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Modeling and Computational Simulation of Dilution and Biochemical Materials Balance Equations for Partially Emptied Batch Reactors

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Abstract

Sequencing batch reactors (SBRs) including aerobic SBRs and anaerobic SBRs (ASBRs) are partially emptied batch reactors that are widely used as bioprocesses in pollution control. We present dilution and biochemical materials balance modeling equations and simulation results for the partially emptied batch reactors, especially for ASBR treatment of low-strength wastewater. The simulated substrate and microbial concentrations for both dilution and materials balance equations follow the same pattern during both feeding and reaction times. However, the results of the materials balance equations show microbial activities during feeding as well as during reaction times and were found to be more appropriate for the biologic system in which substrate removal is associated with microbial growth. Furthermore, the simulation results point to the need to foster high microbial accumulation in the system during startup to optimize the process performance and the need to operate the system at a short reaction time, especially for low substrate concentrations. The results were found to be in agreement with the results of prior laboratory studies.

Index Entries: Aerobic-SBRs; Anaerobic-SBRs; ASBR; biochemical-reaction kinetics; dilution equations; kinetic modeling; materials balance equations; Monod equations; numerical simulation; partially emptied batch-reactors; sequencing-batch-reactors.

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Introduction

The partially emptied batch reactor process has been used in many engineering applications including biologic treatment of wastewaters for pollution control. The partially emptied batch reactor processes include the aerobic sequencing batch reactor (aerobic SBR or simply SBR) and the anaerobic sequencing batch reactor (ASBR or anaerobic SBR). Unlike the continuous-flow processes, the partially emptied batch reactors are high-rate processes with high-performance characteristics owing to their ability to retain high concentrations of microbes in the system without a need for an external solid-liquid separation unit.

In many engineering inventions, initial efforts are usually spent on investigating the system performance to ensure that the system will meet some societal needs before the physics of how the system performs are investigated. In a previous report, the lead author presented one of the first studies on the performance of the ASBR process *(1)*. There have been many other reports in the literature on the application and performance of the ASBR process, especially for the treatment of municipal, industrial, and hazardous wastes including the treatment of low-strength wastewater in tropical regions *(2–11)*.

We present in this article kinetics equations and simulation results especially for ASBR treatment of low-strength substrate at various hydraulic retention times (HRTs) and at 35°C. We also provide comparisons of simulation results from dilution equations and from materials balance equations during feeding time and their overall prediction of the concentrations of substrate and microbes in the reactor during both feeding and reaction time. The kinetics equations and results of the simulation will help advance knowledge and application of the partially emptied anaerobic reactor process.

Model Development

The operating principles of SBR processes involve four sequential steps: feed, react, settle, and decant. The duration of feeding time is usually short in comparison with the duration of reaction time. For a partially emptied batch reactor, during decant only a predetermined volume of the reactor is emptied, not the entire reactor volume. The volume fed to the reactor during the feeding step must be equal to the volume that was decanted to maintain constant working volume and HRT. Figure 1 presents the operating principles of the SBR processes with some of the variables used for developing the model equations. The nomenclature at the end of the article lists the variables used.

Dilution Equations for SBR Processes During Feed Step

Substrate Concentration During Feeding Based on Dilution

An important characteristic of the SBR processes is that substrate concentration and fluid volume in the reactor are at their lowest individual

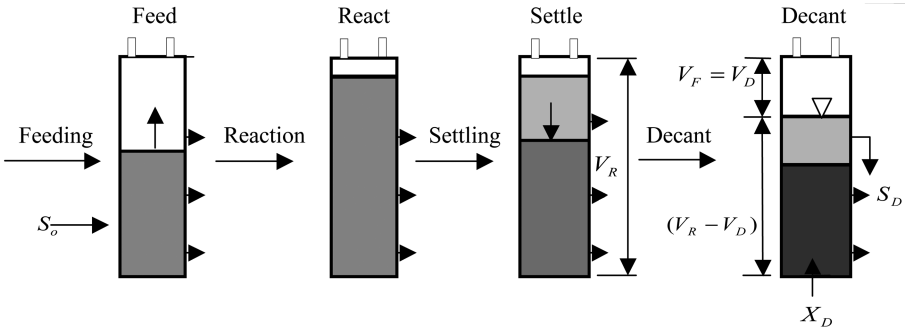

Fig. 1. Schematic of four steps in ASBR operation with some variables used in developing biologic kinetics equations.

value at the end of the react step through the start of the feed step. Substrate concentration in the reactor at any time during the feed step (S_F) owing to dilution can be represented by

$$S_F = (V_o S_D + V_t S_0)\left(\frac{1}{V_o + V_t}\right) = [(V_R - V_D)\, S_D + V_t S_0]\left(\frac{1}{V_o + V_t}\right) \quad (1)$$

in which V_t is the volume of raw substrate fed to the reactor at the time of interest, V_R is the total reactor volume, and V_o is the volume of substrate in the reactor at the end of decant ($V_R - V_D$). Similarly, substrate concentration at the end of the feed step (S_{EF}) can be represented by

$$S_{EF} = (V_D S_0 + V_o S_D)\left(\frac{1}{V_R}\right) = [V_D S_0 + (V_R - V_D)\, S_D]\left(\frac{1}{V_R}\right) \quad (2)$$

Microbial Concentration During Feeding Based on Dilution

Another important characteristic of the SBR processes is the fact that microbial concentration in the reactor is at its highest value at the end of the decant step through the beginning of the feed step whereas fluid volume is at its lowest value at the end of the decant step through the beginning of the feed step. During feeding, microbial concentration in the reactor decreases owing to dilution with raw substrate and can be represented by

$$X_F = (V_o X_D + X_o V_t)\left(\frac{1}{V_o + V_t}\right) = [(V_R - V_D)\, X_D + X_o V_t]\left(\frac{1}{V_o + V_t}\right) \quad (3)$$

Neglecting microbial concentration in the raw feed (X_o), Eq. 3 becomes

$$X_F = V_o X_D\left(\frac{1}{V_o + V_t}\right) = [(V_R - V_D)\, X_D]\left(\frac{1}{V_o + V_t}\right) \quad (4)$$

At the end of the feed step, microbial concentration in the SBR system may be represented by

$$X_{EF} = V_o X_D\left(\frac{1}{V_o + V_t}\right) = [(V_R - V_D)\, X_D]\left(\frac{1}{V_R}\right) \quad (5)$$

Materials Balance Equations for SBR Processes

Materials Balance Equations for Microbes During Feed Step

During the feed step, reactor fluid volume increases whereas microbial concentration decreases, but the changes occur simultaneously. A mass balance (accumulation rate = input rate – output rate + growth rate) gives

$$\frac{d(VX)}{dt} = Q X_o - 0 + V r_x \tag{6}$$

Using product rule of differentiation, we have

$$V\frac{dX}{dt} + X\frac{dV}{dt} = Q X_o + V r_x \tag{7}$$

Dividing all the terms by volume V, we have

$$\frac{dX}{dt} + \frac{X}{V}\frac{dV}{dt} = \frac{Q}{V} X_o + r_x \tag{8}$$

Rearranging terms, we have

$$\frac{dX}{dt} + \frac{XQ}{V} = \frac{Q}{V} X_o + r_x \quad \text{or} \quad \frac{dX}{dt} = \frac{Q}{V}(X_o - X) + r_x \tag{9}$$

