the reactor is well insulated.

Evaluated over all of the optimization problems studied, the maximum P_{sur} is 68.2 MWh/y, corresponding to power surplus productivity $\gamma_{p} = 1.14 \text{ (MWh/y)/LU}$.

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Appendix A. Mathematical models

Values of model parameters having constant values are given in Appendix C.

A.1. Model of the AD process

The mathematical model of the AD processes in the reactor is a modification of the model in Hill (1983b), adapted to the pilot reactor (Haugen et al., 2013a). The model is based on material balances

of biodegradable volatile solids, volatile fatty acids, acidogens and methanogens, and a calculation of the produced methane gas flow. The model is summarized below.

Material balances:

$$\dot{S}_{\rm bvs} = \left(B_0 S_{\rm vs_{in}} - S_{\rm bvs}\right) \frac{F_{\rm feed}}{V} - \mu k_1 X_{\rm acid} \tag{A.1}$$

$$\dot{S}_{\rm vfa} = \left(A_{\rm f}B_0S_{\rm vs_{in}} - S_{\rm vfa}\right)\frac{F_{\rm feed}}{V} + \mu k_2 X_{\rm acid} - \mu_c k_3 X_{\rm meth} \tag{A.2}$$

$$\dot{X}_{\text{acid}} = \left(\mu - K_d - \frac{F_{\text{feed}}/b}{V}\right) X_{\text{acid}}$$
(A.3)

$$\dot{X}_{\text{meth}} = \left(\mu_c - K_{dc} - \frac{F_{\text{feed}}/b}{V}\right) X_{\text{meth}}$$
(A.4)

Methane gas production:

$$F_{\text{meth}} = V \mu_c k_5 X_{\text{meth}} \tag{A.5}$$

Reaction rates:

$$\mu = \mu_m \frac{S_{bvs}}{K_s + S_{bvs}} \tag{A.6}$$

$$\mu_c = \mu_{mc} \frac{S_{\rm vfa}}{K_{\rm sc} + S_{\rm vfa}} \tag{A.7}$$

$$\mu_m = \mu_{mc} = 0.013T_{\text{reac}} - 0.129 \ (20^{\circ}\text{C} < T_{\text{reac}} < 60^{\circ}\text{C}) \tag{A.8}$$

A.2. Model of reactor temperature

The mathematical model able to predict T_{reac} is based on energy balance model of the pilot reactor (Haugen et al., 2013a). For easy reference in the present paper, the model is reviewed here:

$$\dot{T}_{\text{reac}} = \frac{1}{c\rho V} [P_{\text{heat}} + c\rho F_{\text{feed}}(T_{\text{infl}} - T_{\text{reac}}) + G(T_{\text{amb}} - T_{\text{reac}})]$$
(A.9)

The corresponding steady-state version of this model is

$$P_{\text{heat}} = c\rho F_{\text{feed}}(T_{\text{reac}} - T_{\text{infl}}) + G(T_{\text{reac}} - T_{\text{amb}})$$
(A.10)

which is combined with the heat exchanger model as described below.

In Eq. (A.10), *G* is calculated assuming that the reactor is a vertical cylinder of diameter *d* and height *h*. Their ratio is $k_{hd} = h/d$, which can be regarded as an optimization variable. In the context of selected optimization problems described in previous sections, it was found that $k_{hd} = 1$ is optimal, and therefore $k_{hd} = 1$ is used throughout this paper.

For simplicity, it is assumed that the heat conduction takes place at all sides of the cylinder. The area-specific heat transfer conductivity, *U*, is assumed equal to that of the pilot reactor (Haugen et al., 2013a).

A.3. Model of heat exchanger temperatures

The mathematical modeling of the heat exchanger shown in Fig. 1 assumes that the liquid flows are equal to the feed flow, F_{feed} , in all pipelines.

It is assumed that the heat exchanger consists of two homogeneous volumes: the product volume and the heating medium volume, respectively. The energy balances are:

$$c\rho V_{\rm p} T_{\rm infl} = c\rho F_{\rm feed} (T_{\rm feed} - T_{\rm infl}) + G_{\rm hx} (T_{\rm hx_{out}} - T_{\rm infl})$$
(A.11)

$$c\rho V_{\rm h} \dot{T}_{\rm hx_{out}} = c\rho F_{\rm feed} (T_{\rm reac} - T_{\rm hx_{out}}) + G_{\rm hx} (T_{\rm infl} - T_{\rm hx_{out}})$$
(A.12)

In this paper, the steady-state version of this model is used in the analysis, i.e. the time-derivatives are set to zero. Eliminating $T_{hx_{out}}$ from the resulting steady-state equations yields

$$T_{\rm infl} = \frac{1 + g_{\rm hx}}{1 + 2g_{\rm hx}} T_{\rm feed} + \frac{g_{\rm hx}}{1 + 2g_{\rm hx}} T_{\rm reac}$$
(A.13)

where

$$g_{\rm hx} = \frac{G_{\rm hx}}{c\rho F_{\rm feed}} \tag{A.14}$$

Some special cases of Eq. (A.13) are:

