Model description

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1. Model's base

The simplified Pump Mixed Anaerobic Digestion Model is based on S.Weinrich R4 model. R4 model is a simplified version of ADM-1 model. Biogas is directly produced from organic matter polymers (carbohydrates, proteins, and lipids) without mentioning acetogenesis, acidogenesis, or hydrolysis steps. It does not include any inhibition steps; the kinetics of every process consists of a first-order rate equation. Gas products consist of carbon dioxide, methane, and water vapor (due to simplification). Structure
of the model is shown in Petersen's matrix in table 1.

Table 1. Petersen matrix of R4 model [1]

Component → Process ↓	S_{CH4}	S_{IC}	S_{IN}	S_{H2O}	X_{Ch}	X_{Pr}	X_{Li}	X_{Bac}	$S_{gas,ch4}$	$S_{gas,co2}$	Rate
Fermentation X_{Ch}	0.2482	0.6809	-0.0207	-0.0456	-1			0.1372			$k_{Ch}X_{Ch}$
Fermentation X_{Pr}	0.3221	0.7954	0.1689	-0.4588		-1		0.1723			$k_{Pr}X_{Pr}$
Fermentation X_{Li}	0.6393	0.5817	-0.0344	-0.4152			-1	0.2286			$k_{Li}X_{Li}$
Decay X_{Bac}					0.18	0.77	0.05	-1			$k_{dec}X_{Bac}$
Phase transition CH_4	-1								$\frac{V_{liq}}{V_{gas}}$		$k_La(S_{CH4}-16K_{H,CH4}\cdot P_{CH4})$
Phase transition CO_2		-1								$\frac{V_{liq}}{V_{gas}}$	$k_La(S_{IC}-44KH_{,CO2}\cdot P_{CO2})$

The total pressure of biogas consists of the methane, carbon dioxide, and water vapor partial pressures. Each of them can be calculated through applying the gas law. However, the original model contains a mistake and changed indexes for gases. This inaccuracy is essential to the model's integrity, so it has been kept intentionally. For instance, for methane partial pressure the equation is:

$$p_{CH4} = S_{gas,ch4}\frac{RT}{16} \tag{1}$$

Similarly for carbon dioxide, the equation has a form:

$$p_{CO2} = S_{gas,co2}\frac{RT}{44} \tag{2}$$

The stream of produced biogas is similar to the classic ADM-1 model:

$$q_{gas} = k_p(P_{gas} - P_{atm})\frac{P_{gas}}{P_{atm}} \tag{3}$$

2. Pump Mixed Anaerobic Digestion Model

The model's development included dividing the digester into 3 sections. The Upper one (S1) is the only part of the digester that is connected to the gas phase – for this section only phase transition equations are applied. Also, S1 is the only part that takes the fresh feedstock. The middle part (S2) acts as a buffer between sections S1 and S2. There are no additional outputs or inputs in mass balance equations for any component in section S2. The last section, S3, is directly connected to the pump so it

can recirculate the stream. Moreover, it is the only section connected with the reactor's output. This approach has been used before by Postawa et al. [2]. The whole concept is depicted by figure 1.

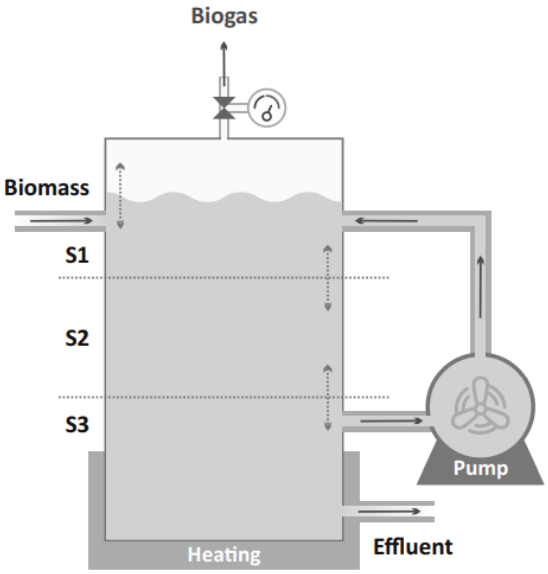

Figure 1. The concept of the Pump Mixed Anaerobic Digestion Model [2]

The general mass balance equation for the component in the liquid phase of the reactor in model R4 has a form:

$$\frac{dC_x}{dt} = \frac{F_{in} \cdot C_{x_{in}} - F_{out} \cdot C_x}{V_m} + \sum_{i=1}^{n} v_i \cdot R_i \tag{4}$$

The sum in the 1st equation involves reaction rates for each component.

In order to include all liquid components transfer and the sectioning due to pump influence, the mass balance equation for section S1 is:

$$\frac{dC_x}{dt} = \frac{F_{in} \cdot C_{x_{in}} - 0}{\frac{V_m}{3}} + \sum_{i=1}^{n} v_i \cdot R_i - lLt_{S1-S2-C_x} + lLt_{S3-S1-C_x} \cdot k_{pump} \tag{5}$$

Two last parts of the 2nd equation involve the transfer driven by the concentration gradient between 1st and 2nd sections and the transfer from the bottom of the reactor is driven by the mechanical work of the pump. The general form of lLt equation is:

$$lLt_{S1-S2-C_x} = kLl_{12} \cdot (C_{x-S1} - C_{x-S2}) \tag{6}$$

The form is dedicated to S1-S2 transfer, but it is analogous to other sections' transfers.

