

Optimization of An Unstructured First-Order Kinetics Model of Cyclically Operated Bioreactors

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Abstract

A procedure for the optimization of an unstructured first-order kinetics model of cyclically operated biological reactors for the biodegradation of a single pollutant is developed using a combination of analytical and numerical tools. Asymptotic analytical profiles for the substrate and biomass for each steady cycle are obtained that allows the formulation of an analytical design equation that relates the concentration of the pollutant at the end of a steady cycle to all the operating parameters of the bioreactor such as space-time, pollutant feed concentration, filling time and ratio of minimum to maximum reactor volume. This analytical design equation is used for the systematic construction of practical bifurcation diagrams showing the variations of the pollutant concentration at the end of a cycle with the bioreactor operating parameters. The design equation also allows the formulation of a variety of optimization problems such as the maximization of volumetric efficiency as well as the minimization of the end-of-cycle pollutant concentration. In all cases it is shown that optimal parameter values sets exist. Implications of these results for the optimization of waste-treatment facilities are discussed.

Subject Headings: biological treatment; bifurcations; dynamic models; optimization.

Introduction

The use of sequencing batch reactors (SBRs) in the treatment of liquid wastes is an established technology. Since its development by Irvine and co-workers (Dennis and Irvine, 1979; Irvine and Busch, 1979; Chiesa and Irvine, 1985), the SBR technology has been used successfully with activated sludge systems. The SBR is perfectly suited for small wastewater flows (< 10 MGD) while it performs satisfactorily even in large applications (Irvine *et al.*, 1987). In an SBR configuration, the wastewater is fed continuously for a determined period of time. It goes through a sequence of treatment processes in the same basin and is drawn out periodically. The operation of an SBR proceeds in cycles. Each cycle consists usually of five distinct periods: a filling phase during which the bioreactor is fed with untreated waste, a batch phase also known as the react-phase, a settle phase which involves settling of biomass, a drawn-down phase during which parts of the reactor contents are drawn down, and finally an idle phase. The SBR has been shown to have a number of advantages over continuously operated activated sludge systems. One primary advantage is the possibility of cycling between anoxic and aerobic periods of operation, achieving in this way organic matter, nitrogen and phosphorus removal (Wilderer *et al.*, 2001). Other advantages include quiescent or carefully controlled mixing during settling, no need for separate clarifier and the ability to discharge treated wastewater only after effluent limitations have been met (Wilderer *et al.*, 2001). Moreover, it has been shown (Baltzis *et al.*, 1989) that even if settling of solids is not considered, cyclically operated bioreactors, under most operating conditions, achieve the same level of treatment in a much smaller volume than equivalent continuous stirred tank reactors (CSTRs), providing SBRs with superior volumet-

ric efficiency.

Although the use of SBRs is a well established technology, it is expected that the continuous understanding of the dynamics of the bioreactor can lead to better operation policies and improved efficiencies. It is also true that stringent environmental regulations have increased the need for the optimization of the operation of existing treatment units, since building new facilities may require substantial capital expenditures.

The optimization of cyclically operated reactors such as SBR units is a subject that has and is still being studied in the literature. One of the early works in the subject was carried out by Lund and Seagrave (1971) for a variable volume CSTR with the simple case of first order irreversible reaction. The authors showed that this mode of operation generally results in higher efficiencies when compared to equivalent constant-volume CSTRs, under both isothermal and adiabatic conditions. As for SBR units, a variety of approaches were used in the literature for the optimization task. The most common strategy consists in making use of calibrated mathematical models of varying complexity that faithfully represent reaction kinetics, reactor dynamics and operational constraints of the process. Demuynck *et al.* (1994), for instance, studied the optimization of a SBR for nitrogen removal. The authors used, for this purpose, the Nitrification Denitrification Biological Excess Phosphorus Removal (NDBEPR) model of Wentzel *et al.*(1992) to optimize SBR time scheduling. The authors concluded that a sequence of short aerobic/anoxic phases perform better than the usual sequence of one aerobic phase followed by one anoxic phase. Coelho *et al.* (2000), on the other hand, carried out an optimization of a SBR for the nitrification process. The authors used a variation of the well-known activated sludge No.1 model (ASM1) (Henze *et al.*, 1987)

to optimize the total batch time using the feed rate profiles, the filling time, and the aerobic reaction time as decision variables. The authors showed that the choice of non conventional fill strategies such as symmetric pulses can lead to an increase in the productivity of the unit. Using the same model, Hvala *et al.*(2001) studied the optimization of an SBR using a split-feed operating mode with input load partitioned into two parts and with two successions of aerobic-anoxic phases. The decision variables were the duration of batch phases and the time of the second input addition. The authors compared the results of the model with that of a pilot plant and found overall satisfactory agreements. Artan *et al.*(2002) studied the optimization of SBR for simultaneous nitrogen and phosphorus removal using the activated sludge model (ASM2d) (Henze *et al.*, 1995). The authors carried out a substantial evaluation of the major process configurations with different aerobic, anoxic, anaerobic sequences, and filling conditions. Recently, Sin *et al.*(2004) presented a systematic approach to determine the optimal operation strategy for nitrogen and phosphorus removal of SBRs using a calibrated ASM2dN model (Insel *et al.*, 2003). The methodology developed was based on using a grid of possible scenarios to simulate the effect of the key degrees of freedom in the SBR system.

While the majority of these cited examples have shown the merit of the model-based approach for the optimization of SBRs, nevertheless this approach suffers from some drawbacks that are associated with the nature of the models used. The models are generally characterized with a high level of parameterization (Carstensen *et al.*, 1995) and the difficulty to estimate the parameters (Ayesa *et al.*, 1995), especially for applications where sufficient data is not available for calibration and where process conditions are time varying. These drawbacks have led to an other approach for the optimization of SBRs. This method is

based on on-line modeling (Vanrolleghem and Coen, 1995) and on-line parameter estimation (Marsili-Libelli and Giovannini, 1997) leading to adaptive optimization as was carried out by Katsogiannis *et al.*(1999) for a nitrifying process. However the use of such black-box models, that are entirely based on input-output data, necessarily overlooks the effect of the physical, biological or chemical process knowledge in the model structure.

Besides the model-based approach and the (black-box) input-output models, other approaches were also used for the optimization of SBRs. These include methods such as multivariate statistical methods (MVS), artificial neural network (ANN) and the use of hybrid models (Ger-naey *et al.*, 2004). Simple unstructured models were also used for the optimization task. This later approach, which is adopted in this paper, was applied extensively by Baltzis and co-workers for a variety of applications. The authors developed lumped models for SBRs based on mass balances of the total liquid, the different substrates and the biomass. The resulting models consist of systems of few ordinary differential equations that may lend themselves to easy mathematical manipulations. Using this approach, Dikshitulu *et al.*(1993), for instance, developed an unstructured model for a SBR to investigate a single pollutant removal by two competing cultures, and showed the effects of the SBR operating conditions on the coexistence of pure and simple competitors. Lenas *et al.*(1994), on the other hand, used a simple unstructured model to perform optimization studies for phenol biodegradation using *Pseudomonas putida* culture. The authors carried out appropriate experimental validation, studied the multiplicity behavior that characterized the operation of the bioreactor and optimized the bioreactor volumetric efficiency. A similar unstructured model and similar techniques were used by Baltzis *et al.* (1996) to

carry out optimization studies of an SBR for the biodegradation of mixed (dissimilar) wastes. The results of these studies clearly pointed out to the existence of optimal parameter value sets. However, there is still room for further understanding of the optimization problem of SBRs, which is the subject of this study.

This paper focuses on the simple case of the biodegradation of a single pollutant in a cyclically operated bioreactor. Using an unstructured kinetic model similar to the one used by previous authors (Lenas *et al.*, 1994), the objective of the paper is to provide a better insight into the optimization problem. Unlike the previous studies, in which only numerical tools were used, the objective of this study is to derive analytical conditions that can guide better the optimization task. The procedure consists in deriving the explicit analytical profiles for substrate and biomass concentrations for each steady cycle of operation, assuming first order kinetics for the biodegradation. These profiles are combined to derive an analytical equation that involves all the operating parameters of the bioreactor. The resulting relation which we call the "design equation" is used to construct practical bifurcation diagrams showing the variations of the concentration of the pollutant at the end of cycle with any of the operating parameters of the bioreactor. The design equation is subsequently used to formulate and readily solve a variety of optimization problems, including the maximization of bioreactor productivity and the minimization of end-of-cycle pollutant concentration.

