A distributed model of solid waste anaerobic digestion: sensitivity analysis

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Abstract A distributed model of anaerobic digestion of solid waste was developed to describe the balance between the rates of polymer hydrolysis and methanogenesis during the anaerobic conversion of rich and lean wastes in batch and continuous-flow reactors. Waste, volatile fatty acids (VFAs), methanogenic biomass and sodium concentrations are the model variables. Diffusion and advection of VFAs inhibiting both polymer hydrolysis and methanogenesis were considered. A sensitivity analysis by changing the key model parameter values was carried out. The model simulations showed that the effective distance between the areas of hydrolysis/acidogenesis and methanogenesis is very important. An initial spatial separation of rich waste and inoculum enhances the methane production and waste degradation at high waste loading if relatively low VFA diffusion into the methanogenic area is taking place. When both hydrolysis and methanogenesis are strongly inhibited by high levels of VFA, fluctuations in biomass concentration are thought to be responsible for initiating the expansion of methanogenic area over the reactor space.

Keywords Anaerobic digestion; distributed model; inhibition; mass transfer; sensitivity analysis; solid waste

Introduction

During anaerobic digestion of solid waste a balance between the rates of polymer hydrolysis and methanogenesis is extremely important. If the production rate of VFAs by polymer hydrolysis and acidogenesis exceeds their consumption rate an increased level of VFAs (low pH) may inhibit the whole process. In the anaerobic digestion of the organic fraction of municipal solid waste (OFMSW), with imperfect mixing conditions, methanogenic bacteria require sites where they will be protected from rapid acidogenesis. To describe this process, lean and rich wastes were considered by Kalyuzhnyi et al. (2000) and Martin (2000). Lean wastes were favorable for the survival of methanogens. One-dimensional distributed models of solid waste anaerobic digestion taking into account diffusion and advection of VFAs were developed recently (Vavilin et al., 2002a,b). This approach considers the bioreactor as an excitable media that promotes VFA and biomass concentration waves from an area where methanogenesis is initiated (local VFA depression) to the total reactor volume. A distributed model of solid waste anaerobic digestion in a 1-D bioreactor with leachate recirculation and pH adjustment which takes into account the initial spatial distributions of the rich and lean wastes and biomass concentrations and which is based on partial differential equations is described here. The distributed model was used to analyze the balance between the rates of polymer hydrolysis/acidogenesis and methanogenesis during the anaerobic digestion of OFMSW in batch and continuous-flow reactors. A sensitivity analysis of the model for changes in key parameter values was carried out.
**Methods**

Lysimeter experiments (height 60 cm) were run at 25°C for more than 500 days with sorted grey waste and unsorted old municipal waste (MSW). Leachate recirculation with and without pH adjustment was used. Experimental data of VFAs concentration and methane production were used for model calibration. A detailed description of all experimental methods was published earlier (Jokela et al., 2001). For comparison, previously published experimental data on anaerobic digestion of OFMSW (Barlaz et al., 1989; Lagerkvist and Chen, 1992) and food waste (FW) (Cho et al., 1995) were also used.

Polymer hydrolysis/acidogenesis and methanogenesis were included in the model as possible rate-limiting steps of the overall anaerobic digestion process. Rich (FW) and lean (non-FW) solid wastes were considered in the model. Lean waste such as digested sludge or well decomposed refuse, which are usually used as inoculum, are more favourable for the survival of methanogens. The following system of six parabolic partial differential equations in which \( Z \) is the vertical coordinate of the 1-D reactor of height \( 0 \leq Z \leq L \) was considered:

\[
\frac{\partial W_1}{\partial T} = -k_1 W_1 f_1(S), \\
\frac{\partial W_2}{\partial T} = -k_2 W_2 f_2(S), \\
\frac{\partial S}{\partial T} = D_S \frac{\partial^2 S}{\partial Z^2} - q \frac{\partial S}{\partial Z} + \chi_1 k_1 W_1 f_1(S) + \chi_2 k_2 W_2 f_2(S) - \rho_m g(S) \frac{SB}{K_S + S}, \\
\frac{\partial B}{\partial T} = D_B \frac{\partial^2 B}{\partial Z^2} - q \alpha \frac{\partial B}{\partial Z} + Y \rho_m g(S) \frac{SB}{K_S + S} - k_d B, \\
\frac{\partial P}{\partial T} = A(1 - Y) \rho_m g(S) \frac{SB}{K_S + S}, \\
\frac{\partial N}{\partial T} = D_N \frac{\partial^2 N}{\partial Z^2} - q \frac{\partial N}{\partial Z},
\]