As was previously mentioned, there is no fresh input or output in the 2nd section. By applying that the mass balance for section S2 is:

$$\frac{dC_x}{dt} = \frac{0 - 0}{\frac{V_m}{3}} + \sum_{i=1}^{n} v_i \cdot R_i + lLt_{S1-S2-C_x} - lLt_{S2-S3-C_x} \tag{7}$$

There is no direct impact of the pump in section S2, just a concentration gradient. Signs before transfer equations indicate the direction of the component's flow [2].

Taking into consideration the last section of the reactor, S3, the proposed form is:

$$\frac{dC_x}{dt} = \frac{0 - F_{out} \cdot C_x}{\frac{V_m}{3}} + \sum_{i=1}^{n} v_i \cdot R_i + lLt_{S2-S3-C_x} - lLt_{S3-S1-C_x} \cdot k_{pump} \quad (8)$$

Mentioned changes increase the number of ODE equations by 3 times (except for gas-phase transition equations). The model is presented by the files in the Pump Mixed Anaerobic Digestion folder. Initial values of used parameters are shown in table 2. Some physiochemical parameters such as Henry's gas constant were calculated for each gas product depending on the operating temperature,

Table 2. Initial values of model's parameters

Parameter	Value
k_ch	0.25
k_pr	0.2
k_li	0.1
k_dec	0.02
k_{La}	200
k_p	50000
k_1_2	0.0403
k_2_3	0.337
k_3_1	0.204
k_pump	0.249

Applied experimental values were achieved using pig slurry as a feedstock with HRT 12 under atmospheric pressure and mesophilic temperature conditions. All parameters are described in Indata file.

3. Sensitivity analysis

Before proper model optimization, it is essential to verify which parameter has the biggest influence on methane production (the most desired gas product). This step required sensitivity analysis. Certain chosen operating parameters (for the last stage of the thesis) and model parameter values, included in Indata file, were increased by 1%. The impact of the parameter's value on methane production has been verified by calculating the reference value of methane before the change and after increasing the parameter value. Then the change was calculated in the form of absolute error. The whole approach was introduced by Danielsson [3]. The sensitivity analysis described above can be presented in form of a pseudo-code:

- Read indata from file
- Select initial values
- Calculate the reference gas value for the unchanged system, f(x)
- For each chosen parameter do:
  -increment parameter value by 1%
  -calculate the new value of produced gas, f(1.01x)
  -calculate the difference (sensitivity)
  $|f(1.01x) - f(x)|$
- Plot result

Sensitivity analysis is included in the Pump Mixed Anaerobic Digestion model's folder [3].

4. Model's parameters optimization

Based on sensitivity analysis results certain model parameters (k_p, k_{1_2}, k_{2_3}, and k_pump) were chosen to optimize their values. Two optimization methods were used (genetic algorithm and fmincon function with global search option) in order to compare their accuracy and the required time for finding the solution. The objective function was the sum of relative errors between theoretical

and experimental values of the amount of produced biogas, the percentage content of methane and percentage content of carbon dioxide:

$$Z = \sum_{i=1}^{n} \left| \frac{F_{biog\_mod_n} - F_{biog\_exp_n}}{F_{biog\_exp_n}} \right| + \left| \frac{C_{CH4\%\_mod_n} - C_{CH4\%\_exp_n}}{C_{CH4\%\_exp_n}} \right| + \left| \frac{C_{CO2\%\_mod_n} - C_{CO2\%\_exp_n}}{C_{CO2\%\_exp_n}} \right| \quad (9)$$

The model's optimization is presented in the model optimization folder. Used methods are presented in separate files using the same objective function (objectivity file). Applied experimental data in equation Z were the average results of data collected in steady-state conditions for HRT 12. The optimization process should be repeated for each mixing period of the pump (10, 20, or 30 min).

5. Operating parameters optimization

The last stage of this work was to optimize the operating parameters of the biogas plant (temperature and feedstock stream values) in order to maximize biogas production and methane content as the most desired product. Optimized values of the model's parameters obtained by the genetic algorithm method were used for this stage, each different for a specific pump mixing period. The genetic algorithm function was the chosen method of optimization. The objectivity function was calculated from 2 separate functions (max. content of methane and max. biogas stream). The general form of the objectivity function is:

$$Z = -(pCH4g + c \cdot q\_gas) \quad (10)$$

The value of the c factor depends on the range of results of separate objective functions. Used values of c are presented in table 3.

Table 3. Values of c factor used in objectivity function

Mixing period	c
10	0.1136
20	0.2126
30	0.0716

The whole approach is included in the parameter optimization folder. Max_pCH4 is the function to maximize methane percentage content, max_q_gas is the function to maximize the biogas stream. Optimalisation_modelv2 file includes all ODE equations.

References

[1] S. Weinrich, M. Nelles, *Systematic simplification of the Anaerobic Digestion Model No.1 (ADM1) – Model development and stoichiometric analysis*, Bioresource Technology 333(2021)

[2] K. Postawa, J. Szczygieł, E. Wrzesińska-Jędrusiak et al., *The pump mixed anaerobic digestion of pig slurry: new technology and mathematical modeling*, Waste Management 123(2021), p.111-119

[3] O. Danielsson, *Modeling and simulation of anaerobic manure digestion into biogas*, Master's Thesis in Applied Physics, Department of Physics & Engineering Physics, Chalmers University of Technology, Sweden, 2014