Nonlinear State Estimation of Packed-Bed Tubular Reactors

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Packed-bed tubular reactors are characterized by nonlinear behavior, limited on-line measurements, and stiff dynamics. Because of the limited number of temperature and composition sensors normally available, state estimation algorithms would be a desirable part of the reactor control system. However, to complicate matters, the thermal transients are usually several orders of magnitude slower than the concentration transients, thus leading to very stiff distributed parameter modeling equations. In spite of a number of reported state estimation studies of this class of problems, a good understanding of the structure of the problem has not come forth, and the previously published results have important practical limitations. In this note we shall illustrate how recently developed, general, theoretical results (Soliman and Ray, 1978) can be profitably applied to this problem and help elucidate the structure of these state estimation problems.

To illustrate the essential features of the problem, we shall choose to study a simple reactor in which a first-order, irreversible, exothermic reaction is taking place. We shall assume a pseudohomogeneous axial dispersion model for the reactor

$$\frac{\partial x_1(z,t)}{\partial t} = \frac{1}{Pe_H}\frac{\partial x_1^2}{\partial z^2} - \frac{\partial x_1}{\partial z} + BDa_0 x_2 e^{-\gamma/x_1} - H(x_1 - x_{1c}) + \xi_1(z,t) \quad (1)$$

$$\epsilon\frac{\partial x_2(z,t)}{\partial t} = \frac{1}{Pe_M}\frac{\partial^2 x_2}{\partial z^2} - \frac{\partial x_2}{\partial z} - Da_0 x_2 e^{-\gamma/x_1} + \xi_2(z,t) \quad (2)$$

$$\left.\begin{aligned}\frac{1}{Pe_H}\frac{\partial x_1}{\partial z} &= x_1 - 1\\ \frac{1}{Pe_M}\frac{\partial x_2}{\partial z} &= x_2 - 1\end{aligned}\right\} z = 0 \quad (3)$$

$$\frac{\partial x_1}{\partial z} = \frac{\partial x_2}{\partial z} = 0; \quad z = 1 \quad (4)$$

Normally, $\epsilon << 1$ holds for packed-bed reactors. The quantities ξ_1 and ξ_2 formally represent additive random noise to the process model.

If we assume temperature measurements at m_1 spatial positions z_k^*, $k = 1, 2, \ldots m_1$, and concentration measurements at m_2 spatial locations z_k^{**}, $k = 1, 2, \ldots m_2$, then these sensors take the form

$$y_{1k} = x_1(z_k^*, t) + \eta_{1k}(t) \quad k = 1, 2, .. m_1 \quad (5)$$

$$y_{2j} = x_2(z_j^{**}, t) + \eta_{2j}(t) \quad j = 1, 2, .. m_2 \quad (6)$$

where the $\eta_{ij}(t)$ are random measurement errors.

Most of the previous studies of this class of problems (for example, Goldman and Sargent 1971; Joffe and Sargent, 1972; McGreavy and Vago, 1972; Sørensen, 1977; Jutan et al., 1977) have taken the following approach. First, discretize (in space) and linearize the system equations and then apply classical lumped parameter Kalman filtering theory to the resulting linear equations, where $\epsilon = 0$ is assumed for the concentration equations. This approach suffers from several disadvantages:

1. The linearized state estimator will not give good results for highly nonlinear systems and for large disturbances from the nominal steady state.

2. There is the danger that essential features of the problem will be lost through brute force discretization. A theoretical analysis of the full partial differential equations is safer and is to be preferred.

3. There is a similar danger in just setting $\epsilon = 0$ and applying the state estimation theory to the degenerate equations. This procedure usually gives incomplete and sometimes even incorrect results (for example, Haddad and Kokotovic, 1971). In particular, the estimator resulting from setting $\epsilon = 0$ does not allow dynamic estimates of the fast variables (x_2 here) or the proper treatment of composition measurements.

Two papers (Ajinkya et al., 1974; Ramirez, and Clough, 1976) have appeared in which the full distributed nature of the problem is treated. In the first paper, only the catalyst activity profile was estimated, while the gas phase concentrations were not estimated but measured. Thus, the problem of two time scales did not arise. In the second paper, state estimation of concentration was attempted using an incorrect algorithm, and rather poor filter performance was reported. A third recent paper describes studies of distributed parameter observers applied to the packed-bed estimation problem (Zeitz, 1977) and reports reasonable estimates with sufficient temperature measurements.

