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# A mathematical model for a hybrid anaerobic reactor

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#### Abstract

A mathematical model for a hybrid anaerobic reactor (HAR), which uses self-immobilized anaerobic bacterial granules under completely fluidized condition, has been developed. Stoichiometry of glucose fermentation into methane has been considered in this model. The model includes: (1) a biofilm model which describes substrate conversion kinetics within a single granule; (2) a bed fluidization model which describes the distribution of biogranules within the fluidized bed and (3) a reactor model which links the above two to predict the substrate and products concentration profile along the reactor height. Product and pH inhibition for each group of bacteria has been considered in the kinetic model. The spatial distribution of each group of anaerobic bacteria within granules has been found to play a vital role in bringing about the conversion. Experiments were conducted in the reactor using a synthetic effluent containing glucose as the carbon source to study the treatment efficiency. The model was simulated first assuming a 3-layered distribution [MacLeod, F.A., Guiot, S.R., Costerton, J.W., 1990. Layered structure of bacterial aggregates produced in an upflow anaerobic sludge bed and filter reactor. Applied and Environmental Microbiology 56, 1598–1607.] of anaerobic bacteria within granules and then homogeneous distribution [Grotenhuis, J.T.C., Smit, M., Plugge, C.M., Yuansheng, X., van Lammeren, A.A.M., Stams, A.J.M., Zehnder, A.J.B., 1991. Bacterial composition and structure of granular sludge adapted to different substrates. Applied and Environmental Microbiology 57, 1942–1949.] of anaerobic bacteria. The predictions of model simulation with the assumption of layered structure closely represented the experimental data.

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# 1. Introduction

A hybrid anaerobic reactor (HAR) developed at the Department of Biochemical Engineering and Biotechnology, IIT Delhi, India, uses self-immobilized anaerobic bacterial granules under completely fluidized condition. In the HAR, no carrier particle is used for the granule formation. In this reactor, the upflow liquid velocity used is well above the minimum fluidization velocity (>4 m/h) of the granules. This technology applies the positive aspects of upflow anaerobic sludge blanket (UASB) reactor (i.e. using self-immobilized granules) and anaerobic fluidized bed reactor (AFBR) (using higher superficial velocity). To study the sensitivity of the process to various operating parameters and to optimize the design of this reactor. A

sound knowledge of the conversion brought about by the biogranules and the system hydraulics is required for this purpose.

The distribution of different groups of microbial community within these self-immobilized granules plays an important role in bringing about the substrate conversion. The structure of the granules developed in the UASB reactor has been extensively studied. Biogranules having layered structure of different groups of anaerobic bacteria were developed when the substrate used to grow them was very easily degradable and water soluble such as carbohydrates (MacLeod et al., 1990; Guiot et al., 1992; Lens et al., 1995; Tagawa et al., 2000, Batstone et al., 2004). Homogeneous structure of biogranule was observed when substrates, which are either difficult to degrade or in particulate form, was used (Grotenhuis et al., 1991; Fang et al., 1995; Wu et al., 2001; Batstone et al., 2004). The flow inside an anaerobic fluidized bed reactor has been modelled using axial dispersion model (Lin, 1991; Buffiere et al.,

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 $<sup>0301\</sup>text{-}4797/\$$  - see front matter C 2007 Elsevier Ltd. All rights reserved. doi:10.1016/j.jenvman.2007.01.036

1998; Seok and Komisar, 2003). Some authors have modelled them as completely mixed reactor as well (Hirata et al., 2000). This paper presents the model development for the HAR and the validation of model predictions with the experimental data generated through laboratory and pilot scale experiments.

# 2. Model development

The model consists of the following elements:

- a. a biofilm model which describes the substrate conversion kinetics within the individual granule;
- b. a bed fluidization model which describes the distribution of biogranules inside the fluidized bed volume;
- c. a reactor flow model, which links the biofilm and the bed fluidization models to yield substrate concentration as a function of axial position (height) within the reactor.

### 2.1. Biofilm model

Glucose was used as the model substrate. Stoichiometric equations described by Denac et al. (1986) were employed here. The coefficients are given as COD yields (i.e. kg COD of product formed per kg COD of glucose consumed).

