

**Keywords** Anaerobic digestion; ADM1; Haldane; Monod; Optimization; Biokinetic constants

## Introduction

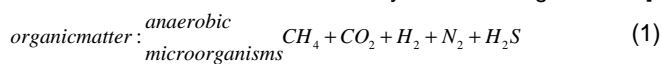
Anaerobic digestion (AD) modeling is an established method for assessing anaerobic wastewater treatment for design, systems analysis, operational analysis, and control. Anaerobic treatment of domestic wastewater is a relatively new, but rapidly maturing technology, especially in developing countries, where the combination of low cost, and moderate-good performance are particularly attractive. The anaerobic digestion is a biochemical process in which bacteria biodegrade organic matters into biogas (methane and carbon dioxide), (Figure 1). During anaerobic digestion, complex biological, chemical, and physical processes take place in a bioreactor system that is influenced by several process protocols and strategies [1]. The anaerobic degradation of organic matter is a complicated biological process; therefore, many technical reviews were published as Kasiri [2]. The conversion of organic matter consists of several independent, consecutive and parallel reactions in which a close-knit community of bacteria cooperates to form a stable, self-regulating fermentation

estimation of biogas rate. After, operation conditions are defined in terms of an acceptable range of VFA (volatile fatty acids). The last section presents a parametric study where effects of different constants were shown via numerical optimization, which can be applicable to several AD bioreactors. Finally, we present in the conclusion a predictive method of best values for a given numerical simulation.

## Modeling

Anaerobic digestion of highly concentrated organic pollutants was used in AD. This process is a very complicated and involved hundreds of possible intermediate compounds and reactions, each of which catalyzed by specific enzymes or catalysts. Many of the transformations can be accomplished by one of several alternative metabolic pathways, and biochemists and microbiologists continue with their attempts to define and describe more precisely the various mechanisms. The overall

biochemical reaction can be illustrated by the following scheme [1]:



The experimental data cannot give a detailed insight into the biological process, since the measurements lump together several

## Numerical Implementation

We describe in this section the details of the implementation strategies used in the construction of the code, and we report the first numerical case test by which the convergence of ~~code~~ ~~code~~ obtained accurately and give currently available numerical results. The first numerical test shows that the one-step AD code gives well pro les

performed a curve fit and then interpreted the best-fit parameter values. In fact, they underlined that the applied kinetics were found to affect the outcome of the regression study. Similarly, we used this numerical technique to optimize the dilution rate of the one-stage AD process [20]. Compared to one-stage AD simulation where we had less initial biokinetic constants values, the 3-stages AD simulation, used in numerical case tests and given in Table 2, presents a more complex problem than for non-inhibitory substrates because one fits simultaneously to the equation set (5) kinetic constants, combined growth data to the Monod equation, are not so easily employed for inhibitory models such as the Haldane equation because only a portion of the curve can be linearized. In our case, optimization numerical code with the Hook and Jeeves method (golden number) has been performed to get the best identification. This method is robust when varying the initial conditions.

The main calculation step was to determine the parameter set for each substrate 1 and 2  $K_1, K_2, K_I$  that minimized the differences between the simulation results of the model for a given initial conditions. This allowed us to choose the optimal parameter sets that had the minimum errors in each estimation step. The mathematical model developed was programmed using the iterative integration scheme with least-squares methodology [23]. Other constant parameters ( $K_1, K_2, \mu_{max}, y_b$  and  $y_p$ ) are then varied to show effect on the kinetic of AD and to estimate the biogas production rates with respect to dynamic model (3-steps ADM1).