In contrast to earlier estimation algorithms, our recent results, reported in more generality and mathematical detail elsewhere (Soliman and Ray, 1978), allow the estimation problem to be decomposed into two time scales with two state estimators, one for the fast variables alone and one for the slow variables. In addition, our results allow, for the first time, the proper inclusion of concentration measurements into the filtering equations for $\epsilon \to 0$. To illustrate these results, the resulting state estimator for the packed-bed reactor system (1) to (6) takes the form

Fast estimator:

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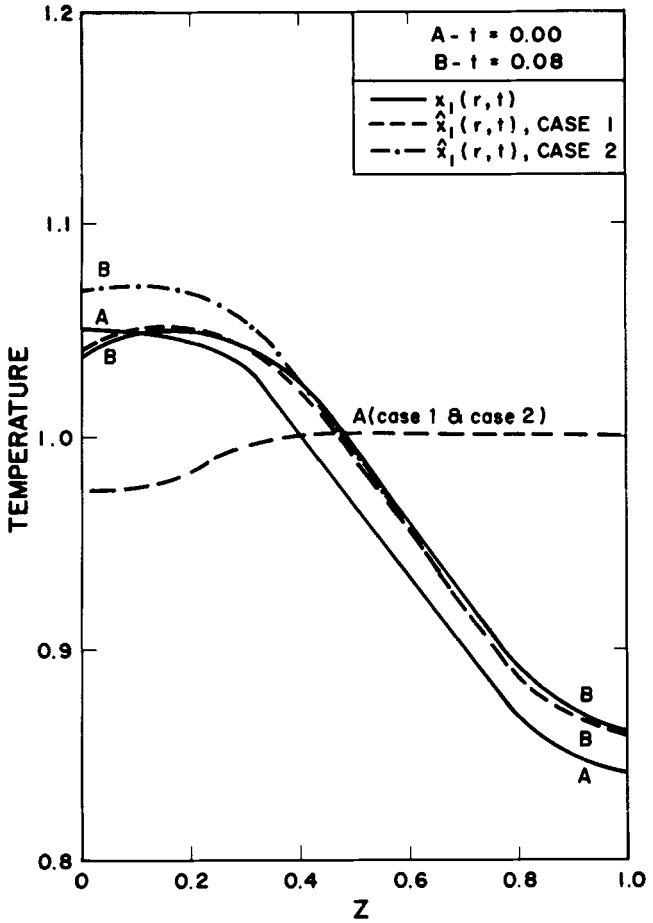

Fig. 1. Temperature estimates from the slow filter for two different levels of measurement information.

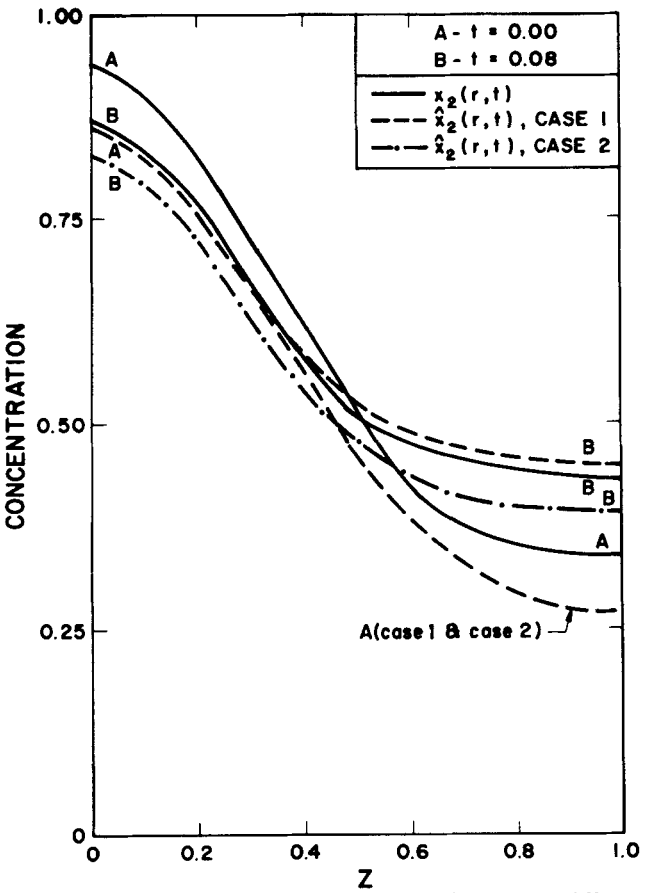

Fig. 2. Concentration estimates from the slow filter for two different levels of measurement information.

$$\frac{\partial \hat{x}_2(z,\tau)}{\partial \tau} = \frac{1}{Pe_M}\frac{\partial^2 \hat{x}_2}{\partial z^2} - \frac{\partial \hat{x}_2}{\partial z} - Da_0 x_2 e^{-\gamma/\hat{x}_1} + \sum_{i=1}^{m_2} \hat{P}^{22}(z, z_i^{**}, \tau) Q_{22}[y_{2i}(\tau) - \hat{x}_2(z_i^{**}, \tau)] \quad (7)$$

$$\frac{1}{Pe_M}\frac{\partial \hat{x}_2}{\partial z} = \hat{x}_2 - 1 \quad z = 0 \quad (8)$$

$$\frac{\partial \hat{x}_2}{\partial z} = 0 \quad z = 1 \quad (9)$$

where $\tau = t/\epsilon$ is an expanded time scale for the fast estimates.

