ROBUST 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. This turns out to be proportional output feedback in the case of anaerobic digestion, where the measurement is the methane production rate. The robustness properties of the feedback controller are also investigated. For situations of large, measurable changes in the organic load of the bioreactor, a feedforward measurement is incorporated in the control law, leading to improved robustness margin. *Copyright © 2002 IFAC*

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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:

$$\frac{dx}{dt} = -Dx + \mu(s)x$$

$$\frac{ds}{dt} = D(S_0 - s) - \frac{1}{Y_{x/s}}\mu(s)x \tag{1}$$

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 via a control Lyapunov function approach. The robustness properties of the feedback controller are examined in Section 4. Finally, Section 5 develops a feedforward / feedback controller with improved robustness margin.

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):

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

The output of the system is the methane production rate,

$$Q = Y\mu(s)x \qquad (3)$$

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:

$$\begin{cases} \mu(s_s) = D_s \\ x_s = Y_{x/s}(S_0 - s_s) \end{cases} \qquad (4)$$

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:

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

For the following values of the parameters:

$S_0 = 10000 \, mg/l$, $K_S = 100 \, mg/l$, $\mu_{max} = 0.5 \, d^{-1}$,
$K_I = 4000 \, mg/l$, $Y_{x/s} = 0.05 \, mg/mg$,
$Y = 0.00746 \, ll_{reactor}^{-1} d^{-1}$
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 $Q_s = 1.337205 \, ll_{reactor}^{-1} d^{-1}$.

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:
$\lambda_1 = -\mu(s_s)$
$\lambda_2 = -\frac{d\mu(s_s)}{ds}(S_0 - s_s)$. Since $\mu(s) > 0$ for all s,

local asymptotical stability is guaranteed as long as $\frac{d\mu(s_s)}{ds}(S_0 - s_s) > 0$. 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.
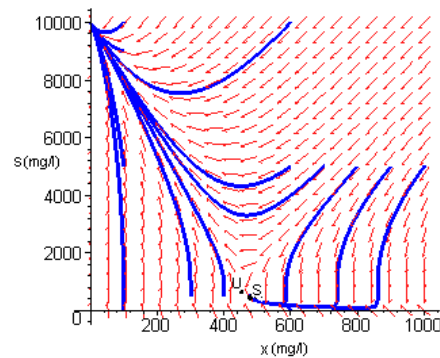

Fig.1. Phase portrait of the open-loop dynamics

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:

$$x_1 = \ln\left(\frac{x}{Y_{x/s}(S_0 - s_s^{des})}\right)$$

$$x_2 = \ln\left(\frac{s}{s_s^{des}}\right) \tag{6}$$

where s_s^{des} is a design steady state value for s (e.g. from equation (5)). Transformation (6) maps the open first quadrant <u>onto</u> 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:

$$\frac{dx_1}{dt} = (1-u)\mu(s_s^{des} e^{x_2})$$

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

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:

$$\dot{V} = \left\{ \left[x_1 - \left(\frac{S_0}{s_s^{des}} - 1\right)x_2 e^{x_1 - x_2}\right](1 - ue^{-x_1}) \right.$$

$$\left. + u[x_1(e^{-x_1} - 1) + x_2(e^{-x_2} - 1)] \right\}\mu(s_s^{des} x_2) \tag{10}$$

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:

$$\frac{dx}{dt} = \left(1 - \frac{x}{Y_{x/s}(S_0 - s_s^{des})}\right)\mu(s)x$$

$$\frac{ds}{dt} = \frac{(s_s^{des} - s)\mu(s)x}{Y_{x/s}(S_0 - s_s^{des})} \tag{14}$$

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.
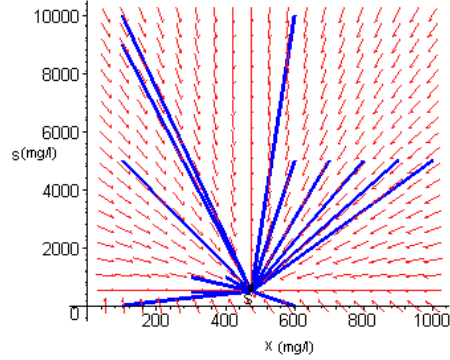

