## **EVALUATION OF A MECHANISTIC MATHEMATICAL MODEL OF A PACKED-BED ANAEROBIC REACTOR TREATING WASTEWATER**

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Abstract - A mechanistic mathematical model is proposed and evaluated for simulating the performance of a bench-scale packed-bed anaerobic reactor that uses polyurethane foam as biomass support. The model developed under rational criteria was based on the study of mass transfer and also considering biochemical kinetics, the hydrodynamic characteristics of the reactor. The data generated by the model adhered well to the experimental data obtained from the operation of the reactor applied to the treatment of a glucosebased substrate. The liquid-phase mass transfer coefficient was found to be the main parameter in the model, and its precise estimation is essential for the model to be successfully applied. Additionally, a case study was used in order to verify the applicability of the model for designing full-scale reactors. The simulations performed permitted to demonstrate the importance of the choice of convenient liquid superficial velocity and polyurethane foam matrix size which have direct influence on the solid- and liquid-phase mass transfers resistance and, consequently on the volume of the designed reactor.

*Keyword* - Wastewater treatment, anaerobic process, packed-*bed* reactor, HAIB reactor, performance simulation

## **1. INTRODUCTION**

Most of the anaerobic reactor configurations containing immobilized sludge have been developed essentially based on empirical criteria. The predominance of empirical over rational criterion arises as a consequence of the variety and complexity of interactive processes occurring in such heterogeneous units.

According to Wentzel and Ekama (1997), two extremes in mathematical models can be identified: empirical and mechanistic. The mechanisms and processes are ignored in the empirical ("black box") approach, while the mechanistic models are based on some fundamental phenomena. Both approaches can be useful for design and simulation purposes, but the mechanistic one provides more reliable bases for optimization than the empirical approach. On the other hand, mechanistic models demand wide knowledge about chemical, physical and biological aspects of the system. Such knowledge is not always available and, sometimes, the parameters required cannot be estimated.

Mechanistic models can be very complicated, especially in anaerobic digestion, due to the many interactions, such as inhibition microbial by intermediary products formed and competition for substrate. In this case, a complex model can be used for better understanding the system, but its use for simulation can be limited. Such limitation derives from the difficulty of estimating all parameters involved. Moreover, the mechanistic model derived is frequently too complex and difficult to be solved. The proposition of a mechanistic model presupposes the existence of reliable methods for estimating its parameters. Otherwise, even a well conceived model would be useless, if the required parameters were not accessible.

This work aims to supply elements for modeling a packed-bed anaerobic reactor, the Horizontal-Flow Anaerobic Immobilized Biomass (HAIB) reactor, under rational criteria. A simple mechanistic mathematical model was tested to simulate the performance of a labscale bioreactor used to treat a glucose-based synthetic substrate. Such a model was based on the study of phenomena as mass transfer, biochemical kinetics and hydrodynamic characteristics.

## 2. EXPERIMENTAL EQUIPMENT

A 2-liters horizontal-flow anaerobic immobilized biomass (HAIB) reactor was composed by a glass tube of 1.0 m with 0.05 cm diameter and length to diameter ratio (L/D) of 20 (Fig. 1). A perforated tube (0.9 cm of diameter) for gas collection was installed along the reactor in its upper part. Intermediate sampling ports were allocated along the reactor at L/D of 4, 8, 12 and 16.

A performance test was carried out in a previous work (Zaiat *et al.*, 1997a) using a synthetic substrate composed of glucose as the main carbon source (chemical oxygen demand-2090 mg COD. $l^{-1}$ ). The hydraulic detention time ( $\theta_h$ ) was 8 hours and temperature was controlled at 30°C. The reactor was filled with polyurethane foam cubic particles, previously inoculated with anaerobic biomass. Data of chemical oxygen demand (COD) along the reactor

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