Simplified anaerobic digestion model for organic waste

Xingjian Zhang-Schneider 05/24

May 5, 2025

Introduction

Anaerobic digestion is a microbially driven process that converts organic matter into biogas, primarily methane and carbon dioxide, as well as digestate, in the absence of oxygen. The Single-Step Degradation Model (SSDM) describes the time-dependent degradation of a single substrate and its conversion into biogas within a batch anaerobic digester. We closely follow the modeling approach proposed by Fedailaine et al. (see [2]), with the SSDM representing a simplified version that retains the core structure while omitting certain complexities. Mathematically, the SSDM can be formulated as an initial value problem, where a system of ordinary differential equations captures the temporal evolution of substrate concentration, biogas production, and digestate accumulation, based on defined initial conditions such as the starting concentrations of substrate. In our approach, we omit intermediate metabolic steps and microbial species interactions, focusing instead on the macroscopic dynamics from substrate to gas.

When to use?

- To estimate the amount of biogas and digestate produced over time from a given feedstock

- When detailed modeling of microbial pathways or intermediate compounds is not required

Key assumptions

- The digester is modeled as a sealed batch reactor with no continuous inflow or outflow

- Perfect mixing is assumed, ensuring uniform conditions throughout the reactor

- Microbial growth is modeled using a range of kinetic expressions including Monod, Haldane, Contois, Teissier, Moser, Chen Hashimoto, Andrews, and Ierusalimsky models to explore their impact on system behavior and evaluate which model best fits different substrate conditions and degradation dynamics.

Model setup

We assume a sealed batch reactor with no continuous inflow or outflow, where the initial feedstock is loaded at the beginning and the contents remain undisturbed until the process is complete. Furthermore, since the retention time is short, we assume that biomass loss is negligible and can be excluded from the model. Under these assumptions, the mass balance for the biomass simplifies to:

$$\frac{dB}{dt} = \mu B, \tag{1}$$

where B is the biomass concentration in g/L and μ is the specific microbial growth rate in 1/day. Various empirical models have been developed to describe the microbial growth rate μ. An overview is provided by Emebu et al. (see [1]). In our approach, we consider kinetic expressions including those by Monod, Haldane, Contois, Teissier, Moser, Chen–Hashimoto, and Andrews.

The mass balance for biogas assumes a constant yield coefficient Y_b for biogas formation, leading to the equation:

$$\frac{dG}{dt} = Y_b \mu B, \tag{2}$$

where $G(t)$ is the cumulative biogas concentration in g/L.

For the mass balance on the substrate, we assume that the homogeneous substrate S is converted through anaerobic digestion into biogas (a mixture of CH_4, CO_2, H_2 and NH_3) and biomass, which is considered as the digestate. The substrate consumption is then given by:

$$\frac{dS}{dt} = -\mu B - Y_b \mu B. \tag{3}$$

The unit for all three right-hand sides is $\frac{g}{L \cdot \text{day}}$. The task is to compute the biomass concentration $B(t)$, the cumulative biogas concentration $G(t)$ and substrate consumption $S(t)$ over time such that they satisfy the dynamics defined by equations (1)-(3) with specified initial concentrations at $t = 0$. This can be equivalently formulated as an initial value problem, stated as follows:

Problem (Simplified AD-model). Find the functions $B(t)$, $G(t)$ and $S(t)$, defined on the time interval $t \in [t_1, t_2]$ such that

$$\frac{dB}{dt} = \mu B,$$

$$\frac{dG}{dt} = Y_b \mu B,$$

$$\frac{dS}{dt} = -\mu B - Y_b \mu B,$$

holds with given initial values $B_0 := B(0)$, $G_0 := G(0)$ and $S_0 := S(0)$.

Models for microbial growth rate

Emebu et al. provide an overview of microbial growth kinetics (see [1]).

1. Monod Kinetics (Classic model for microbial growth as a function of substrate concentration):

$$\mu = \mu_{\max} \frac{S}{K_S + S},$$

where $\mu_{\max}$ is the maximum specific growth rate in $1/d$. K_S is the half-saturation constant in g/L and S is the substrate concentration in g/L.

2. Linear Kinetics (Proportionality between growth rate and substrate):

$$\mu = kS,$$

where k is the linear rate constant.

3. Haldane Kinetics (Substrate Inhibition):

$$\mu = \mu_{\max} \frac{S}{K_S + S} \frac{K_I}{K_I + S},$$

where K_I is the inhibition constant in g/L.

4. Contois Kinetics (Growth depends on both substrate and biomass):

$$\mu = \mu_{\max} \frac{\frac{S}{B}}{K_C + \frac{S}{B}},$$

where K_C is the Contois constant and B is the biomass concentration in g/L.

5. Teissier Kinetics (Empirical model similar to Monod kinetic):

$$\mu = \mu_{\max} \left(1 - \exp(-\frac{S}{K_T}) \right),$$

where K_T is the Teissier constant in g/L.

6. Moser Kinetics (Generalized Monod with exponent):

$$\mu = \mu_{\max} \frac{S^n}{K_S + S^n},$$

where n is the Moser exponent.

7. Chen-Hashimoto Kinetics (Use retention time):

$$\mu = \mu_{\max} \frac{\frac{S}{S_0}}{k_{\mathrm{CH}} + \left(\frac{S}{S_0}\right)\left(1 - \frac{S}{S_0}\right)},$$

where S_0 is the biodegradable influent substrate concentration and k_{CH} is the Chen-Hashimoto constant.

8. Andrews Kinetics (Haldane-type):

$$\mu = \mu_{\max} \frac{S}{K_S + S + \frac{S^2}{K_I}}.$$

References

[1] Samuel Emebu, Jiří Pecha, and Dagmar Janáčová. Review on anaerobic digestion models: Model classification & elaboration of process phenomena. *Renewable and Sustainable Energy Reviews*, 160:112288, 2022.

[2] Maamar Fedailaine, Karima Moussi, Mohamed Khitous, Sabah Abada, Meryem Saber, and Nassima Tirichine. Modeling of the anaerobic digestion of organic waste for biogas production. *Procedia Computer Science*, 52:730–737, 2015.