KINETIC MODELLING AND PERFORMANCE PREDICTION OF A HYBRID ANAEROBIC BAFFLED REACTOR TREATING SYNTHETIC WASTEWATER AT MESOPHILIC TEMPERATURE

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Abstract

A modelling study on the anaerobic digestion process of a synthetic medium-strength wastewater containing molasses as a carbon source was carried out at different influent conditions. The digestion was conducted in a laboratory-scale hybrid anaerobic baffled reactor with three compartments and a working volume of 54 L, which operated at mesophilic temperature (35 ºC). Two different kinetic models (one model was based on completely stirred tank reactors (CSTR) in series and the other an axial diffusion or dispersion model typical of deviations of plug-flow reactors), were assessed and compared to simulate the organic matter removal or fractional conversion. The kinetic constant (k) obtained by using the CSTR in series model was 0.60 ± 0.07 h^{-1}, while the kinetic parameter achieved with the dispersion model was 0.67 ± 0.06 h^{-1}, the dispersion coefficient (D) being 46. The flow pattern observed in the reactor studied was intermediate between plug-flow and CSTR in series systems, although the plug-flow system was somewhat predominant. The dispersion model allowed for a better fit of the experimental results of fractional conversions with deviations lower than 8% between the experimental and theoretical values. By contrast, the CSTR in series model predicted the behaviour of the reactor somewhat less accurately showing deviations lower than 10% between the experimental and theoretical values of the fractional conversion.

Keywords: Modelling; hybrid anaerobic baffled reactor; synthetic wastewater; CSTR in series model; dispersion model.

1. Introduction

In recent years, anaerobic technology has been applied to the treatment of many medium and high-strength industrial wastewaters. Taking into account the slow growth of many anaerobic microorganisms, particularly methanogenics, the main objectives of the efficient reactor design should be high retention time of bacterial cells with very little loss of microorganisms from the bioreactor [1, 2]. The technological challenge to improve anaerobic digestion lies in enhancing bacterial activity together with good mixing to ensure adequate contact between the cells and their substrate [3, 4].

The anaerobic baffled reactor (ABR) consists of a cascade of baffled compartments where the wastewater flows upward through a bed of anaerobic sludge after being transported to the bottom of the compartment. The ABR does not require the sludge to granulate in order to perform effectively, although granulation can occur over time [5, 6]. Experiments with lab-scale reactors have shown that the ABR is very stable under shock loads due to its compartmentalised structure [6, 7, 8]. In addition, the ABR has many potential advantages, i.e. no requirement of biomass with unusual settling properties and low capital and operating costs coupled with mechanical simplicity [6].

In the present study, a hybrid anaerobic baffled (HABR) reactor or multistage biofilm reactor with three compartments was used. This reactor configuration can be considered as a combination of the anaerobic baffled reactor (ABR) and upflow anaerobic fixed bed (UAFB) system which include the advantages of the ABR systems and anaerobic filters. These properties are: better resilience to hydraulic and organic shock loadings, longer biomass retention times; lower sludge yields, and the ability to partially separate between the various phases of anaerobic catabolism [6, 9]. The latter causes a shift in bacterial population allowing increased protection against toxic materials and higher resistance to changes in environmental parameters such as pH and temperature. The greatest advantage of this reactor configuration is probably its ability to separate acidogenesis and methanogenesis longitudinally down the reactor, allowing the reactor to behave as a two-phase system without the associated control problems and high costs.

Kinetic studies are helpful for reproducing the empirical behaviour of the anaerobic process and understanding the metabolic routes of biodegradation, while simultaneously saving time and money [10]. However, the development of an up-to-date model of organic matter anaerobic degradation is complex with considerable difficulties due to the high number of variables affecting the anaerobic system [11, 12].

A model was developed for the anaerobic digestion of a glucose-based medium in an innovative high-rate reactor known as the periodic anaerobic baffled reactor (PABR). In this model, each compartment is considered as two variable volume interacting sections, with constant total volume, one compartment with high solids and the other one with low solid concentrations, with the gas and liquid flows influencing the material flows between the two sections. For the simulation of glucose degradation, the biomass was divided into acidogenic, acetogenic and methanogenic groups of microorganims. The model succeeded in predicting the reactor performance as the organic loading rate was gradually increased [13]. Another kinetic model for predicting the behaviour of the PABR was developed based on batch experiments using glucose as substrate [5]. The PABR may be operated as an upflow anaerobic sludge blanket (UASB) reactor, an ABR or at an intermediate mode. The key assumption of this model was that the hydraulic behaviour of a PABR was equivalent to the behaviour of CSTRs in series as regards the dissolved matter. The model adequately predicted the experimental behaviour of this glucose-fed PABR and was also used to examine the performance of this reactor as a function of the operating conditions, both for constant and varying loading rates. It was shown that the reactor would best be operated as a UASB or an ABR [5].

Another kinetic model was recently developed for explaining the performance of a four-compartment ABR, incorporating granular sludge biomass and operating at different hydraulic retention times (HRT) in the range of 3 to 24 hours using dilute aircraft de-icing fluid with total chemical oxygen demand (COD) concentrations in the range of 300-750 mg/L. However, the first-order empirical model initially developed for describing the reactor performance did not adequately predict the total COD removal efficiency in the reactor with unsatisfactory results between the experimental and theoretical values [14].

A mathematical model of the baffled reactor performance was developed and applied using a concept of completely mixed reactors operating in series to describe the performance of a modified laboratory-scale (150 L) ABR using molasses wastewater as substrate [15]. This reactor had three chambers and a final settler. The first two compartments each had a 10 cm layer of plastic media (Pall rings with a specific surface area of 142 m^2/m^3) near the liquid surface. The third chamber had the upper half filled with a modular corrugated block. This kinetic analysis focussed on the granular sludge bed, with total mass of granular sludge as the main parameter. The model results were in good agreement with the experimental data [15].

However, despite the advantages offered by the hybrid anaerobic baffled reactors few mathematical analyses have been reported to date for modelling the kinetic behaviour of these reactors and for simulating the variation of the total COD removal efficiency under several operating conditions. Therefore, the main objective of this work was to compare two different kinetic models: a model based on the concept of completely stirred tank reactors (CSTR) in series and an axial diffusion or dispersion model, typical of deviations of plug-flow reactors, in the anaerobic treatment of synthetic wastewater containing molasses as a carbon source. These mathematical models have not been reported up to now in the literature to describe the kinetic performance of this specific type of hybrid reactor operating under varying HRTs, organic loading rates and influent substrate concentrations. The anaerobic hybrid reactor used was composed of three sequential compartments, where each one formed a packed bed using Pall rings (PVC) as a medium for supporting the biofilm formation.

