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Decomposition Modeling

Modeling Chemical and Biological Processes of Solid Waste Anaerobic Digestion

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MILESTONES

- Anaerobic digestion model No.1 (ADM1)
- Balance between polymer hydrolysis and methanogenesis as the rate-limiting steps
- Key factors for kinetics (waste composition, moisture, pH, particle size, temperature, microorganisms,...)
- Inhibition phenomenon
- Mass transfer processes
- Stimulation of degradation rate (leachate recirculation and pH adjustment, inoculation,…)

Many attempts have been made to apply simple models like first-order equation to describe the rate of solids degradation in landfills but the fit was often poor

The main purpose of the presentation is to show the factors potentially affecting decomposition dynamics which should be included into the model

There are a number of famous mathematical models of anaerobic digestion systems of a continuous-flow stirred-tank reactor (CSTR).

The IWA Anaerobi? Digestion Model No. 1 is the result of four years collaborative work by the international experts in anaerobic process analysis, modeling and simulation

Scientific and Technical Report No. 13

Anaerobic Digestion Model No. 1

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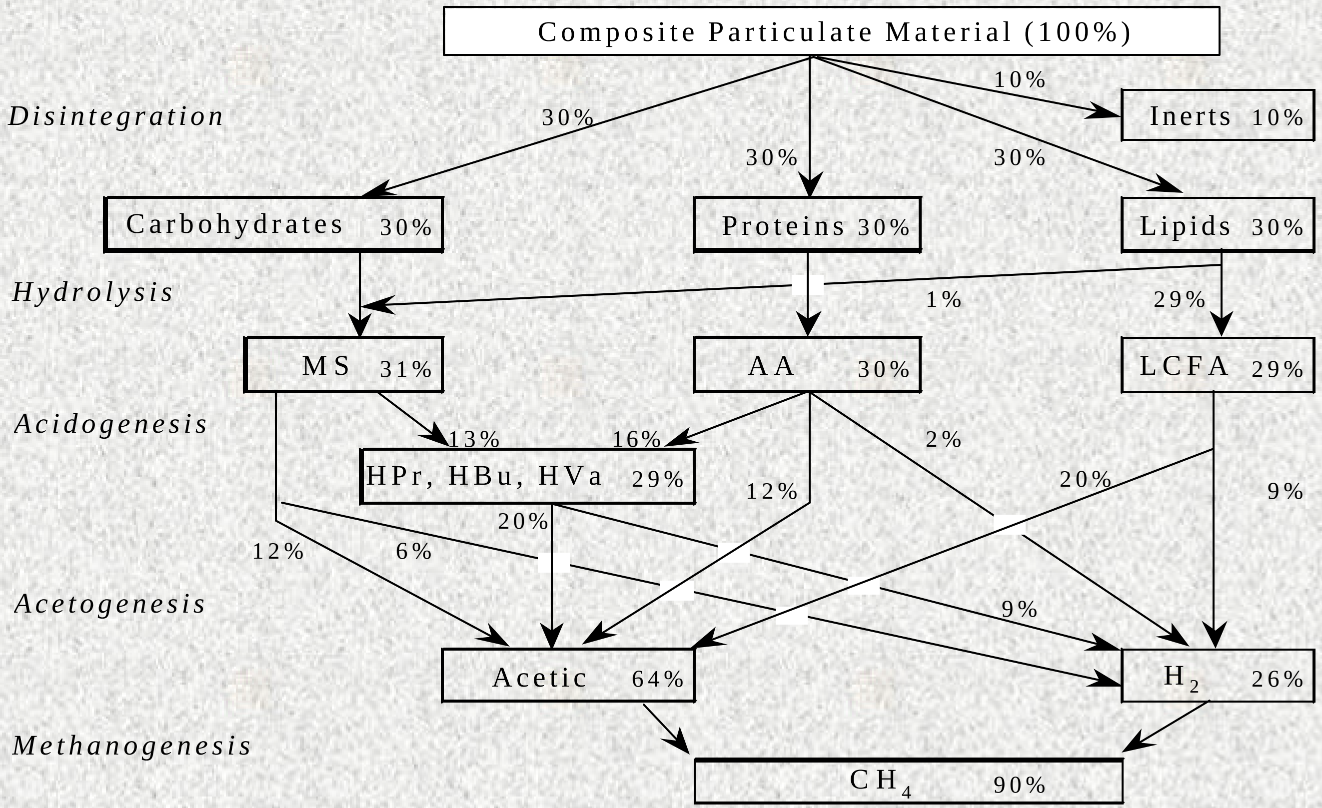
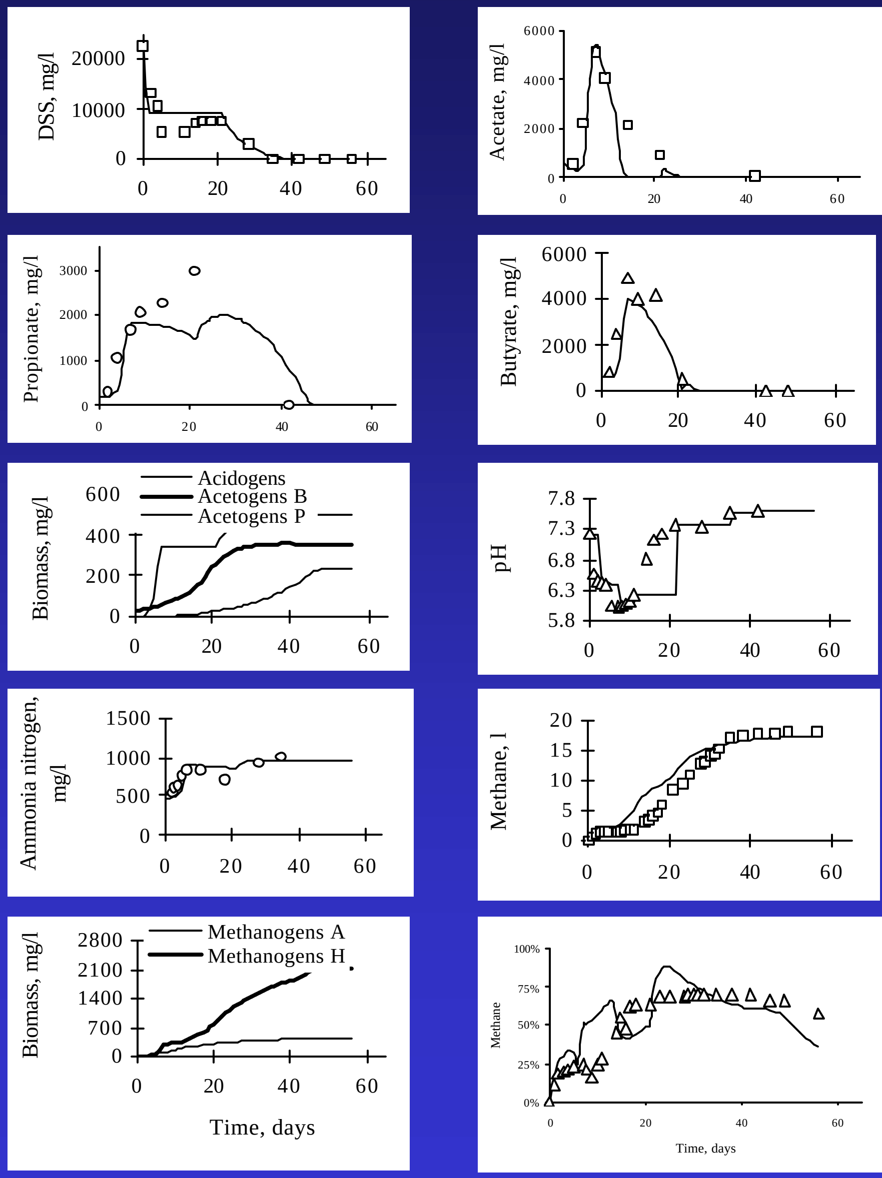
ANAEROBIC DIGESTION MODEL N1



COD flux for a particulate composite comprised of 10% inerts, and 30% each of proteins, carbohydrates and lipids (in terms of COD). Propionic acid (10%), butyric acid (12%) and valeric acid (7%) are grouped in the figure for simplicity.

