



HAL
open science

Modelling of an acidogenic anaerobic fixed-bed reactor with the Anaerobic Digestion Model number 1 discretized by the Method of Lines

Pamela T Couto, Gabriel Capson-Tojo, Renaud Escudié, D.M.F. Lima, W.K. Moreira, R. Ribeiro, Eric Trably, M. Zaiat, Jean-Philippe Steyer

► To cite this version:

Pamela T Couto, Gabriel Capson-Tojo, Renaud Escudié, D.M.F. Lima, W.K. Moreira, et al.. Modelling of an acidogenic anaerobic fixed-bed reactor with the Anaerobic Digestion Model number 1 discretized by the Method of Lines. 6th International Conference on Monitoring and Control of Anaerobic Digestion Processes, Sep 2023, Leipzig, Germany. hal-04466641

HAL Id: hal-04466641

<https://hal.inrae.fr/hal-04466641>

Submitted on 19 Feb 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Modelling of an acidogenic anaerobic fixed-bed reactor with the Anaerobic Digestion Model number 1 discretized by the Method of Lines

Couto P.T.^{a,b}, Capson-Tojo G.^b, Escudie R.^b, Lima D.M.F.^c, Moreira W.K.^a, Ribeiro R.^d,
Trably E.^b, Zaiat M.^a, Steyer J-P.^b

^aBiological Processes Laboratory, São Carlos School of Engineering, University of São Paulo, 1100 João Dagnone Avenue, 13563-120 São Carlos, SP, Brazil

^bINRAE, Univ Montpellier, LBE, 102 Avenue des Etangs, 11100 Narbonne, France

^cDepartment of Civil Engineering, Federal University of Sergipe, 49100-000 São Cristóvão, SE, Brazil

^dEnvironmental Biotechnology Laboratory, Faculty of Animal Science and Food Engineering, University of São Paulo, 225 Duque de Caxias Norte Avenue, 13635-900 Pirassununga, SP, Brazil

Keywords: AFBR; Anaerobic Digestion; Hydrogen; ADM1; Method of Lines.

Research related with green hydrogen production has increased over the years due to the eminent necessity of renewable sources of energy. In this context, the development of mathematical models has contributed to a better understanding of the metabolic pathways involved in anaerobic digestion (AD), thus facilitating the simulation in other scenarios, such as fermentative processes. The most widely used model to describe AD is the Anaerobic Digestion Model #1 (ADM1), which includes biochemical and physicochemical equations in its structure. In this work, a mesophilic (25 °C) anaerobic fixed-bed reactor (AFBR) for hydrogen production from glucose (2000 mg COD·m⁻³) was operated during 60 days. This reactor had a total volume of 3.5 L, a length of 0.7 m, and was composed of three parts, a mixed zone (0.1 m), a bed zone (0.5 m) and an effluent zone (0.1m). According to hydrodynamics tests, the AFBR behaved as a plug-flow reactor, thus the substrate and products inside the reactor changed their concentrations along time and space, resulting in a system of partial differential equations (PDE) to be solved to model the profiles of state variables along the reactor. Diffusion-convection was assumed in the mixed and effluent zones, and diffusion-convection-reaction in the bed zone. Analyzing the experimental data, reactions considering the main metabolic pathways involved were implemented in the ADM1, to describe the reaction in the bed zone. Those are: *glucose* → *acetate* + H₂, *glucose* → *lactate*, *glucose* → *acetate* + *ethanol* + H₂ and *glucose* → *butyrate*, *lactate* → *butyrate* + H₂, *lactate* → *acetate* + *ethanol* + H₂, *lactate* → *propionate*. These equations differ from the ADM1 originally implemented by the IWA Task group, because the fermentation occurring in the AFBR was an acidogenic reactor process, i.e., it is an incomplete AD process, where acids are accumulated. For the PDEs, the Danckwerts boundary conditions were assumed, allowing flow continuity in the initial and final sections of the reactor. The components concentration at the entrance of the reactor were updated daily according to the measurements. The model was implemented in the software Matlab R2021b and the solution of the PDE system was carried out using the method of lines (MOL). This method consists in discretizing the space using finite difference techniques such as five biased-upwind points to calculate the first derivative (convection) and five centralized points for the calculation of the second derivative (diffusion). Subsequently, the integration in time was performed by the integrator ODE15s, used to solve stiff ODEs systems, as in the case of ADM1. The model was able to describe the experimental data for substrate consumption, volatile fatty acids concentrations, and hydrogen production during the reactor operation. However, more accurate results were achieved after optimizing free parameters. These results indicate that including the assumed metabolic pathways and discretizing the reactor were relevant for improving the model predictions. These modifications are potentially applicable for anytype of real wastewaters treated using plug-flow bioreactors.