•
$$g_{hx} = 0$$
, i.e. no heat exchange:
 $T_{infl} = T_{fact}$ (A.15)

• $g_{hx} = \infty$, i.e. an extremely high, or ideal, heat exchange:

$$T_{\text{infl}} = \frac{1}{2} (T_{\text{feed}} + T_{\text{reac}}) \tag{A.16}$$

Combining Eq. (A.13) with Eq. (A.10) gives

$$P_{\text{heat}} = \frac{1 + g_{\text{hx}}}{1 + 2g_{\text{hx}}} c\rho F_{\text{feed}}(T_{\text{reac}} - T_{\text{feed}}) + G(T_{\text{reac}} - T_{\text{amb}})$$
(A.17)

where P_{heat} is in J/d.

A.3.1. Power savings due to using preheating with heat exchanger

The saving in P_{heat} due to using an heat exchanger can be calculated as the difference in P_{heat} given by Eq. (A.17) with $g_{\text{hx}} = 0$ and with the assumed value of g_{hx} . Assuming T_{reac} is the same in both cases, the saving is

$$\Delta P_{\text{heat}} = \frac{g_{\text{hx}}}{1 + 2g_{\text{hx}}} c \rho F_{\text{feed}}(T_{\text{reac}} - T_{\text{feed}})$$
(A.18)

Considering the special case of G = 0 (perfect reactor insulation) and $g_{hx} = \infty$ (perfect heat exchange),

$$\Delta P_{\text{heat}} = \frac{1}{2} c \rho F_{\text{feed}} (T_{\text{reac}} - T_{\text{feed}})$$
(A.19)

Compared with Eq. (A.17), the savings is *half* of the power demand without preheating. In other words, for a perfectly insulated reactor, preheating with a perfect heat exchanger halves the external power needed to retain the reactor at a given T_{reac} .

A.4. Power calculations

The power surplus is calculated as

$$P_{\rm sur} = P_{\rm meth} - P_{\rm heat} - P_{\rm agit} - P_{\rm supply} - P_{\rm sep} - P_{\rm feed} \tag{A.20}$$

where P_{sur} is in MWh/y. The individual terms in Eq. (A.20) are:

$$P_{\rm meth} = E_{\rm meth} F_{\rm meth} [kWh/y]$$
(A.21)

$$P_{\text{supply}} = k_{\text{supply}} F_{\text{feed}_{\text{raw}}} [\text{kWh/y}]$$
(A.22)

$$P_{\rm sep} = k_{\rm sep} F_{\rm feed_{\rm raw}} [kWh/y]$$
(A.23)

$$P_{\text{feed}} = \rho g h F_{\text{feed}}[J/d] \tag{A.24}$$

where

$$F_{\text{feed}} = k_{\text{s}} F_{\text{feed}_{\text{raw}}} \tag{A.25}$$

$$P_{\text{agit}} = k_{\text{agit}} F_{\text{feed}_{\text{raw}}} [kWh/y] \tag{A.26}$$

Appendix B. Abbreviations

AD = Anaerobic digestion. BVS = Biodegradable volatile solids. COD = Chemical oxygen demand. CSTR = Continuous stirred tank reactor. HRT = Hydraulic retention time. LU = Livestock unit (head or cow). NLP = Nonlinear programming. sCOD = Soluble COD. SRT = Solids retention time. STP = Standard temperature and pressure; 0 °C, 1 bar. tCOD = Total COD. UASB = Upflow anaerobic sludge blanket. VFA = Volatile fatty acids. VS = Volatile solids.

Appendix C. Nomenclature and values of constants

The nomenclature is in alphabetical order.

 $A_f = 0.25 (g VFA/L)/(g BVS/L)$ is acidity constant.

b = SRT/HRT [d/d] is retention time ratio.

 $B_0 = 0.69 \text{ (g BVS/L)/(g VS/L)}$ is biodegradability constant.

c = 1000 J/(kg K) is specific heating capacity of reactor liquid.

 $E_{\text{meth}} = 9.95 \text{ kWh/m}^3$ is specific energy contents of methane gas at STP conditions (calculated from the ideal gas law).

 F_{feed} [m³/d] is influent or feed flow or load rate, assumed equal to effluent flow (constant volume).

 $F_{\text{feed}_{\text{raw}}}$ [m³/d] is raw diluted dairy waste fed to the separator. F_{meth} [L CH₄/d] is methane gas flow.

 $g = 9.81 \text{ kg m/s}^2$ is gravity constant.

 $g_{\rm hx}$ [1] is defined as the heat transfer conductivity coefficient of the heat exchanger.