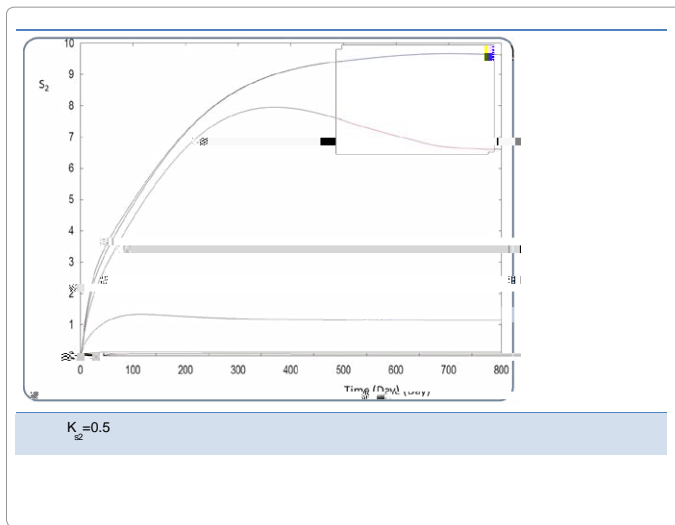
## Numerical Case Test

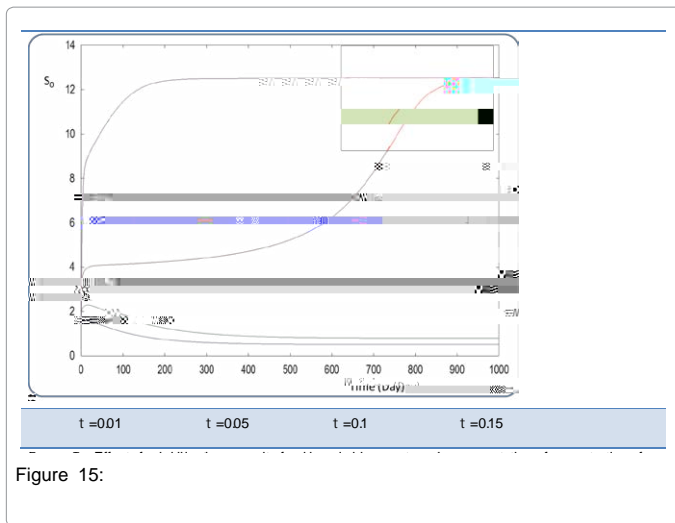
Here we present several numerical simulations for 3-steps ADM1 set of equations (5), for which we applied half-explicit Runge-Kutta methods. In fact, all examples were studied, discretized and evaluated for each small step of time (0.1 day), and where convergence criterion was based on satisfying an averaged squared error. The dilution parameter  $D$  was set as an optimal constant as described in previous works [20].

Before doing the calculation, we have to initialize  $S_0$  in and introduce different constant values that will be needed. The first case test that we had run is summarized in Table 2. It contains all basic values that are necessary to perform simulation and to get the temporal quantities of different substrates and biomass concentrations and therefore the biogas production rate.

In the following, the goal was the determination of the evolution of biogas production rate ( $Q$ ) of an AD bioreactor over a long period. Generally, the variable  $Q$  increases sharply at the beginning of the process and reaches a quasi-constant value when the methanisation

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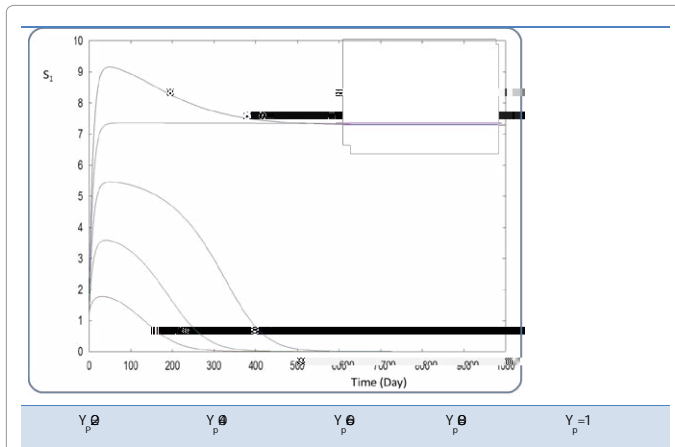
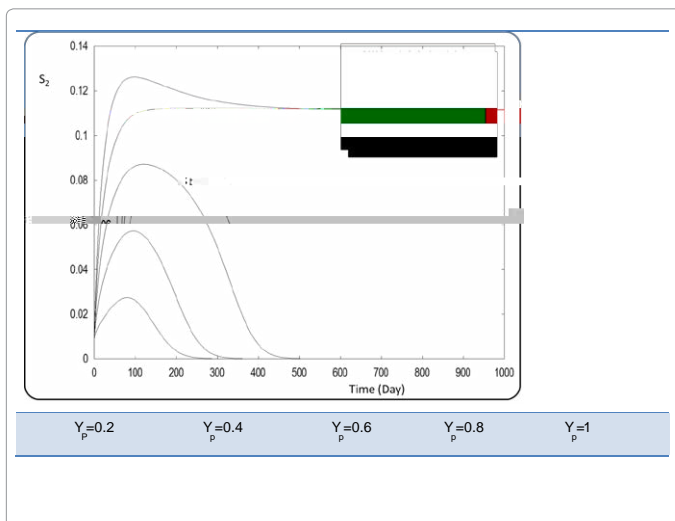


Figure 21: (IIHFWR IYRODWLOH VRO LGV IUDFWLRQ LQ WKH LQAXHQW <S RQ WKH FRQFHQWUDWLRQ of soluble volatile solids S1 (g/l).







21. Noykova N, Müller TG, Gyllenberg M, Timmer J (2002) Quantitative analyses