2. Materials and methods

2.1. Experimental set-up

The hybrid anaerobic baffled reactor was composed of three sequential compartments, which were fabricated from Plexiglas. The reactor dimensions were 58 cm long, 24 cm wide and 44 cm high, with a total working volume of 54 L. The wastewater had an upflow mode inside each stage. The baffle spacing was determined by keeping the compartments the same size, the ratio between the up-corner and down-corner being 4:1. The height and width of baffles were 38 and 6 cm respectively. The baffles inside the reactor were used to direct the flow of wastewater in an upflow mode through a series of compartments where each one formed a packed bed using Pall Rings as a media for supporting the biofilm formation. The main characteristics of Pall Rings as a microorganism support medium were: material, PVC; nominal size, 25 mm; height, 25 mm; thickness, 1 mm; surface area, 206 m^2/m^3; and 90% porosity. This kind of packing resulted in increased process efficiency and a decrease in clogging as reported in previous works [16]. A diagram of the hybrid anaerobic baffled reactor used is given in Figure 1.

The initial porosity of the beds was 77% and after the immobilization of anaerobic cells they had a similar porosity (65%). Each compartment of the reactor was filled up to 64% of its active volume with the pall packing and equipped with sampling ports that allowed liquid samples to be withdrawn. A peristaltic pump (model “Omega”, FPUDVS2000 Series) was used to feed the bioreactor. The reactor was covered with a water jacket keeping the operational temperature at 35ºC ± 0.5 ºC.

2.2. Synthetic wastewater

The reactor was fed with synthetic wastewater containing molasses as a carbon source. Synthetic wastewater was used in the present work with the aim of avoiding and minimising variations in wastewater composition between experiments. In addition, real wastewater with the same characteristics is not always available to be used in the laboratory. A fresh batch was made every day by diluting molasses with tap water to achieve the total COD concentration required for each loading rate. The characteristics of the molasses used were (mean values ± standard deviations) : pH, 7.6±0.3; COD (total COD throughout the paper), 1124±35 mg/L; BOD_5: 411±12 mg/L; Kjeldahl nitrogen, 16.6±0.5 mg/L; total phosphate, 0 mg/L; Ca^{2+}, 59.2±1.8 mg/L; K^+, 3.1±0.1 mg/L; alkalinity, 196±6 mg/L; total sugars, 47.4±1.5%; free sugars, 18.7±0.6%; non-fermentable sugars, 6.0±0.2%; total dissolved solids (TDS), 38±1%. These values summarize the main features of the molasses obtained by diluting 1 g of raw molasses into 1 L of distilled water. The COD:N ratio of the wastewater used was 67:1. Only during the start-up period were urea and ammonium phosphate used as sources of nitrogen and phosphorus, respectively. A total dose of 925 mL of a micronutrient and trace metal solution was added only at the beginning of the start-up period of the reactor. The composition of this micronutrient and trace metal solution was: $CoCl_2 \cdot 6H_2O$, 0.25 mg/L; H_3BO_3, 0.05 mg/L; $FeCl_2 \cdot 2H_2O$, 2 mg/L; $MnCl_2 \cdot 4H_2O$, 0.5 mg/L; $ZnCl_2$, 0.05 mg/L; $CuCl_2$, 0.15 mg/L; $Na_2MoO_4 \cdot 2H_2O$, 0.01 mg/L; $NiCl_2 \cdot 6H_2O$, 0.01 mg/L; Na_2SeO_3, 0.01 mg/L; $AlCl_3 \cdot 6H_2O$, 0.05 mg/L; $MgCl_2$, 1 mg/L; $MgSO_4 \cdot 7H_2O$, 0.3 mg/L; $CaCl_2 \cdot 2H_2O$, 0.18 mg/L [9]. These nutritious substances were used to favour the growth of the biofilm on the surface media. During the start-up period, COD:N:P ratio was 100:5:1. When a steady-state condition was achieved, the COD:N:P ratio changed to 350:5:1. In order to prevent the build-up of a localized acid zone in the reactor, sodium bicarbonate was used for supplementing the alkalinity. $NaHCO_3$ is the only chemical which gently shifts the equilibrium to the desired value without disturbing the physical and chemical balance of the sensitive microbial population [17].

2.3. Reactor inoculum

The microorganisms used as inoculum in the reactor originated from the sludge of the ABR system treating non-alcoholic beer wastewater of the Berinuscher Company located in Shiraz, Iran. The basic characteristics of the anaerobic inoculum used were (mean values ± standard deviations): total acidity, 178±6 g acetic acid/m^3; total solid content, 69.5±2.1 kg/m^3; volatile solid content, 28.3±0.3 kg/m^3; bicarbonate alkalinity, 1374±45 g $CaCO_3$/m^3; and pH, 7.3±0.3. A total volume of 19 L of the above-mentioned inoculum was added to the reactor and distributed among compartments before starting the experiments.

2.4. Experimental procedure

At the beginning of the start-up, the reactor was run in a batch mode. During this time, sludge was acclimated to the synthetic wastewater by using influent COD concentrations in the range of 0.5 to 1.5 g/L. This initial period lasted 45 days. The continuous operation of the system was started using an initial COD concentration of 3000 mg/L at a HRT of 2 days, which was equivalent to an organic loading rate (OLR) of 1.5 kg COD/m^3 d. A COD removal efficiency of 70% was achieved at this level. When there was no fluctuation in different parameters such as COD and volatile fatty acids (VFA) in each compartment, then the OLR increased to 3 kg COD/m^3 d (HRT = 1 day) as the input flow-rate increased. The reactor was operated at this OLR for 45 days.

A COD removal efficiency of 91.6% was achieved at this OLR. An alkalinity value of 900 mg/L in the form of $CaCO_3$ was added at this stage. COD removal profile and pH variations trend were monitored during this period. It was observed that the COD decreased from 980 to 540 mg/L, from 710 to 340 mg/L and from 460 to 250 mg/L in the compartments 1, 2 and 3, respectively. As could also be observed, there were some irregularities in the pH value variations during the first few days, but as time went by microbial selection and zoning were encouraged inside the reactor, with the acidogenesis in compartments closer to the inlet. Specifically, pH values ranged between 6.5–6.8, 6.4–7.3 and 6.5–7.6 in compartments 1, 2 and 3, respectively, during this start-up period (45 days).

Two sets of experiments were carried out. A first group of experiments was performed to study the influence of reducing the HRT on the system performance. The reactor was fed with diluted molasses containing 3000 mg COD/L at two different HRTs of 16 h and 8 h, which were equivalent to OLRs of 4.5 and 9 kg COD/m^3 d. The COD and volatile fatty acid (VFA) concentration changes in all compartments and reactor effluents were monitored.

In the second part of the experiments, the effect of different OLRs was studied by varying the COD of the influent substrate at a constant retention time. Specifically, the reactor was fed with diluted molasses containing 3000, 4500 and 6000 mg COD/L at a constant HRT of 16 h. The amount of COD eliminated and VFA concentration changing profiles were obtained. All samples were analysed in triplicate and the final results expressed as means.

The operating conditions studied for the two sets of experiments carried out were selected taking into account the operational conditions evaluated previously in other ABRs treating different wastewaters.