G[(J/d)/K] is thermal conductivity of the reactor.

 G_{hx} [(J/d)/K)] is thermal conductivity between the heating medium side and the product side of the heat exchanger. γ_{meth} [(m³ CH₄/d)/(m³/d)] is gas productivity:

$$\gamma_{\rm meth} = \frac{F_{\rm meth}}{F_{\rm feed}} \tag{C.1}$$

 $\gamma_{\rm P}$ [(MWh/y)/LU] is power surplus productivity:

$$\gamma_{\rm P} = \frac{P_{\rm sur}}{N_{\rm LU}} \tag{C.2}$$

h [m] is lift height of reactor influent.

 $HRT = F_{feed}/V$ [d] is hydraulic retention time.

 $k_{\text{agit}} = 243.3 \text{ (kWh/y)/(m^3/d)}$ is power coefficient of agitator. $k_{\text{hd}} \text{ [m/m]}$ is ratio of reactor height to reactor diameter. $k_{\text{f}} \text{ [1]}$ is wet fraction of raw (non-separated) feed passing through the separator and being fed to the reactor.

 $k_{\rm w}$ [MWh/y] is energy conversion constant.

 $k_{\rm s} = 0.70 \,({\rm m}^3/{\rm d})/({\rm m}^3/{\rm d})$ is separation constant.

 $k_{supply} = 24.33 \text{ (kWh/y)/(m^3/d)}$ is power coefficient of supply pump.

 $k_{\text{sep}} = 121.7 \text{ (kWh/y)/(m^3/d)}$ is power coefficient of separator. $k_1 = 3.89 \text{ g BVS (g acidogens/L)}$ is a yield constant.

 $k_2 = 1.76$ g VFA (g acidogens/L) is a yield constant.

 $k_3 = 31.7$ g VFA (g methanogens/L) is a yield constant.

 $k_5 = 26.3 \text{ L/g}$ methanogens is a yield constant.

 $K_s = 15.5$ g BVS/L is Monod half-velocity constant for acidogens.

 $K_{sc} = 3.0$ g VFA/L is Monod half-velocity constant for methanogens.

 $K_d = 0.02 \text{ d}^{-1}$ is specific death rate of acidogens.

 $K_{dc} = 0.02 \text{ d}^{-1}$ is specific death rate of methanogens.

L CH₄ is litres of methane gas at STP (standard temperature and pressure), i.e. temperature 0 °C and pressure 1 bar. L is litres of liquid.

 μ [d⁻¹] is reaction (growth) rate of acidogens.

 μ_c [d⁻¹] is reaction (growth) rate of methanogens.

 μ_m [d⁻¹] is the maximum reaction rate for acidogens.

 μ_{mc} [d⁻¹] is the maximum reaction rate for methanogens.

n is the number of optimization variables.

 $N_{\rm LU}$ is number of lifestock units (LU).

 N_{x_i} [1] is number of grid intervals, or subintervals, for optimization variable x_i .

OLR $[g VS L^{-1} d^{-1}] = [kg VS m^{-3} d^{-1}]$ is organic loading rate:

$$OLR = \frac{S_{vs_{in}}F_{feed}}{V}$$
(C.3)

 P_{agit} [kWh/y] is power consumption of the agitator.

 P_{heat} [kWh/y] is power consumption of the electrical heater, i.e. power supplied to the reactor by the electrical heater.

 P_{meth} [kWh/y] is usable power of the methane gas.

 P_{feed} [kWh/y] is power consumption of the feed pump related to lifting the feed up to the reactor inlet, typically provided by a displacement pump.

 P_{supply} [kWh/y] is power consumption of the supply pump, which is typically a monopump.

 P_{sep} [kWh/y] is power consumption of the feed separator.

 P_{sur} [MWh/y] is power surplus.

 ρ [kg/m³] is density of reactor liquid.

*S*_{bvs} [g BVS/L] is concentration of BVS in reactor influent.

 S_{vfa} [g VFA/L] is concentration of VFA acids in reactor.

 $S_{vs_{in}}$ [g VS/L] is concentration of VS in reactor influent.

 $SRT = b \cdot HRT [d]$ is solids (biomass) retention time.

 T_{amb} [°C] is ambient (air) temperature.

 T_{feed} [°C] is temperature of reactor feed.

 T_h [°C] is "hot" side temperature of the heat exchanger.

 T_{infl} [°C] is temperature of reactor feed.

 T_p [°C] is "cold" side temperature of the heat exchanger.

 T_{reac} [°C] is reactor temperature.

 $U = 6.50 \cdot 10^4 ((J/d)/K)/m^2$ is specific thermal conductivity of the reactor, assumed equal to that of the pilot reactor. In Haugen et al. (2013b), *U* is denoted *G*_s.

 $V[m^3]$ is effective volume of reactor liquid.

y is year.

Appendix D. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.compag.2015.01. 001.

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