Fig.2. Phase portrait of the closed-loop system (14)

4. ROBUSTNESS PROPERTIES OF THE FEEDBACK CONTROL LAW

In the case of direct measurement of the methane production rate $Q = Y\mu(s)x$, the control law derived in the previous section is completely insensitive to errors in $\mu(s)$, in terms of achieving global stability. Of course, the computed s_s^{des} (e.g. from equation (5)) will depend on the parameters in $\mu(s)$ (like K_s and K_I) and will no longer be optimal in the presence of parameter errors. For the particular parameter values given in Section 2, which are representative of a typical anaerobic digestion process, it is found that a 50% error below the nominal values of K_s and K_I corresponds to 1.24% and 1.17% biogas loss respectively and that a 50% error above the nominal values corresponds to 0.63% and 0.22% biogas loss.

The situation is different in the presence of errors in S_0. Suppose that a design value S_0^{des} is used in the control law (13), i.e.

$$D = \frac{1}{YY_{x/s}(S_0^{des} - s_s^{des})}Q \qquad (15)$$

whereas the true substrate concentration in the process is S_0. Then the resulting closed-loop dynamics will follow:

$$\frac{dx}{dt} = \left(1 - \frac{x}{Y_{x/s}(S_0^{des} - s_s^{des})}\right)\mu(s)x$$

$$\frac{ds}{dt} = \frac{\left[(S_0 - S_0^{des}) + s_s^{des} - s\right]}{Y_{x/s}(S_0^{des} - s_s^{des})}\mu(s)x \qquad (16)$$

From (16) it is seen that the closed-loop system's equilibrium will be at $\begin{cases} x_s = Y_{x/s}(S_0^{des} - s_s^{des}) \\ s_s = s_s^{des} + (S_0 - S_0^{des}) \end{cases}$

Notice that x_s equals the design value of biomass concentration, but there will be an offset of the substrate from the design conditions by an amount equal to the error in S_0. The problem is that, if S_0 is significantly lower than its design value S_0^{des}, s_s may be negative and therefore physically unrealistic.

<u>Case 1</u>: If $s_s^{des} + (S_0 - S_0^{des}) > 0$, then the system (16) can be transformed via the coordinate transformation:

$$x_1 = \ln\left(\frac{x}{Y_{x/s}(S_0^{des} - s_s^{des})}\right)$$

$$x_2 = \ln\left(\frac{s}{S_0 - S_0^{des} + s_s^{des}}\right) \qquad (17)$$

resulting in:

$$\frac{dx_1}{dt} = (1 - e^{x_1})\mu((S_0 - S_0^{des} + s_s^{des})e^{x_2})$$

$$\frac{dx_2}{dt} = -(1 - e^{-x_2})e^{x_1}\mu((S_0 - S_0^{des} + s_s^{des})e^{x_2}) \qquad (18)$$

which is globally asymptotically stable, as can be easily seen through the Lyapunov function (9).

<u>Case 2</u>: If $s_s^{des} + (S_0 - S_0^{des}) < 0$, the trajectories of the system (16) will still be straight lines. However, they will not reach the physically unrealistic equilibrium point. Instead, they will terminate on the x-axis, which corresponds to process shut down (x=const., s=0, $D = 0$).

Figures 2 and 3 depict representative phase portraits for S_0^{des} =10000 mg/l and the rest of the parameters as in Section 2. In Figure 3, $S_0 = 11000\ mg/l$ and this corresponds to Case 1, where the effect of the error in S_0 is just a shift in the steady-state value of s. In Figure 4, for $S_0 = 8000\ mg/l$ and this corresponds to Case 2, where the error in S_0 brings the system to shut down.

