Global Stabilization of Continuous Bioreactors

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Abstract: This paper studies the problem of designing controllers for enlarging the stability region of continuous stirred microbial bioreactors. A specific application is in anaerobic digestion, where the stability region can be very small if the operating steady state is selected to maximize the methane production rate. A control Lyapunov function approach is followed to construct a globally stabilizing state feedback control law in continuous time. This turns out to be proportional output feedback in the case of anaerobic digestion, where the measurement is the methane production rate. The control law is implemented in discrete time under zero-order hold. Stability analysis of the resulting closed-loop system is performed using the same control Lyapunov function, leading to an upper bound on the sampling period for guaranteed stability over a given region. Numerical simulation results indicate that closed-loop stability under sampled-data control is global, irrespective of the size of the sampling period.

Keywords: Stabilization, Lyapunov methods, Robust stability, Bio control, Nonlinear analysis, Process control.

1. INTRODUCTION

Continuous stirred microbial bioreactors, often called chemostats, cover a wide range of applications; specialised "pure culture" biotechnological processes for the production of specialty chemicals (proteins, antibiotics etc.) as well as large-scale environmental technology processes of mixed cultures such as wastewater treatment. The dynamics of the chemostat is often adequately represented by a simple dynamic model involving two state variables, the microbial biomass x and the limiting organic substrate s. For control purposes, two operating variables are usually considered, the dilution rate D which is the manipulated input, and the feed substrate concentration S_0 which is a load variable. A general model for microbial growth on a limiting substrate in a chemostat is of the form:

$$\begin{aligned} \frac{dx}{dt} &= -Dx + \mu(s)x \\ \frac{ds}{dt} &= D(S_0 - s) - \frac{1}{Y_{x/s}}\mu(s)x \end{aligned} \tag{1}$$

where $\mu(s)$ is the specific growth rate, and $Y_{x/s}$ is a biomass yield factor. One important example is anaerobic digestion, which finds many applications e.g. in wastewater treatment, sludge management, energy from biomass, etc.
The purpose of this work is to study the problem of robust global stabilization of a bioreactor whose dynamics follows (1), the motivation coming from control problems in anaerobic digestion processes. Section 2 provides some background on anaerobic digestion and explains the nature of the control problem. In Section 3, a simple feedback controller is derived in continuous time via a control Lyapunov function approach, which guarantees global stability of the bioreactor over the entire first quadrant. In Section 4, the same control Lyapunov function is used for stability analysis for the digital implementation of the control law, under zero-order hold. Finally, in Section 5, numerical simulation results are presented, to study the effect of the size of the sampling period on closed-loop stability and performance.

2. EXAMPLE: ANAEROBIC DIGESTION

Anaerobic digestion is a complex biochemical process, in which organic compounds are mineralised to biogas (a useful energy product), consisting primarily of methane and carbon dioxide, through a series of reactions mediated by several groups of microorganisms. Under normal (or balanced) operation, the rate of production of the intermediates is matched by their consumption rate; hence there is very little accumulation of these compounds. However, disturbances such as an increase in the concentration of organic compounds in the feed (organic overload), an increase in feed flow rate (hydraulic overload), presence of toxins in the feed, and temperature fluctuations, can cause an imbalance in the process (Switzenbaum et al., 1990), which results in accumulation of volatile organic acids. These acids cause a drop in the pH, inhibiting methanogenesis and the reactor fails. Such a failure has major consequences in the process economics since digester recovery can be a very cumbersome and costly process. For this reason, the development of appropriate control schemes for anaerobic digesters has received significant attention in recent years (Perrier and Dochain, 1993; Pind et al., 2003).

2.1 Mathematical model of anaerobic digestion.

For the description of anaerobic digestion, the mathematical model (1) can be used. This system of equations describes methanogenesis, the ultimate step in anaerobic digestion, which is rate limiting and is usually the most sensitive step. In other words, it is assumed that the bioconversion of organics into fatty acids (hydrolysis and acidification) has fast kinetics. Then x and s in (1) represent the methanogen and volatile fatty acid concentrations respectively. The specific growth rate is assumed to follow the Andrews kinetics (substrate inhibition) (Graef and Andrews, 1974):

$$\mu(s) = \frac{\mu_{\max} s}{K_S + s + \dfrac{s^2}{K_I}} \tag{2}$$

The output of the system is the methane production rate,

$$Q = Y\mu(s)x \tag{3}$$

where Y is a yield factor for methane production.