Process Model

The operation of a classical SBR, described schematically in Fig.1, consists in alternating the reactor volume between a minimum and a maximum values by adjusting the input and output flow rates. A fraction of the reactor contents is periodically harvested and replenished with fresh medium through generally stepwise changes in the flow rates. As was mentioned in the introduction, the operation of SBRs generally goes through five phases described as fill, react, settle, drawn-down and idle/waste sludge. Reactions in SBRs occurs during the first two phases, and in classical SBR technology the extent of the remaining three phases is large which, in actuality, make SBRs discontinuous systems where each cycle is almost independent of the others. Some experimental studies (Dikshitulu *et al.*, 1993; Baltzis *et al.*, 1996) have, however, demonstrated that SBRs can be further optimized when they operate continuously following a repeated pattern. The results of these studies have shown substantial advantages of this mode of operation when proper operating conditions are selected. In this paper we consider a special case of SBR where there are no settle and idle phases and where the reaction occurs through out the cycle. The operation of the unit studied in this paper, is assumed to occur through the steps of Fig.2 that shows schematic variations of the reactor volume with time. Initially i.e. at time $t = t_0$ the bioreactor contains an amount of liquid waste of volume $V = V_0$. From $t = t_0$ to $t = t_1$ (phase I), the reactor is fed with the untreated waste while there is no stream exiting the reactor. Consequently the volume of the suspension increases with time. When the reactor volume reaches its maximum value of $V = V_m$, the filling stops. Between times t_1 and t_2 the bioreactor operates in a batch mode with a constant volumetric hold up equal to V_m . The period of time from t_1 to t_2 is the second phase (phase II) of the cycle. Following

this phase, parts of the reactor contents are drawn-down, while there is no feed flow rate. During this phase the volume of the reactor contents decrease with time. At the end of this phase (III) ($t = t_3$), the reactor volume returns to its initial value of V_0 . At this instant the reactor outlet phase is shut off, the inlet is opened and the cycle starts repeating itself. Assuming that the density of the suspension in the reactor to be constant at all times and equal to that of the medium fed to the vessel, the assumption of constant flow rates imply linear changes in the volume of the reactor contents during phases I and III of the cycle. The following expressions for the flow rates and volumes can be therefore written for the three phases of the cycle:

$$\text{Phase I : } t_0 \leq t \leq t_1, Q_f = Q_{fI}, Q_e = 0, V = V_0 + Q_f(t - t_0) \quad (1)$$

$$\text{Phase II : } t_1 < t \leq t_2, Q_f = 0, Q_e = 0, V = V_m \quad (2)$$

$$\text{Phase III : } t_2 < t \leq t_3, Q_f = 0, Q_e = Q_{eIII}, V = V_m - Q_{eIII}(t - t_2) \quad (3)$$

where Q_f and Q_e are respectively the reactor inlet and outlet flowrates. Q_{fI} is the value of Q_f during the phase I and Q_{eIII} is the value of Q_e during the phase III of the cycle.

Having described the volumetric variations of the reactor contents we turn the attention to the derivation of the mathematical model of the unit. A number of simplifying assumptions are made for the derivation of the unstructured kinetic model. We first assume that the untreated waste stream contains a single pollutant and the biomass used consists of either a pure culture or a functional population for which the relative composition of species is constant. The maintenance requirements for the biomass are assumed to be negligible and the growth of the culture is assumed to be rate-limited only by the availability of the pollutant. The reaction, on the other hand, is assumed to take place during all the

three phases of the cycle, and the same first order kinetics are used to describe the biodegradation during the cycle. This assumption implies that the nature of the biodegradation is the same in the three phases of the unit. This may not be true in all actual cases of SBR applications. However and on line with the experimental works of Dikshitulu *et al.*(1993), Lenas *et al.*(1994) and Baltzis *et al.*(1996), this assumption simplifies to a great deal the resulting mathematical model.

By writing the mass balances for liquid volume, substrate and biomass, the following ordinary differential equations are obtained for the reactor, assuming that the biomass is not externally fed, (Lenas *et al.*, 1994)

$$dV/dt = Q_f - Q_e \quad (4)$$

$$dX/dt = (\mu(S) - Q_f/V)X \quad (5)$$

$$dS/dt = (Q_f/V)(S_f - S) - (X/Y)\mu(S) \quad (6)$$

S is the pollutant concentration, S_f the pollutant feed concentration, X the biomass concentration, $\mu(S)$ the specific growth rate, and Y is the yield coefficient (assumed constant). The system equations are rendered dimensionless using the following variables

$$\bar{V} = V/V_m, \quad \bar{t} = tQ_{fI}/V_m, \quad \bar{Q}_f = Q_f/Q_{fI}, \quad \bar{Q}_e = Q_e/Q_{fI} \quad (7)$$

$$\bar{X} = X/(YS_{ref}), \quad \bar{D} = Q_{fI}/(\mu_{ref}V_m), \quad \bar{S} = S/S_{ref}, \quad \bar{S}_f = S_f/S_{ref} \quad (8)$$

\bar{D} is a dimensionless measure of the inverse of space time, \bar{Q}_f and \bar{Q}_e are respectively the reactor dimensionless inlet and outlet flow rates. They can be defined, for each phase, in a similar way to Eqs.(1-3).

S_{ref} and μ_{ref} are, on the other hand, reference quantities, respectively for the substrate S and the growth rate $\mu(S)$. Both S_{ref} and μ_{ref} are related to the kinetic constants, explicit in the selected expression for $\mu(S)$. Examples of these quantities are provided in a later section. The model in dimensionless form is given by

$$d\bar{V}/d\bar{t} = \bar{Q}_f - \bar{Q}_e \quad (9)$$

$$d\bar{X}/d\bar{t} = (\bar{\mu}(\bar{S})/\bar{D} - \bar{Q}_f/\bar{V})\bar{X} \quad (10)$$

$$d\bar{S}/d\bar{t} = (\bar{S}_f - \bar{S})\bar{Q}_i/\bar{V} - \bar{\mu}(\bar{S})\bar{X}/\bar{D} \quad (11)$$

Following the reasoning used by the authors (Lenas *et al.*, 1996; Baltzis *et al.*, 1996), it can be shown that the three dimensional model (Eqs. 9-11) is equivalent to the following system of two equations,

$$d\bar{X}/d\bar{t} = (\bar{\mu}(\bar{S})/\bar{D} - R/(w + \bar{t}))\bar{X} \quad (12)$$

$$d\bar{S}/d\bar{t} = R(\bar{S}_f - \bar{S})/(w + \bar{t}) - \bar{\mu}(\bar{S})\bar{X}/\bar{D} \quad (13)$$

where $w = V_0/V_m$ is the ratio of minimum to maximum volume of reactor contents. The constant R , on the other hand, takes the value of unity for the first phase of cycle i.e. $0 \leq \bar{t} \leq 1 - w$ and zero for the subsequent two phases i.e. $1 - w \leq \bar{t} \leq (1 - w)/f_1$ where f_1 is the fraction of the cycle allocated to filling the reactor.

For the rest of the paper the bioreactor model described by Eqs.(12-13) is analyzed.

Results and Discussion

In the first step, the long term behavior of the reactor is determined. Adding the two equations (Eqs.12-13) yields,

$$d(\bar{X} + \bar{S})/d\bar{t} = R(\bar{S}_f - (\bar{S} + \bar{X}))/(w + \bar{t}) \quad (14)$$

The integration of this equations results in

$$\bar{X}(t) + \bar{S}(t) - \bar{S}_f = C/(w + \bar{t})^R \quad (15)$$

with C being a constant. As has been discussed by Dikshitulu *et al.*(1993), it follows from Eq.15 that after transients decay (\bar{t} large), and the system reaches a pseudo steady state (i.e. the volume and concentration profiles repeat identically), the following relation holds

$$\bar{X}(t) + \bar{S}(t) = \bar{S}_f \quad (16)$$

Substituting this equation in Eq. 13 yields the following differential equation describing the steady cyclic behavior of the reactor,

$$d\bar{S}/d\bar{t} = R(\bar{S}_f - \bar{S})/(w + \bar{t}) - \bar{\mu}(\bar{S})(\bar{S}_f - \bar{S})/\bar{D} \quad (17)$$

The biomass concentration profile is given, on the other hand, by Eq.16. The expression for the dimensionless growth rate $\bar{\mu}$ can take on a number of forms. For instance, for Monod kinetics the expression of μ is

$$\mu = \mu_{max}S/(K_S + S) \quad (18)$$

Choosing $S_{ref} = K_S$ and $\mu_{ref} = \mu_{max}$ as reference quantities, to define

the dimensionless variables (Eqs.7-8), the dimensionless growth rate becomes

$$\bar{\mu} = \bar{S}/(1 + \bar{S}) \quad (19)$$

Substituting in the model equation (Eq.17) and expanding yields

$$(1 + \bar{S})d\bar{S}/d\bar{t} = R(\bar{S}_f - \bar{S})(1 + \bar{S})/(w + \bar{t}) - \bar{S}(\bar{S}_f - \bar{S})/\bar{D} \quad (20)$$