The conclusion from the foregoing analysis is that the feedback control law is robust for errors in S_0 such that: $s_s^{des} > (S_0^{des} - S_0)$. Otherwise, it brings the

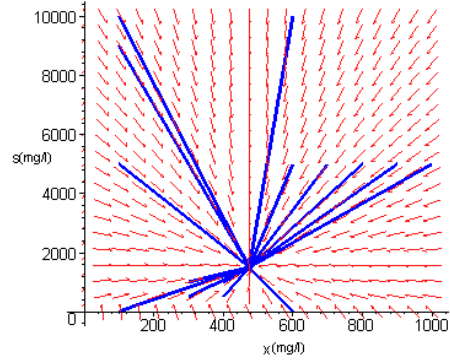system to shut down, which is completely undesirable.
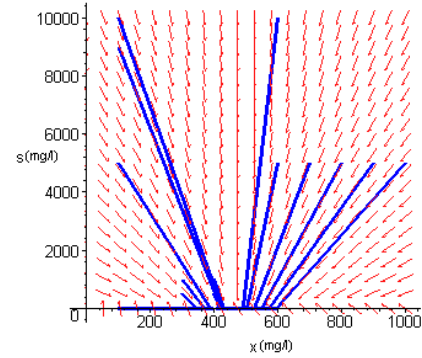

Fig.3. Phase portrait for $S_0 = 11000\ mg/l$

Fig.4. Phase portrait for $S_0 = 8000\ mg/l$

5. FEEDFORWARD /FEEDBACK CONTROL

If it is anticipated that the error in S_0 could be large enough to violate the robustness condition of the previous section, the control law will need to be modified to prevent shut down. One possibility is to measure the feed substrate concentration on-line and use it as a feedforward measurement in the control law. The measurement of S_0 is feasible using a Total Organic Carbon (TOC) analyzer.

Consider the control law (12) or (13), where S_0 is now the on-line measurement of the feed substrate concentration and, therefore, the control law now involves both feedback and feedforward action. Then, the resulting closed-loop system is still given by (14), even though now S_0 is a function of time, with $S_0(t) > 0$ for all $t > 0$. In the event that S_0 remains constant, the closed-loop system's equilibrium will be at: $\begin{cases} x_s = Y_{x/s}(S_0 - s_s^{des}) \\ s_s = s_s^{des} \end{cases}$. As long

as $S_0 > s_s^{des}$, the equilibrium will be in the first quadrant and the closed-loop system will be globally stable as a result of the analysis of section 3.

The situation where $S_0(t)$ is time-varying but bounded requires further attention. Suppose that S_0^{des} is the value of S_0 for which the reactor has been designed to operate. Then the difference

$$z(t) = S_0(t) - S_0^{des} \qquad (19)$$

represents a bounded but, in general, non-vanishing perturbation to the system. To be able to analyze the

effect of this perturbation, consider the coordinate transformation:

$$x_1 = \ln\left(\frac{x}{Y_{x/s}(S_0^{des} - S_s^{des})}\right)$$

$$x_2 = \ln\left(\frac{s}{s_s^{des}}\right) \tag{20}$$

Under this transformation, (14) transforms into:

$$\frac{dx_1}{dt} = \left(1 - \frac{e^{x_1}}{1 + \frac{S_0(t) - S_0^{des}}{S_0^{des} - s_s^{des}}}\right)\mu(s_s^{des} e^{x_2})$$

$$\frac{dx_2}{dt} = (e^{-x_2} - 1)\frac{e^{x_1}}{1 + \frac{S_0(t) - S_0^{des}}{S_0^{des} - s_s^{des}}}\mu(s_s^{des} e^{x_2}) \tag{21}$$

Now assume that:

$$\left|\frac{S_0(t) - S_0^{des}}{S_0^{des} - s_s^{des}}\right| \leq L \ , \quad \text{for all } t > 0 \tag{22}$$

where $L < \frac{1}{3}$. Then

$$\frac{d}{dt}\left(\frac{1}{2}x_2^2\right) = x_2(e^{-x_2} - 1)\frac{e^{x_1}}{1 + \frac{S_0(t) - S_0^{des}}{S_0^{des} - s_s^{des}}}\mu(s_s^{des} e^{x_2}) \leq 0 \tag{23}$$