Time profiles of sorted houshold waste (SHW) degradation



Symbols: data
(Salminen & Rintala)
Curves:
(the <METHANE>model)
http: methane.da.ru

Rapid increase in VFA concentration (low pH) efficiently inhhibits the polymer hydrolysis

The rates of polymer hydrolysis and methanogenesis as a product of several functions

$$P = P_m \cdot FT \cdot FL \cdot FI \cdot B$$

FT, *FL*, *FI* , functions describing the temperature dependence, mechanism of substrate limitation and inhibition;

B , biomass concentration of hydrolytic/acidogenic or methanogenic bacteria

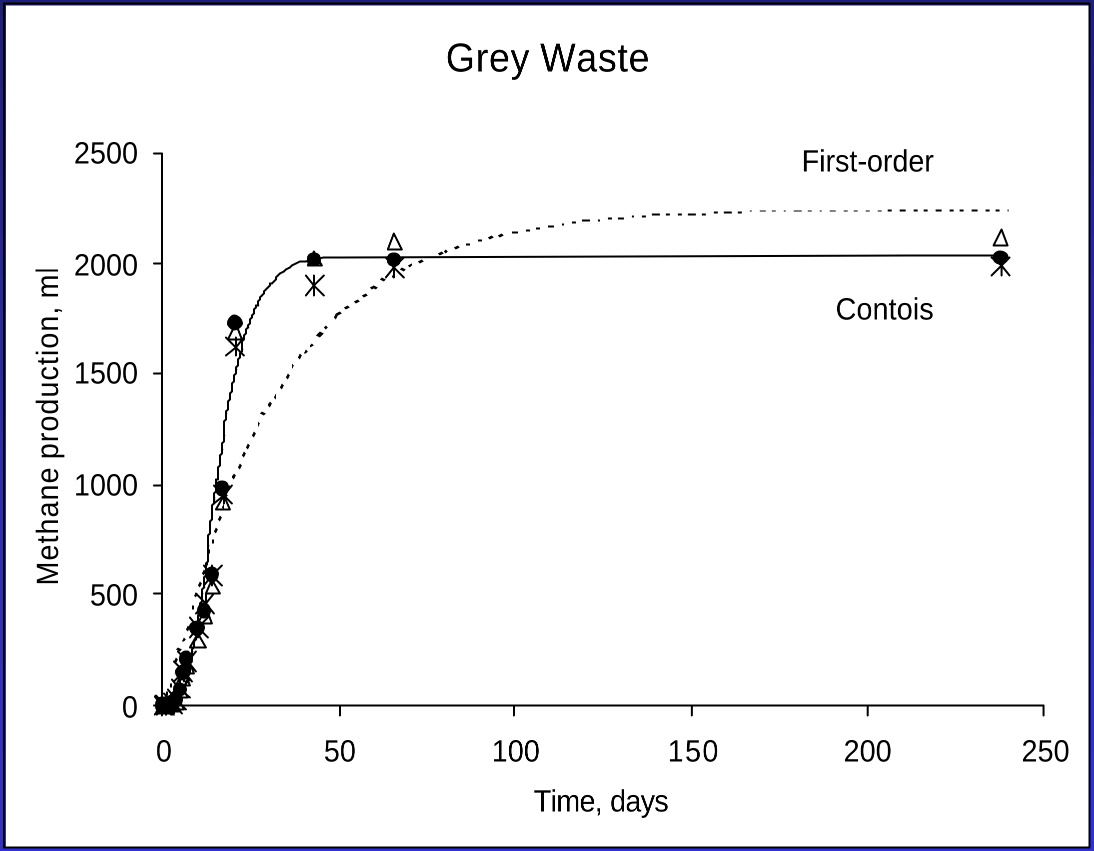
SUBSTRATE LIMITATION

First-order hydrolysis kinetic as the limiting case of surface- related kinetics *(Vavilin et al., 1996)*

$$r_{BH} = -\overline{r_H} \frac{k B_H}{1 + k B_H} \frac{X}{K_X + X} \approx -k_h X \quad (B_H >> 1/k;\ X << K_X,\ k_h = \overline{r_H} / K_X)$$

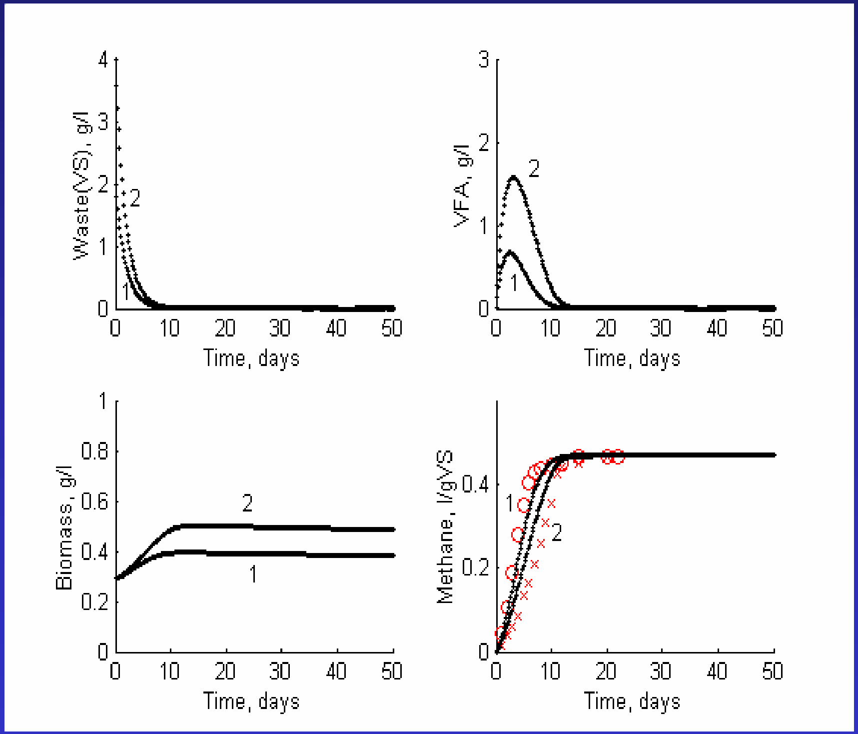
Monod model for methanogenesis $$r_{BM} = -\overline{r_M} \frac{S B_M}{K_S + S}$$