This first order differential equation is known in the literature as Abel equation of type 1 (Kamke, 1977). Unfortunately it does not have an analytical solution, except under some specific conditions which can be shown not to be satisfied for this equation. The same observation holds if a substrate inhibited expression is chosen for $\bar{\mu}$,

$$\bar{\mu}(\bar{S}) = \bar{S}/(1 + \bar{S} + \gamma\bar{S}^2) \quad (21)$$

In an attempt to derive analytical profiles for substrate \bar{S} and biomass \bar{X} concentrations, we will solve the differential equation for relatively small values of \bar{S} i.e. values of \bar{S} for which the growth rate μ is almost linear in S i.e. $\bar{\mu}(\bar{S}) \simeq \bar{S}$. In this case the differential equation (Eq. 17) becomes for the first phase of the cycle i.e. $R=1$,

$$d\bar{S}/d\bar{t} = (\bar{S}_f - \bar{S})/(w + \bar{t}) - \bar{S}(\bar{S}_f - \bar{S})/\bar{D} \quad (22)$$

This is a Riccati type equation (Kamke, 1977) that can be solved explicitly. Introducing the following change of variables, $\bar{Z} = 1/(\bar{S} - \bar{S}_f)$, yields the following solution

$$\bar{Z}(\bar{t}) = (w + \bar{t})\exp(-\bar{S}_f\bar{t}/\bar{D})(C_1 - Ei(\bar{t})\exp(-\bar{S}_fw/\bar{D})/\bar{D}) \quad (23)$$

Where

$$Ei(\bar{t}) = \int_{\bar{S}_f w / \bar{D}}^{\bar{S}_f (w + \bar{t}) / \bar{D}} e^{\xi} / \xi d\xi \quad (24)$$

and C_1 is a constant. The profiles for substrate \bar{S} and biomass \bar{X} are given therefore by

$$\bar{S}(t) = \bar{S}_f + 1/\bar{Z}(t) \quad (25)$$

while

$$\bar{X}(t) = \bar{S}_f - \bar{S}(t) \quad (26)$$

The constant C_1 in Eq. 23 is determined from the condition

$$\bar{S}(\bar{t} = 0) = \bar{S}_r \quad (27)$$

where \bar{S}_r is the residual substrate concentration i.e. the value that the substrate concentration reaches at the end of a steady cycle. Substituting Eq. 27 into Eq.23 yields,

$$C_1 = 1/(w(\bar{S}_r - \bar{S}_f)) \quad (28)$$

For the two remaining phases of the cycle, i.e. $R = 0$, the differential equation (Eq. 17) becomes,

$$d\bar{S}/d\bar{t} = -\bar{S}(\bar{S}_f - \bar{S})/\bar{D} \quad (29)$$

Introducing again the variable $\bar{Z} = 1/(\bar{S} - \bar{S}_f)$, the integration of Eq.

(29) yields,

$$\bar{Z}(t) = -1/\bar{S}_f + C_2 \exp(-\bar{S}_f \bar{t}/\bar{D}) \quad (30)$$

where C_2 is a constant that is determined by matching both solutions (Eq.23 and Eq.30) at $\bar{t} = 1 - w$ i.e. the end of the first phase and the start of the two other phases of the cycle. This yields

$$C_2 = -\exp(-\bar{S}_f w/\bar{D}) Ei(1 - w)/\bar{D} + 1/(w(\bar{S}_r - \bar{S}_f)) + \exp(\bar{S}_f(1 - w)/\bar{D})/\bar{S}_f \quad (31)$$

with

$$Ei(1 - w) = \int_{\bar{S}_f w/\bar{D}}^{\bar{S}_f/\bar{D}} e^\xi/\xi d\xi \quad (32)$$

At the end of the cycle i.e. $\bar{t} = (1 - w)/f_1$, the substrate concentration \bar{S} must satisfy the condition $\bar{S} = \bar{S}_r$ i.e. $\bar{Z} = 1/(\bar{S}_r - \bar{S}_f)$, to ensure a cyclic operation. Substituting this condition in Eq.30, and rearranging yields the following equation

$$\begin{aligned} \int_{\bar{S}_f w/\bar{D}}^{\bar{S}_f/\bar{D}} e^\xi/\xi d\xi &= -\exp(\bar{S}_f(w + (1 - w)/f_1)/\bar{D})\bar{S}_r\bar{D}/(\bar{S}_f(\bar{S}_r - \bar{S}_f)) \\ &+ (\bar{D}/\bar{S}_f)\exp(\bar{S}_f/\bar{D}) + (\bar{D}/w(\bar{S}_r - \bar{S}_f))\exp(\bar{S}_f w/\bar{D}) \end{aligned} \quad (33)$$

This equation involves all the parameters $\bar{S}_f, \bar{D}, w, f_1, \bar{S}_r$ of the model. This condition should always be satisfied to ensure the cyclic operation of the bioreactor. We will show how this "design" equation can be the starting point for a variety of analysis and results.

Pollutant concentration at the end of cycle

We first start with the study of the bifurcation behavior of the model. The design equation (Eq. 33) can be solved for \bar{S}_r to yield,

$$\bar{S}_r = \bar{S}_f + \frac{1 - \frac{\exp(-\frac{\bar{S}_f(1-w)}{Df_1})}{w}}{-\frac{1}{\bar{S}_f} - \frac{\exp(-\frac{\bar{S}_f(w+\frac{1-w}{f_1})}{D})Ei(1-w)}{D} + \frac{\exp(-\frac{\bar{S}_f(1-w)(1-\frac{1}{f_1})}{D})}{S_f}} \quad (34)$$

This equation allows the construction of bifurcation diagrams showing the variations of \bar{S}_r with any of the operating parameters (\bar{D} , w , f_1 , \bar{S}_f). To construct the bifurcation diagram, the integral term $Ei(1-w)$ (Eq. 32) can be evaluated using any standard integration rule such as Simpson rule (Press *et al.*, 1989). Figure 3 shows the variations of \bar{S}_r with the inverse of space-time \bar{D} , for $\bar{S}_f = 0.5$, $f_1 = 0.25$ and $w = 0.5$. The figure shows a monotonic increase in \bar{S}_r up to the wash-out line i.e. $\bar{S} = \bar{S}_f$ and $\bar{X} = 0$. A safe operation of the bioreactor is possible for values of \bar{D} , smaller than the one corresponding to wash-out conditions. The washout state occurs in SBRs when the conditions are such that the amount of biomass lost during the drawdown phase is not compensated for during the first two phases of the cycle. The expression for \bar{D} at the washout state i.e. ($\bar{D}_{washout}$) can be obtained analytically. Setting $\bar{S}_r = \bar{S}_f$ in Eq. 34 yields,

$$w = \exp[-\bar{S}_f(1-w)/(\bar{D}f_1)] \quad (35)$$

Solving for \bar{D} yields the following useful relation for the wash-out condition

$$\bar{D}_{washout} = \bar{S}_f(w-1)/(f_1 \ln(w)) \quad (36)$$

From this equation it can be seen that $\bar{D}_{washout}$ is proportional to \bar{S}_f . Increasing \bar{S}_f would, as expected, increase the domain of safe operation of bioreactor as shown in Fig. 4a. $\bar{D}_{washout}$ is also proportional to $1/f_1$. Increasing the filling time would decrease the safe operation of bioreactor, as shown in Fig.4b. Finally, $\bar{D}_{washout}$ can be seen (Fig. 4c) to increase with increasing values of w , reaching the asymptotic value of $\bar{D}_{washout} = \bar{S}_f/f_1$ as w approaches the value of 1.

The variations of \bar{S}_r with filling time f_1 are shown in Fig.5. It can be seen that the end-of-cycle pollutant concentration increases monotonically with f_1 until the washout line is reached. Figure 6 shows, on the other hand, the portrait as function of \bar{S}_f , for $f_1 = 0.25$, $w = 0.5$ and $\bar{D} = 0.4$. It can be seen that when the rest of parameters are fixed, the end-of cycle pollutant concentration decreases monotonically with \bar{S}_f . Finally, Figure 7 shows the bifurcation diagram as function of w , for $\bar{S}_f = 0.5$, $f_1 = 0.25$ and $\bar{D} = 0.1$. The figure shows a non-monotonic behavior. It can be seen that the end-of-cycle pollutant concentration decreases with w and reaches a minimum value at $w = 0.201$ before increasing towards the wash-out line. The diagram of Fig. 7 suggests the existence of optimum values of some of the operating parameters. The optimization issue is discussed in the following section.