2.2 Optimal steady state for methane production

Apart from the washout steady state ($x = 0$, $s = S_0$), the bioreactor's steady states are calculated from the equations:

$$\left\{ \begin{array}{l} \mu(s_s) = D_s \\ x_s = Y_{x/s}(S_0 - s_s) \end{array} \right\} \tag{4}$$

For a given feed, there is a value of the dilution rate that maximises the methane production rate. The steady state that corresponds to the maximization of methane production rate, i.e. $Q = YY_{x/s}\mu(s_s)(S_0 - s_s)$, draws technical interest. The methane production rate is maximized when:

$$\frac{dQ}{ds_s} = 0 \Leftrightarrow \frac{d\mu(s_s)}{ds}(S_0 - s_s) = \mu(s_s)$$

Solving the above equations for $\mu(s)$ given by (2), it is found that the optimal steady state is:

$$s_s^{opt} = \frac{S_0}{1 + \sqrt{1 + \dfrac{S_0}{K_S}\left(1 + \dfrac{S_0}{K_I}\right)}} \tag{5}$$

For the following values of the parameters:

$S_0 = 10000\ mg/l, K_S = 100\ mg/l, \mu_{\max} = 0.5\ d^{-1}$,

$K_I = 4000\ mg/l, Y_{x/s} = 0.05\ mg/mg$,

$Y = 0.00746\ ll^{-1}_{reactor} d^{-1}$

the optimal steady state from equation (5) is $s_s = 506.714\ mg/l$. This corresponds to $x_s = 474.664\ mg/l$, $D_s = 0.377635\ d^{-1}$ and

$Q_s = 1.337205\ ll^{-1}_{reactor} d^{-1}$.

The above numerical values of the parameters and the resulting optimal steady state conditions will be used in the numerical calculations throughout this paper.

2.3 Local asymptotic stability

The eigenvalues of the linearization of (1) are: $\begin{array}{l} \lambda_1 = -\mu(s_s) \\ \lambda_2 = -\dfrac{d\mu(s_s)}{ds}(S_0 - s_s) \end{array}$. Since $\mu(s) > 0$ for all s, local asymptotical stability is guaranteed as long as $\dfrac{d\mu(s_s)}{ds}(S_0 - s_s) > 0$. This condition is satisfied for the optimal steady state given by equation (5).

2.4 The need for control

Figure 1 depicts the phase portrait of the system dynamics under constant dilution rate *D*, in particular for $D = D_s = 0.377635\, d^{-1}$, which is the optimal steady state value. In the diagram, the points S and U represent the corresponding stable and the unstable steady states of the reactor, which are the solutions of equations (4). Notice that the optimal steady state S is locally stable but the stability region is very small. This makes the optimal operation of the biochemical reactor very sensitive to disturbances.
The goal of control is the stabilization of the system in the sense of enlargement of the stability region.

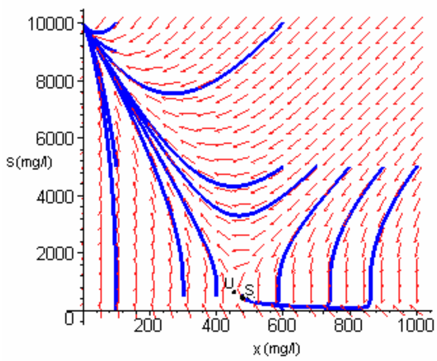


Fig. 1: Phase portrait of the open-loop dynamics

3. FEEDBACK CONTROLLER SYNTHESIS: A CONTROL LYAPUNOV FUNCTION APPROACH

Consider the dynamic system (1) with $D \in [0,+\infty)$, $x \in (0,+\infty)$, $s \in (0,+\infty)$ where $\mu : R^+ \to R^+$ is a smooth function with $\mu(0)=0, \mu(s)>0$ for all $s>0$. Also, consider the coordinate transformation:

$$\begin{aligned} x_1 &= \ln\left(\frac{x}{Y_{x/s}(S_0 - s_s^{des})}\right) \\ x_2 &= \ln\left(\frac{s}{s_s^{des}}\right) \end{aligned} \tag{6}$$