Assuming negligible microbial concentration in the feed substrate (X_o), Eq. 9 becomes

$$\frac{dX}{dt} = -\frac{Q}{V} X + r_x \tag{10}$$

Using the relations $V = V_o + V_t$, in which $V_t = Q_t$, Eq. 10 becomes

$$\frac{dX}{dt} = \frac{-QX}{V_o + Q_t} + r_x \tag{11}$$

In the previous equations, r_x is the net microbial growth rate. It is the microbial growth rate minus microbial death rate ($r_x = r_g - r_d$). Using the mixed-order Monod biochemical kinetics expression for microbial growth rate and first-order rate expression for the microbial death rate, Eq. 11 becomes

$$\frac{dX}{dt} = \frac{-QX}{V_o + Q_t} + \hat{\mu}\frac{SX}{K_s + S} - K_d X \tag{12}$$

Mass Balance for Microbes During React Step

During the react step, flow into the reactor is zero; therefore, Q in Eq. 12 will be zero, resulting in Eq. 13:

$$\frac{dX}{dt} = \frac{\hat{\mu} SX}{K_s + S} - K_d X \tag{13}$$

Materials Balance for Substrate During Feed Step

Substrate concentration in a partially emptied batch reactor system is at its lowest value at the end of the react step through the beginning of the feed step. Reactor fluid volume is at its lowest value at the end of the decant step through the beginning of the feed step. During feeding, the change (increase) in substrate concentration and in reactor fluid volume occurs simultaneously. A mass balance on substrate (accumulation rate = input rate – output rate – decay rate) gives

$$\frac{d(VS)}{dt} = QS_o - 0 - Vr_s \tag{14}$$

When we apply the product rule of differentiation as before, Eq. 14 gives

$$V\frac{dS}{dt} + S\frac{dV}{dt} = QS_o - Vr_s \quad \text{or} \quad \frac{dS}{dt} + \frac{S}{V}\frac{dV}{dt} = \frac{Q}{V}S_o - r_s \tag{15}$$

Substituting $dV/dt = Q$ into Eq. 15 gives

$$\frac{dS}{dt} + \frac{S}{V}Q = \frac{Q}{V}S_o - r_s \quad \text{or} \quad \frac{dS}{dt} = \frac{Q}{V}(S_o - S) - r_s \tag{16}$$

Using the relation $V = V_o + V_t$, in which $V_t = Q_t$, Eq. 16 can be written in the following form:

$$\frac{dS}{dt} = \frac{Q}{V_o + Qt}(S_o - S) - r_s \tag{17}$$

Using the mixed-order Monod biochemical rate expression for substrate decay (r_s), Eq. 17 becomes

$$\frac{dS}{dt} = \frac{Q}{V_o + Qt}(S_o - S) - \frac{\hat{\mu}}{Y}\frac{SX}{K_s + S} \tag{18}$$

Materials Balance for Substrate During React Step

During the react step, substrate flow rate is zero; therefore, Eq. 18 becomes

$$\frac{dS}{dt} = \frac{\hat{\mu}}{Y}\frac{XS}{K_s + S} \tag{19}$$

Simultaneous Substrate Removal and Microbial Growth Model

An important aspect of biologic treatment is relating substrate removal to microbial growth. To simulate substrate and microbial concentrations based on dilution during feeding, Eqs. 1 and 4 were solved independently followed by simultaneous simulation of Eqs. 13 and 19 for substrate and microbial concentrations during the reaction step. To simulate substrate and microbial concentrations based on the materials balance approach,

Table 1
Sequencing Characteristics for Various HRTs *(1)*

Sequencing characteristic	Reactor (HRT, h)			
	1 (48)	2 (24)	3 (16)	4 (12)
Number of sequences per day	6	6	6	6
Length of sequence (h)	4	4	4	4
Volume of feed per sequence (L)	0.5	1.0	1.5	2.0
Volume of feed per day (L)	3	6	9	12
Volume decanted per sequence (L)	0.5	1.0	1.5	2.0
Volume remaining after decant (L)	5.5	5.0	4.5	4.0
Volume decanted per day (L)	3	6	9	12
Length of feeding time (min)	5	10.5	16.87	11.22
Length of reaction time (min [h])	189.5 (3.16)	179.5 (2.99)	171.1 (2.85)	180.8 (3.0)
Length of settling time (min)	40	40	40	40
Length of decanting time (min)	5.5	10	12	8

Eqs. 12 and 18 were simulated simultaneously, which gives substrate and microbial concentration during feeding through the end of the react step.

Numerical Simulation

In this article, we simulate the performance of the partially emptied batch reactor equations for ASBR treatment of low-strength wastewater (synthetic milk waste) at various HRTs at 35°C. The simulation is performed for substrate concentrations (COD) of 1000, 800, 600, and 400 mg/L, each at system HRTs of 48, 24, 16, and 12 h, which were previously studied in the laboratory by Ndon and Dague *(1)*. Tables 1 and 2 present the input variables for the model simulation obtained from the previous study.

The substrate concentrations reported in Table 2 are quasi-steady-state concentrations analyzed at the end of reaction just before the settle step. Therefore, these substrate concentrations are assumed to stay unchanged until feeding begins. Similarly, the microbial concentrations reported in Table 2 are quasi-steady-state concentrations analyzed at the end of reaction just before the settle step. However, the microbial concentration is a function of reactor fluid volume. Therefore, the microbial concentrations reported in Table 2 are used to determine the concentration after the decant step based on fluid volume remaining in the reactor after decant.

Kinetic constants reported by Lawrence and McCarty *(12)* for anaerobic treatment of synthetic milk waste at 20°C were used to determine the corresponding constants at 35°C using the well-known relationship for determining kinetic constants at various temperatures $_{KT} = K_{20}\theta^{(T-20)}$, in which $\theta = 1.04$ *(13)*. Table 3 presents values of the kinetic constants used in the kinetic simulation.

Table 2
Effluent Substrate Concentrations
and Mixed-Liquor Volatile Suspended Solids Concentrations
for Each Raw Substrate Concentration Treated
and Raw Substrate Feeding Rate for Various HRTs *(1)*

	Reactor (HRT, h)			
	1 (48)	2 (24)	3 (16)	4 (12)
Effluent soluble COD "S_D" (mg/L)				
1000 Feed COD (mg/L)	14	35	50	80
800 Feed COD (mg/L)	33	30	36	67
600 Feed COD (mg/L)	28	28	23	43
400 Feed COD (mg/L)	16	19	21	23
Feeding rate (L/min)	0.1	0.095	0.089	0.178
MLVSS concentrations before decant step "X_D" (mg/L)[a]				
1000 Feed COD (mg/L)	9070	8020	6490	6130
800 Feed COD (mg/L)	8900	8230	8020	5980
600 Feed COD (mg/L)	8130	8610	7960	6320
400 Feed COD (mg/L)	8270	8960	7690	6640

[a]MLVSS, mixed-liquor volatile suspended solids.