Optimization of Reactor Operation

Having constructed the bifurcation diagrams, the design equation (Eq.33) can be used explicitly for optimization studies of the bioreactor. We formulate the optimization problem in the following way

$$\max(\text{or min})F(\bar{S}_f, w, \bar{D}, f_1, \bar{S}_r) \quad (37)$$

$$\text{subject to (Eq.33)} \quad (38)$$

$$\text{and subject to } \bar{D} < \bar{D}_{washout} \quad (\text{Eq.36}) \quad (39)$$

where F represents a given objective function. The first constraint (Eq. 38) is the design equation while the second constraint (Eq. 39) is added to ensure that the optimum results correspond to the safe operation of the bioreactor. In the following section we provide specific examples of the optimization problem. The first problem to be solved is the maximization of the bioreactor volumetric productivity. The volume supplied to the reactor in each cycle, taking $t_0 = 0$, is $Q_{fI}t_1$. This volume is also equal to what is taken from the reactor i.e. $Q_{eIII}(t_3 - t_2)$. Since the length of each cycle is t_3 then a per unit volumetric productivity can be defined as $P := Q_{fI}t_1/t_3 = Q_{fI}f_1$. In dimensionless form, \bar{P} can be written as

$$\bar{P} := Q_{fI}f_1/(\mu_{ref}V_m) = \bar{D}f_1 \quad (40)$$

Before solving the actual optimization problem we first show an example of the trend expected for the objective function \bar{P} with one of the decision variables i.e. w . For instance, for values of $\bar{S}_f = 0.5$, $f_1 = 0.25$

and $\bar{S}_r = 0.01$, Figure 8 shows the detailed profile of \bar{P} versus w . It can be seen that the profile shows a clear maximum of 0.070 that occurs at $w = 0.148$. This suggests the existence of optimal parameter value sets. Next the optimization problem (Eqs. 37-39) is solved. For each value of filling time f_1 , the optimum productivity \bar{P}_{opt} and the corresponding optimum value of w_{opt} are obtained and are shown respectively in Figs. 9(a-b). The values of \bar{S}_f and \bar{S}_r are taken to be 0.5 and 0.01 respectively. The results of Fig.9 indicate that for each values of f_1 , optimum values of \bar{P} (i.e. of \bar{D}) and w do exist. The trend of Figs.9(a-b) also indicates that the optimum values of productivity \bar{P} and those of w do decrease with the filling time. Therefore when the value of w is chosen, the highest productivity is achieved for short filling times. The effect of substrate feed concentration \bar{S}_f on the optimum productivity are shown in Fig.10. It can be seen that for a given filling time, an increase in \bar{S}_f would shift the optimum productivity to larger values. However the corresponding optimum values of (w) would shift to smaller values. For example, for $f_1 = 0.25$ the optimum values of productivity for $\bar{S}_f = 0.1$ is 0.0203 and occurs at $w = 0.266$. For the same filling time and for $\bar{S}_f = 0.3$, the optimum values of productivity is at the larger value of 0.0465 but occurs at a lower value of $w = 0.172$. The effect, on the other hand, of the end-of-cycle pollutant concentration \bar{S}_r is shown in Figs.11(a-b). As it can be seen from the figures, the end-of-cycle pollutant concentration has important effect on the optimum productivity. An increase in the values of \bar{S}_r pushes the maximum value of productivity to larger values. The optimum values of w also increase with \bar{S}_r . For instance, for $f_1 = 0.5$ and $\bar{S}_r = 0.01$ the optimum value of P and w are respectively 0.063 and 0.10. For the same filing time and a larger value of $\bar{S}_r = 0.03$, the optimum productivity increases to 0.079 while the optimum value of w

increases to 0.163.

The second optimization problem to be solved is the minimization of the end-of-cycle pollutant concentration \bar{S}_r for given values of productivity. We have shown previously in Fig.7 an example of the expected profile of \bar{S}_r with w . It was seen that the profile of \bar{S}_r is characterized by the presence of a clear minimum, suggesting also the existence of optimal parameter value sets. Figures 12(a-b) show the results of the optimization problem. The optimum values of \bar{S}_r and those of w are plotted against the filling time f_1 , for $\bar{S}_f = 0.5$ and for various values of \bar{D} . It can be seen from Fig.12(a-b) that optimum values of \bar{S}_r and w are found for each value of f_1 . Moreover, it can be observed from Fig.12(a-b) that both optimum values of \bar{S}_r and w increase with increasing values of f_1 . However, it can be seen from Fig. 12(a) that for values of f_1 larger than a break point, the optimum values of w correspond to the trivial value of $w = 1$. The effect of \bar{D} on the optimum values of \bar{S}_r are also shown in Fig.12(a-b). It can be seen that for each value of f_1 , increasing \bar{D} (or the productivity), would push to larger values both the optimum values of \bar{S}_r and those of w . For instance, for a productivity of $P = 0.08$ i.e. ($\bar{D} = 0.4, f_1 = 0.2$), the optimum end-of-cycle concentration \bar{S}_r is 0.0178 and occurs at the optimum value of $w = 0.184$. For a larger productivity, $P = 0.12$ i.e. ($\bar{D} = 0.6, f_1 = 0.2$), the optimum \bar{S}_r is 0.078 and occurs at $w = 0.349$.

Finally, it should be noted that the results of the optimization part carried out on this first order kinetics model can be considered as an extension of the work of Lund and Seagrave (1971) for variable volume CSTRs. However, the mentioned study, for the case of isothermal operation, was limited to the optimization of the reactor yield using only the filling time as a decision variable. Our study, on the other hand, has covered both the maximization of reactor productivity as well as

the minimization of end cycle pollutant concentration. Moreover, the decision variables used in this study were not limited to the filling time and included a total of five variables. i.e. $(\bar{S}_f, \bar{S}_r, \bar{D}, f_1, w)$.

Practical Implications

The first order kinetics model for SBRs, studied in this paper, involves a number of simplifying assumptions and may be too idealized to represent the operation of actual cyclically operated treatment units, for which the generally used models are highly structured and the kinetic expressions are quite complex. However, it is also true that the analysis of the many rigorous models available in the literature for SBRs is generally limited to numerical investigation, and their complexity renders any analytical manipulations almost impossible. The contribution of this study is to show how the investigated simple model can provide a useful analytical insight into the effect of key operating parameters/decision variables in SBRs. These include substrate feed concentration, space-time, filling time and ratio of minimum to maximum reactor volume as well as the end-of-cycle pollutant concentration.

For this purpose, the integration of the model equations has enabled the derivation of a useful algebraic equation that describes the cyclic operation of the bioreactor, and that involves all the parameters of the bioreactor. This equation can be used for a rough and qualitative analysis of the bioreactor operation. In this regard, we have shown that this design equation can be used to construct practical diagrams showing the long term variations of the end-of-cycle pollutant concentration with any of the operating parameters. This analysis has shown, for instance, that the the ratio of minimum to maximum reactor volume plays a key role in the performance of the bioreactor, and there

exist values of this ratio for which the end-of-cycle pollutant can be minimized. The design equation was also useful in deriving the conditions that can ensure the safe operation of the SBR by preventing the occurrence of washout conditions. A simple relation was derived that sets the allowable (i.e. safe) variations in space-time (and implicitly in the feed flow rate and maximum volume) as function of substrate feed concentration, ratio of minimum to maximum volume and filling time. This relationship shows that the allowable inverse of space-time is directly proportional to both the substrate feed concentration and to the inverse of filling time, while it varies in a complex but increasing trend with the ratio of minimum to maximum reactor volume.

The design equation was also used to study the optimization of the unit. Two practical optimization problems were solved. The first one dealt with the maximization of productivity of the reactor. It was shown that optimal parameter value sets exist. The obtained trends indicate that when the ratio of minimum to maximum value of reactor volume is selected, then an increase in productivity can be achieved by decreasing the filling times. On the other hand, for a given filling time, increasing the substrate feed concentration would increase the optimal values of productivity but decrease those of ratio of minimum to maximum values of reactor volume. The second optimization problem dealt with the minimization of end-of-cycle pollutant concentration for given productivity. For given values of filling time, optimal values of parameter sets were also shown to exist. Moreover, it was shown that for given filling time, increasing the productivity would increase the optimum values of both the end-of cycle pollutant concentration as well as the ratio of minimum to maximum reactor volume.

The quantitative results of this paper (either the analytical relations or the numerical investigation) may not be directly extrapolated to actual

SBR units. Nevertheless the qualitative behavior found for the effect of various decision variables is consistent with the experimental results of more complex applications, such as microbial competition (Dikshittulu *et al.*,(1993)) and the biodegradation of mixed wastes (Baltzis *et al.*,(1996)) in SBRs. Moreover, the current simple model could be further improved in a number of ways, while hopefully, still be amenable to some kind of analytical manipulations. One such improvement would be to relax the assumption of identical biodegradation kinetics for the different phases of the cycle. In this regard, it is possible to include two separate sets of kinetic equations for the fill phase which is generally anoxic and the react phase which is generally oxic. This however requires further investigations.