2.5. Analytical methods

The total COD concentration was measured by using a semi-micro method [18]. Alkalinity was determined in accordance with the standard method 2320 B of APHA [19]. The concentration of VFA was determined by using HPLC according to Björnsson et al. [20]. Total and volatile solids were determined according to the method number 2540 B [19]. The pH was determined with a Crison, model basic 20 pH-meter. Phosphate was measured by spectrophotometry (880 nm) using the normalized method 4500 P [19]. Kjeldahl nitrogen was determined according to the standard method number 4500-B [19]. Finally, Ca^{2+} and K^{+} were measured by atomic absorption spectrophotometry.

2.6. Software used

SigmaPlot software (version 9.0) was used to elaborate all the graphs and Figures of this study and to perform the statistical analyses. Mathcad software (version 14) was used to solve the mathematical equations corresponding to the two models assessed.

3. Results and Discussion

3.1. Operational behaviour of the HABR

A previous study reported the operational performance of the HABR under different experimental conditions [9]. Specifically, during the start-up period (first 45 days of operation), pH fluctuations were observed because there was no microbial selection or zoning, but as the experiments progressed, results showed that phase separation had occurred inside the reactor. COD removal percentages of 91.5%, 91.5%, 90.0% and 88.3% were achieved at organic loading rates of 3.0, 4.5, 6.75 and 9.0 kg COD/m^3 day, respectively. A decrease in HRT from 24 h to 16 h had no effect on COD removal efficiency. When HRT decreased to 8 h, COD removal efficiency was still 84.7%. The VFA/alkalinity ratio can be used as a measure of process stability [20]: when this ratio is less than 0.3-0.4 (equiv. acetic acid/equiv. $CaCO_3$) the process is considered to be operating favourably without acidification risk. As could be observed the ratio values were lower than the suggested limit value for all HRTs and OLRs studied in the present work, showing the high stability of this reactor for all the operating conditions assessed. Recirculation ratios of 0.5 and 1.0 had no effect on COD removal but other factors such as the volatile fatty acid (VFA) content were affected. The effect of toxic shock was also investigated and results showed that the main advantage of using this bioreactor lies in its compartmentalized structure [9].

3.2. Mathematical modelling

The fractional conversion or organic matter removal efficiency (per one) can be defined as the ratio between the amount of COD eliminated and the COD fed [21]. Figures 2 and 3 show the variation of the fractional conversion in the three compartments of the HABR for the first set of experiments corresponding to HRTs of 16 h and 8 h respectively, and a constant influent substrate concentration (S_0) of 3000 mg COD/L. As can be seen in Figure 2, the steady-state fractional conversion or removal efficiency (per one) increased from 0.788 to 0.872 and to 0.917 for the compartments 1, 2 and 3 of the reactor during the assay corresponding to a HRT of 16 h (S_0 = 3000 mg/L). A small decrease in the fractional conversion was observed when the HRT decreased to 8 h (Figure 3). To be specific, the values of the conversion were

0.734, 0.795 and 0.847 for compartments 1, 2 and 3 of the reactor, respectively. Therefore, a decrease in the final conversion of around 7% was observed when the HRT dropped from 16 h to 8 h.

Figure 4 illustrates the effect of the influent substrate concentration (S_0 = 3000, 4500 and 6000 mg/L) on the fractional conversion for the three compartments of the reactor when this operated at a constant HRT of 16 h. For the S_0 values of 3000, 4500 and 6000 mg COD/L, the steady fractional conversions for compartments 1 and 3 ranged between 0.818 and 0.918, 0.777 and 0.899 and 0.699 and 0.885, respectively. Therefore a decrease in the conversion of only 3% was appreciated when the influent substrate concentration doubled from 3000 to 6000 mg COD/L, which demonstrated how effective this reactor configuration was against medium and high-strength wastewaters.

In order to predict the fractional conversion or organic matter removal efficiency (per one) for HABR, two different models were assessed and compared: a completely stirred tank reactor (CSTR) in series model and an axial diffusion or dispersion model, typically used for deviations of plug-flow systems.

When a stream of material flows steadily through a reactor or tank, where it takes part in some process such as chemical or biological reaction, or simple mixing, it is usual to make use of one of the following assumptions for the purpose of calculation [22]:

a) The fluid in the tank is completely mixed, so that its properties are uniform and identical with those of the outgoing stream. This assumption is frequently made as the basis of calculation in stirred reactors.

b) Elements of fluid which enter the reactor at the same moment move through it with constant and equal velocity on parallel paths, and leave at the same moment. This type of behaviour is usually referred to as “piston flow” or “plug flow” and is normally assumed when considering flow through packed reactors, catalytic reactors, etc.

It is clear that there are many cases in which neither type of flow corresponds exactly to the experimental facts [21-23]. It is of great importance to investigate the discrepancies between the assumed and actual behaviour of these reactors, and where necessary to allow for them in making kinetic calculations.

In the present study and given that the reactor used was a HABR with packing medium in the three compartments, the hydrodynamic flow should be explained on the basis of a plug flow model. The possible deviation of the behaviour of a plug-flow model can be explained by the concurrence of two main factors: both liquid and gaseous phases (biogas) circulate in the same direction and, in addition, due to the fact that the upward velocity of the gas is much higher than the upward velocity of the liquid (approximately 0.95 m/day), causing an airlift effect, which results in a mix of the liquid phase and consequently in a deviation of the plug-flow hydrodynamic model. As a consequence, either the CSTR in series model and the dispersion or axial diffusion model are assayed and compared to predict the COD removal efficiency or fractional conversion in the HABR.

3.2.1. CSTR in series model

This model assumes that the HABR is made up of three completely mixed tanks with equal volume and connected in series. As was previously pointed out, the mix in each tank is caused by the airlift effect generated by the produced biogas and circulation of the liquid phase. Assuming that the steady-state conditions are achieved for each reactor and that the substrate degradation follows a first-order kinetics, the following COD balance can be set out:

$$q \cdot S_{n-1} = q \cdot S_n + k \cdot S_n \cdot V \qquad (1)$$

where: q is the volumetric flow-rate of the feed or influent; S_n is the COD in the bioreactor or tank n; S_0 is the influent or inlet COD; V is the bioreactor volume and k is the kinetic constant of the process.

Defining the hydraulic retention time τ as the quotient: $\tau = V/q$ and the fractional conversion (X) for any bioreactor (n) by the expression: $X_n = 1 - (S_n/S_0)$, the following three equations can be established for a system with three CSTRs in series:

$$X_1 = 1 - 1/(1 + k \cdot \tau) \qquad (2)$$

$$X_2 = 1 - 1/(1 + k \cdot \tau)^2 \qquad (3)$$

$$X_3 = 1 - 1/(1 + k \cdot \tau)^3 \qquad (4)$$

The value of the kinetic constant, k, was determined from the experimental results (Figures 2-4) by mathematical adjustment (non-linear regression) using Mathcad software (version 14) based on the condition that the value of the sum of the squares of the differences between the experimental and theoretical values should be at a minimum. In this way, the value obtained for the kinetic constant, k, with its standard deviation was $0.60 \pm 0.07\ h^{-1}$.