(1)

**Initial conditions**

\[ W(Z,0) = \sigma(Z); \ S(Z,0) = \phi(Z); \ B(Z,0) = \psi(Z); \ N(Z,0) = \xi(Z) \]

(2)

**Boundary conditions**

\[ \frac{\partial S(0,T)}{\partial Z} = \frac{q}{D_S} (S(0,T) - S(L,T)); \quad \frac{\partial B(0,T)}{\partial Z} = \frac{q}{D_B} (B(0,T) - B(L,T)) \]

(3)

\[ N(0,T) = \frac{23}{60} \frac{S(L,T)}{1 + [H^+] / K_a} \]

(4)

\[ \frac{\partial B(L,T)}{\partial Z} = \frac{\partial S(L,T)}{\partial Z} = \frac{\partial N}{\partial Z} = 0 \]

(5)

where \( W_1 \equiv W_1(Z,T) \geq 0; \ W_2 \equiv W_2(Z,T) \geq 0; \ S \equiv S(Z,T) \geq 0; \ B \equiv B(Z,T) \geq 0; \ N \equiv N(Z,T) \geq 0 \) are the rich and lean solid wastes, total VFA, methanogenic biomass, and sodium concentrations, respectively; \( \partial P/\partial T = \partial P/\partial T(Z,T) \geq 0 \) is the methane production rate; \( 0 \leq T < +\infty \) is time; \( k_1, k_2 \) are the first-order hydrolysis rate constants; \( \rho_m \) is the maximum specific rate of VFA utilization; \( k_d \) is the specific biomass decay coefficient; \( \chi_1, \chi_2 \) are stoichiometric coefficients; \( A = 16/60 \) is the mass fraction of methane in biogas; \( K_s \) is the half-saturation
constant for VFA utilization; \( Y \) is the biomass yield coefficient; \( D_S, D_B \) and \( D_N \) are the diffusion coefficients for VFA, biomass and sodium, respectively; \( q \) is the volumetric liquid flow rate per unit surface area (specific liquid flow rate); \( \alpha \) is the fraction of biomass transferred by liquid flow; \([H^+]\) is the proton ion concentration; and \( K_a \) is the VFA (acetic acid) dissociation constant.

If there is no leachate recirculation in the batch reactor, the boundary conditions (3) transform into:

\[
\frac{\partial S(0,T)}{\partial Z} = \frac{\partial B(0,T)}{\partial Z} = 0
\]  

(6)

In this case, the equation for sodium concentration should be excluded from the model (1). In a continuous-flow system with influent waste, the corresponding boundary conditions for waste should be written as:

\[
\frac{\partial W(0,T)}{\partial Z} = \frac{q}{D_W} (W(0,T) - W_{in}(0,T)); \quad \frac{\partial W(L,T)}{\partial Z} = 0
\]  

(7)

where \( D_W \) is the diffusion coefficient for waste and \( W_{in} \) is the influent waste concentration.