whereas the quantity

$$\frac{d}{dt}\left(\frac{1}{2}x_1^2\right) = \left\{x_1(1 - e^{x_1}) + \frac{x_1 e^{x_1}\frac{S_0(t) - S_0^{des}}{S_0^{des} - s_s^{des}}}{1 + \frac{S_0(t) - S_0^{des}}{S_0^{des} - s_s^{des}}}\right\}\mu(s_s^{des} e^{x_2}) \tag{24}$$

will be ≤ 0 as long as

$$x_1 \leq \ln\left(1 - \frac{2L}{1+L}\right) \tag{25}$$

or $\qquad x_1 \geq \ln\left(1 + \frac{2L}{1-3L}\right) \tag{26}$

From the above, using standard arguments of the theory of non-vanishing perturbations (Khalil, 1996, Chapter 5), it follows that for any initial conditions,

$$\lim_{t\to\infty} x_2(t) = 0$$

and there exists a time $T \geq 0$ such that

$$|x_1(t)| \leq b \ , \forall t \geq T \tag{27}$$

where

$$b = \max\left\{-\ln\left(1 - \frac{2L}{1+L}\right), \ln\left(1 + \frac{2L}{1-3L}\right)\right\} \tag{28}$$

In other words, the solutions of (21) are uniformly ultimately bounded, with x_2 asymptotically approaching zero.
Consequently, the final value of the substrate concentration will equal its design value, $\lim_{t\to\infty} s(t) = s_s^{des}$, whereas the ratio of the biomas divided by its design value will be ultimately bounded as follows:

$$e^{-b} \leq \frac{x(t)}{Y_{x/s}(S_0^{des} - s_s^{des})} \leq e^b \tag{29}$$

for every initial condition within the open first quadrant.

Numerical simulations were performed under pure feedback action (FB) and combined feedforward and feedback action (FF/FB), when the system is initially at steady state with $S_0 = S_0^{des} = 10000\,mg/l$ but S_0 undergoes a step change to a new value.
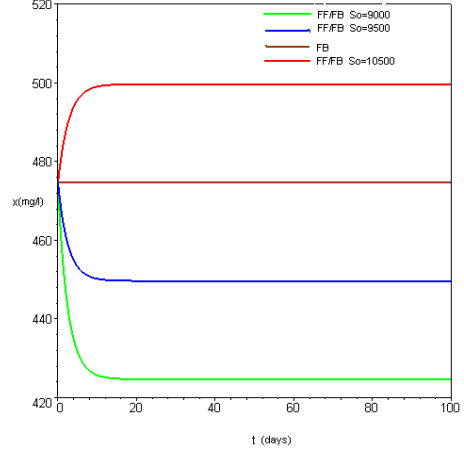Figures 5, 6 and 7 compare the responses of x, s and Q for some representative final values of S_0.

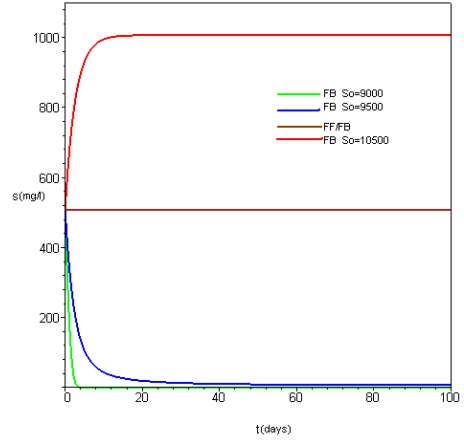Fig.5.Responses of x for representative values of S_0

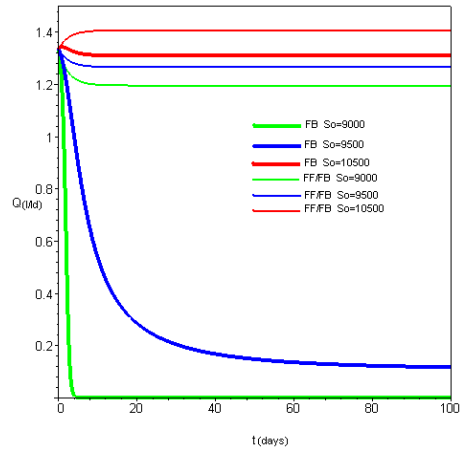Fig.6.Responses of s for representative values of S_0

Fig.7. Response of Q for representative values of S_0

It is seen from Figures 5 and 6 that, as predicted by the analysis, in a step change in S_0, the steady state of x is unaffected under FB control, whereas the steady state of s is unaffected under FF/FB control.

