A MATHEMATICAL MODEL OF ANAEROBIC WASTE WATER REACTOR

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Introduction. The anaerobic waste water treatment is a complex process with multiple interactions between substrates and microorganisms at different scales. The process presents serious operational problems because there are several microorganisms growing in food chains where the excreted metabolites from some ones are the substrate for other species. The usually operational conditions are pH=7, temperature 35°C, and residence time between 10 to 30 days.
The process produces a gas mixture roughly 65 to 70 % of methane. This gas mixture has a heating value between 650 to 750 BTU/ft^3; lower than natural gas heating value. It is produced with a yield of 1 to 18 ft^3/lb of organic matter. Hydrogen is produced as an intermediate product and is converted in hydrogen sulfide, then pH fall.
One of the operational problems in this process is that high organic substrate concentrations causes buildup of volatile acid, then methane bacteria are inhibited by acid pH.

Model. This model considers three phases in the bioreactor: a solid organic matter, a liquid phase where microorganisms live and a gas phase. The insoluble organic matter is solubilized by liquefaction by extracellular hydrolytic enzymes; this step is fast enough and is not a limiting of the rate of overall reaction.
The soluble organics are consumed by acid producing bacteria, they are facultative anaerobic heterotrophs. These reactions produce bacteria cells, volatile acids, CO_2, H_2, and other compounds, and has relative rapid rate.
Then, another bacteria species, methanogenic bacteria use the H_2 produced to form methane, carbon dioxide and cells (see figure).
The gas phase contains the carbon dioxide, the methane and the hydrogen produced by the different microorganisms' species. Their profile concentrations can be calculated as:
Methane concentration:

$$\frac{dCH_{4g}}{dt} = k_l a_v \left(CH^*_4 - CH_{4g}\right)$$

Carbon dioxide concentration:

$$\frac{dCO_{2g}}{dt} = k_l a_v \left(CO^*_2 - CO_{2g}\right)$$

Hydrogen concentration:

$$\frac{dH_{2g}}{dt} = k_l a_v \left(H^*_2 - H_{2g}\right)$$

In the liquid phase profiles concentration are given by:
Hydrogen concentration:

$$\frac{dH_2}{dt} = \frac{1}{Y_{\frac{x2}{H2}}} \mu_2 x_2 - k_l a_v \left(H^*_2 - H_{2g}\right) - k_H H_2$$

Methane concentration:

$$\frac{dCH_4}{dt} = \frac{1}{Y_{x_2/CH_4}} \mu_2 x_2 - k_l a_v (CH_4 - CH_{4g})$$

Volatile acid concentration:

$$\frac{dHC}{dt} = \frac{F}{V}(HC_0 - HC) + \frac{1}{Y_{HC/x_1}} \mu_1 x_1 - \frac{1}{Y_{x_2/HC}} \mu_2 x_2 - \frac{Ka\, HC}{H^+}$$

The solubilized substrate concentration in liquid phase:

$$\frac{dS}{dt} = \frac{F}{V}(S_0 - S) + R_S - \frac{\mu_1 x_1}{Y_{x_1/S}}$$

The acid producing bacteria concentration is:

$$\frac{dx_1}{dt} = \frac{F}{V}(x_{10} - x_1) + \mu_1 x_1 - k_{d1} x_1$$

The methane producing bacteria concentration is:

$$\frac{dx_2}{dt} = \frac{F}{V}(x_{20} - x_2) + \mu_2 x_2 - k_d t - k_{d2} x_2$$

Substrate concentration in the solid phase:

$$\frac{dS_s}{dt} = \frac{F}{V}(S_{s0} - S_s) - R_s$$

Where:

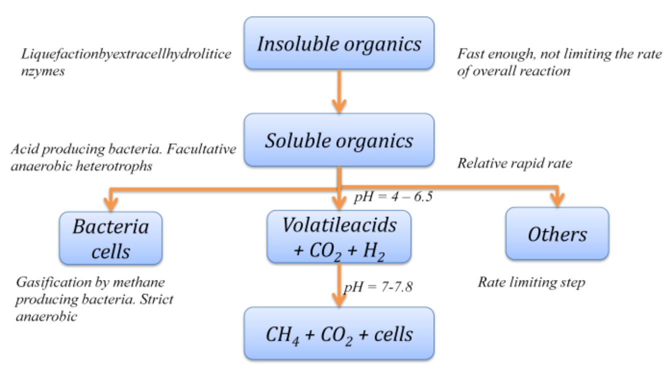
$$R_s = \frac{v_{max}\, S_s}{K_m + S_s} E$$

$$\mu_1 = \frac{\mu_{max}\, S}{K_{S1} + S}$$

$$R_2 = \mu_2 = \mu_{max} \left[\frac{1}{\frac{1+Ks}{HC} + \frac{HC}{Ki}} \right]$$

$$R_d = -k_d t$$

$$R_i = -k_i x_i$$



Conclusions. The model results can help to make a better control of the parameters than affect the operation of these bioreactors.

References.1. Bayley, James; Ollis, David. (1977). *Biochemical engineering fundamentals. McGraw Hill.*