Flow-Rate Control of a Continuous Stirred Tank Reactor

Start-Up and Large Disturbances

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Abstract

The non-linear character of the dynamics of a continuous stirred tank reactor is analysed in case of flow rate control. Analysis is made of a simple process model for continuous ethanol production using immobilized yeast, but the results carry over to most reactions with immobilized catalyst. An analytical solution of the bilinear state equations are given. The solution has a structure that makes it easy to calculate the evolution of reachable sets from different initial states. The insight obtained from analysis of reachability is used to derive a time-optimal control strategy. A bang-bang control law is obtained with a simple switch curve in the state space. It is found that start-up and large disturbances call for reversed control actions compared to control around the working point. The structure of the process model suggests application of exact linearization. However, analysis shows that such a transformation becomes singular in this case. Exact linearization is therefore of less value in this application.

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Flow-rate Control of a Continuous Stirred Tank Reactor
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Introduction

The continuous stirred tank reactor is a very general component that is used also in biotechnology applications. Enzymes in living cells act as catalysts, and they may be immobilized, recycled or continuously growing at the dilution rate. For biotechnology processes media concentrations and enzyme activity often vary considerably and feedback control is required for good economy. Continuous ethanol fermentation using alginate entrapped yeast was studied in the laboratory. The concentrations of the substrate sugar and the product ethanol were measured on-line and utilized for controlling the flow-rate through the fermentor, as described in a series of papers, (Axelsson *et al.*, 1982; Mattiasson *et al.*, 1983; Mandenius *et al.*, 1987). The linear controllers used were designed to compensate for the time-delays introduced in the sensors. Good control was shown for set point changes and in response to small disturbances, both with product and substrate concentration as controlled variable.

Models for the process are however nonlinear, actually bilinear, and for large disturbances nonlinear controllers are required. This paper shows that it is possible to use the structure of the solutions to describe the reachable sets of the system. Limitted controllability is found on a line in the state space, actually related to reaction invariants. See eg. (Fjeld *et al.*, 1974; Waller and Mäkilä, 1981).

In the next section these reachable set expressions are then used to obtain a time optimal controller. The expressions are also compared with a lack of controllability obtained using the Lie brackets of differential geometry. The final section describes the transformations needed when applying exact linearization. The lack of controllability shows up as singularities in the transformations.

Process dynamics

Normalized mass balance equations for the continuous tank are

$$\begin{cases} \dfrac{dS}{dt} = -S + (1-S)u \\ \dfrac{dE}{dt} = S - Eu \end{cases} \tag{1}$$

where S, E and u are sugar, ethanol and flow rate through the reactor, respectively. Note that these are non-negative quantities. Let

$$\begin{cases} z_1 = 1 - S \\ z_2 = 1 - S - E \end{cases} \tag{2}$$

which gives

$$\begin{cases} \dfrac{dz_1}{dt} = -(1+u)z_1 + 1 \\ \dfrac{dz_2}{dt} = -uz_2 \end{cases} \tag{3}$$

Integration of the equations gives

$$\begin{cases} z_1(t) = e^{-t}v(t)z_1(t_0) + w(t) \\ z_2(t) = v(t)z_2(t_0) \end{cases} \tag{4}$$

where

$$\begin{aligned} v(\tau) &= \phi(t, t-\tau) \\ w(t) &= \int_{t_0}^{t} e^{-\tau} v(\tau) d\tau \\ \phi(t,s) &= e^{-\int_s^t u(\tau)d\tau} \end{aligned} \tag{5}$$

Reachable Sets

The state-space is not completely reachable since $v(t) \in (0, \infty)$, and $z_2(t_0) = 0$ implies $z_2(t) = 0$ for any input signal. No trajectories pass the line $z_2 = 0$.

It is further interesting to regard the implication of the input u being limited to the interval $[0, d]$, as in the current real process. Denote by $\Omega(t, z(t_0))$ the subset of the state space that can be reached at time t from the point $z(t_0)$. In order to characterize Ω all possible $z_1(t)$ values are determined for a given $z_2(t)$ value, i.e. from (4) it follows that $v(t)$ is given by $z_2(t)$ and possible $w(t)$ values are obtained via $v_{[t_0,t]}$ from all possible input signals $u_{[t_0,t]}$.