Acidogenesis:

$$C_{6}H_{12}O_{6} \rightarrow 0.028CH_{3}(CH_{2})_{2}COOH + 0.053CH_{3}CH_{2}COOH + 0.614CH_{3}COOH + 0.302H_{2}$$
(2.1)

Acetogenesis:

$$CH_3CH_2COOH \rightarrow 0.571CH_3COOH + 0.429H_2, \qquad (2.2)$$

 $CH_3(CH_2)COOH \rightarrow 0.8CH_3COOH + 0.2H_2.$ (2.3)

Methanogenesis:

 $CH_3COOH \rightarrow CH_4,$  (2.4)

$$H_2 + CO_2 \to CH_4. \tag{2.5}$$

The biofilm model was developed by assuming a 3layered structure as proposed by MacLeod et al. (1990) as well as a homogeneous structure (Grotenhuis et al., 1991; Fang et al., 1995; Wu et al., 2001). In addition to that, the following assumptions were made:

- 1. granules are spherical in shape;
- 2. bulk liquid phase mass transfer resistance for the substrate is negligible;
- 3. substrate transport within the biofilm/granule is described by Fick's first law;
- 4. the reaction within the biofilm follows Monod kinetics;
- 5. steady state conditions exist.

## 2.1.1. Growth kinetics

2.1.1.1. Acidogenesis. The Monod relationship was used to describe the growth kinetics of acidogenic bacteria

$$\mu_g = \frac{\mu_{\max,g}g}{k_{s,g} + g},\tag{2.6}$$

where  $\mu$  is the specific growth rate (1/s),  $\mu_{\text{max}}$ , the maximum specific growth rate (1/s),  $k_s$  the Monod saturation constant (kg COD/m<sup>3</sup>), g the glucose concentration (kg COD/m<sup>3</sup>) and subscript "g" denotes acidogens.

2.1.1.2. Acetogenesis. For propionic acid and butyric acid degradation, Monod kinetics with competitive inhibition by acetic acid and pH inhibition were used

$$\mu_p = \frac{\mu_{\max,p}p}{k_{s,p}(1 + (a/k_{i,p})) + p} I_{pH},$$
(2.7)

$$\mu_b = \frac{\mu_{\max,b}b}{k_{s,b}(1 + (a/k_{i,b}) + b} I_{\rm pH}, \qquad (2.8)$$

where *a* is the acetate concentration (kg COD/m<sup>3</sup>), *b* the butyrate concentration (kg COD/m<sup>3</sup>), *p* the propionate concentration (kg COD/m<sup>3</sup>),  $k_i$  the inhibition coefficient (kg COD/m<sup>3</sup>) and subscript "*p*" and "*b*" denote propionate and butyrate degrading acetogens.

 $I_{\rm pH}$  is pH inhibition factor described by Michaelis pH function normalized to give a value of 1.0 as centre value (Angelidaki et al., 1993; Batstone et al., 2002)

$$I_{\rm pH} = \frac{1 + 2 \times 10^{0.5(\rm pH_{\rm LL}-\rm pH_{\rm UL})}}{1 + 10^{(\rm pH-\rm pH_{\rm UL})} + 10^{(\rm pH_{\rm LL}-\rm pH)}}.$$
(2.9)

2.1.1.3. *Methanogenesis*. For acetate degradation, Monod growth kinetics with pH inhibition was assumed

$$\mu_{a} = \frac{\mu_{\max,a}a}{k_{sa} + a} I_{\rm pH}, \tag{2.10}$$

where subscript "a" denotes acetate utilizing methanogens.

#### 2.1.2. Biofilm model for 3-layered structure

In this model biogranules are considered to have three layers (Fig. 1). The outer layer consists of *acidogens*, middle layer consists of *acetogens* and *hydrogen utilizing methanogens* and the inner layer consists of *aceticlastic methanogens*.

General steady state mass balance for a component within a biogranule can be written as follows:

Rate of component in - rate of component out

= Accumulation + Consumption – Production.

At steady state, accumulation = 0. The component degradation and production terms in the mass balance equation describe the kinetics of corresponding component degrading/producing microbial group.

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