Table 3
Kinetic Constants for Anaerobic Treatment
of Synthetic Milk Waste at Various Temperatures

Temperature	$\hat{\mu}$ (d^{-1} [h^{-1}])	K_s (mg/L COD)	Y (lb MLVSS/lb COD)[a]	K_d (d^{-1} [h^{-1}])
20°C (from ref. *12*)	0.38 (0.016)	24.3	0.37	0.07 (0.0029)
35°C (calculated values)	0.68 (0.03)	43.7	0.67	0.13 (0.005)

[a]MLVSS, mixed-liquor volatile suspended solids.

Numerical Method for Simulating the Simultaneous Equations

Herein we use the first-order Runge-Kutta numerical method (also called the Euler's method) to simulate the simultaneous equations. Equations 13 and 19 can be written in the Euler's numerical iterative form as shown in Eqs. 20 and 21, respectively.

$$X(t+\Delta t) = X(t) + h\left[\frac{\hat{\mu}X(t)S(t)}{(K_s + S(t))} - K_d X(t)\right] \tag{20}$$

$$S(t+\Delta t) = S(t) - h\left[\frac{\hat{\mu}X(t)S(t)}{Y(K_s + S(t))}\right] \tag{21}$$

In Eqs. 20 and 21, h is a time step or the step size. It is the incremental time at which solutions are to be generated. Equation 21 can be simplified into Eqs. 22 and 23 and Eq. 20 can be simplified into Eqs. 24 and 25, respectively.

$$(\Delta S)_i = \left[\frac{-\hat{\mu} X_i S_i}{Y(K_s + S_i)}\right] \Delta t \tag{22}$$

$$S_{i+1} = S_i + (\Delta S)_i \tag{23}$$

$$(\Delta X)_i = -Y(\Delta S)_i - K_d X_i \Delta t \tag{24}$$

$$X_{i+1} = X_i + (\Delta X)_i \tag{25}$$

In Eqs. 22–25, i denotes the previous time at which the value of each of the variables (substrate and microbes) are known, and $i + 1$ denotes the current time at which the value of each of the variables has to be computed or simulated. Using the same approach, Eq. 18 can be simplified into Eqs. 26 and 27 and Eq. 12 can be simplified into Eqs. 28 and 29, respectively. All simulations were performed by setting up spreadsheets that solve the stated equations.

$$(\Delta S)_i = \left\{\left[\frac{Q}{(V_o + Qt)}\right](S_o - S_i) - \left[\frac{\hat{\mu} X_i S_i}{Y(K_s + S_i)}\right]\right\} \Delta t \tag{26}$$

$$S_{i+1} = S_i + (\Delta S)_i \tag{27}$$

$$(\Delta X)_i = \left\{\left[\frac{-QX_i}{(V_o + Qt)}\right] + \hat{\mu}\frac{S_i X_i}{K_s + S_i} - K_d X_i\right\} \Delta t \tag{28}$$

$$X_{i+1} = X_i + (\Delta X)_i \tag{29}$$

Results and Discussion

Substrate Concentrations

Substrate concentrations from the materials balance equations (Eqs. 12 and 18 simulated using Eqs. 26–29) for feeding through the end of the reaction step are illustrated in Fig. 2 for the various HRTs and the various raw substrate concentrations. As expected, Fig. 2 shows increasing substrate concentration during feeding and decreasing substrate concentration during reaction time. Also as illustrated in Fig. 2, substrate concentrations in the reactor at the end of feeding were significantly lower than the raw substrate concentrations in the feed flow. In addition, the long-HRT systems showed lower substrate concentrations at the end of feeding than the short-HRT systems. This could be a result of the dilution of the raw substrate by the reactor content since the system is a partially emptied process. In particular, the long-HRT systems were associated with a smaller feed volume of raw substrate during the feed step as well as a larger volume of previously treated substrate remaining in the reactor at the end of the

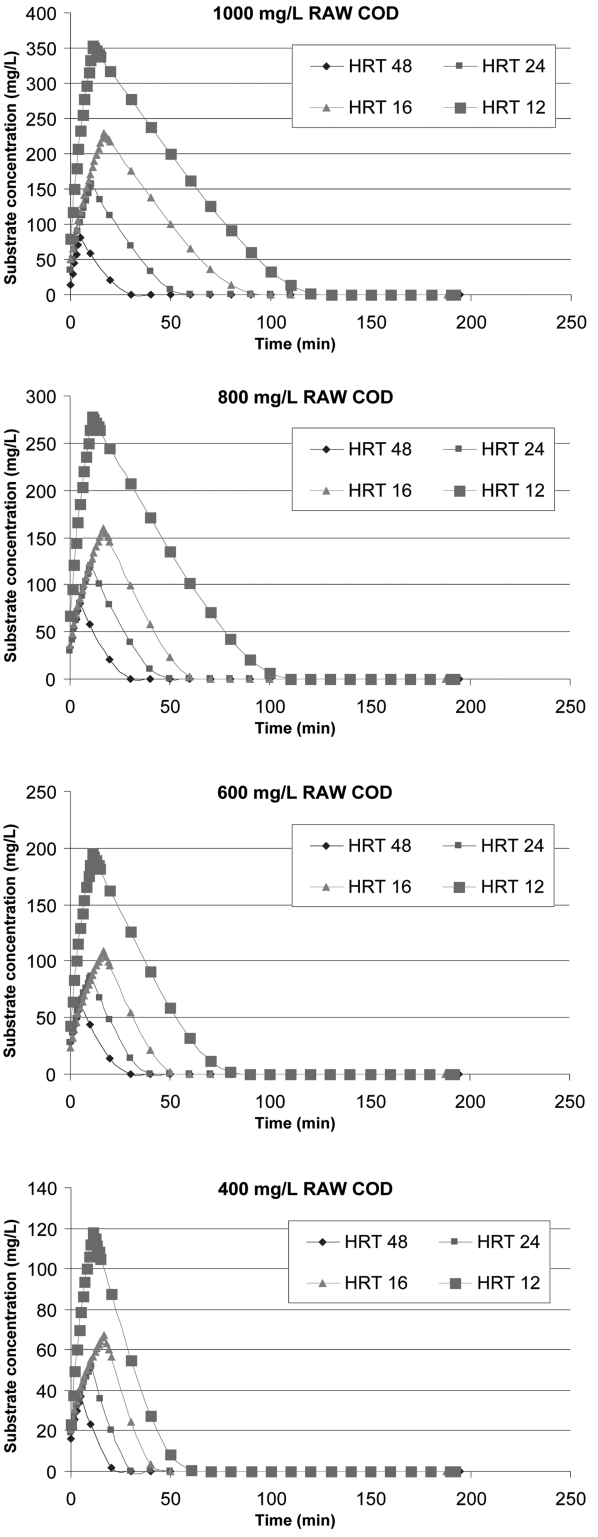

Fig. 2. Substrate concentration profile during feeding and reaction time at various HRTs at 35°C.

decant step, in comparison with the short-HRT systems. That is, short-HRT systems had higher hydraulic loading in comparison with long-HRT systems. These findings are in agreement with the results of previous reports *(1)*.

The results also showed higher concentrations of substrate in the reactor at the end of feeding for higher raw substrate concentrations. As illustrated in Fig. 2, a longer reaction time was required to achieve complete destruction of the substrate at higher raw substrate concentrations and at shorter HRTs. From the results, it would be appropriate to operate the system at a shorter reaction time (more cycles per day) when treating low concentrated substrates. This will result in more treatment cycles per day.