Appendix I. References

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Appendix II: Nomenclature

D	inverse of space-time (1/s)
F	objective function (Eq. 37)
f_1	fraction of cycle time devoted to filling reactor
K_S	kinetic constant (kg/m^3) (Eq.18)
P	volumetric efficiency of reactor per unit time (m^3/s)
Q_e	flow rate of exiting treated waste (m^3/s)
Q_{eIII}	value of Q_e during phase III (m^3/s)
Q_f	feed flow rate of untreated waste (m^3/s)
Q_{fI}	value of Q_f during phase I of cycle (m^3/s)
R	scalar equal to 1 for $0 \leq \bar{t} \leq 1 - w$ and equal to 0 for $1 - w \leq \bar{t} \leq (1 - w)/f_1$
S	pollutant concentration (kg/m^3)
S_{ref}	reference value for S (kg/m^3)
t	time (h)
t_0	start time of the cycle (s)
t_1	end time of phase I of cycle (s)
t_2	end time of phase II of cycle (s)
t_3	end time of cycle (s)
V	reactor volume (m^3)
V_m	maximum value of V for $t_1 \leq t \leq t_2$ (m^3)
V_o	minimum value of V at t_0 and t_3 (m^3)
w	ratio of minimum to maximum value of V
X	biomass concentration (kg/m^3)
Y	yield coefficient (kg dry biomass/kg pollutant)
$\bar{Z}(t)$	intermediate variable equal to $1/(\bar{S} - \bar{S}_f)$

Greek Symbols

γ	dimensionless kinetic parameter (Eq.21)
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μ_{ref} reference quantity for $\mu(S)$ (1/s)
 $\mu(S)$ specific growth rate (1/s)
 μ_m maximum specific growth rate (1/s)

Subscripts

f feed
 r end-of-cycle
 $\bar{(\cdot)}$ dimensionless value of (\cdot)

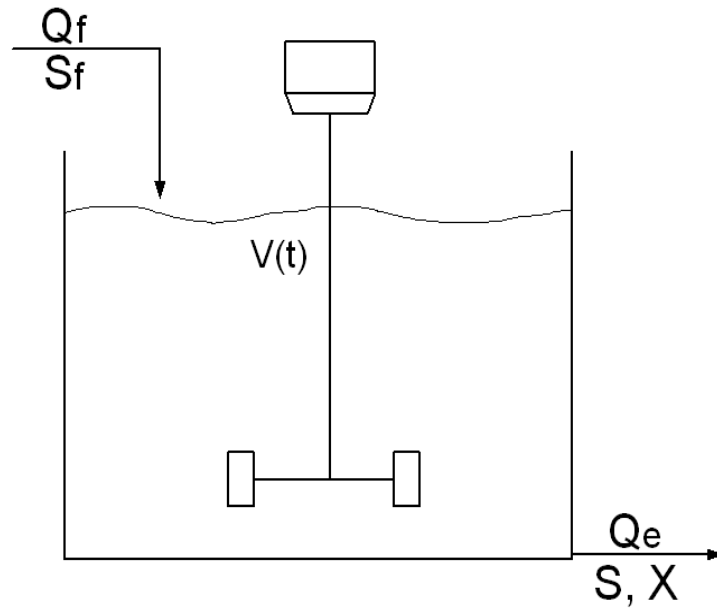


Figure 1. Schematic diagram of the bioreactor with variable volume.

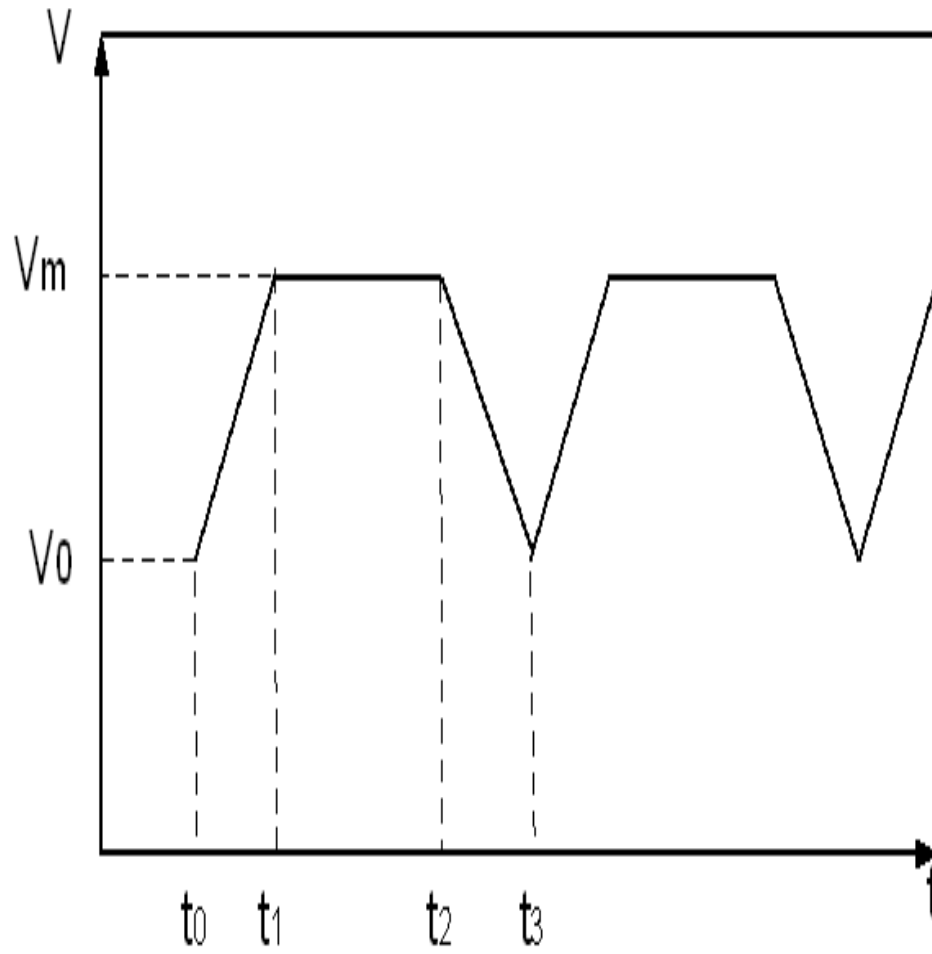


Figure 2. Schematic diagram showing the variation of the reactor contents volume during the operation of the studied SBR.

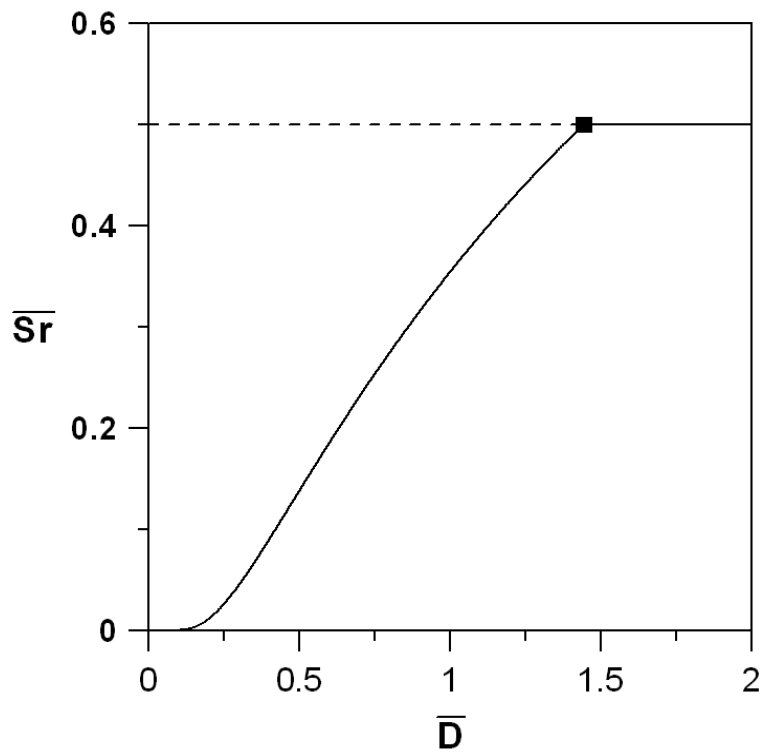


Figure 3. Bifurcation diagram showing the variations of the dimensionless pollutant concentration at the end of cycle with the dimensionless measure of inverse of space-time for $\bar{S}_f = 0.5$, $f_1 = 0.25$, $w = 0.5$. solid - stable branch; dash - unstable; square - bifurcation point.