A CSTR in series model was also found to be applicable for studying the hydrodynamic behaviour of a bench-scale horizontal flow anaerobic immobilized sludge (HAIS) reactor filled with porous ceramic spheres (5 mm diameter). This reactor operated at HRTs in the range of 2-7 hours using tracers with different characteristics (bromophenol blue, dextran blue, eosin Y, etc.) (Table 1)[24].

On the other hand, the value of the kinetic constant, k, obtained with this model in the present work is much higher than the specific substrate utilization rate coefficient obtained in an ABR with three chambers (0.012 h^{-1}) processing molasses wastewater (9-38 g COD/L) at OLRs of between 5-25 kg COD/m^3 d (Table 1) [15]. By contrast, this constant value is only slightly higher than the specific rate constant obtained in the modelling of the anaerobic digestion of wastewater generated in orange juice production (0.46 h^{-1}) using CSTR systems (Table 1) [25]. Finally, the value of k in the present study is of the same order of magnitude as the maximum specific rate of substrate consumption (0.70 h^{-1}) achieved in the methanogenesis from acetate using a periodic ABR under increasing organic loading conditions (2700 to 10500 mg/L) (Table 1) [13].

3.2.2. Validation of the CSTR in series model

The proposed equations (2-4) were validated by comparing the theoretical curves obtained with the corresponding experimental data of the fractional conversions for the different operational conditions studied. Figure 5 shows the comparison of the experimental fractional conversion data with the theoretical curves obtained using the CSTR in series model for all the experiments carried out: those corresponding to HRTs of 16 h and 8 h at a constant S_0 value of 3000 mg COD/L and those corresponding to increasing influent substrate concentrations of 3000, 4500 and 6000 mg COD/L and a constant HRT of 16 h. Figure 6 shows a comparison of the experimental data of fractional conversion and theoretical data obtained with this model for all the experiments carried out. As can be seen in both sets of experiments, deviations equal to or lower than 10% between the experimental and simulated values of the fractional conversion were obtained. However, a clear trend was observed in this model: the theoretical fractional conversions obtained with the model were slightly higher than the experimental values for almost all cases studied. Therefore, this simple model based on a single parameter (such as the kinetic constant) allows for the adequate reproduction of the fractional conversion values, which demonstrates that the kinetic parameter obtained represents approximately the activity of the different microorganisms involved in the anaerobic process. Table 2 summarizes the most significant statistical parameters (such as the non-linear regression coefficient (R), coefficient of determination (R^2), standard error of estimate, normality test (Shapiro-Wilk), W statistic and significance level) derived from the adjustment of the experimental data to this CSTR in series proposed model. The high values obtained for R and R^2 and the low values of the standard errors of estimates for the two HRTs studied (8 and 16 h) demonstrated the goodness of the model proposed.

3.2.3. Axial diffusion or Dispersion model

Assuming steady-state conditions in a bioreactor of length L for which a fluid flows with a constant rate u and the feed is axially mixed with a dispersion coefficient, D, and considering a first-order kinetics for substrate consumption, the following expression can be obtained [21]:

$$(D/u\cdot L)\mathrm{d}^2X/\mathrm{d}z^2 - \mathrm{d}X/\mathrm{d}z + k\cdot\tau\cdot(1-X) = 0 \qquad (5)$$

where X is the fractional conversion (per one), τ is the hydraulic retention time, z is the non dimensional length ($z = l/L$) and ($D/u\cdot L$) is the dispersion coefficient and is equal to the inverse of the Peclet number.

Equation (5) can easily be converted into the following equation:

$$X = 1 - [4\cdot a\cdot \exp(u\cdot L/(2\cdot D))/[(1+a)^2\cdot \exp(a\cdot u\cdot L/(2\cdot D)) - (1-a)^2\cdot \exp(-a\cdot u\cdot L/(2\cdot D))]] \quad (6)$$

where $a = [1 + 4\cdot \mathrm{k}\cdot\tau(\mathrm{D}/(\mathrm{u}\cdot\mathrm{L}))]^{0.5}$ and k is the kinetic constant of the process.

In conclusion, the dispersion model has two parameters which need to be calculated: the kinetic constant (k) and the dispersion coefficient (D).

According to the characteristics of this model and the experimental design used in the present study, it is foreseeable that the dispersion model fits the experimental results obtained better than the CSTR in series model. By solving equation (6) with the above-mentioned Mathcad software, the following values for these parameters were obtained: $k = 0.67 \pm 0.06$ h^{-1} and $D = 46$, therefore, the Peclet number, N, being equal to 0.02.

Taking into account the value of the dispersion coefficient obtained (46), the flow pattern is intermediate between the plug-flow and completely stirred reactors (CSTR), although it comes nearer to the plug-flow model. Consequently, the values of the kinetic constant obtained with both models are quite similar.

A dispersion model was also found to be highly suitable for describing the anaerobic digestion of municipal wastewater in a novel outside cycle reactor developed based on the characteristics of an expanded granular sludge bed (EGSB) reactor [26]. The standard deviation of the simulated data (concentration of the effluent suspended solids) was less than 6% (Table 1) [26]. The flow pattern and behaviour of an acidogenic UASB reactor was also successfully simulated with the dispersion model. The axial dispersion coefficient was identified as the most important factor in the dispersion modelling of this reactor [27]. The axial dispersion model was also found to be appropriate for studying the hydrodynamic pattern of a fluidised bed reactor [28] and a rotating disc anaerobic reactor digesting acetic acid as substrate [29]. The feasibility of the dispersion model simulating the process performance in anaerobic filters was also reported in the literature [30].

Finally, similar small Peclet numbers (0.01-1.5) to those obtained in the present study (0.02) were found in the deep-biofilm kinetics of substrate utilization during acetate fermentation in anaerobic filters [31]. An axial dispersion model coupled with deep biofilm kinetics can be better used to estimate the removal efficiency in this type of reactors, as is also concluded in this work [31].

3.2.4. Validation of the Dispersion model

This newly proposed model was validated by comparing the simulated curves obtained by means of equation (6) with the experimental values of the fractional conversion for all the experiments carried out (Figure 7). The slight deviations obtained (less than 8% in all cases) demonstrate the suitability of the proposed dispersion model and suggest that this model describes the anaerobic digestion process of this wastewater in the HABR more accurately than the CSTR in series model. All the statistical parameters summarized in Table 2 indicate that, compared with the CSTR in series model, the dispersion model slightly gives more accurate predictions of the reactor performance than the CSTR in series model. Between the two flow hypotheses, plug-flow appears to match the performance data more closely than the CSTR hypothesis according to the statistical parameters evaluated.