Figures 3–6 compare the effect of dilution (Eqs. 1 and 4 during the feed step followed by Eqs. 13 and 19 at the react step) and the effect of biochemical materials balance equations (Eqs. 12 and 18 for the feed step through the end of the react step) on substrate concentrations at the various raw substrate concentrations and HRTs. As discussed earlier, Eqs. 13 and 19 are simulated using Eqs. 22–25, and Eqs. 12 and 18 are simulated using equations 26–29.

As expected, Figs. 3–6 show increasing substrate concentration during feeding for both the dilution curves and the materials balance curves. However, the materials balance curves show lower substrate concentrations in the reactor at the end of feeding and during reaction time than the dilution curves. The lower substrate concentration from the materials balance equations can be attributed to biologic utilization of substrate during the feeding time since the dilution equations ignore the impact of biologic reaction during feeding.

The predicted results also show higher concentrations of substrate in the reactor at the end of feeding for higher raw substrate concentrations. As Figs. 3–6 show, at each raw substrate concentration fed to the reactor, the predicted substrate concentrations at the end of feeding were higher in the short–HRT systems than the long–HRT systems. This can be attributed to higher hydraulic loading to the short-HRT systems in comparison with the long-HRT systems.

Microbial Concentrations

Microbial concentrations from the materials balance equations (Eqs. 12 and 18 simulated using Eqs. 26–29) for feeding through the end of the reaction step are illustrated in Fig. 7 for the various HRTs and raw substrate concentrations. As expected, Fig. 7 shows decreasing microbial concentrations during feeding. This is in agreement with the operational characteristics of the partially emptied batch reactor process. Operationally, microbial concentrations are at highest levels in the partially emptied batch reactor process at the end of the decant step and decrease during feeding owing to dilution with raw flow.

Figure 7 also shows higher microbial concentrations in the long-HRT systems at the end of feeding, which is an accurate prediction of low micro-

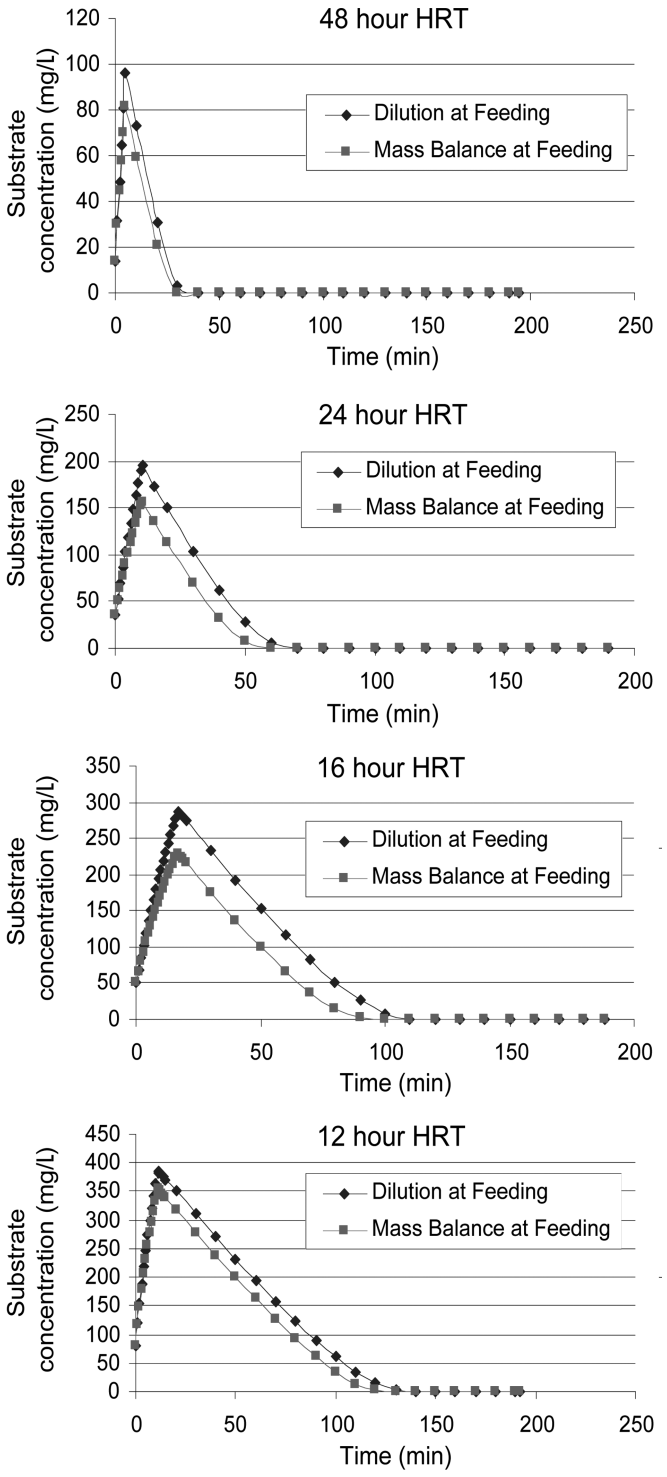

Fig. 3. Substrate concentration profile during feeding and reaction time at various HRTs and at raw substrate concentration of 1000 mg/L.