Therefore introduce two extreme input signals

$$\begin{aligned} u^+(s) &= \begin{cases} d & s \in [0, \tau_1] \\ 0 & s \in (\tau_1, t] \end{cases} \\ u^-(s) &= \begin{cases} 0 & s \in [0, t-\tau_1] \\ d & s \in (t-\tau_1, t] \end{cases} \end{aligned} \tag{6}$$

satisfying the $v(t)$ constraint by

$$v(t) = e^{-\tau_1 d} \tag{7}$$

It is straight forward to calculate the corresponding functions v^+, and v^-, and for any possible v function it actually holds that

$$v^-(\tau) \le v(\tau) \le v^+(\tau), \qquad \tau \in [0, t] \tag{8}$$

and thus similarly for the corresponding w functions:

$$w^-(\tau) \le w(\tau) \le w^+(\tau), \qquad \tau \in [0, t] \tag{9}$$

It can also be shown that for any w function fulfilling (9) there exists a corresponding input function u. Introduce by (4) the corresponding extremal z_1^+

and z_1^- functions. Now all possible $z_2(t)$ values together with their corresponding possible $z_1(t)$ values form the desired Ω set. All possible $z_2(t)$ values are obtained by letting τ_1 in (7) sweep the interval $\tau_1 \in [0, t]$. Since z_1^+ and z_1^- are the extreme values the boundary of Ω is generated by the (z_1^+, z_2) and (z_1^-, z_2) curves. Actually this requires $z_1 \geq 0$, i. e. $S \leq 1$. Back transformation gives the corresponding (S, E)-reachable sets shown in Figure 1. It should be noted that it also follows that the points on the boundary of the set are reached using control signals with only one switching point.

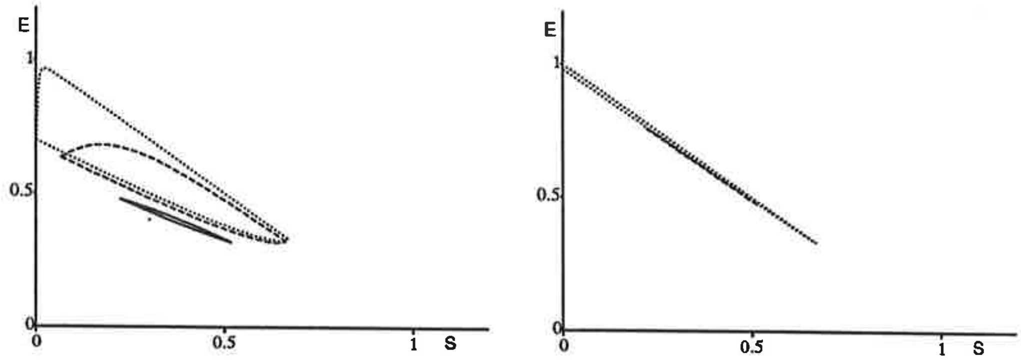

Figure 1. The reachable set as a function of time (left diagram: t=0, 0.3, 1.5, 5 and right diagram: t=0, 0.3, 5) for two different initial states.

Time Optimal Control

The reachable sets Ω can be used to develop optimal control strategies for different control objectives. In this section control to a set-point E_r in product concentration E is studied, and the criterion is chosen to be minimum time. As seen from the Figure 1. the sets increase their maximal E-value as time increases. For small t the maximum occurs at the lowest S-value, while the line $E = E_r$ is a tangent to the boundary curve, if a longer time is needed. The first case means that $u = 0$ is optimal, while the optimal control in the second case starts with a maximal u then switching to zero at time τ_1. Those starting values that correspond to a tangent in the leftmost point, i.e. a switching at $\tau_1 = 0$ generate a switching curve in the state space. Simple calculations show that this curve is the line

$$E = E_r(1 - S) \tag{10}$$

The reachable sets have their minimal point for maximal S, at least above the maximal possible stationary $E = \frac{1}{1+d}$. This corresponds to maximal control signal during the whole time interval, which is thus the optimal strategy when starting from $E > E_r$. In summary it is thus proven that the following strategy is time-optimal:

$$u = \begin{cases} 0 & E_r(1 - S) < E < E_r \\ d & \text{otherwise} \end{cases} \tag{11}$$

In Figure 2. is shown the time-optimal elimination of a small and large disturbance. Both state space trajectories and resulting time functions are shown, and for comparison a simulation of a proportional controller is given in Figure 3. Notice for the large disturbance case that the time-optimal regulator starts off in the opposite direction as compared to the proportional regulator.

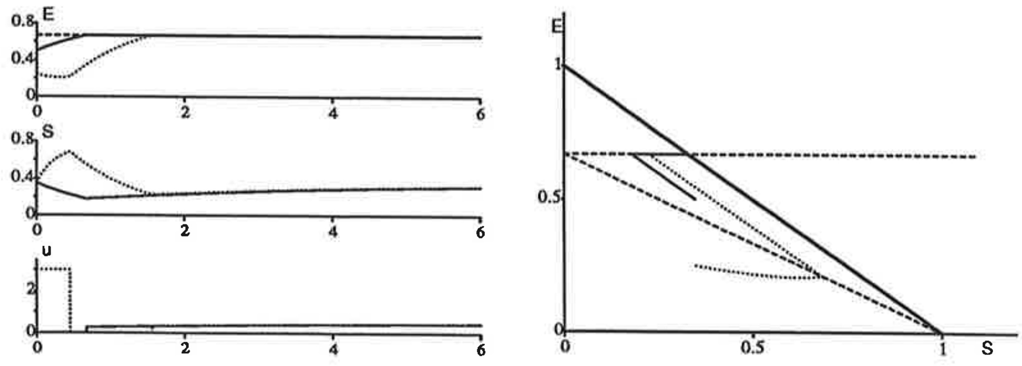

Figure 2. Time optimal elimination of a small and a large disturbance.

