THE EFFECT OF DISCRETIZATION ON THE PI CONTROL OF A TUBULAR REACTOR MODEL WITH AXIAL DIFFUSION

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Received: Aug. 6, 1994

Abstract

Various nonlinear behaviors, including chaos, may result from a tubular reactor with an exothermic reaction when a PI controller is added. In this paper, we show that for this highly nonlinear system the stable gains are very sensitive to the number of states used for controller design. The region of successful control is determined as a function of \(k_P\), \(k_I\), and the number of spatial discretizations.

Keywords: tubular reactor model.

Introduction

Traditionally, distributed parameter systems (DPS) have been approximated by finite dimensional systems in order to design adequate controllers. One of the most popular methods for making this approximation is finite differencing. While the basic finite difference premise of truncating a Taylor series expansion of the spatial derivatives is almost trivial, there is a lack of literature on how many discretizations are necessary to retain enough spatial information such that a stabilizing controller can be developed. Researchers who have designed controllers for DPS seem to have chosen only enough spatial states to accurately model the nonlinear uncontrolled system (Zweitering, 1992; Cetinkunt, 1991; Alatiqi, 1991). Choosing a small number of discretizations will result in a low order design model thus facilitating controller design and also give the added benefit of a low order controller.

An additional problem with previous controllers designed for DPS is that their performance has been tested on the discretized system and not on the actual system. This essentially eliminates any questions about the adequacy of the spatial modeling. After achieving successful control of the design model it is then assumed that this controller will also control the real plant. However, acceptable results from this approximate finite dimensional closed loop system may not be indicative of closed loop stability for
the full infinite dimensional system (Bontsema, 1988). When the finite difference approximation error exceeds the robustness margin of the controller, eigenvalue spillover may occur resulting in closed loop instability (Balas, 1978). In order to reduce this error, it is necessary to increase the number of spatial states, thus the order of the design model.

In this paper we show the relationship between the stable controller gains and the number of spatial discretizations used to design the controller. The performance of the controller, as measured by the rate of convergence to the set point, is also determined as a function of spatial states.

**PI Control of a Tubular Reactor**

The system is a model of the material and energy balances (Eq. (1)) for a non-catalytic tubular reactor with axial backmixing developed by Pellegrini et al. (1992). Heat from the exothermic first order reaction is removed by a constant temperature coolant $\theta_c$.

\[
\frac{\partial \zeta}{\partial t} = -\frac{\partial \zeta}{\partial \xi} + \frac{1}{Pe_M} \frac{\partial^2 \zeta}{\partial \xi^2} + \kappa_0 \tau (1 - |\zeta|) \exp \left( -\frac{E}{RT_{ad} \theta} \right),
\]

\[
\frac{\partial \theta}{\partial t} = -\frac{\partial \theta}{\partial \xi} + \frac{1}{Pe_T} \frac{\partial^2 \theta}{\partial \xi^2} + NTU (\theta - \theta_c) + \kappa_0 \tau (1 - |\zeta|) \exp \left( -\frac{E}{RT_{ad} \theta} \right).
\]

(1)

The corresponding boundary and initial conditions for this system are:

\[
\left( \zeta - \frac{1}{Pe_M} \frac{\partial \zeta}{\partial \xi} \right)_{\xi=0} = 0, \quad \left( \theta - \frac{1}{Pe_M} \frac{\partial \theta}{\partial \xi} \right)_{\xi=0} = \theta_0^*,
\]

\[
\left. \frac{\partial \zeta}{\partial \xi} \right|_{\xi=1} = 0, \quad \left. \frac{\partial \theta}{\partial \xi} \right|_{\xi=1} = 0.
\]

In the above set of equations, $\zeta$ is the conversion, $\theta$ is the nondimensionalized temperature, and $\xi$ represents the spatial dimension. It is assumed that the reader is familiar with the standard notation used in Eq. (1).

The first step taken in analyzing this system is to reduce the set of partial differential equations to a set of ordinary differential equations by using central differences. The system is discretized using $N$ grid points for the $\xi$ variable:
\[
\frac{\partial \zeta_i}{\partial t} = -\frac{(\zeta_{i+1} - \zeta_{i-1})}{2\Delta \xi} + \frac{1}{\text{Pe}_M} \frac{(\zeta_{i+1} - 2\zeta_i + \zeta_{i-1})}{\Delta \xi^2} + \kappa_0\tau (1 - \zeta_i) \exp \left( -\frac{E}{R\Delta T_{ad}\theta_i} \right),
\]
\[
\frac{\partial \theta_i}{\partial t} = -\frac{(\theta_{i+1} - \theta_{i-1})}{2\Delta \xi} + \frac{1}{\text{Pe}_T} \frac{(\theta_{i+1} - 2\theta_i + \theta_{i-1})}{\Delta \xi^2} - \text{NTU} (\theta_i - \theta_c) + \kappa_0\tau (1 - \zeta_i) \exp \left( -\frac{E}{R\Delta T_{ad}\theta_i} \right).
\]