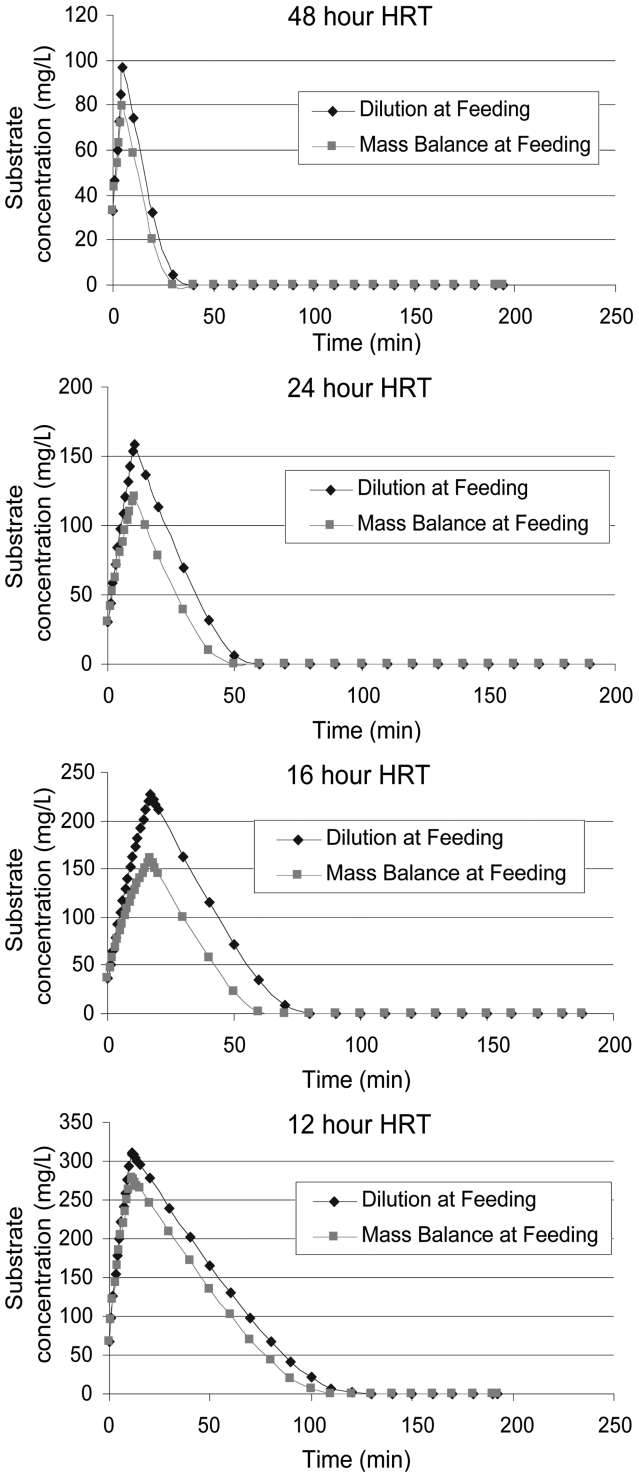

Fig. 4. Substrate concentration profile during feeding and reaction time at various HRTs and at raw substrate concentration of 800 mg/L.

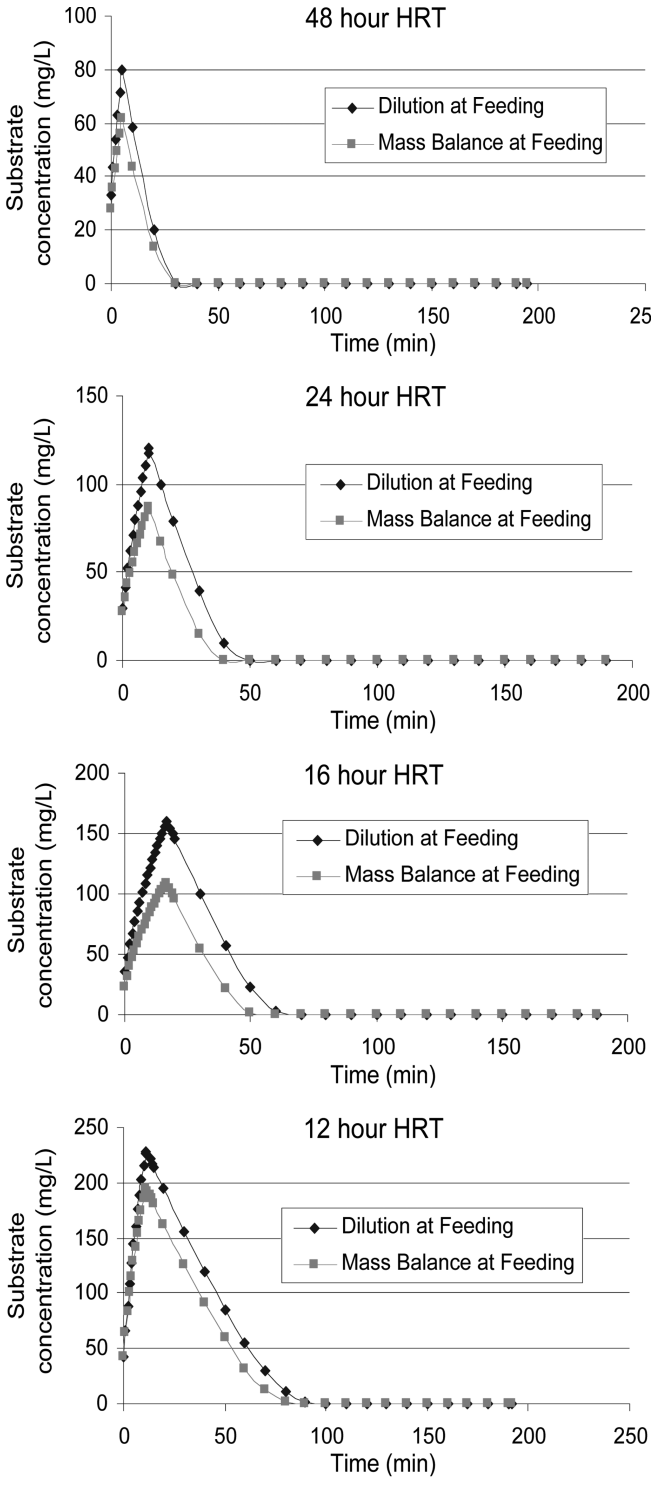

Fig. 5. Substrate concentration profile during feeding and reaction time at various HRTs and at raw substrate concentration of 600 mg/L.

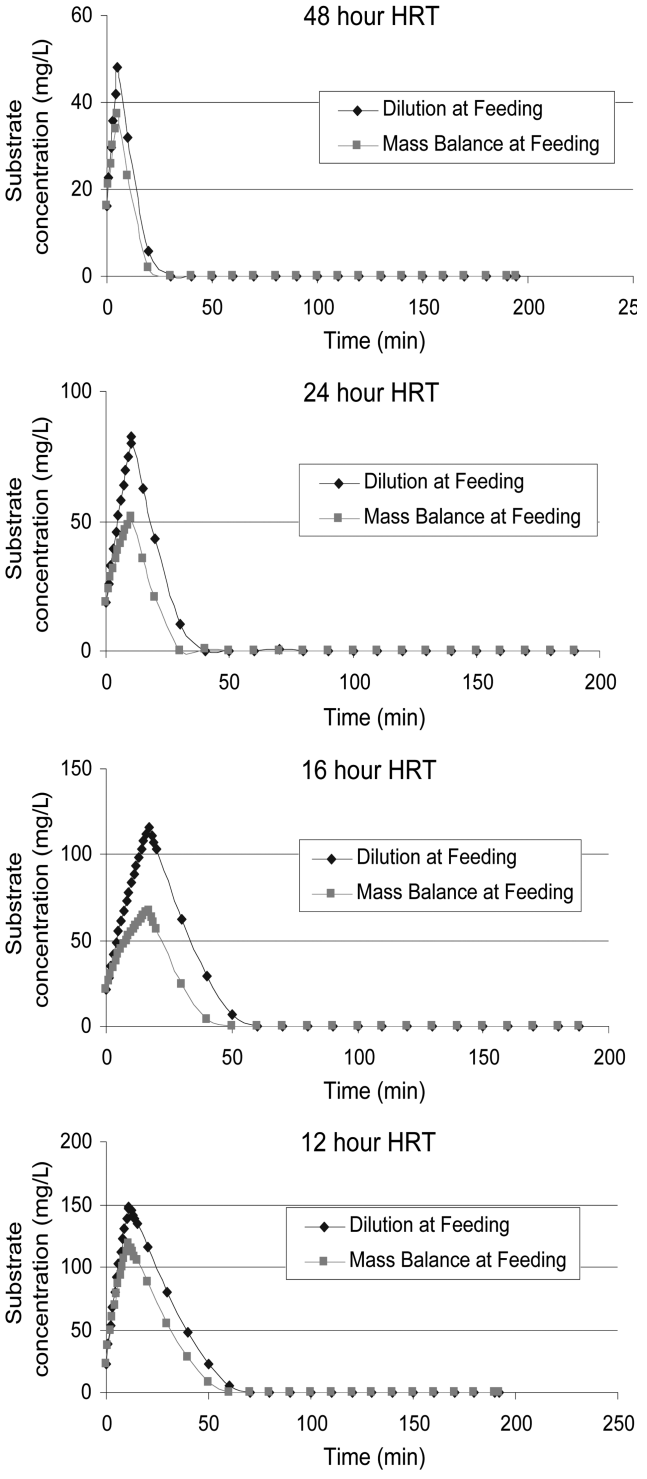

Fig. 6. Substrate concentration profile during feeding and reaction time at various HRTs and at raw substrate concentration of 400 mg/L.