4. Conclusions

The performance of a hybrid anaerobic baffled reactor treating molasses-based synthetic wastewater was evaluated using two different kinetic models: a model of CSTR in series and an axial diffusion or dispersion model. These models were assessed and compared with the aim of simulating the organic matter removal or fractional conversion under different operational conditions. The kinetic constant (k) obtained by using the CSTR in series model was 0.6 h^{-1}, while the kinetic parameter of the dispersion model and the dispersion coefficient (D) were 0.67 h^{-1} and 46, respectively.

The flow pattern and hydrodynamic behaviour observed in the hybrid reactor studied was intermediate between plug-flow and CSTR in series systems, although the plug-flow system was slightly predominant. The dispersion model allowed a slight better fit of the experimental results of fractional conversions with deviations lower than 8% between the experimental and theoretical values. On the basis of results obtained a study using real molasses-based wastewater will be made in the future.

Acknowledgements

The authors gratefully acknowledge the financial support of the Water Research Center of Greentech (Co. Ltd.), Shiraz, Iran. The authors also thank Dr. Anahita Parsnejad for her help.

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Table 1

Comparison of the kinetic constants obtained in the present work with other values reported in the literature

Substrate	Reactor type	Model used	Kinetic constant	Reference
Synthetic wastewater	Hybrid anaerobic baffled reactor	CSTR in series	0.60 h^{-1}	Present study
Synthetic wastewater	Horizontal flow anaerobic immobilised sludge (HAIS) reactor	CSTR in series	0.45 h^{-1}	[24]
Molasses	ABR	CSTR in series	0.012 h^{-1}	[15]
Wastewater from orange juice production	CSTRs	CSTR in series	0.46 h^{-1}	[25]
Acetate	Periodic ABR	CSTR in series	0.70 h^{-1}	[13]
Synthetic wastewater	Hybrid anaerobic baffled reactor	Dispersion model	0.67 h^{-1}	Present study
Municipal wastewater	Outside cycle reactor	Dispersion model	0.45 h^{-1}	[26]

Table 2

Statistical parameters used in evaluating models performances

Parameter	CSTR in series model HRT = 8 h	CSTR in series model HRT = 16 h	Dispersion model
Non linear regression coefficient (R)	0.9995	0.9996	0.9998
Coefficient of determination (R^2)	0.9993	0.9994	0.9996
Standard error of estimate	0.0123	0.0138	0.0004
Normality test (Shapiro-Wilk)	Passed (P=0.3720)	Passed (P=0.5544)	Passed (P=0.0001)
W Statistic	0.8876	0.9231	0.6809
Significance level	0.0001	0.0001	0.0001

FIGURE CAPTIONS

Figure 1. Diagram of the hybrid anaerobic baffled reactor (HABR) and its baffles with dimensions (cm).

Figure 2. Variation of the fractional conversion in the three compartments of the HABR for the experiment corresponding to an HRT = 16 h.

Figure 3. Variation of the fractional conversion in the three compartments of the HABR for the experiment corresponding to an HRT = 8 h.

Figure 4. Effect of the influent substrate concentration on the fractional conversion in the three compartments of the HABR.

Figure 5. Variation of the experimental and theoretical values of the fractional conversion (obtained with the CSTR in series model) with the hydraulic retention time.

Figure 6. Comparison of the experimental and theoretical values of the fractional conversion (obtained with the CSTR in series model) for all the experiments carried out.

Figure 7. Comparison of the experimental and theoretical values of the fractional conversion obtained with the dispersion model for all the experiments carried out.