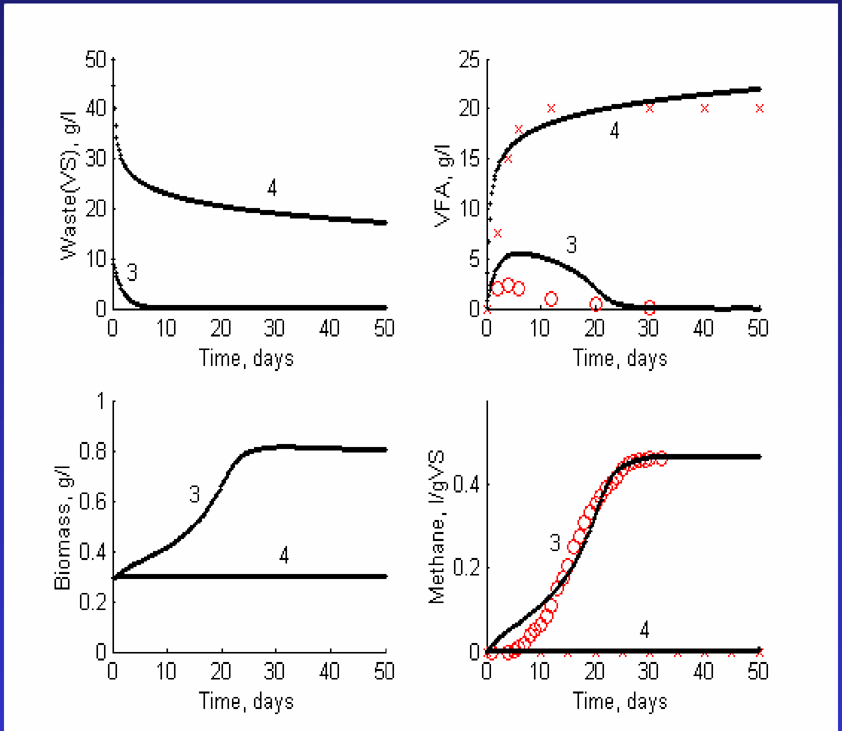
The Contois and first-order models (lines) and experimental data (symbols) of methane production from the grey waste for the triplicate data (Jokela et al. 2001)



The surface - related kinetics as well as the Contois kinetics of polymer hydrolysis fitted to experimental data better than the traditional first-order kinetics

Simulations of municipal food waste anaerobic digestion *(data: Cho et al., 1995)* with the various initial loadings: (1) ***2gVS/l***, (2) ***4gVS/l***, (3) ***10 gVS/l***, (4) ***50 gVS/l***





Methanogenesis was inhibited at 10gVS/l (3); but, at 50gVS/l (4) both methanogenesis and hydrolysis were inhibited by high VFA concentration. No methane production was observed in this case

INHIBITION FUNCTIONS

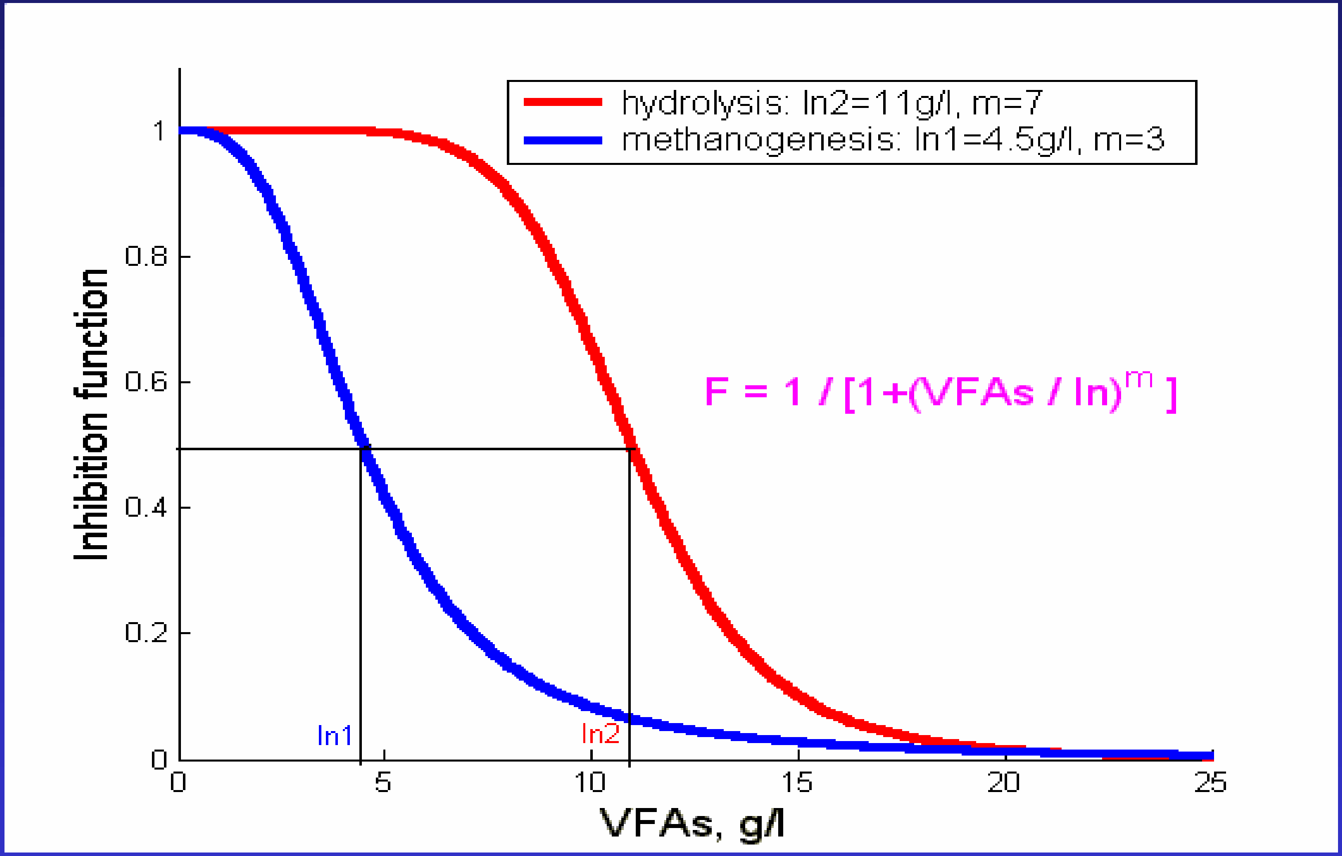
Dimensionless functions *f(S)* and *g(S)* characterise strong or weak inhibition of hydrolysis and methanogenesis by VFA (pH)

$$f(S) = \frac{1}{1 + \left(\frac{S}{K_f}\right)^{m_f}} \qquad g(S) = \frac{1}{1 + \left(\frac{S}{K_g}\right)^{m_g}}$$

where K_f, K_g are the inhibition constants and m_f, m_g are the degree indexes.