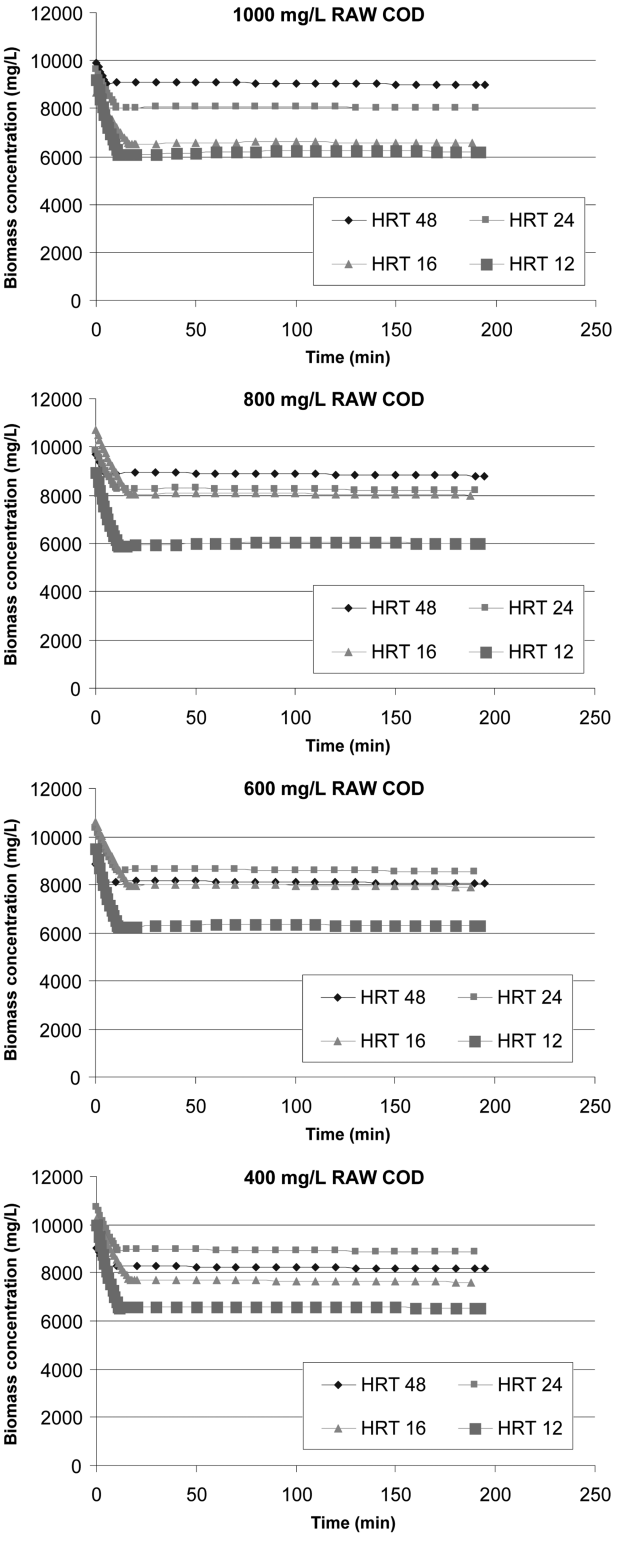

Fig. 7. Microbial concentration profile during feeding and reaction time at various HRTs at 35°C.

bial loss at long HRTs owing to low hydraulic loading applied to long-HRT systems. This finding is in agreement with results of prior studies *(1)*. In particular, Fig. 7 shows relatively steady microbial concentrations in the reactor during the react step. An important implication of these facts is that it is necessary to achieve high microbial content in the ASBR system during seeding (system startup) to optimize the process performance, because little microbial growth is expected, especially at low substrate concentrations.

Figures 8–11 compare the effect of dilution (Eqs. 1 and 4 during the feed step followed by Eqs. 13 and 19 at the react step) and the effect of biochemical materials balance equations (Eqs. 12 and 18 for the feed step through the end of the react step) on microbial concentrations at the various raw substrate concentrations and HRTs. As expected, the concentration of microbes decreased during feeding owing to increasing fluid volume. Figures 8–11 show relatively identical predicted concentrations of microbes in the reactors for both dilution and materials balance equations during feeding. The predicted microbial concentrations based on materials balance are related to substrate consumed during both feeding and reaction times, but the dilution equations at feeding time do not include the relationship between substrate consumption and cell production. Therefore, the reason for the identical concentrations of microbes predicted by the materials balance equations during feeding in comparison with the predicted microbial concentrations by the dilution equation can be owing to the short feeding time not being sufficient for microbial biosorption of the substrate and subsequent metabolism for synthesis of new cells.

As illustrated in Figs. 8–11, the materials balance equation predicts relatively higher concentrations of microbes during the reaction time than the dilution equation, especially at higher raw substrate concentrations. This could be owing to higher substrate removal predicted by the materials balance equations being converted to new cells during the reaction step in comparison to the dilution model. It also indicates new cell production occurring during the reaction step in comparison with the feeding step. Furthermore, at each raw substrate concentration, the short-HRT systems showed relatively higher microbial concentrations. This could be owing to the higher hydraulic loading applied to short-HRT systems that results in higher substrate loading that gets converted to microbes, which is in agreement with the results of prior studies *(1)*.

Conclusion

Generally, the predicted substrate and microbial concentrations for both dilution and materials balance equations follow the same pattern during both feeding and reaction times. However, the results of the materials balance equations were found to be more appropriate for the biologic system in which substrate removal is associated with microbial growth. Therefore, in using the partially emptied batch reactor in biologic treatment, this study shows that microbial activities are important during feeding as well as reaction times.