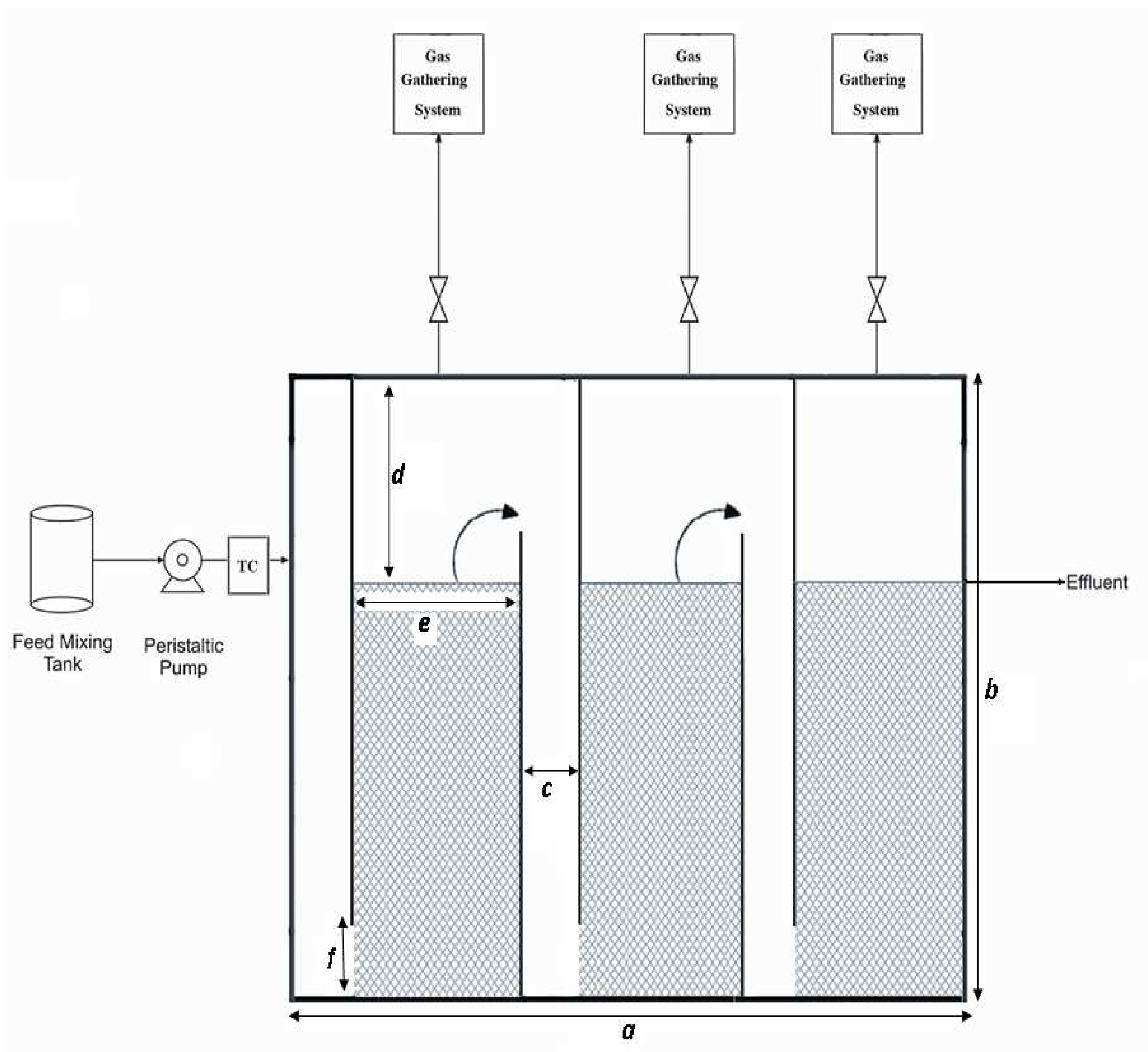

Figure 1

a = 58 cm; b = 44 cm; c = 1.5 cm; d = 6 cm; e = 18 cm; f = 2.5 cm

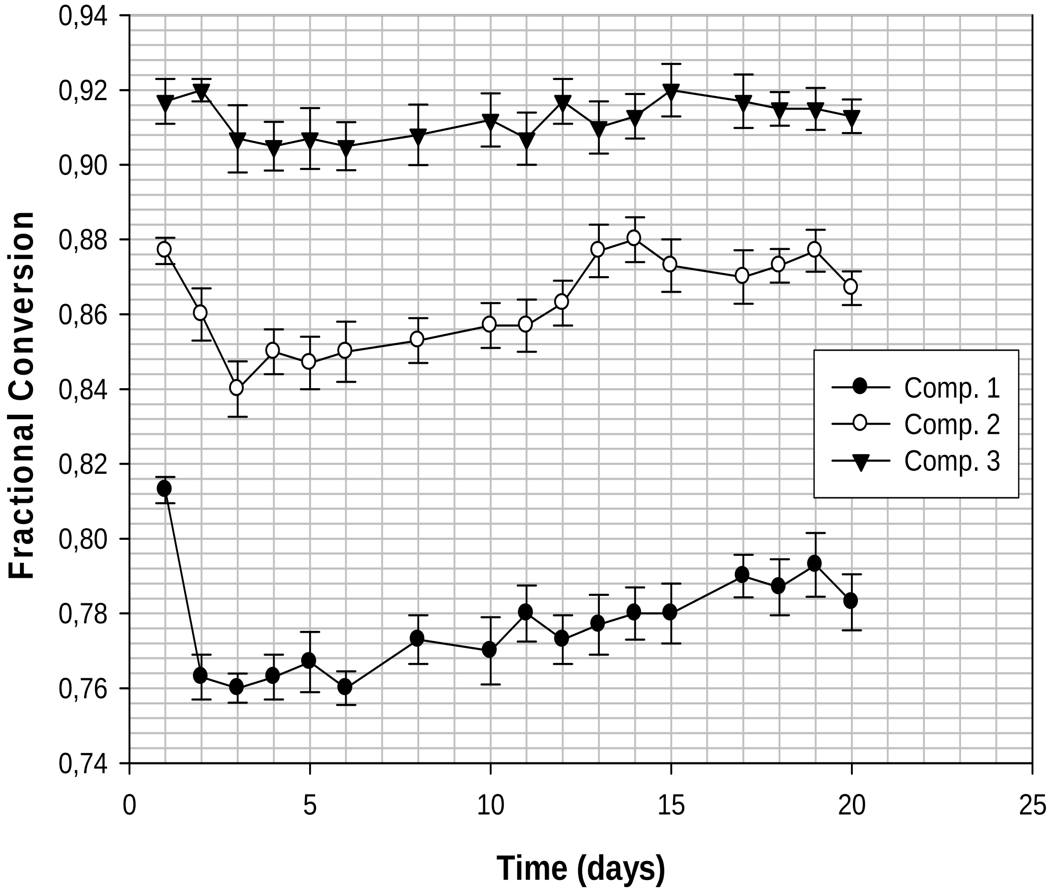
0,94
0,92
0,90
0,88
0,86
0,84
0,82
0,80
0,78
0,76
0,74
Fractional Conversion
0
5
10
15
20
25
Time (days)
Comp. 1
Comp. 2
Comp. 3

Figure 2

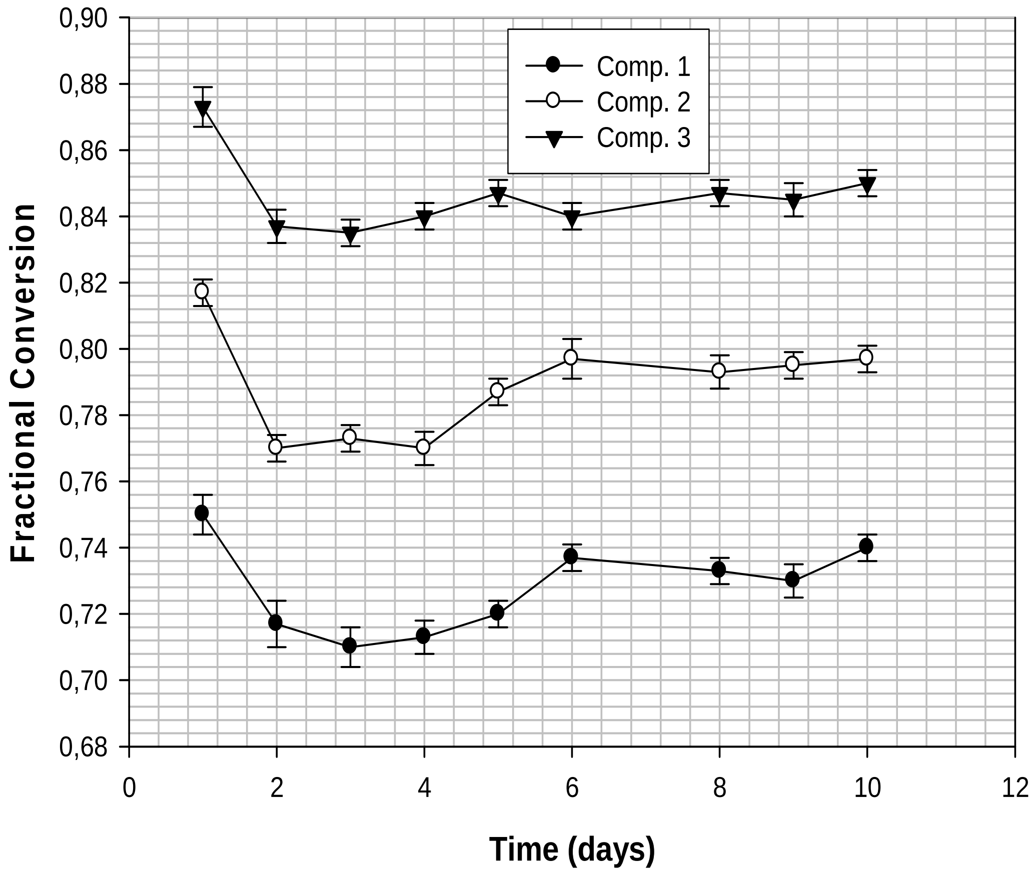
Comp. 1
Comp. 2
Comp. 3
Fractional Conversion
0,90
0,88
0,86
0,84
0,82
0,80
0,78
0,76
0,74
0,72
0,70
0,68
0
2
4
6
8
10
12
Time (days)