INHIBITION FUNCTIONS FOR MFW

(methanogenesis is inhibited by VFA much stronger than hydrolysis)

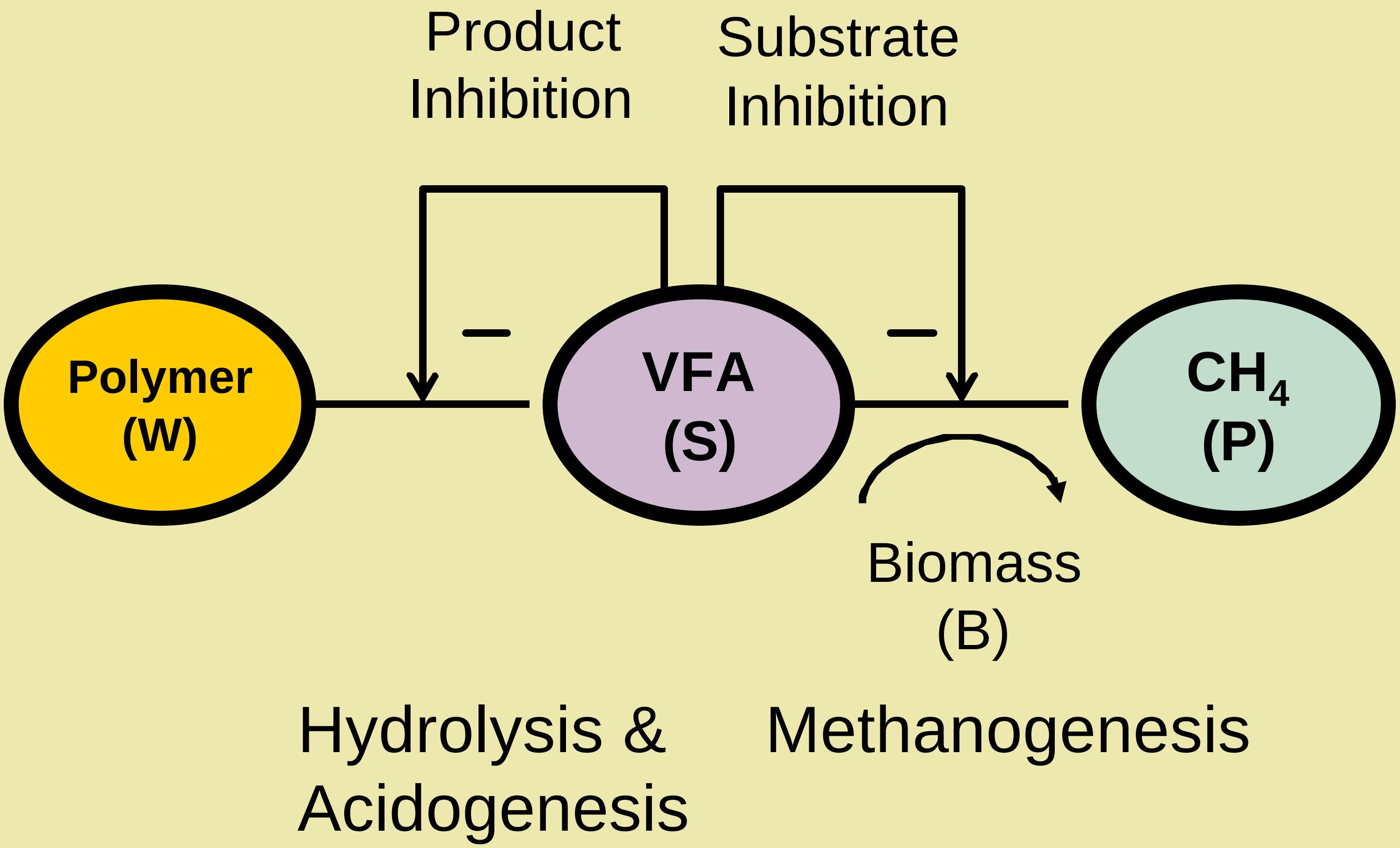


Sharp and smooth inhibition functions correspond to hydrolysis and methanogenesis, respectively

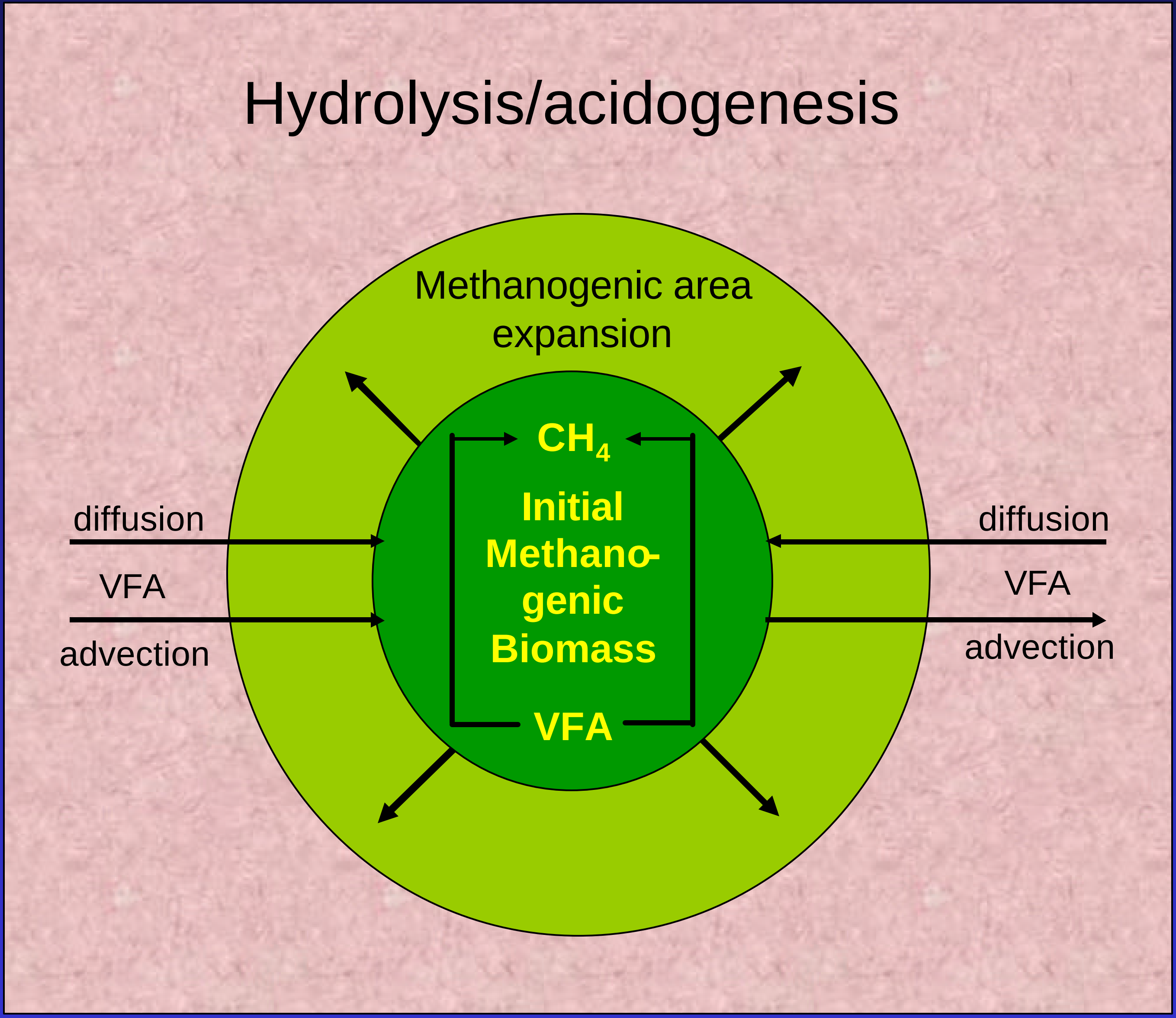
The effects of mass transfer and acid inhibition are cruicial for anaerobic digestion (AD) of solid waste. A balance between the rates of polymer hydrolysis and methanogenesis is extremely important