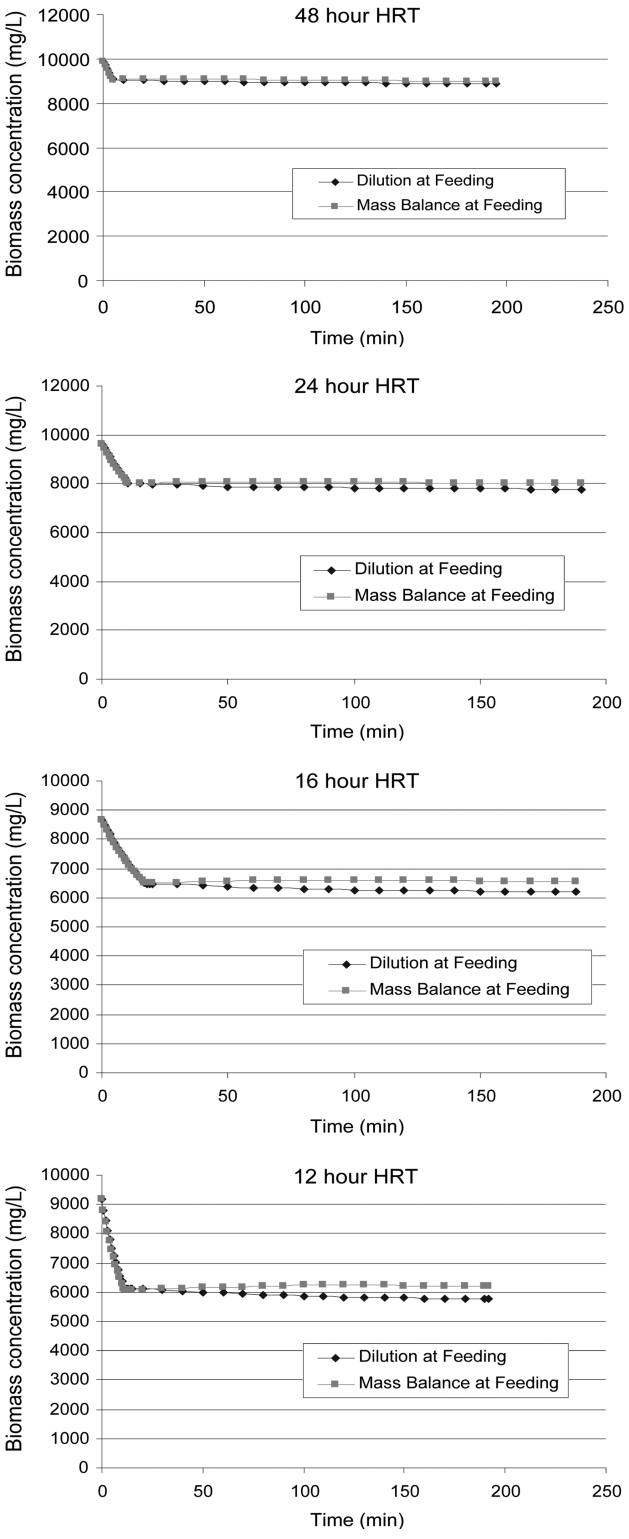

Fig. 8. Microbial concentration profile during feeding and reaction time at various HRTs and at raw substrate concentration of 1000 mg/L.

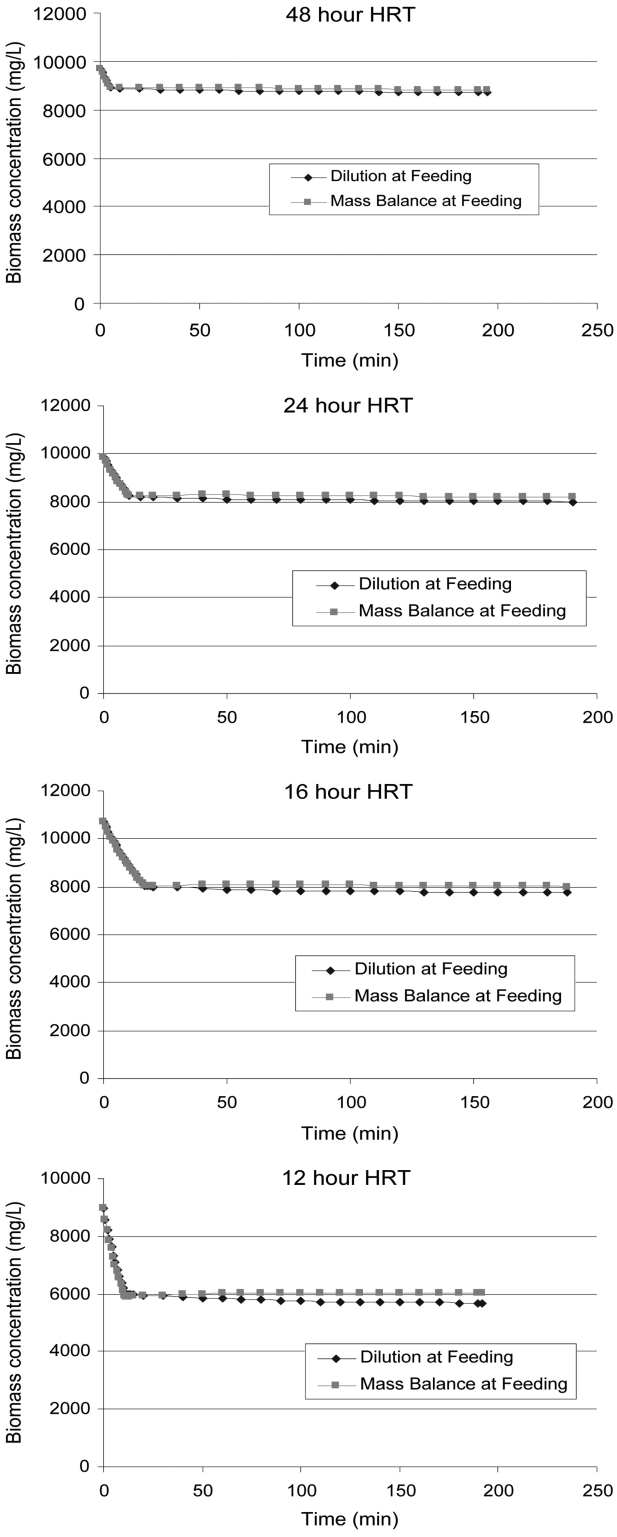

Fig. 9. Microbial concentration profile during feeding and reaction time at various HRTs and at raw substrate concentration of 800 mg/L.