Slow estimator:

$$\frac{\partial \hat{x}_1(z,t)}{\partial t} = \frac{1}{Pe_H}\frac{\partial^2 \hat{x}_1}{\partial z^2} - \frac{\partial \hat{x}_1}{\partial z} + BDa_0 \hat{x}_2 e^{-\gamma/\hat{x}_1} - H(\hat{x}_1 - x_{1c}) + \sum_{i=1}^{m_1} P^{11}(z, z_i^*, t) Q_{11}[y_{1i}(t) - \hat{x}_1(z_i^*, t)] + \sum_{j=1}^{m_2} P^{12}(z, z_j^{**}, t) Q_{22}[Y_{2j}(t) - \hat{x}_2(z_j^{**}, t)] \quad (10)$$

$$0 = \frac{1}{Pe_M}\frac{\partial^2 \hat{x}_2(z,t)}{\partial z^2} - \frac{\partial \hat{x}_2}{\partial z} - Da \hat{x}_2 e^{-\gamma/\hat{x}_1} + \sum_{i=1}^{m_2} \hat{P}^{22}(z, z_i^{**}, t) Q_{22}[y_{2i}(t) - \hat{x}_2(z_i^{**}, t)] \quad (11)$$

with boundary conditions given by Equations (3) and (4). The filter parameters P^{11}, P^{12}, P^{22}, and $\hat{P}^{22}$ are obtained by solving a set of partial differential Riccati equations containing least-squares weighting parameters Q_{11} and Q_{22} which represent error statistics. Note that while the fast estimator gives only dynamic concentration estimates, the slow estimator gives slow estimates of both temperature and concentration. For some applications, only the slow estimator would be required if the time scale of interest was minutes rather than a few seconds. Thus, one may choose the level of complexity desired in a particular application.

To demonstrate the state estimator performance with practical levels of measurement, numerical simulations were carried out for the following set of parameters:

$$Pe_M = Pe_H = 30, \quad BDa_0 = 12\,000, \quad Da_0 = 20\,000,$$
$$\gamma = 10, \quad H = 2, \quad x_{1c} = 0.8, \quad \text{and} \quad \epsilon = 0.01$$

Two different cases are presented here:

Case 1: there are three temperature sensors in the bed [$z^{*T} = (0.25, 0.5, 1.0)$] and one concentration sensor at the reactor exit.

Case 2: no concentration measurements are possible, but temperature measurements are available as in case 1.

In both cases, random errors were added to the sensor signals from a Gaussian random number generator having zero mean and standard deviation, $\sigma = 0.02$.

Although the fast filter worked well for cases where more concentration measurements were available (for example, Soliman and Ray, 1978), for the results shown here, the fast filter did not converge. This is not surprising in case 2, where there are no concentration measurements, since one would not expect the fast concentration dynamics to be observable without direct concentration measurements. For case 1, it is likely that a single exit concentration sensor is not sufficient for system observability.

The slow filter performance, shown in Figures 1 and 2, was quite acceptable in both cases. Note that both the temperature and the quasi-steady-state concentration estimates converge quickly to the true profiles in case 1, while for case 2 the estimates are less accurate but reasonable.

This example suggests that slow state estimates will perform acceptably, even in the case of no direct concentration measurements, but will perform significantly better with one or more composition sensors. The fast state estimator, which would be needed to follow fast concentration dynamics, requires more than one concentration sensor for good performance. However, in many applications the fast estimator would not be required, particularly if feed concentration were not a control variable.

Presently work is underway in our laboratory to test these algorithms on-line in real time with pilot scale reactors.

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NOTATION

B = dimensionless heat of reaction
Da_0 = reference Damköhler number
H = dimensionless heat transfer coefficient
P = differential sensitivity filter parameter
Pe_H = Peclet number for heat transfer
Pe_M = Peclet number for mass transfer
Q = filter parameter
t = dimensionless time
x_1 = dimensionless reactant temperature
x_{1c} = dimensionless coolant temperature
x_2 = dimensionless reactant concentration
y_1 = temperature measurement
y_2 = concentration measurement
z = dimensionless length along the reactor

Greek Letters

γ = dimensionless activation energy
η = measurement error
ξ = model error
ϵ = ratio of reactor residence time and thermal time constant
τ = t/ϵ

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The Expansion of a Fluidized Bed Containing Biomass

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Much interest has been shown recently in treating wastewater by passing it through a fluidized bed of particles on which a bacterial film is growing. The possibilities of such systems were first demonstrated by Freidman et al. (1971) in their work on the importance of bacterial growth in beds of activated carbon. Beds of coal and sand have