Distributed mathematical models describing dynamics of biochemical processes in reactor space should be developed to analize the effects of mass transfer on the rate of anaerobic digestion

Simplified kinetic model of solid waste anaerobic digestion



Spatial Reaction Zones



The conditions of a mass transfer-based acceleration of methane production in the reactor

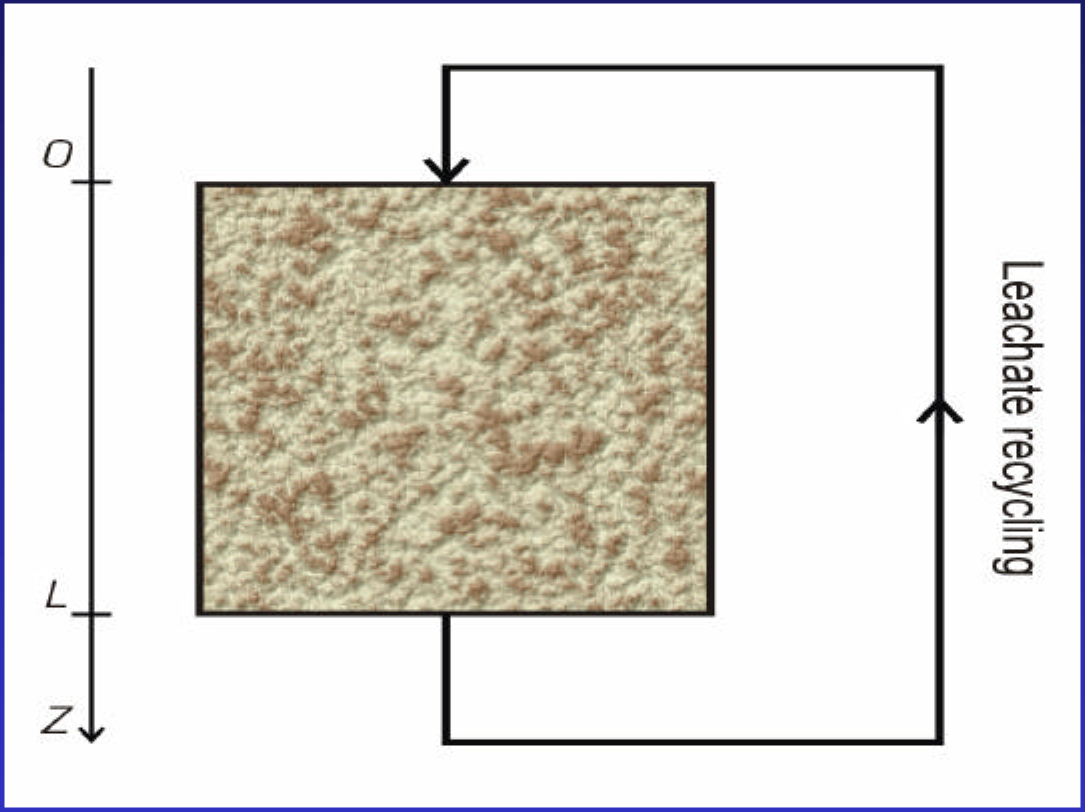
when intensity of VFA utilization in methanogenic area Θ *is sufficient for the complete digestion of incoming acid flow*

$$J_{\Theta} + \int_{\Theta} R_H(X,T)\,dX < \int_{\Theta} R_M(X,T)\,dX$$

where R_H is the rate of VFA production by hydrolysis; R_M is the rate of VFA consumption by methanogens; J_T is the incoming VFA flow through boundaries of T due to diffusion and advection.

An increase of the initial hydrolysis rate and a decrease of the initial methanogenesis rate above and below the critical values, respectively, causes an inhibition, first of methanogenesis and then of hydrolysis

BATCH REACTOR WITH LEACHATE RECIRCULATION



Z , vertical coordinate; *L*, reactor depth;
q, volumetric liquid flow rate per unit surface area

1-D DISTRIBUTED MODEL with saturated water flow

$$
\begin{cases}
\dfrac{\partial W}{\partial T} = -k \cdot W \cdot f\left(S\right), \\[2ex]
\dfrac{\partial S}{\partial T} = \dfrac{\partial}{\partial Z}\left(D_S \cdot \dfrac{\partial S}{\partial Z}\right) - q \cdot \dfrac{\partial S}{\partial Z} + c \cdot k \cdot W \cdot f\left(S\right) - u_m \cdot g\left(S\right) \cdot \dfrac{S \cdot B}{K_S + S}, \\[2ex]
\dfrac{\partial B}{\partial T} = \dfrac{\partial}{\partial Z}\left(D_B \cdot \dfrac{\partial B}{\partial Z}\right) - q \cdot a \cdot \dfrac{\partial B}{\partial Z} + Y \cdot u_m \cdot g\left(S\right) \cdot \dfrac{SB}{K_S + S} - k_d B, \\[2ex]
\dfrac{\partial P}{\partial T} = A \cdot (1 - Y) \cdot u_m \cdot g(S) \cdot \dfrac{SB}{K_S + S}, \\[2ex]
\dfrac{\partial N}{\partial T} = \dfrac{\partial}{\partial Z}\left(D_N \cdot \dfrac{\partial N}{\partial Z}\right) - u \cdot \dfrac{\partial N}{\partial Z},
\end{cases}
$$

W, solid waste; *S*, VFA; *B*, biomass; *N*, sodium; dP/dT, methane production rate; *T*, time; D_S, D_B, D_N diffusion coefficients of VFA, biomass and sodium, respectively

BOUNDARY CONDITIONS

(with pH adjustment)

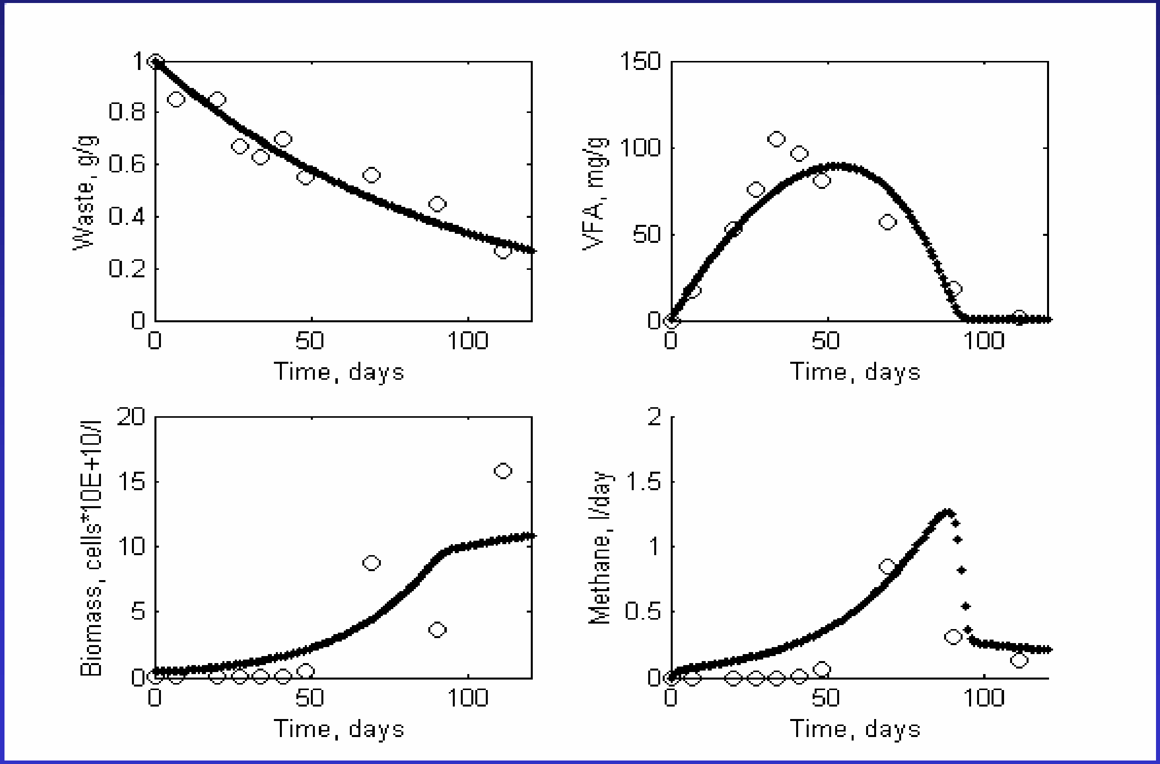
$$\frac{\partial S(0,T)}{\partial Z}=\frac{q}{D_S}(S(0,T)-S(L,T)),\quad \frac{\partial S(L,T)}{\partial Z}=0\,, \qquad VFA$$