where s_s^{des} is a design steady state value for s (e.g. from equation (5)). Transformation (6) maps the open first quadrant onto R^2. In particular, it maps the design steady state $\left\{ \begin{array}{c} x_s = Y_{x/s}(S_0 - s_s^{des}) \\ s_s = s_s^{des} \end{array} \right\}$ to the origin. Moreover, to facilitate the derivations, consider the input transformation:

$$D = \mu(s)u \tag{7}$$

Under the transformations (6) and (7), the system (1) becomes:

$$\begin{aligned} \frac{dx_1}{dt} &= (1-u)\mu(s_s^{des}e^{x_2}) \\ \frac{dx_2}{dt} &= \left[u\left(\frac{S_0}{s_s^{des}}e^{-x_2} - 1\right) - \left(\frac{S_0}{s_s^{des}} - 1\right)e^{x_1 - x_2} \right]\mu(s_s^{des}e^{x_2}) \end{aligned} \tag{8}$$

Consider now the control Lyapunov function:

$$V = \frac{1}{2}(x_1^2 + x_2^2) \tag{9}$$

The time derivative of V along the trajectories of (8) is given by:

$$\begin{aligned} \dot{V} = \Big\{ &\left[x_1 - \left(\frac{S_0}{s_s^{des}} - 1\right) x_2 e^{x_1 - x_2} \right](1 - ue^{-x_1}) \\ &+ u[x_1(e^{-x_1} - 1) + x_2(e^{-x_2} - 1)] \Big\} \mu(s_s^{des} x_2) \end{aligned} \tag{10}$$

Since $x(\exp(-x)-1) < 0$ for all $x \neq 0$, it is concluded from (10) that the smooth feedback law:

$$u = e^{x_1} \tag{11}$$

will globally stabilize the origin for system (8).
Transforming the feedback law (11) back to the original coordinates (via (6) and (7)) results in

$$D = \frac{\mu(s)x}{Y_{x/s}(S_0 - s_s^{des})} \tag{12}$$

Notice that from equation (12), it is guaranteed that $D \geq 0$ for all times.

The feedback law (12) is a nonlinear state feedback law and, in general, requires measurement of both biomass and substrate. However, in the case of anaerobic digestion (see Section 2) where the measured biogas production rate is proportional to the product $\mu(s)x$, it becomes a linear output feedback law:

$$D = \frac{1}{YY_{x/s}(S_0 - s_s^{des})}Q \tag{13}$$

It is important to point out that the control law of equation (13) coincides with the constant yield control law (CYCL) of Pullammannappallil et al (1998), where the methane yield (defined as the ratio between the methane production rate and the feed flow rate) was maintained at a constant set-point value. Mailleret and Bernard (2001), using a different approach, arrived at the same control law and provided a rigorous justification of global closed-loop stability. The control law was implemented experimentally in Pullammannappallil et al (1998) and in Mailleret et al. (2003).

The closed-loop system under the feedback law (12) or (13) is:

$$
\begin{aligned}
\frac{dx}{dt} &= \left(1 - \frac{x}{Y_{x/s}(S_0 - s_s^{des})}\right)\mu(s)x \\
\frac{ds}{dt} &= \frac{(s_s^{des} - s)\mu(s)x}{Y_{x/s}(S_0 - s_s^{des})}
\end{aligned}
\tag{14}
$$

The form of the closed-loop system shows that:

i) the closed-loop system's equilibrium is at $x_s = Y_{x/s}(S_0 - s_s^{des})$ and $s_s = s_s^{des}$

ii) $\dfrac{d(s - s_s^{des})}{d(x - Y_{x/s}(S_0 - s_s^{des}))} = \dfrac{s - s_s^{des}}{x - Y_{x/s}(S_0 - s_s^{des})}$, which proves that the system's trajectories represent straight lines on the $s - x$ plane.

Figure 4 depicts a phase portrait of the closed-loop dynamics (14) for the particular parameter values and design conditions of Section 2.