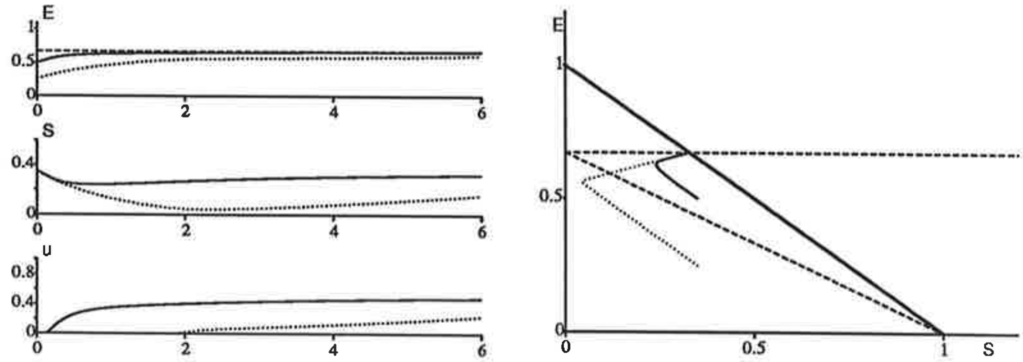

Figure 3. Elimination of a small and a large disturbance using limited proportional control.

Remark on exact linearization

The process model has a structure that at first sight suggests application of exact linearization, (Hunt, Su, and Meyer 1983). However, analysis shows that this methodology is of less value for design of the control law in this case.

The process model could be described as an interaction between a drift field f and a control field g

$$\dot{x} = f(x) + g(x)u(t) \tag{12}$$

where $x_1 = S$, $x_2 = E$ and

$$f(x) = \begin{pmatrix} -x_1 \\ x_1 \end{pmatrix} \qquad g(x) = \begin{pmatrix} 1 - x_1 \\ -x_2 \end{pmatrix} \tag{13}$$

Controllability can be analysed with the aid of Lie brackets (Isidori, 1985). A necessary condition for controllability is that g, f, $[f, g]$, $[f, [f, g]]$, $\ldots$, span the state space. Simple calculations give

$$\begin{aligned} [f, g] &= \frac{dg}{dx} f - \frac{df}{dx} g \\ &= \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} -x_1 \\ x_1 \end{pmatrix} - \begin{pmatrix} -1 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 - x_1 \\ -x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{aligned} \tag{14}$$

and further bracketing $[f,[f,g]],[f,[f,[f,g]]],\dots[g,[f,g]]\dots$ etc., gives no new directions. Thus, the condition for controllability becomes

$$\det\Big(\, g(x),[f,g](x)\,\Big) = \det\begin{pmatrix}1-x_1 & 1\\ -x_2 & -1\end{pmatrix} = -(1-x_1-x_2)\neq 0 \qquad (15)$$

This shows that there is no higher order controllability on the line (15). Further, outside this line the system is controllable.

The fact that the dimension of the controllability space shrinks to one on the line (15) implies, of course, that no non-singular transformation can bring the system to a controllable form.

An example of such a transformation is

$$\begin{aligned} z_1 &= x_1\cdot\frac{1-x_1-x_2}{(1-x_1)^2}\\ z_2 &= x_2\cdot\frac{1}{1-x_1}\end{aligned} \qquad (16)$$

and

$$u=\psi(x_1,x_2,v)=\frac{(1-x_1)^2}{1-x_1-x_2}\cdot v + x_1\cdot\frac{1+x_1}{1-x_1} \qquad (17)$$

which brings the system to the Brunovsky form

$$\dot z = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix} z + \begin{pmatrix}1\\ 0\end{pmatrix} v(t) \qquad (18)$$

Note, that the transformation is singular in two different ways. The stationary points (15) are mapped into a single point in the z-plane, $z=(0,1)$. Further, the control law (17) will be singular if for instance linear state feedback from z is used.

The fact that the control variable is non-negative further complicates application of exact linearization. It is not clear how this limitation should be accounted for.

Concluding remarks

The results of this paper were obtained to describe the reversed control action required for large disturbances and startup of a continuous ethanol fermentation, but they carry over to most reactions with immobilized catalyst in a stirred tank reactor.

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