$$\frac{\partial B(0,T)}{\partial Z}=\frac{q}{D_B}a(B(0,T)-B(L,T)),\quad \frac{\partial B(L,T)}{\partial Z}=0\,, \qquad Biomass$$

$$N(0,T)=\frac{23}{60}S(L,T)\cdot\frac{1}{1+[H^+]/K_d},\quad \frac{\partial N(L,T)}{\partial Z}=0\,, \qquad Sodium$$

Leachate recirculation and pH adjustment during MSW degradation *(data: Barlaz et al., 1989)*

(waste, biomass and VFA values averaged over the reactor volume)



*D_S=1*10 $^{-4}$L^2/day*

*D_B=1*10 $^{-5}$L^2/day*

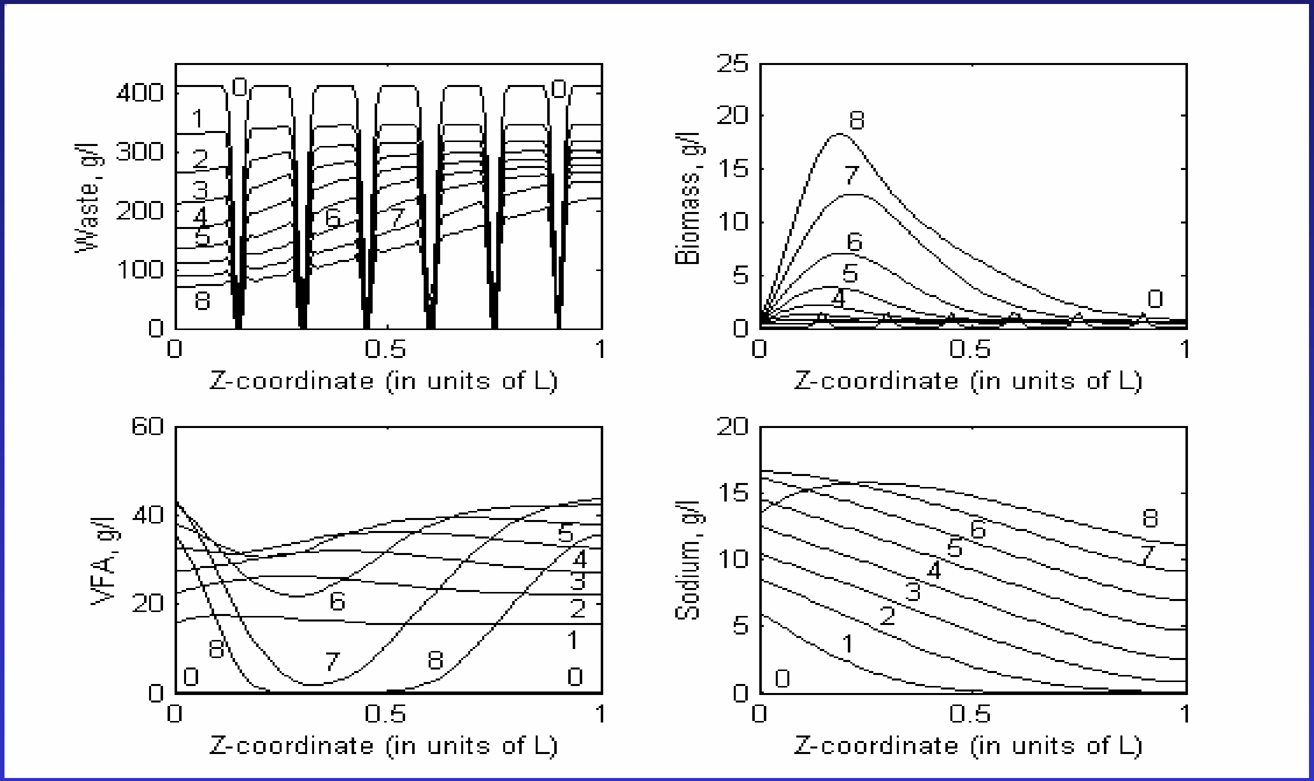
*D_N=1*10 $^{-4}$L^2/day*

q = 1.0 L/day

pH=7.0 (adjusted)

An increase in VFA concentration effectively inhibits methanogenesis as well as hydrolysis/acidogenesis

Time sequence of distributions of waste, VFA, biomass and sodium concentrations through reactor depth *Z* at the low leachate recirculation rate