Three dimensionless functions describe VFA inhibition of hydrolysis \( (f_1(S), f_2(S)) \) and methanogenesis \( (g(S)) \), respectively. These functions can be written in the following explicit form:

\[
f_1(S) = \frac{1}{1 + \left( \frac{I}{K_{f1}} \right)^{m_{f1}}}; \quad f_2(S) = \frac{1}{1 + \left( \frac{I}{K_{f2}} \right)^{m_{f2}}}; \quad g(S) = \frac{1}{1 + \left( \frac{I}{K_g} \right)^{m_g}},
\]  

(8)

where \( I = S \) is the inhibiting concentration of VFA; \( K_{f1} > 0, K_{f2} > 0, K_g > 0 \) are the inhibition constants; \( m_{f1} \geq 1, m_{f2} \geq 1 \) and \( m_g \geq 1 \) are the corresponding inhibition degree indexes. Using the basic model (1) with both wastes (food and non-food), the initial waste, VFA and biomass distributions along the reactor height \( Z \) are simulated using the following functions:

\[
\sigma(Z) = \gamma_1 \left[ 1 - \exp \left( -0.5 \left( \frac{Z - a_1}{\gamma_{21}} \right)^2 \right) \right] \times \ldots \times \left[ 1 - \exp \left( -0.5 \left( \frac{Z - a_n}{\gamma_{2n}} \right)^2 \right) \right],
\]  

(9)

\[
\psi(Z) = \gamma_3 \left[ 1 + \gamma_{41} \exp \left( -0.5 \left( \frac{Z - b_1}{\gamma_{51}} \right)^2 \right) \right] \times \ldots \times \left[ 1 + \gamma_{4m} \exp \left( -0.5 \left( \frac{Z - b_m}{\gamma_{5m}} \right)^2 \right) \right],
\]  

(10)

where \( \gamma_1, \gamma_{21}, \gamma_{22}, \ldots, \gamma_{2n}, \gamma_3, \gamma_{41}, \ldots, \gamma_{4m}, \gamma_{51}, \ldots, \gamma_{5m} \) are the distribution coefficients; \( n \) and \( m \) are the total number of depression/peak zones of waste and biomass, respectively. The functions (9) and (10) describe the case with a multi-depression for rich waste and VFA \( (\sigma(Z); W_1, S) \) and multi-peak for lean waste and biomass \( (\psi(Z); W_2, B) \) distributions along the reactor height \( Z \) (with minima at \( Z = a_i \) and maxima at \( Z = b_j \) correspondingly). The initial methane production rate was assumed to be zero. Numerical simulation based on the above described model was performed using a vector-oriented software (MATLAB, ver. 6.0). A visual calibration of the model against experimental data resulted in the estimated parameter values given in the next section of this paper.

**Results and discussion**

Lean waste. The model dynamics for old MSW digestion without and with leachate recirculation and pH adjustment are shown in Figure 1. For both cases the same kinetic coefficients (Table 1) and initial conditions were used taking into account the different
boundary conditions only. The methane accumulation curves did not differ significantly. Therefore, leachate recirculation with pH adjustment to neutral did not improve the methane production. Based on these results it can be concluded that there was no significant effect of inhibition by VFAs on methanogenesis. The VFAs data were not described well by the model because only total concentration of VFAs was considered and transformations of butyrate, propionate and other acids were not taken into account. Modelling Barlaz’s experimental data (Barlaz et al., 1989), we showed (Vavilin et al., 2003) that, in general, leachate recirculation with pH adjustment is stimulatory to both methanogenesis and waste reduction when inhibition of methanogenesis and hydrolysis/acidogenesis is prevented rapidly from the onset of the process throughout the reactor volume by increasing the liquid flow rate. Old MSW taken from a 10-year-old landfill had a balanced microorganism community with a high population size of methanogenic microorganisms. Methane production alone is described well (results not shown) by a simple first-order equation which is the result of an exponential decay of MSW:

$$P_W = M_Y \left(1 - e^{-k_h T}\right)$$

where $M_Y = 280 \text{ ml/gVS}$ is the maximum methane yield per initial waste mass, $k_h = 0.003 \text{ day}^{-1}$ is the first-order kinetic coefficient of waste hydrolysis. In fact, about the same value of $k_h = 0.0035 \text{ day}^{-1}$ was used in the model simulations (see Table 1). According to the experimental data, after the old MSW prewetting where a rather high quantity of water was added to waste and then drained, a long delay in methane production occurred in spite of

**Figure 1** Time profiles of old MSW, VFAs and biomass concentrations and cumulative methane volume without (1) and with leachate recirculation and pH adjustment (2). Symbols (stars and circles): experimental data corresponding to cases (1) and (2); lines: model predictions. Uniform initial waste and biomass concentration distributions were used. In the case with leachate recirculation a value of $q$ equal to 0.1 L/day was used.