Figure 3

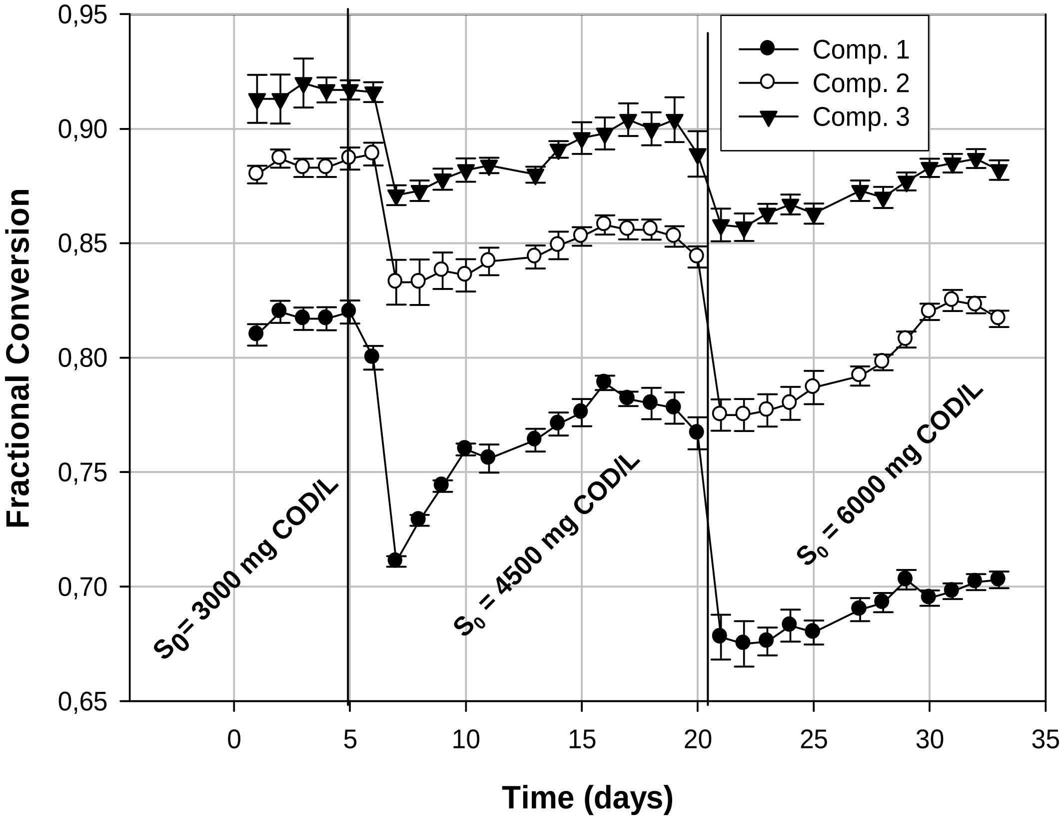
Fractional Conversion
Time (days)
0,95
0,90
0,85
0,80
0,75
0,70
0,65
0
5
10
15
20
25
30
35
Comp. 1
Comp. 2
Comp. 3
S0= 3000 mg COD/L
S0 = 4500 mg COD/L
S0 = 6000 mg COD/L

Figure 4

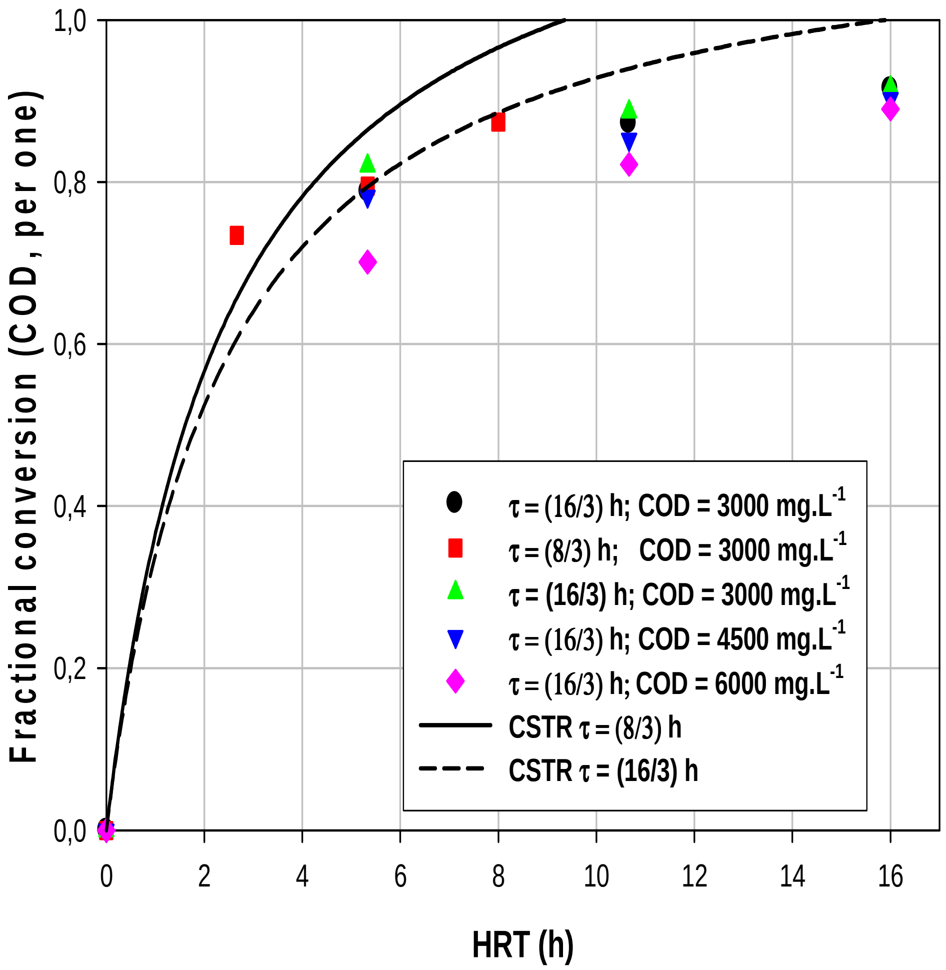
1,0
0,8
0,6
0,4
0,2
0,0
Fractional conversion (COD, per one)
0
2
4
6
8
10
12
14
16
HRT (h)
τ = (16/3) h; COD = 3000 mg.L-1
τ = (8/3) h; COD = 3000 mg.L-1
τ = (16/3) h; COD = 3000 mg.L-1
τ = (16/3) h; COD = 4500 mg.L-1
τ = (16/3) h; COD = 6000 mg.L-1
CSTR τ = (8/3) h
CSTR τ = (16/3) h