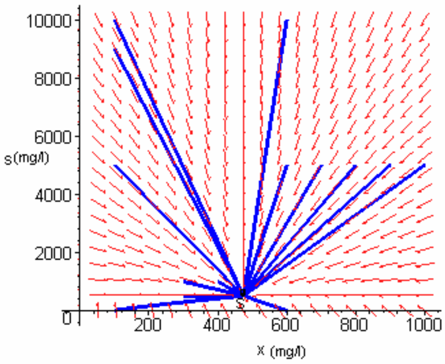


Fig. 2: Phase portrait of the closed-loop system (14)

4. SAMPLED-DATA CONTROL OF THE CONTINUOUS STIRRED BIOREACTOR – STABILITY ANALYSIS

In practice, measurements of the methane production rate $Q = Y\mu(s)x$, are available only at certain instances (sampling times). If the control action is kept constant between two consecutive sampling times then we say that we apply a sample-and-(zero order) hold control policy. The sample-and-(zero order) hold control policy is the usual way of implementing nonlinear feedback laws. Consequently, it is important to study the behaviour of the closed-loop system of the chemostat under a sample-and-hold control policy.

Let a uniform sampling partition $\{0, T, 2T, 3T, ...\}$, i.e., we assume that measurements of the methane production rate $Q = Y\mu(s)x$ are available every T time units. Let $Q_i = Y\mu(s_i)x_i$ be the methane production rate at time iT where i is a non-negative integer and let s_i, x_i be the limiting organic substrate concentration and the microbial biomass, respectively, at time iT. If the feedback law (12) is applied with a zero-order-hold element then we have:

$$D = \frac{\mu(s_i)x_i}{Y_{x/s}\left(S_0 - s_s^{des}\right)}, \text{ for } iT \le t < (i+1)T \tag{15}$$

The stability analysis of the corresponding closed-loop system (1) with (15) is performed via the coordinate transformation (6) and using the control Lyapunov function defined in (9). It can be shown that if $x(iT) = (x_1(iT), x_2(iT))' \in \Omega_R$, $x(t) = (x_1(t), x_2(t))' \in \Omega_R$, where $R > 0$ and $\Omega_R := \left\{ x \in \Re^2 : |x| \le \sqrt{2}R \right\}$ then the following inequalities hold for all $iT \le t < (i+1)T$:

$$\frac{d}{dt}\left(\frac{1}{2}|x(t) - x(iT)|^2\right) \le L(R)|x(t) - x(iT)|^2 + \frac{1}{2}\mu_{\max}^2 \exp\left(4\sqrt{2}R\right)|x(iT)|^2 \tag{16}$$

$$\frac{d}{dt}V(x(t)) \le -\frac{1}{2}\exp\left(-2\sqrt{2}R\right)\mu\left(s_s^{des}e^{x_2(t)}\right)\left[|x(t)|^2 - M(R)|x(t) - x(iT)|^2\right] \tag{17}$$

where

$$L(R) := \frac{1}{2}\left(1 + L_\mu(R)\right) + \frac{1}{2}\left(\frac{S_0}{s_s^{des}} - 1\right)\mu_{\max} \exp\left(2\sqrt{2}R\right) + \left(\frac{S_0}{s_s^{des}} - 1\right)L_\mu(R)e^{2\sqrt{2}R} \tag{18}$$

$$M(R) := 2e^{5\sqrt{2}R} \max\left\{1 ; \mu_{\max}^2 B_\mu^2(R)\right\}\left(1 + e^{\sqrt{2}R}Q^2(R)\right) \tag{19}$$

$$L_\mu(R) := \max\left\{ S|\mu'(S)| : s_s^{des}e^{-\sqrt{2}R} \le S \le s_s^{des}e^{\sqrt{2}R} \right\} \tag{20}$$

$$B_\mu(R) := \max\left\{ \frac{S|\mu'(S)|}{\mu^2(S)} : s_s^{des}e^{-\sqrt{2}R} \le S \le s_s^{des}e^{\sqrt{2}R} \right\} \tag{21}$$

$$\mu_{\max} := \max\{ \mu(s) : 0 \le s \} \tag{22}$$

$$Q(R) := \max\left\{ \frac{S_0}{s_s^{des}}e^{\sqrt{2}R} - 1 ; 1 - \frac{S_0}{s_s^{des}}e^{-\sqrt{2}R} \right\} \tag{23}$$

Using the above inequalities, it can be shown that for every $R > 0$ and if

$$T < \frac{1}{2L(R)}\ln\left(1 + \frac{2L(R)}{\mu_{\max}^2}e^{-4\sqrt{2}R}\left(\frac{1}{1 + M(R)}\right)^2\right) \tag{24}$$

then the optimal steady state for methane production is Locally Asymptotically Stable with region of attraction $\Omega_R := \left\{ x \in \Re^2 : |x| \leq \sqrt{2}R \right\}$ for the closed-loop system (1) with (15).