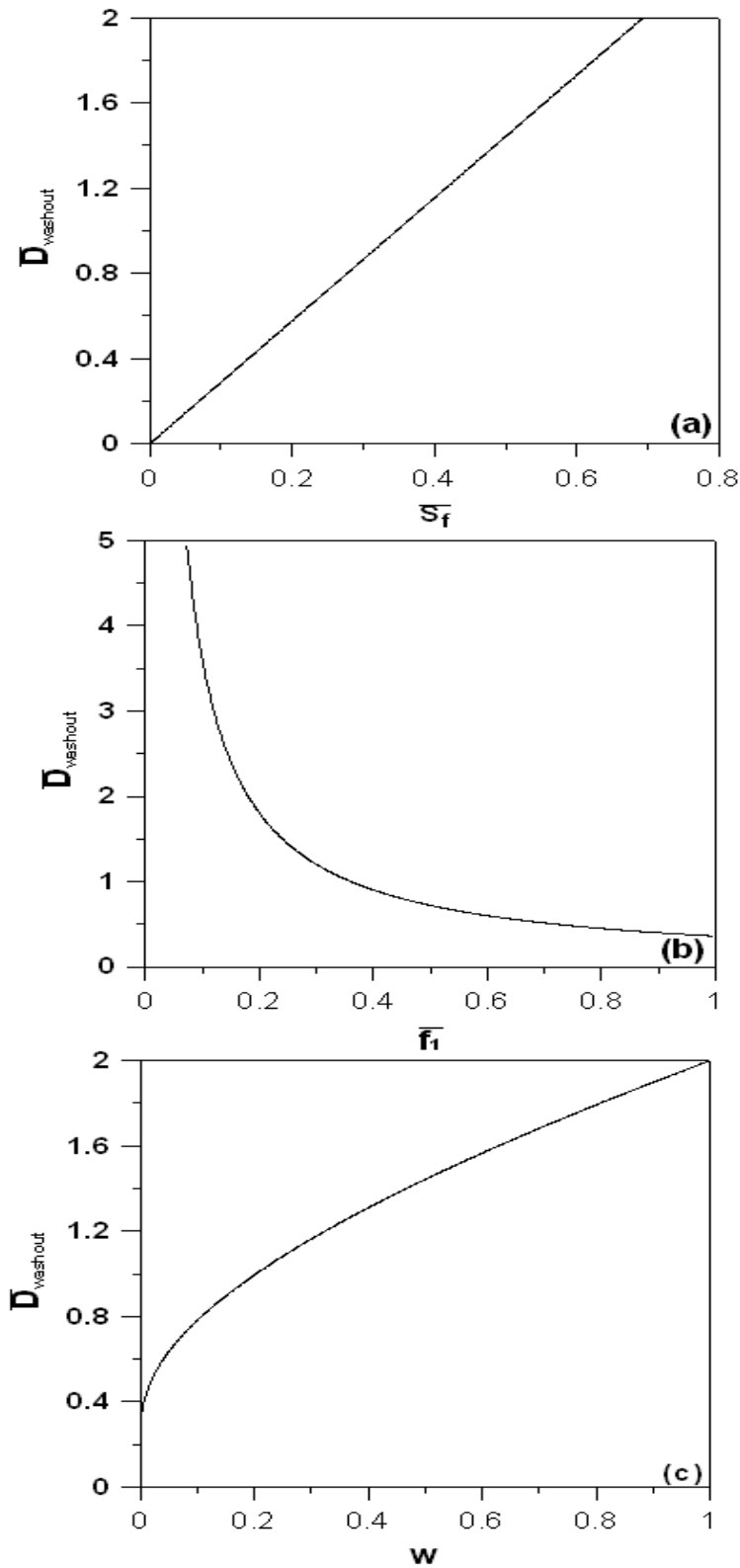


Figure 4. Variations of the $D_{washout}$ with: (a) dimensionless substrate feed concentration for $f_1 = 0.25, w = 0.5$; (b) filling time for $\bar{S}_f = 0.5, w = 0.5$; (c) ratio of minimum to maximum reactor volume for $\bar{S}_f = 0.5, f_1 = 0.25$.

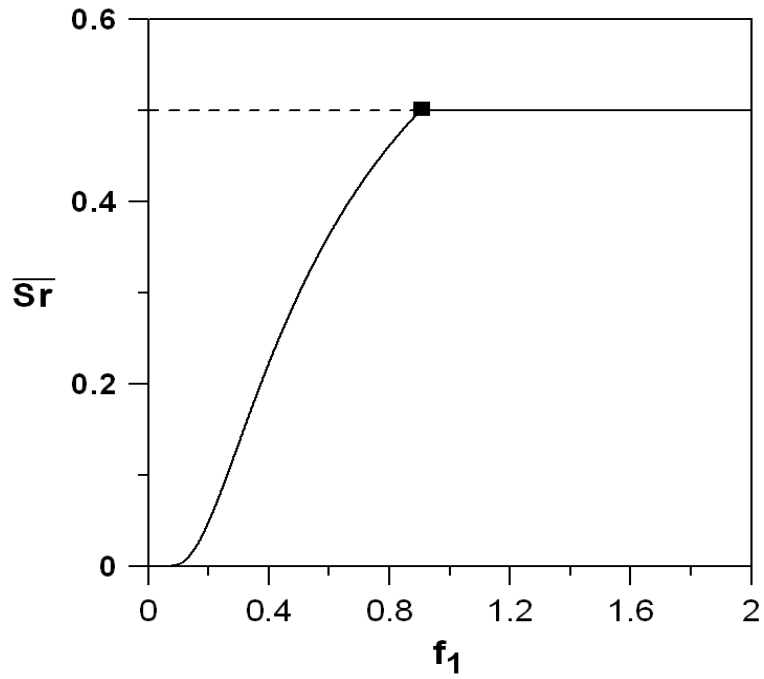


Figure 5. Bifurcation diagram showing the variations of the dimensionless pollutant concentration at the end of cycle with filling time for $\bar{S}_f = 0.5, w = 0.5, \bar{D} = 0.4$. solid - stable branch; dash - unstable; square - bifurcation point.

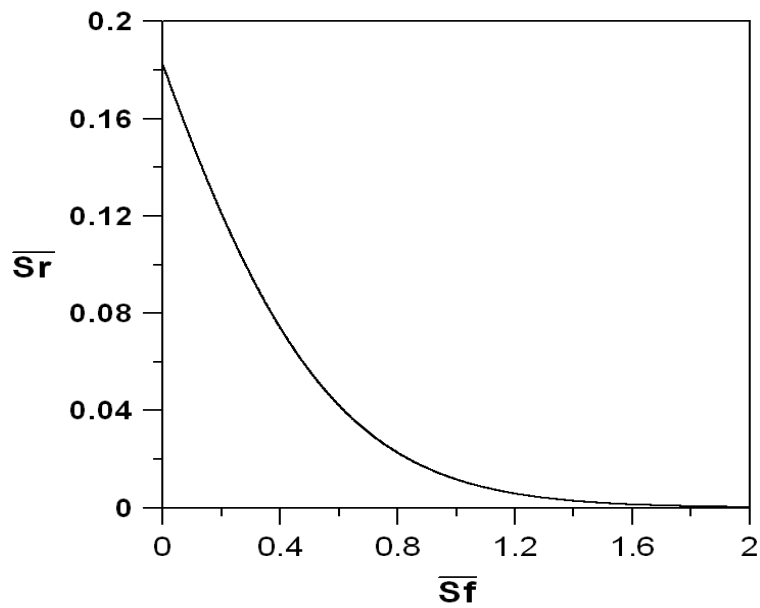


Figure 6. Bifurcation diagram showing the variations of the dimensionless pollutant concentration at the end of cycle with the dimensionless substrate feed concentration for $w = 0.5, f_1 = 0.25, \bar{D} = 0.4$

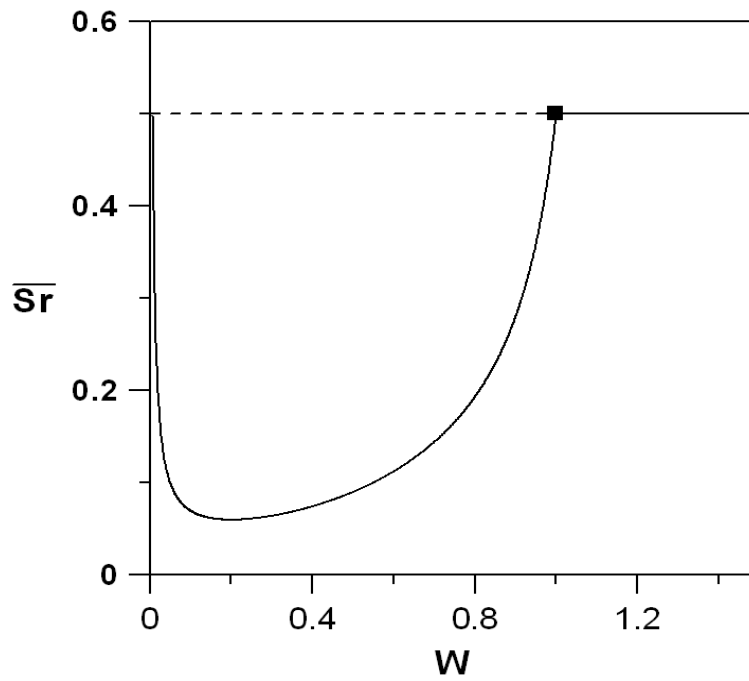


Figure 7. Bifurcation diagram showing the variations of the dimensionless pollutant concentration at the end of cycle with ratio of minimum to maximum reactor volume for $\bar{S}_f = 0.5$, $f_1 = 0.25$, $\bar{D} = 0.1$. solid - stable branch; dash - unstable; square - bifurcation point.