**Table 1** Model parameter values

<table>
<thead>
<tr>
<th>Waste type (reference)</th>
<th>$k \text{ day}^{-1}$</th>
<th>$\rho_m \text{ day}^{-1}$</th>
<th>$K_g \text{ g/l}$</th>
<th>$Y \text{ g/g}$</th>
<th>$X$</th>
<th>$m_1; m_2$</th>
<th>$K_1; K_2 \text{ g/l}$</th>
<th>$D_a \text{ L}^2/\text{day}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSW (Lagerkvist and Chen, 1992)</td>
<td>0.3</td>
<td>1.1</td>
<td>2.0</td>
<td>0.1</td>
<td>0.9</td>
<td>3; 3</td>
<td>5.5; 11.5</td>
<td>$7 \times 10^{-3}$</td>
</tr>
<tr>
<td>Cellulose (Barlaz et al., 1989)</td>
<td>0.011</td>
<td>0.32</td>
<td>1.2</td>
<td>0.12</td>
<td>0.48</td>
<td>3; 3</td>
<td>16; 10</td>
<td>$1 \times 10^{-3}$</td>
</tr>
<tr>
<td>Old MSW (Jokela et al., 2001)</td>
<td>0.0035</td>
<td>0.15</td>
<td>0.5</td>
<td>0.08</td>
<td>0.79</td>
<td>1; 1</td>
<td>20; 8</td>
<td>$1 \times 10^{-4}$</td>
</tr>
<tr>
<td>FW (Cho et al., 1995)</td>
<td>0.55</td>
<td>1.1</td>
<td>0.5</td>
<td>0.08</td>
<td>0.68</td>
<td>7; 3</td>
<td>11; 4.5</td>
<td>$1 \times 10^{-3}$</td>
</tr>
</tbody>
</table>
For model simulations (Figure 2) the same coefficient values (Table 1) were used. At the low initial methanogenic bacteria concentration, appreciable methane production occurred only after 400 days of incubation.

For the grey waste without initial inoculation, methane production did not take place probably because of a very low initial methanogenic biomass concentration. According to Jokela et al. (2002), in batch assays with the grey waste inoculated with digested mesophilic municipal sewage sludge, most of the methane was produced within 11 days.

**Rich waste.** Rather low values of hydrolysis kinetic coefficients were obtained as a result of model calibration for the old MSW (see Table 1). The results of simulations of FW anaerobic digestion are shown in Figure 3. The model describes all experimental data comparatively well taking into account that a 25-fold change of FW loading took place within the experimental period. At an initial FW of 10 gVS/l methanogenesis was suppressed by the relatively high VFA concentration, but at the highest loading of 50 gVS/l both methanogenesis and hydrolysis were totally inhibited by the high VFA concentration (Figures 3 and 4).

**Sensitivity analysis.** Vavilin et al. (2000 a,b) have formalized the conditions of a mass transfer-based acceleration of methane production, when the rate of VFAs utilization in a methanogenic area is sufficient for the complete conversion of the incoming VFAs flow due to diffusion and advection. A balance between the rates of hydrolysis/acidogenesis and methanogenesis should be kept in order for an expansion of the methanogenic area to take place. A sensitivity analysis of the model for changes in key parameter values of FW digestion was carried out. The width of peak/depression in biomass and waste concentrations along the reactor height (i.e., biomass and waste distribution) determines the magnitude of the effective distance between the areas of hydrolysis/acidogenesis and methanogenesis. When such distance becomes less than a critical one, a strong inhibition of methanogenesis takes place (Figure 5a). The methane production increases slightly with an increase of diffusion coefficient value because of a greater VFA diffusion rate from the acidogenic to the methanogenic areas, but when it becomes higher than a critical value, a strong inhibition of methanogenesis takes place also (Figure 5a). It should be noted that the range of changes in parameter values selected for these model simulations was not very large and was equal to up to ±50%. The model was sensitive to the changes in maximum specific rate of VFA consumption and in hydrolysis rate coefficient (Figure 5b), in the inhibition coefficient of methanogenesis and hydrolysis (Figure 5c), and in the initial methanogenic biomass and waste concentrations (Figure 5d). The values of the half-saturation coefficient of VFA