Notice that (24) implies that large regions of attraction (large values for $R > 0$) necessitate more frequent measurements of the methane production rate $Q = Y\mu(s)x$ (smaller sampling period T). Clearly, there is a trade-off between the sampling period and the radius of the region of attraction.

The maximum allowable sampling period is generally larger than the right-hand side of inequality (24), i.e., (24) is a conservative estimate of the maximum allowable sampling period. In the following sections it is shown that the sample-and-hold feedback law (15) is effective even for large values of the sampling period. In order to reduce the conservatism of (24), other control Lyapunov functions (or vector control Lyapunov functions) could be used.

5. SAMPLED-DATA CONTROL OF THE CONTINUOUS STIRRED BIOREACTOR – NUMERICAL SIMULATION RESULTS

Extensive numerical simulation results were obtained for many different initial conditions, far away from the operating steady state. It was observed that:

i) for any initial condition used, and for any sampling period used, trajectories converged to the bioreactor steady state

ii) the control system could tolerate significantly large sampling periods without appreciable loss of performance.

In what follows, three representative cases will be shown.

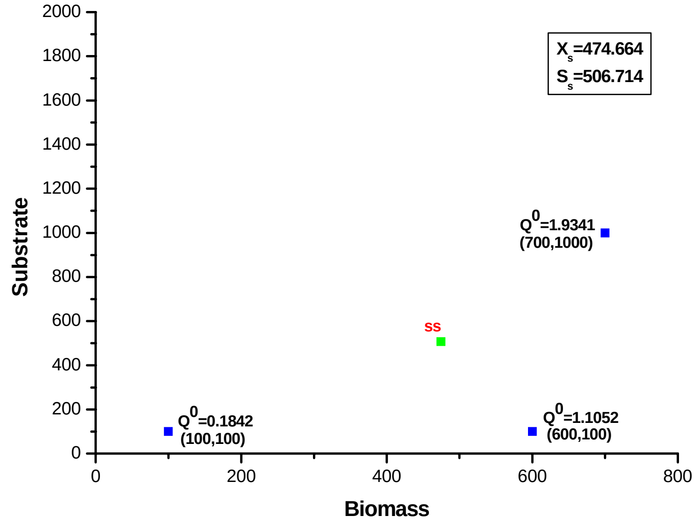


Fig. 3: Biomass and Substrate initial conditions and the bioreactor steady state

Case 1: $x(0) = 600,\ s(0) = 100,\ Q^0 = Y\ \mu(s(0))x(0) = 1.1052$

Case 2: $x(0) = 100,\ s(0) = 100,\ Q^0 = Y\ \mu(s(0))x(0) = 0.1842$

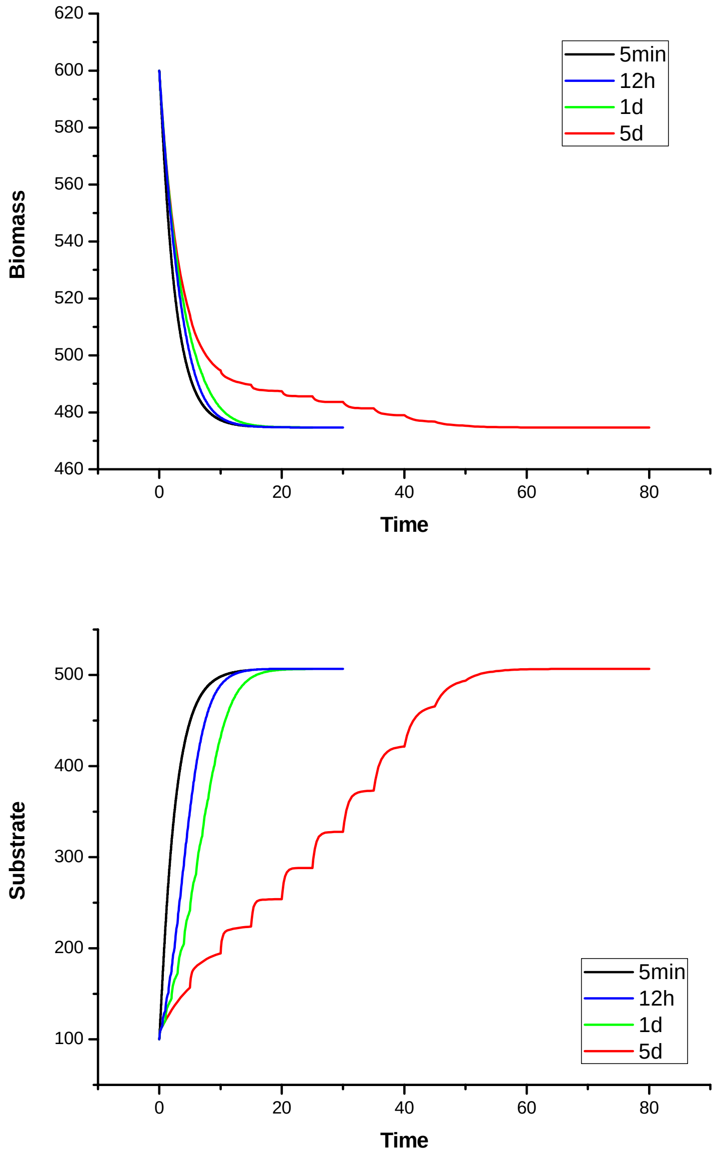
Case 3: $x(0) = 700,\ s(0) = 1000,\ Q^0 = Y\ \mu(s(0))x(0) = 1.9341$

Figures 4 - 9 depict the time responses of the biomass and the substrate concentrations as well as the corresponding phase-space trajectories, for the 3 cases of initial conditions and different values of the sampling period.

<u>Case 1:</u> $x(0) = 600,\ s(0) = 100, \quad Q^0 = Y\ \mu(s(0))\, x(0) = 1.1052$

- initial Q is of similar magnitude as its the steady state value

System can tolerate very large sampling periods. Only for sampling periods of the order of 12 hours and larger, there is appreciable loss of performance.



Sampling Time	Settling Time
5 min	16 days
12 hours	18 days
1 day	20 days
5 days	57 days

Fig. 4: Biomass and Substrate responses for Case1 for different values of the sampling period

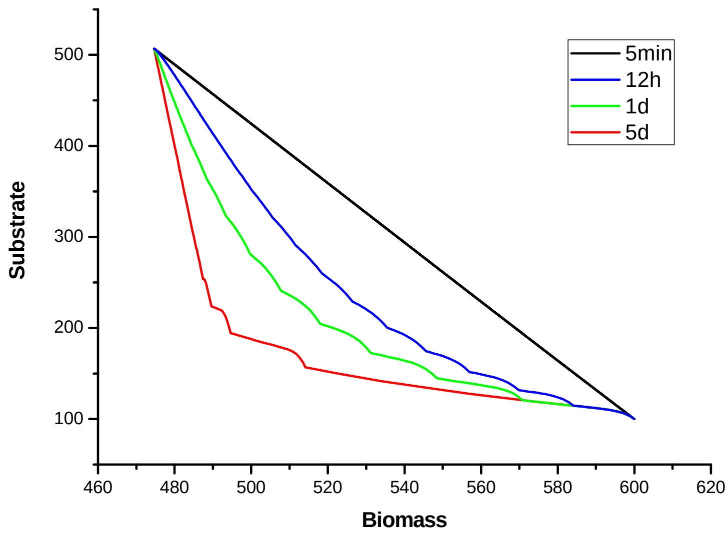
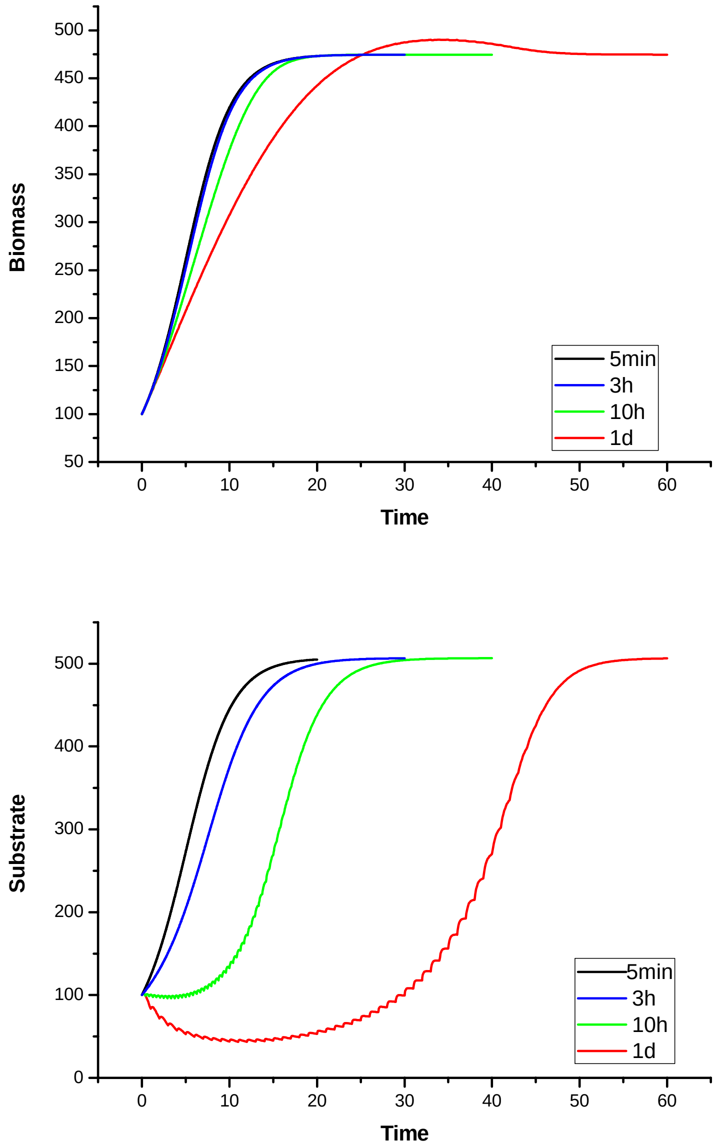