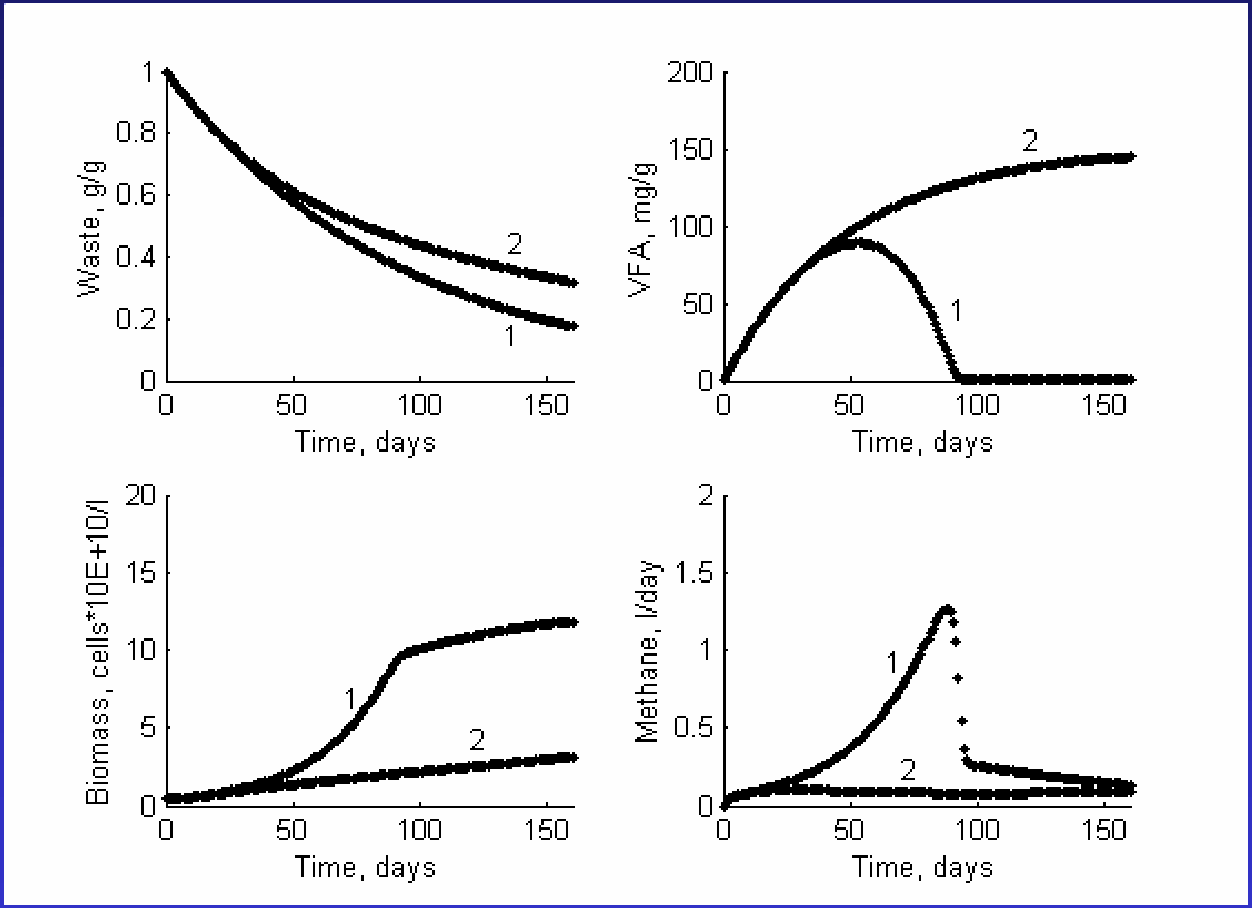


Sequence (Days)

0 (0)
1 (24)
2 (48)
3 (72)
4 (96)
5 (120)

Waste degraded more rapidly at the top of the reactor than the bottom because leachate recirculation with pH adjustment prevents inhibition of methanogenesis and hydrolysis by non-ionized VFA mostly at the reactor top

Concentrations of waste, VFA and biomass averaged over the reactor volume and methane production rate



pH adjusted:

Run1: **7.0**

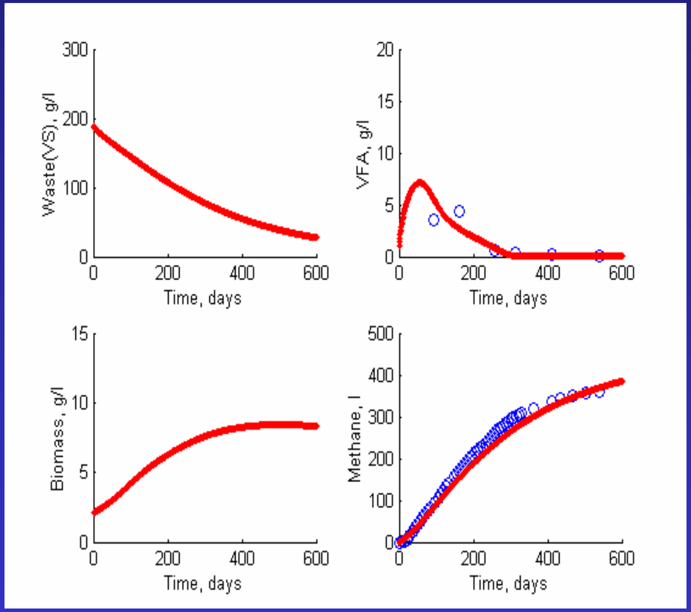
Run2: **5.0**

Without pH adjustment or with pH adjusted to 5.0, a strong inhibition of methanogenesis takes place

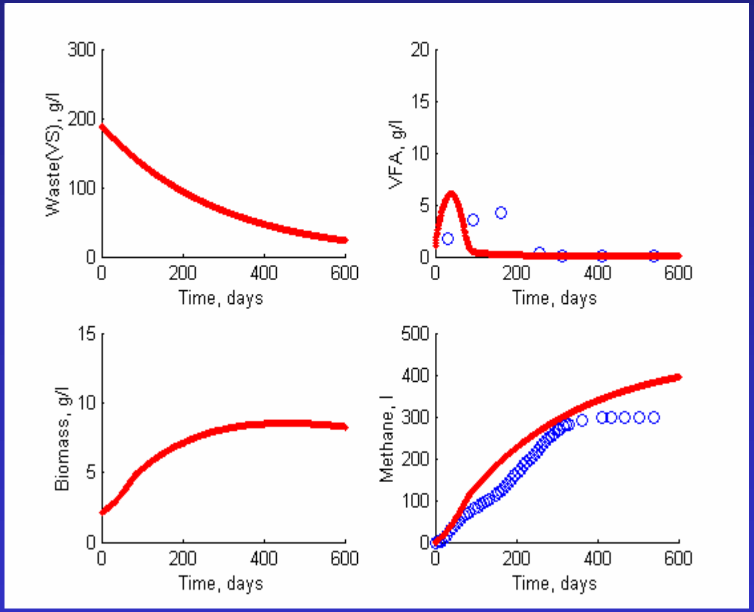
The case without (a) and with (b) leachate recirculation and neutralization for old MSW

(Jokela et al., 2001)

a



b



Leachate recirculation have no much effect on methane production because low VFA concentration did not inhibit methanogenesis significantly

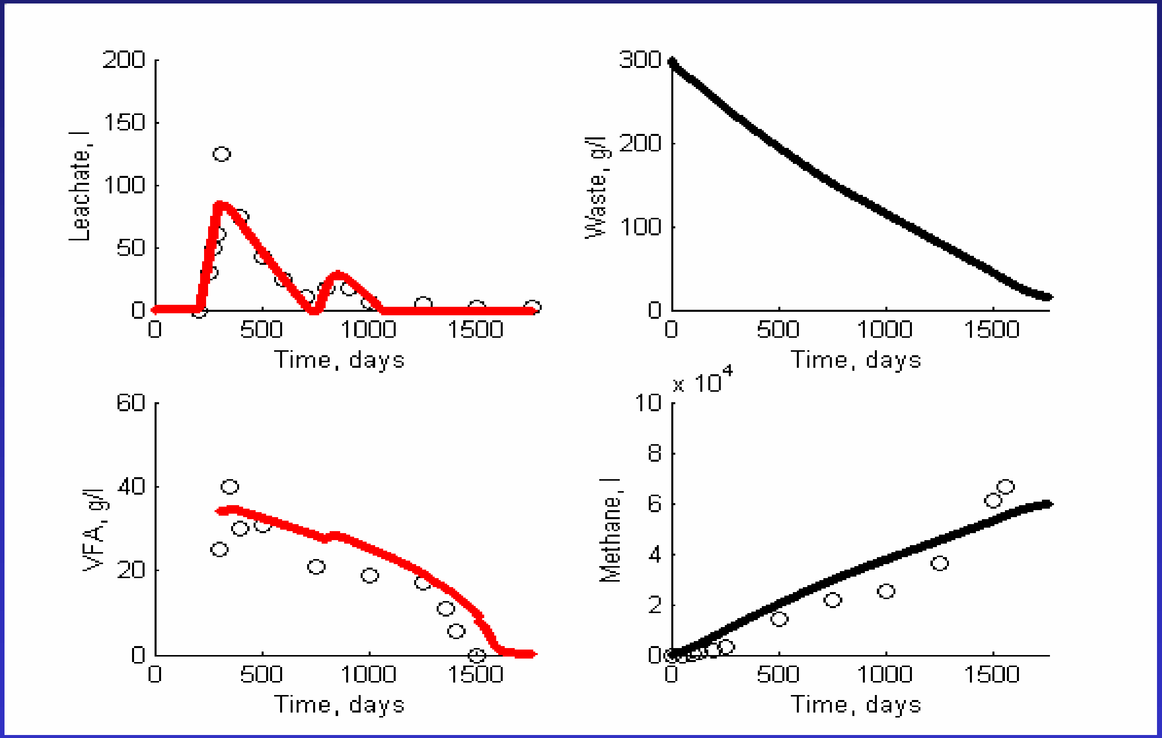
1-D DISTRIBUTED MODEL with unsaturated water flow