(2)

The open loop system is simulated using \( N = 20 \) as the truth model and is shown in Fig. 1. Simulation results with \( N = 5 \) are also shown in Fig. 1 and are indiscernible from the \( N = 20 \) case. All parameter values are the same as in Pellegrini (1992). It is observed that the steady state outlet conversion is close to zero and thus very little reaction is taking place.

In an effort to increase the outlet conversion, a proportional plus integral (PI) controller is added so the output temperature can be driven to a set point resulting in increased conversion. The control scheme measures the outlet temperature \( (\theta \text{ at } \xi = 1) \) and manipulates the feed temperature, \( \theta_0^* \). The controller is described by Eq. (3).

\[
\Delta \theta_0^* = -k_p \Delta \theta_N - k_I \int_0^{t^*} \Delta \theta_N \, dt.
\]

(3)

Fig. 2 shows the values for the proportional and integral gains which should yield successful control based on different number of spatial discretizations. In other words, we select an \( N \) which we assume is sufficient to model the spatial dimension and predict that gains to the right of the line shown will yield a stable controller for the actual infinite dimensional system. Note that as the number of states used in developing the design model is increased, the amount of shift in the border of the region of successful control decreases. Thus Fig. 2 shows the convergence to an adequate number of spatial discretizations for controller design. As can be seen in Fig. 2, if the controller is designed based on too few spatial states, then the allowable proportional gain will be overpredicted and the allowable integral gain will be underpredicted. Thus the real plant will require less proportional gain and more integral gain than predicted by using a low order model.

An example of successful control of the actual plant (simulated using \( N = 20 \) as the truth model) is shown in Fig. 3 for \( k_p = 0.02 \) and \( k_I = 0.5 \).
Fig. 1. Time series of outlet temperature and outlet conversion for the open loop system of Eq. (1) using $N = 20$ as the truth model and $N = 5$ for comparison.
These values for the gains are within the stable region for all $N$ shown in Fig. 2. As shown in Fig. 3, successful control to almost complete conversion is quickly achieved.

For an example of what can happen when too few spatial discretizations are used to determine the controller gains, consider a design model created using five spatial states. From Fig. 2, the values of $k_p = 0.05$ and $k_I = 0.4121$ are well within the stable gain region for this case. However, when the controller developed using these gains is applied to the $N = 20$ truth model, chaotic behaviour as shown in Fig. 4 results. Because the system is nonlinear, the closed-loop system actually exhibits a wide range of periodic and aperiodic behaviour for different values of $k_p$ and $k_I$ (Pellegrini, 1992).

In order to gauge the performance of the PI controller, we examined the amount of time for the closed loop system to achieve steady state. In Figs. 5, 6, and 7 the amount of proportional gain is held fixed at 0.01, 0.03, and 0.05, respectively. The time to steady state is then plotted as a function of integral gain and the number of spatial discretizations used in the design model. In Fig. 5 and 6 it should be noted that there is no significant difference between time to steady state and the order of the design model. It is only in Fig. 7 where we are able to see a complex and dramatic change in time to steady state as a function of $N$. A full explanation for this phenomenon is not available at this time.
Fig. 3. Time series of outlet temperature and outlet conversion for the closed loop system with $N = 20$, $k_p = 0.02$ and $k_r = 0.5$.
Fig. 4. Chaos in closed loop system with \( k_P = 0.05, k_I = 0.4121 \) and \( N = 20 \)

Fig. 5. Time to steady state as a function of \( k_I \) and the number of discretizations used in the design model, \( k_P = 0.01 \)
Fig. 6. Time to steady state as a function of $k_I$ and the number of discretizations used in the design model, $k_P = 0.03$

Fig. 7. Time to steady state as a function of $k_I$ and the number of discretizations used in the design model, $k_P = 0.05$
Conclusion

It has been demonstrated that successful control of a DPS is sensitive to the number of spatial states used in the controller design model. For central difference approximations, the number of spatial states needed for a controller design model is much greater than the number needed for an accurate open loop simulation. When controllers are designed using too low of an order design model, the resulting system may not behave as desired. In the case of nonlinear systems this undesirable behaviour may lead to periodic or chaotic behaviour.

References