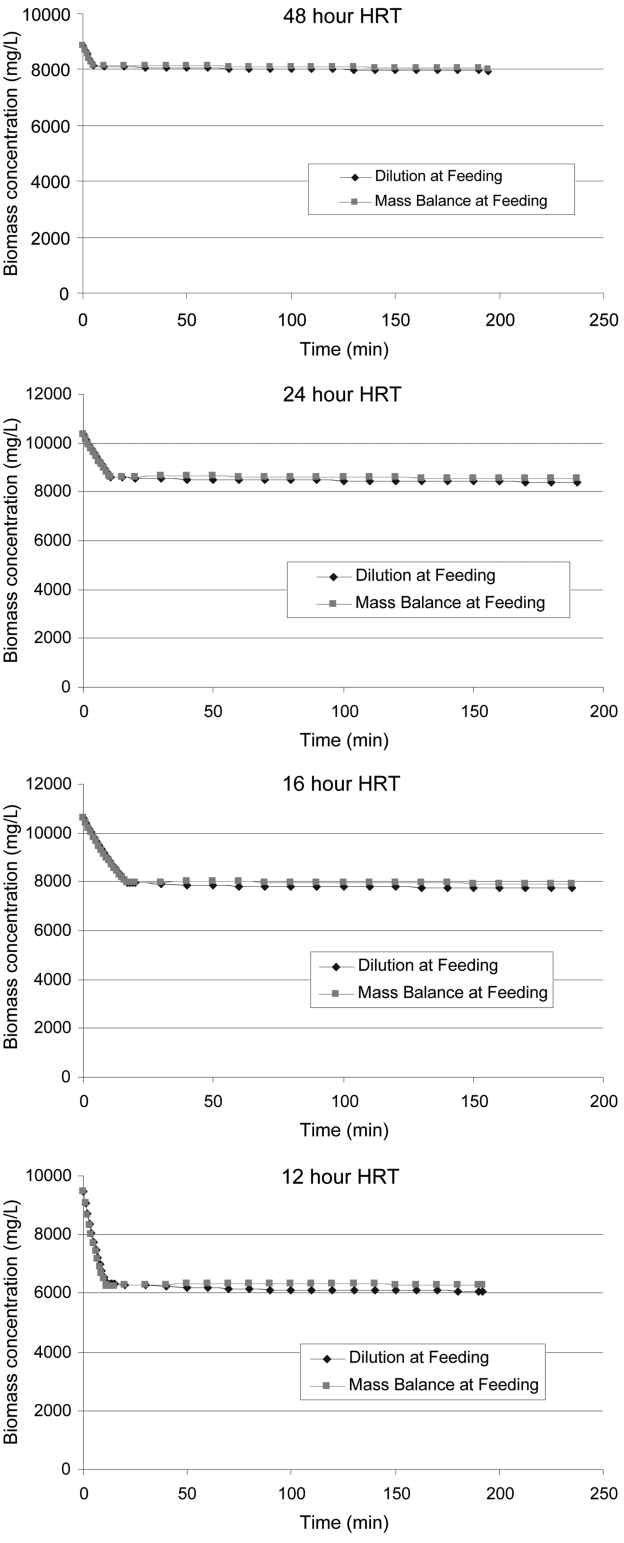

Fig. 10. Microbial concentration profile during feeding and reaction time at various HRTs and at raw substrate concentration of 600 mg/L.

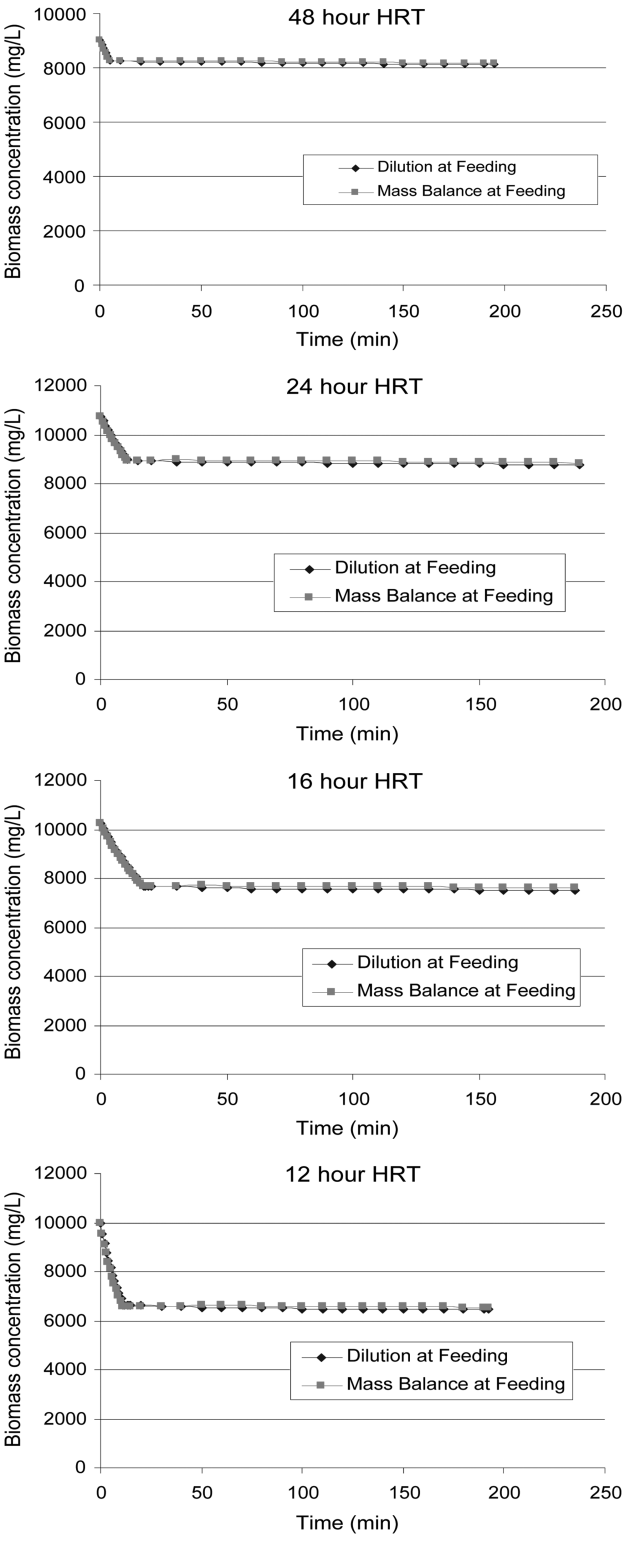

Fig. 11. Microbial concentration profile during feeding and reaction time at various HRTs and at raw substrate concentration of 400 mg/L.

The results also point to the need to achieve high microbial content in the partially emptied batch reactor system during seeding (system startup) to optimize the process performance, because little microbial growth is expected, especially at low substrate concentrations. In addition, the model points to the need to operate the partially emptied batch reactor system at shorter reaction time when treating low concentrated substrates and when operating the system at long HRTs to eliminate or reduce microbial death owing to lack of substrate that may result from unnecessary long reaction time. Such an operation will result in more treatment cycles per day.

Acknowledgment

We wish to express our sincere gratitude to Jin C. Zhao and Marta Larroya Seguan, graduate students in the Department of Civil and Environmental Engineering at San Jose State University, for generating the simulation data and figures.

Nomenclature

K_d = endogenous decay rate (1/time)
K_s = half-saturation constant (mg/L)
Q = influent flow rate (volume/time)
r_d = microbial death rate (mg/[L·time])
r_g = microbial growth rate (mg/[L·time])
r_s = substrate decay rate (mg/[L·time])
r_x = net microbial growth rate ($r_g - r_d$) (mg/[L·time])
S = substrate concentration (mg/L)
S_D = effluent (decanted) substrate concentration (mg/L)
S_{EF} = substrate concentration in reactor at end of feed step (mg/L)
S_F = substrate concentration in reactor during feed step (mg/L)
S_o = influent substrate concentration (mg/L)
V = volume of fluid in reactor at any time during feeding ($V_o + V_t$) (L)
V_D = volume decanted per sequence (L)
V_F = volume of feed per sequence (L)
V_o = volume of fluid remaining after decant step ($V_R - V_D$) (L)
V_R = total reactor fluid volume (L)
V_t = volume of substrate feed at time t during feed step (Q_t) (L)
X = microbial concentration (mg/L)
X_D = microbial concentration at end of decant step (mg/L)
X_{EF} = microbial concentration at end of feed step (mg/L)
X_F = microbial concentration during feed step (mg/L)
X_o = microbial concentration in substrate (mg/L)
X_R = microbial concentration during react step (mg/L)
Y = microbial yield coefficient
ΔS = change in substrate concentration (mg/L)
Δt = change in time (mg/L)
ΔX = change in microbial concentration (mg/L)
$\hat{\mu}$ = maximum specific growth rate (1/s)
$\hat{\mu}/Y$ = maximum specific substrate utilization rate (1/s)

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