The problem with FB control is when the robustness condition $s_s^{des} > (S_0^{des} - S_0)$ is violated, like in the case $S_0 = 9000\ mg/l$, where the system is brought to shut down. For $S_0 = 9500\ mg/l$, the reactor is not shut down because the robustness condition is satisfied, but the final value of the substrate is very small ($s \rightarrow 6.714\ mg/l$), leading to small biogas production ($Q \rightarrow 0.111\ ll_{reactor}^{-1}d^{-1}$). On the other hand, FF/FB control can tolerate much larger deviations.

In all the step changes considered, FF/FB has better performance than FB in the sense that the biogas production Q is larger (see Fig. 7).

Figures 8, 9 and 10 depict the responses of x, s and Q under a sinusoidal variation in S_0 of amplitude 500 mg/l and period 60 d. The system is initially at steady state with $S_0 = S_0^{des} = 10000\ mg/l$ and the average value of S_0 remains the same (10000 mg/l) for $t > 0$:

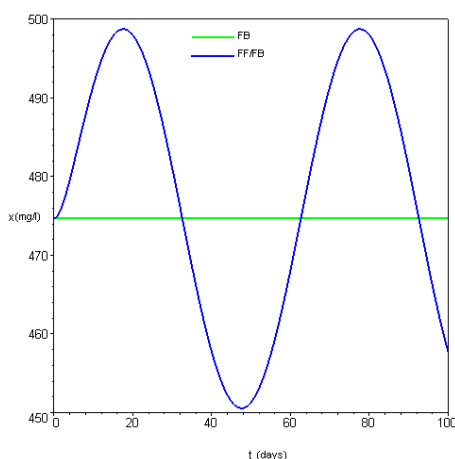$$S_0(t) = 10000 + 500 \sin(\frac{2\pi}{60}t)\ .$$

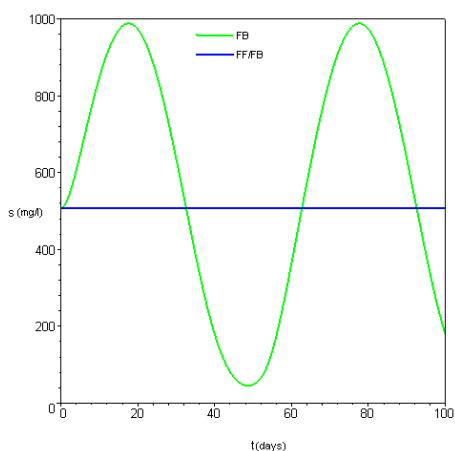Fig.8. Response of x for a sinusoidal change in S_0

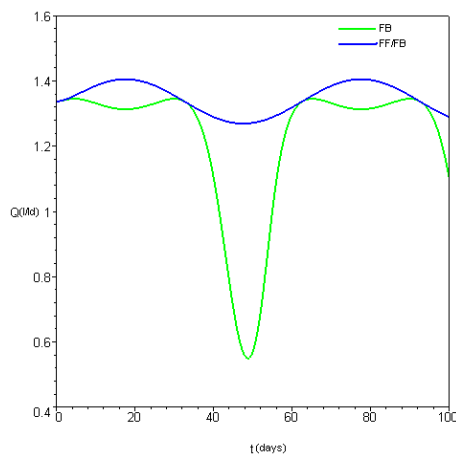Fig.9. Responses of s for a sinusoidal change in S_0

Fig.10. Response of Q for a sinusoidal change in S_0

Even though FF/FB cannot completely eliminate the effect of the discrepancy $S_0(t) - S_0^{des}$, the response of the system is bounded. Also, FF/FB leads to higher biogas production, as shown in Figure 10.

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