(

$$
\begin{cases}
\dfrac{\partial W}{\partial T} = -k\,W\,f(S,q), \\[2ex]
\dfrac{\partial S}{\partial T} = D_S\,\dfrac{\partial^2 S}{\partial Z^2} - K(q)\,\dfrac{\partial S}{\partial Z} + c\,k\,W\,f(S,q) - r_m\,g(S,q)\,\dfrac{B\,(S/q)}{K_S + B\,(S/q)}, \\[2ex]
\dfrac{\partial B}{\partial T} = Y\,r_m\,g(S,q)\,\dfrac{B\,(S/q)}{K_S + B\,(S/q)} - k_d\,B, \\[2ex]
\dfrac{\partial P}{\partial T} = A(1-Y)\,r_m\,g(S,q)\,\dfrac{B\,(S/q)}{K_S + (S/q)}, \\[2ex]
\dfrac{\partial q}{\partial T} = \dfrac{\partial}{\partial Z}\left[D(q)\,\dfrac{\partial q}{\partial Z}\right] - \dfrac{\partial K(q)}{\partial Z} - k\,k\,W\,f(S,q),
\end{cases}
$$

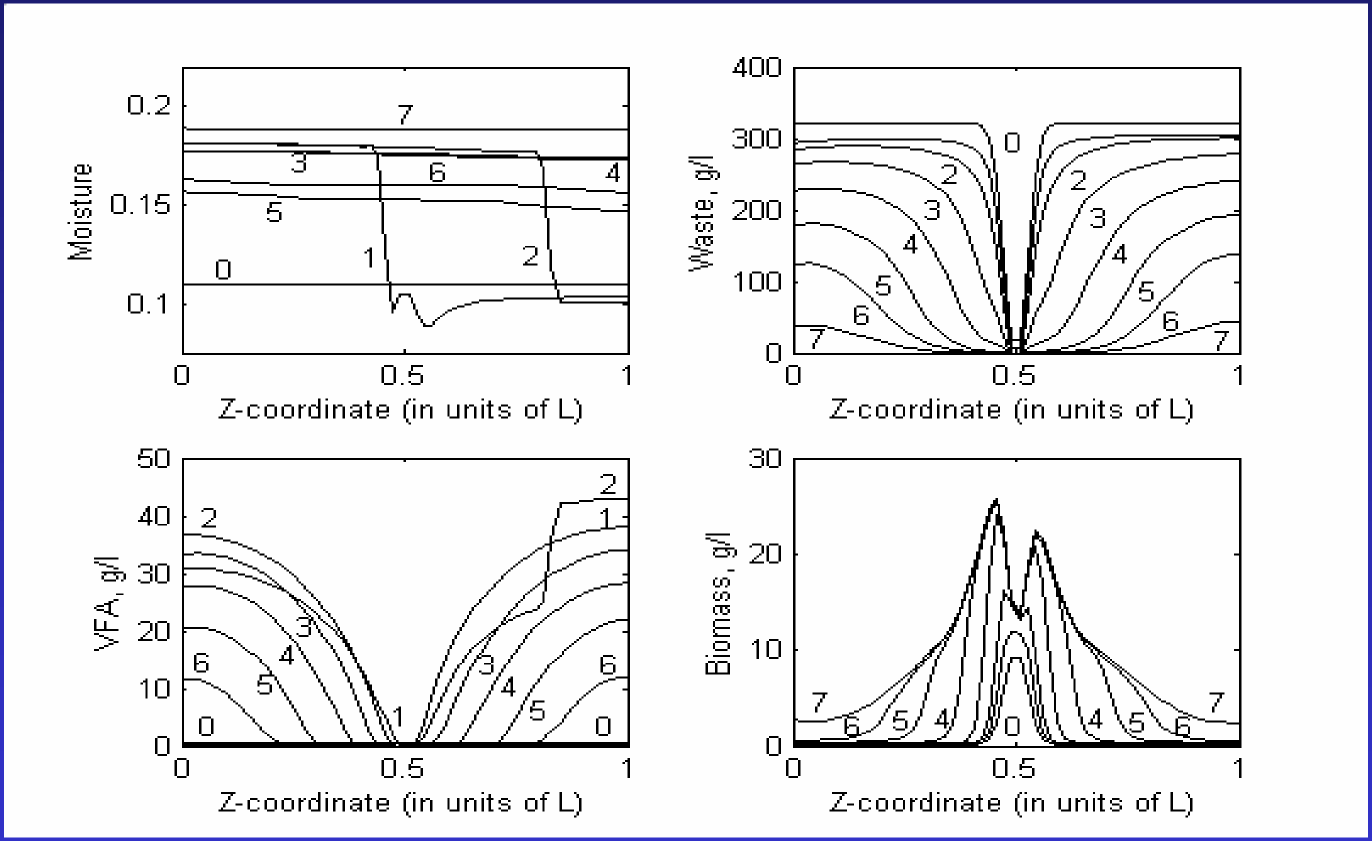
W, solid waste; *S*, VFA; *B*, biomass; θ, moisture; dP/dT, methane production rate; *T*, time; D_S, diffusion coefficient of VFA; $K(\theta)$, $D(\theta)$, hydraulic conductivity and water diffusivity

Simulated landfill column leachate generation during MSW degradation *(data: Pohland et al., 1992)*



Water consumption during hydrolysis/acidogenesis was taken into account to describe the leachate volume drop

Time sequence of distributions of moisture, waste, VFA in leachate, and methanogenic biomass concentrations through reactor depth *Z*



Sequence (Days)

0 (0)
1 (85)
2 (170)
3 (400)
4 (750)
5 (1150)
6 (1450)
7 (1750)

Initially, water passes through the column. At the same time a stronger inhibition occurs at the bottom of the reactor rather than the top

CONCLUSIONS (***answers on some questions***)

- *Waste composition and physical character of placed waste effect* ***polymer hydrolysis rate****; methanogenic biomass concentration is responsible for* ***methanogenesis rate****. A balance of these processes is extremely important to keep a non-acidified leachate*

- *On the basis of distributed models of solid waste anaerobic digestion including* ***diffusion and advection*** *of VFA an expansion of the initial methanogenic areas to the total reactor volume was obtained. However, such a model requires a lot of parameter values to be determined*

- *Advanced decomposition modeling depends on improved understanding of the key processes. The* ***generic model*** *including mass-transfer processes should be developed*

ACKNOWLEDGEMENTS

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