Fig. 5: Phase plane trajectories for Case 1 for different values of the sampling period

<u>Case 2:</u> $x(0)=100,\ s(0)=100,\quad Q^0 = Y\ \mu(s(0))\,x(0) = 0.1842$

- initial Q is small compared to its steady state value

System is less tolerant to large sampling periods. Even for sampling periods of a few hours, there is appreciable loss of performance.



Sampling Time	Settling Time
5 min	20 days
3 hours	31 days
10 hours	40 days
1 day	60 days

Fig. 6: Biomass and Substrate responses for Case2 for different values of the sampling period

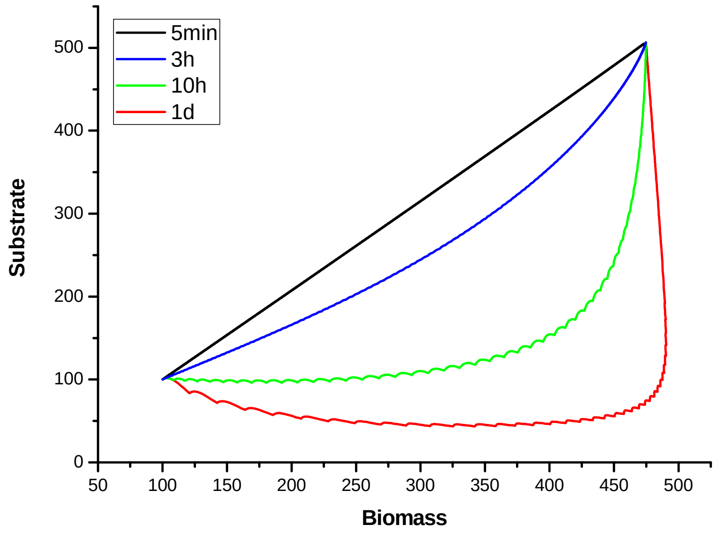
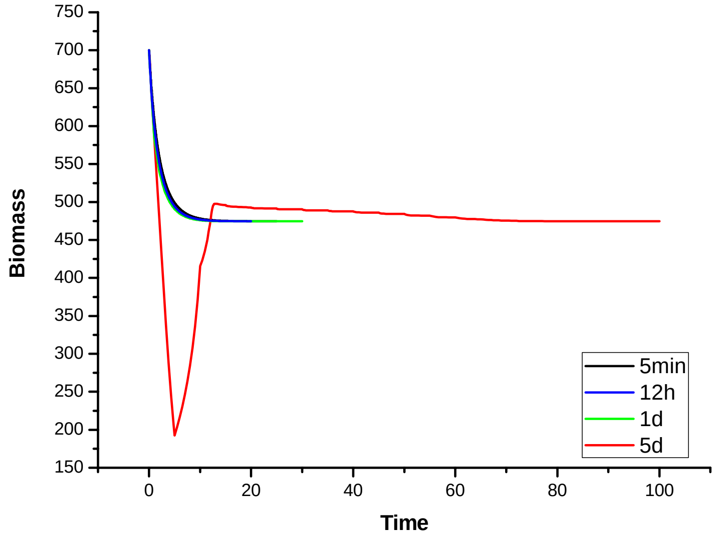