Figure 5

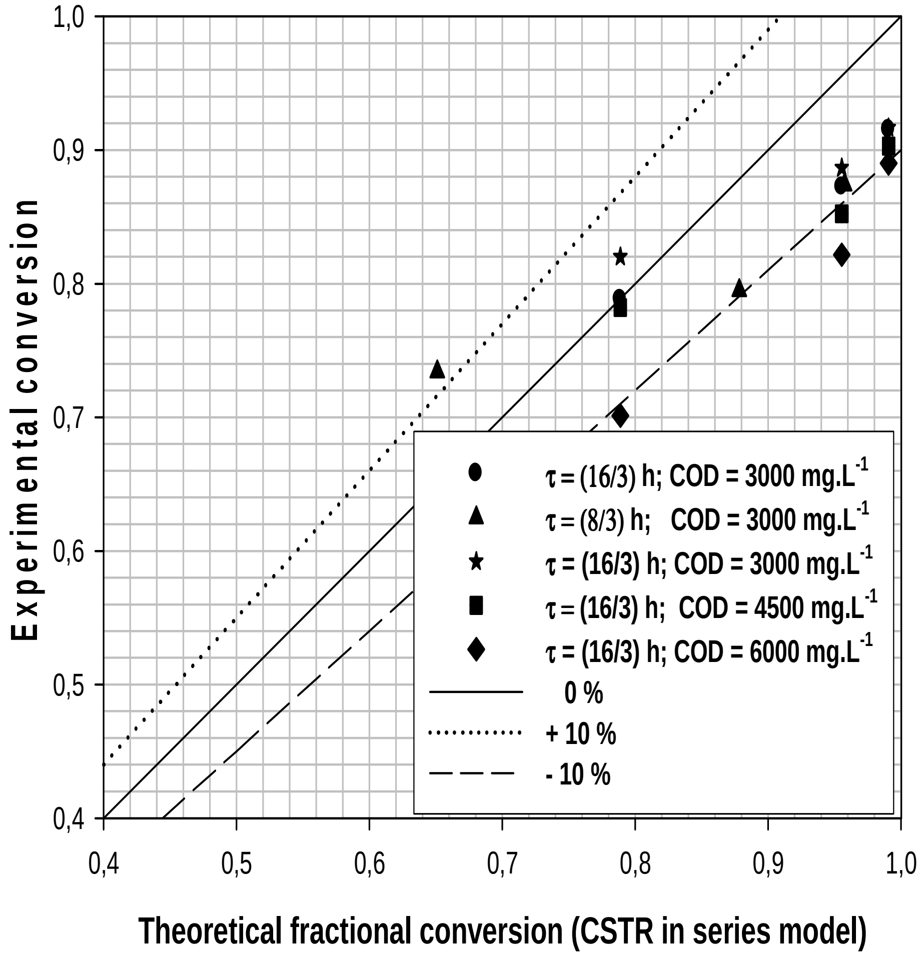
1,0
0,9
0,8
0,7
0,6
0,5
0,4
Experimental conversion
0,4
0,5
0,6
0,7
0,8
0,9
1,0
Theoretical fractional conversion (CSTR in series model)
τ = (16/3) h; COD = 3000 mg.L-1
τ = (8/3) h; COD = 3000 mg.L-1
τ = (16/3) h; COD = 3000 mg.L-1
τ = (16/3) h; COD = 4500 mg.L-1
τ = (16/3) h; COD = 6000 mg.L-1
0 %
+ 10 %
- 10 %

Figure 6

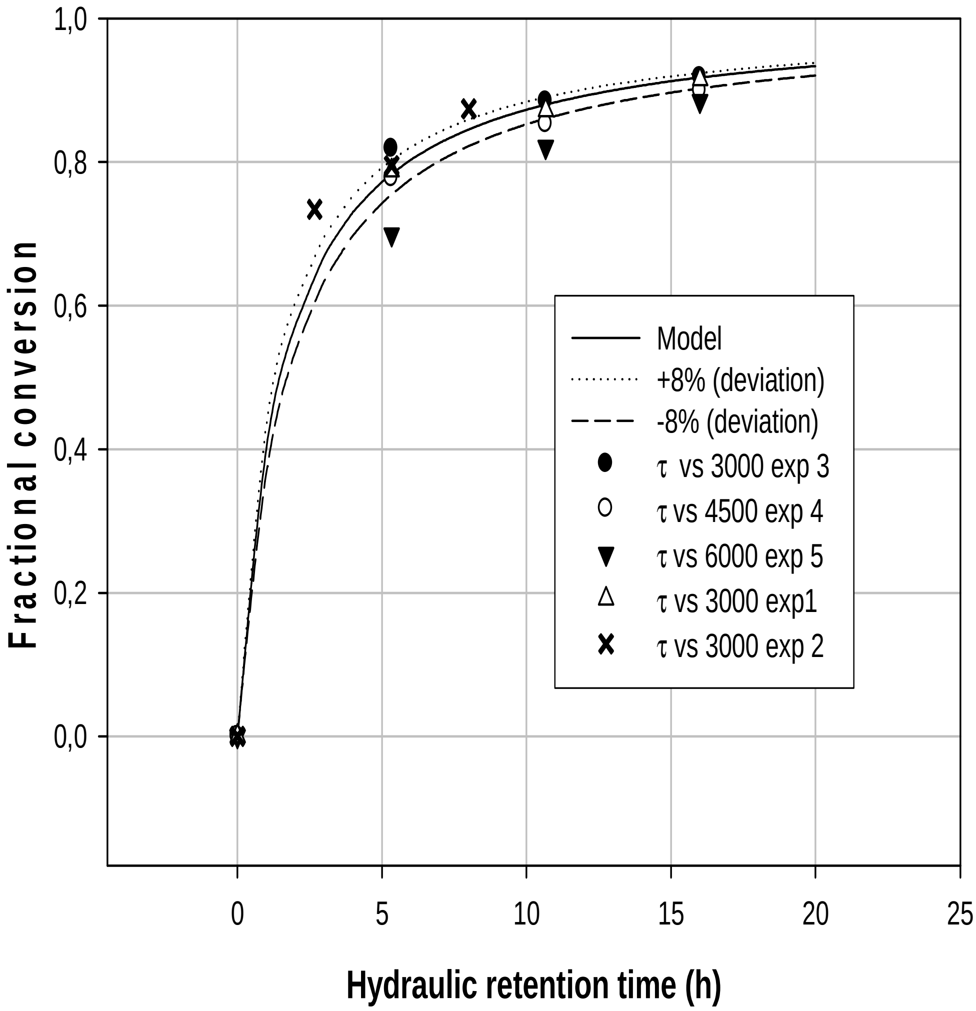
1,0
0,8
0,6
0,4
0,2
0,0
Fractional conversion
0
5
10
15
20
25
Hydraulic retention time (h)
Model
+8% (deviation)
-8% (deviation)
τ vs 3000 exp 3
τ vs 4500 exp 4
τ vs 6000 exp 5
τ vs 3000 exp1
τ vs 3000 exp 2

Figure 7