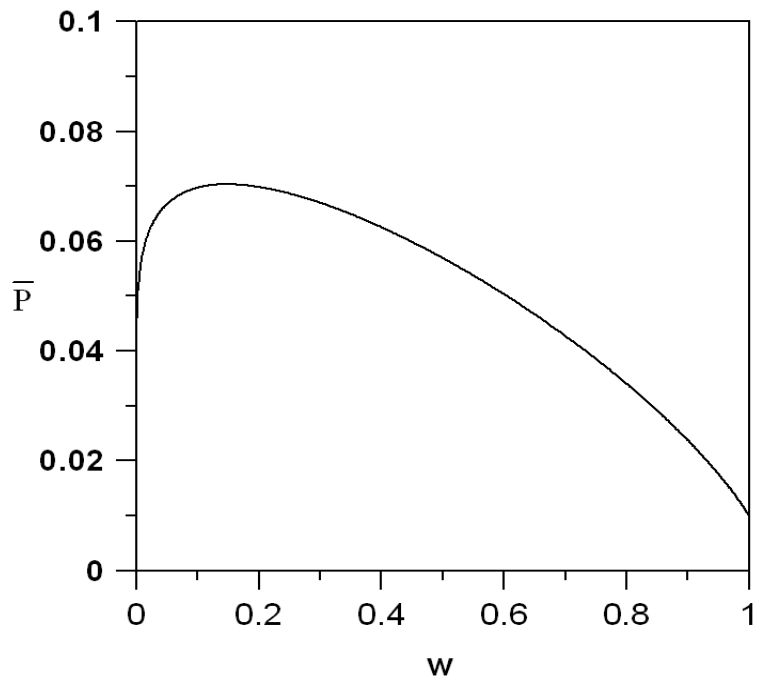


Figure 8. Example of the profile of productivity \bar{P} with w , for $\bar{S}_f = 0.5, \bar{S}_r = 0.01, f_1 = 0.25$.

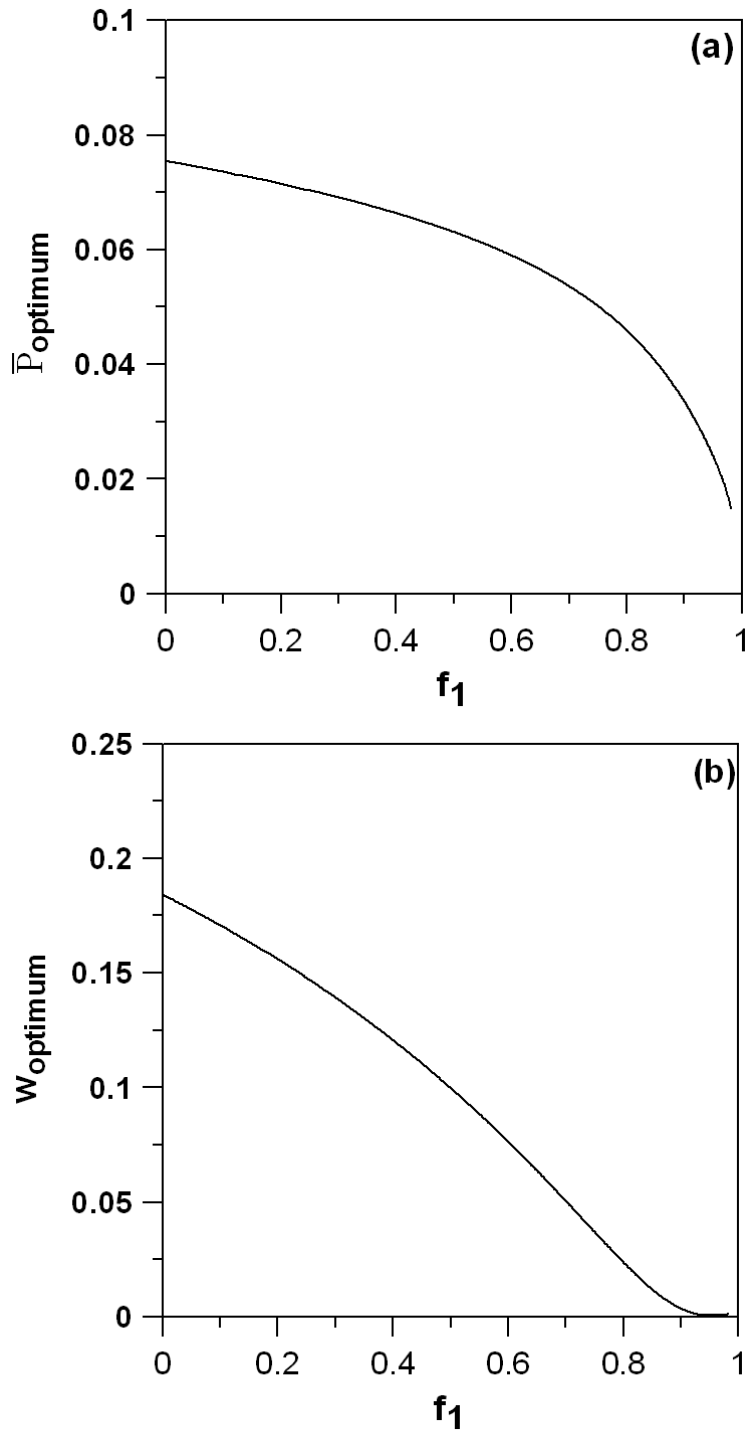


Figure 9. Results of the optimization of the reactor for maximum productivity for $\bar{S}_f = 0.5, \bar{S}_r = 0.01$. (a) Variations of optimum values of dimensionless productivity with filling time; (b) Corresponding variations of optimum values of w with filling time.

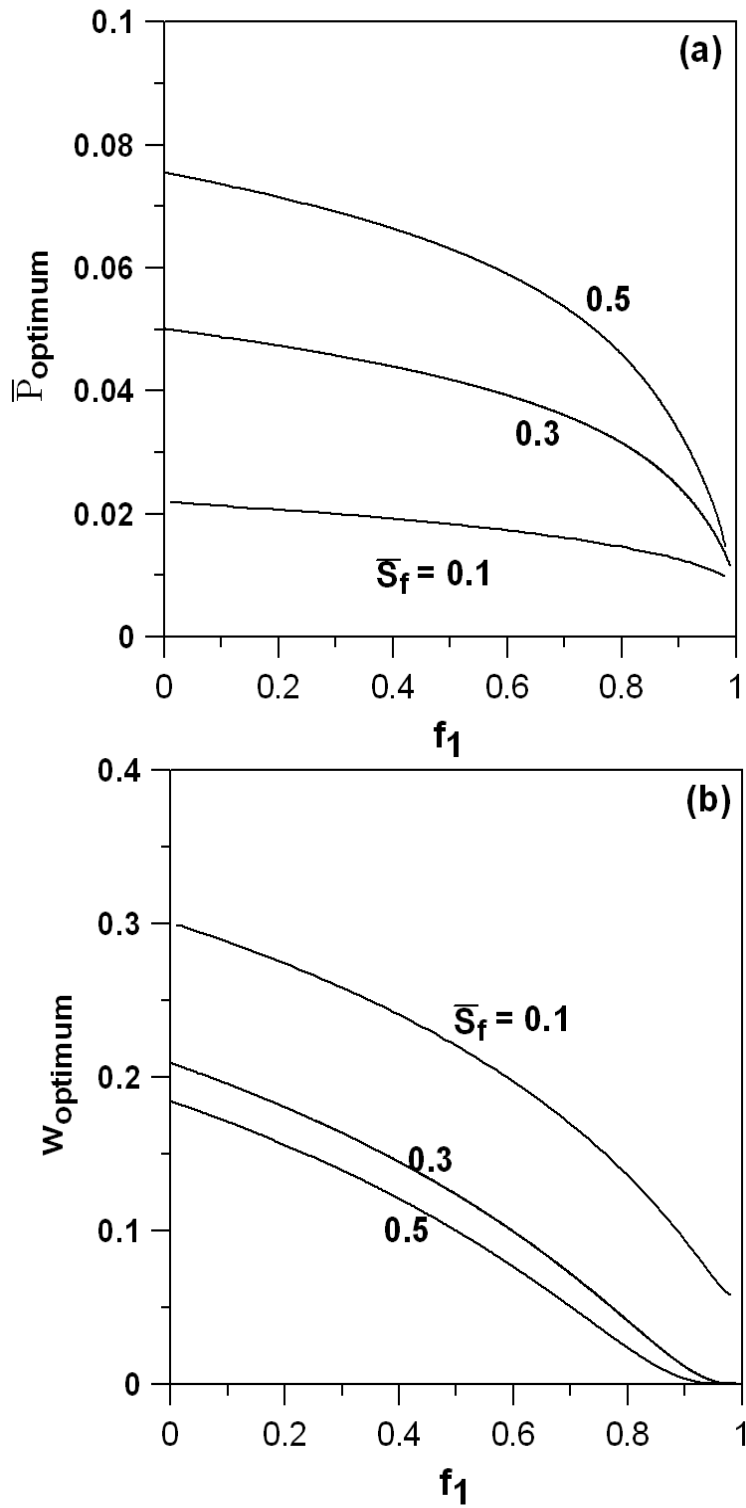


Figure 10. Effect of dimensionless substrate feed concentration on the optimization of bioreactor for maximum productivity for $\bar{S}_r = 0.01$. (a) Variations of optimum values of dimensionless productivity with filling time; (b) Corresponding variations of optimum values of w with filling time.

