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

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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 ºC) 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: $glucose \rightarrow acetate + H_2$, $glucose \rightarrow lactate$, $glucose \rightarrow acetate + ethanol + H_2$ and $glucose \rightarrow butyrate$, $lactate \rightarrow butyrate + H_2$, $lactate \rightarrow acetate + ethanol + H_2$, $lactate \rightarrow propionate$. 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.