![Figure 2](https://iwaponline.com/wst/article-pdf/48/4/147/423319/147.pdf)
consumption as well as the microbial yield coefficient had a low influence on the variables studied (results not shown). All in all, an increase of the initial hydrolysis rate above a critical value causes an inhibition, first of methanogenesis and then of hydrolysis. A decrease of the initial methanogenesis rate below a critical value has the same effect.

**Concentration fluctuations.** For waste and inoculum randomly distributed over the reactor space, only a fraction of the existing initial methanogenic areas can survive and expand in space. Comparing kinetic coefficients obtained for the different case studies (Table 1), a $K_f$ value greater than $K_g$ was used to describe the Lagerkvist and Chen (1992) data. However, it is well known that the inhibition of methanogenesis by high VFA concentration is much stronger than that of hydrolysis/acidogenesis (i.e., $K_f$ should be less than $K_g$). According to the Lagerkvist and Chen data, during a long incubation time of about 100 days there was no change in waste and VFA concentrations because both hydrolysis/acidogenesis and methanogenesis were inhibited by the high initial VFA concentration of 26 g/l (pH ≈ 5.8).

Using uniform or non-uniform concentration distributions of waste and biomass (Eqs (9) and (10)), the deterministic model (1) could not fit the experimental data for $K_f < K_g$. Such an effect when methanogenesis and hydrolysis started after a long delay may be explained because of biomass or VFA concentration fluctuations during the lag-phase of anaerobic digestion of solid wastes. For a chemical system where autocatalysis and inhibition are taking place, this phenomenon is known and the cell automata theory was successfully used to predict it (Vanag, 1996). Experimentally, the effect of concentration fluctuations was reported by Vavilin and Zaikin (1971) who studied an autocatalytic chemical reaction.
Conclusions

The model showed that, during sorted grey waste anaerobic digestion, leachate recirculation with pH adjustment to neutral did not improve the methane production because there was no significant effect of inhibition by VFAs on methanogenesis. According to the model, during rich waste degradation an increase of the initial hydrolysis rate above a critical value causes an inhibition, first of methanogenesis and then of hydrolysis. A decrease of the initial methanogenesis rate below a critical value has the same effect.

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Figure 5 (a–d). Sensitivity of the model variables (W-waste, B-biomass, VFA, CH4) for changes in the values of the following parameters: (eleven parameter values within the ±50% range were used for the model simulations)

(a) VFA diffusion coefficient $D_S$ (dotted lines) and initial width of waste depression zones $\gamma_2$ (solid lines); (b) maximum VFA specific utilization rate $\rho_m$ (dotted lines) and hydrolysis rate constant coefficient $k_1$ (solid lines); (c) methanogenesis inhibition coefficient $K_g$ (dotted lines) and hydrolysis inhibition coefficient $K_f$ (solid lines); (d) initial biomass concentration $\gamma_3$ (dotted lines) and initial waste concentration $\gamma_1$ (solid lines).

The point (0,0) corresponds to the following values of parameters and variables at $T = 20$ days: $\gamma_2 = 0.01$ L, $D_S = 1 \times 10^{-3}$ L$^2$/day, $\rho_m = 1.1$ day$^{-1}$, $k_1 = 0.55$ day$^{-1}$, $K_g = 4.5$ g/l, $K_f = 11$ g/l, $\gamma_3 = 1$ g/l, $\gamma_1 = 340$ g/l, $W_1 = 28.7$ gVS/l, $VFA = 2.4$ g/l, $B = 24$ g/l, $CH_4 = 0.77$ l/gVS.
References