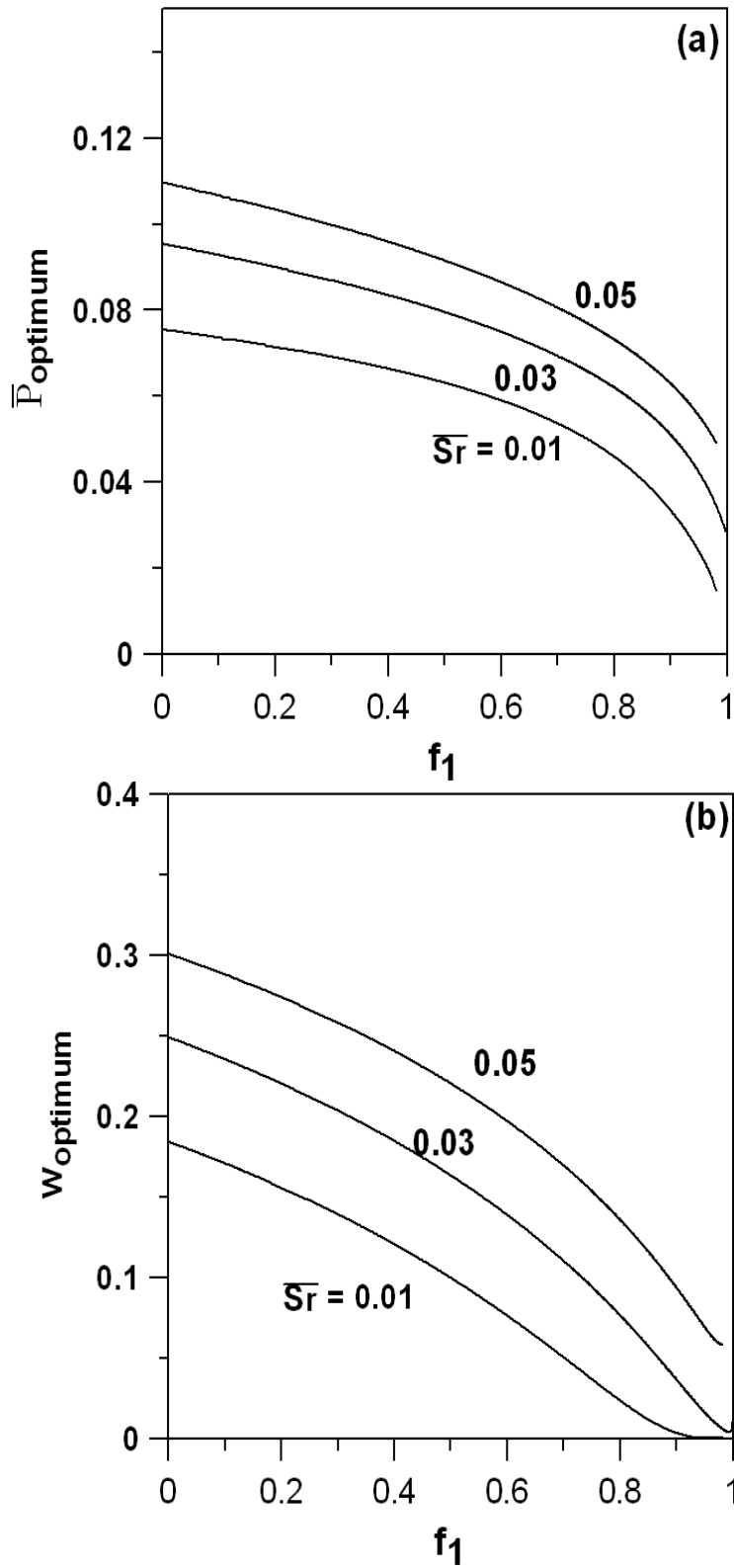


Figure 11. Effect of dimensionless end-of-cycle pollutant concentration on the optimization of bioreactor for maximum productivity for $\bar{S}_f = 0.5$. (a) Variations of optimum values of dimensionless productivity with filling time; (b) Corresponding variations of optimum values of w with filling time.

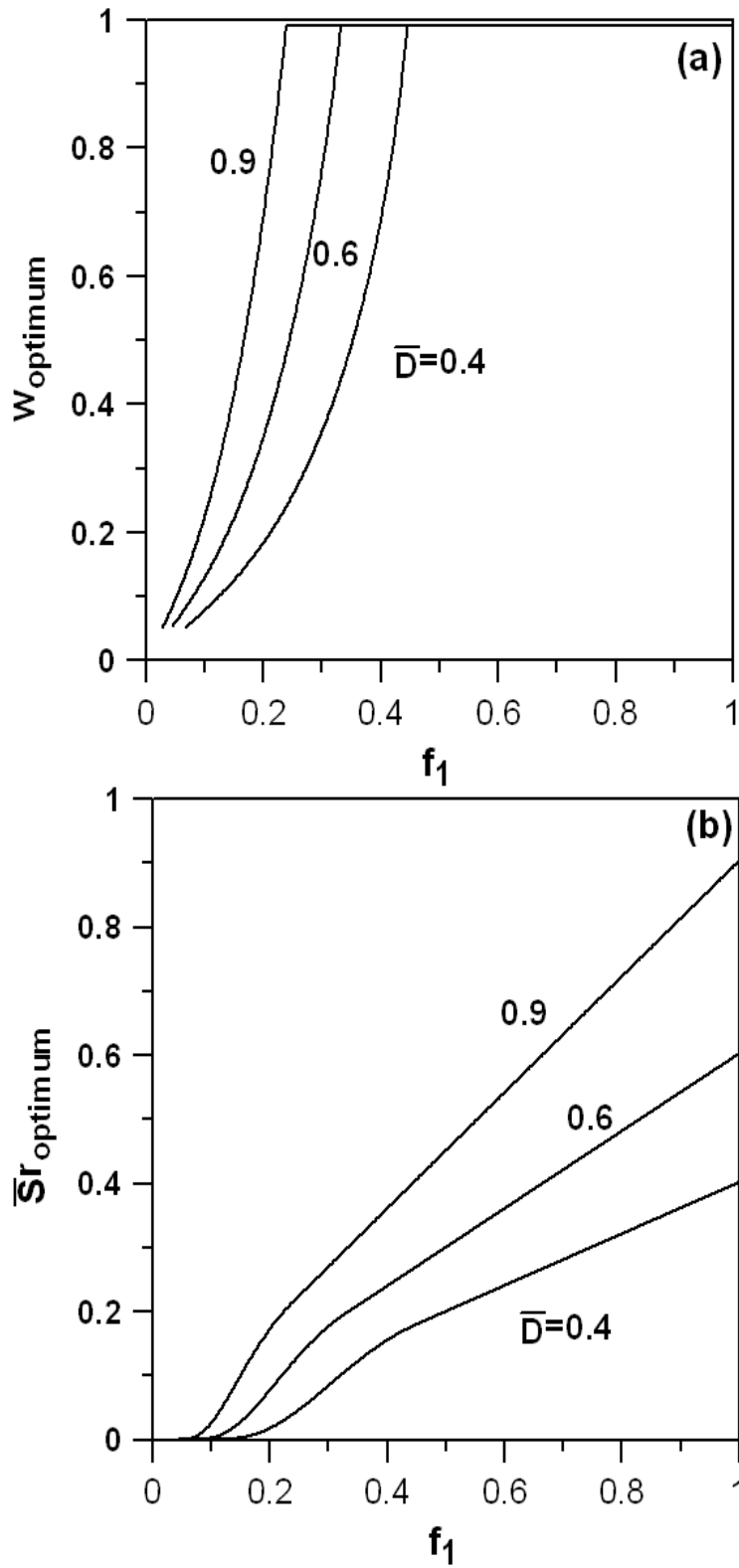


Figure 12. Results of the optimization of the reactor for the minimization of end-of-cycle dimensionless pollutant concentration for $\bar{S}_f = 0.5$. (a) Variations of optimum values of w with filling time. (b) Variations of optimum values of dimensionless end of cycle pollutant concentration with filling time.