Fig. 7: Phase plane trajectories for Case 2 for different values of the sampling period

Case 3: $x(0) = 700,\ s(0) = 1000, \quad Q^0 = Y\,\mu(s(0))\,x(0) = 1.9341$

- initial Q is small compared to its steady state value

System can tolerate large sampling periods as in Case 1. In the event that extremely large sampling periods are used, system is initially directed towards washout conditions, but because washout corresponds to low Q, the system is able to slowly recover.



Sampling Time	Settling Time
5 min	8 days
12 hours	14 days
1 day	18 days
5 days	80 days

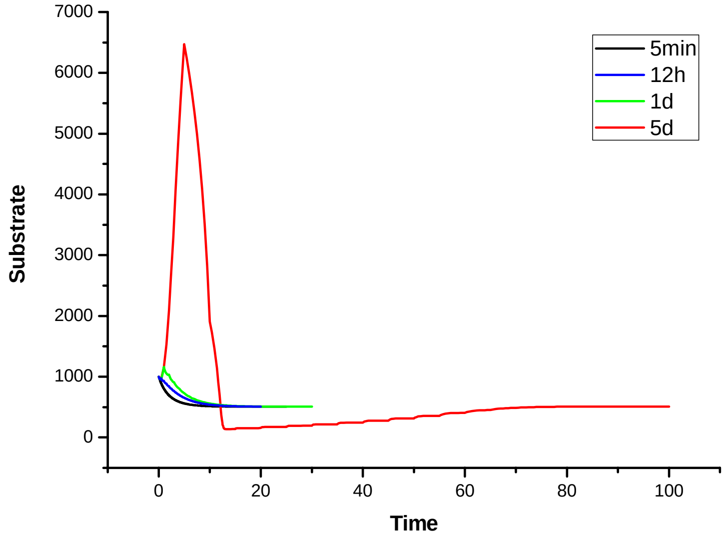


Fig. 8: Biomass and Substrate responses for Case3 for different values of the sampling period

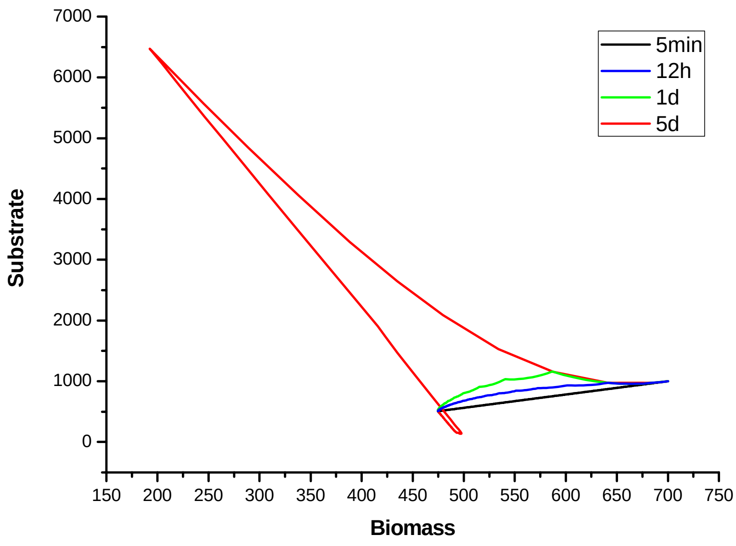


Fig. 9: Phase plane trajectories for Case 3 for different values of the sampling period

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