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SHORT COMMUNICATION

A STUDY OF THE DYNAMIC BEHAVIOR OF DISPERSION-TYPE TUBULAR REACTOR MODELS

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Abstract – The dynamic behavior of dispersion-type tubular reactors, referred to as finite and truncated models depending on the boundary condition representations at the reactor exit, was investigated through numerical simulations. It was found that the dynamic behavior of the two models can be identical or different depending on how the *Péclet* number changes.

Key words: Dispersion-Type Tubular Reactor, Dynamic Behavior, Boundary Condition

INTRODUCTION

In modeling dispersion-type tubular reactors, either steady-state or dynamic, a well-established and popularly used model is one with the gradient boundary condition at the exit set to zero: dc/da = 0. On the other hand, another model, not often used, is one with the gradient set to zero at infinity and the solution is truncated at the real reactor exit.

For steady-state cases, the difference in the behavior of the two models has been compared extensively with various values of *Péclet* number (*Pe*) and *Damköhler* number (*Da*) [Chang et al., 1982]. A comparison of dynamic behavior, on the other hand, has not yet appeared in the literature. We investigate and compare the dynamic behavior of the two models. For brevity, we shall call one model a finite model and the other a truncated model.

FINITE TUBULAR REACTOR MODEL

A well-known general mathematical description of axial dispersion-type tubular reactors is given in dimensionless form by the following partial differential equation:

$$\frac{\partial c}{\partial t} = \frac{1}{Pe}\frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} - f(c). \tag{1}$$

Initial condition: $c(z, 0) = g(z)$ (2)

Boundary conditions:

at the entrance (z=0) $$\frac{1}{Pe}\frac{\partial c}{\partial z} - c(0,t) = -h(t) \tag{3}$$

at the exit (z=1) $$\frac{1}{Pe}\frac{\partial c}{\partial z} = 0 \tag{4}$$

where c(z, t) is the reactant concentration at position z and time t; f(c) the reaction rate term; g(z) the initial concentration distribution in the reactor; and h(t) the feed concentration to the reactor at the inlet.

The analytical solution to this widely used and well-known model when $f(c)=Da \cdot c$ (the first-order reaction) is given in Godsalve and Chang [1980] as

$$c(z,t) = \exp\left[\frac{Pe}{2}z - \left(\frac{Pe}{4} + Da\right)t\right] \cdot \sum_{k=1}^{\infty} \exp\left[-\frac{\alpha_k^2}{Pe}t\right] \cdot \frac{2\alpha_k \cos(\alpha_k z) + Pe \sin(\alpha_k z)}{\alpha_k^2 + \frac{Pe^2}{4} + Pe}$$
$$\left\{\frac{1}{2}\int_0^1 g(z)\exp\left(-\frac{Pe}{2}z\right) \cdot [2\alpha_k \cos(\alpha_k z) + Pe \sin(\alpha_k z)]dz + \alpha_k \int_0^t h(\tau)\exp\left[\left(\frac{\alpha_k^2}{Pe} + \frac{Pe}{4} + Da\right)\tau\right]d\tau\right\} \tag{5}$$

where the eigenvalue α_k is the k^{th} positive root of the transcendental equation:

$$\tan\alpha = \frac{Pe \cdot \alpha}{\alpha^2 - \frac{Pe^2}{4}} \tag{6}$$

TRUNCATED TUBULAR REACTOR MODEL

Although the overwhelming majority of researchers and engineers in the past have used the finite dispersion-type tubular reactor model, some researchers have had reservations about using the exit boundary condition stated above. The main reason seems to be that the reactant going through the reactor cannot see the reactor exit in advance and adjust its concentration gradient to be exactly zero at the exit.

An alternative approach then is to imagine the concentration gradient reaches equilibrium (dc/dz=0 or c=0) only at the end of an infinitely long reactor. Since a tubular reactor is of a finite length, the concentration obtained is truncated at the

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real reactor exit. For this case, the reactor model in dimensionless form becomes

$$\frac{\partial c}{\partial t} = \frac{1}{Pe}\frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} - f(c). \tag{7}$$

Initial condition: $c(z, 0)=g(z)$ (8)

Boundary conditions:

at the entrance (z=0) $$\frac{1}{Pe}\frac{\partial c}{\partial z} - C(0, t) = -h(t) \tag{9}$$

at the exit (z=∞) $$\frac{1}{Pe}\frac{\partial c}{\partial z} = 0 \tag{10}$$

The difference of this model from the former one is the position ($z\to\infty$) of the exit boundary condition. For this model with $f(c)=Da \cdot c$, the analytical solution is rather complicated, but presented again in Godsalve and Chang [1980] as

$$c(z, t) = \exp\left[-\left(\frac{Pe}{4} + Da\right)t\right] \cdot \int_0^\infty G_1(z, t, \xi)g(\xi)d\xi + 2\exp\left(\frac{Pe}{2}z\right)\int_0^t G_2(z, t-\tau)h(\tau)d\tau \tag{11}$$

where

$$G_1(z, t, \xi) = \exp\left[\frac{Pe}{2}(z-\xi)\right] \cdot \left\{\frac{1}{\sqrt{\pi}}\frac{\sqrt{Pe}}{4t}\left(\exp\left[-\frac{Pe(z-\xi)^2}{4t}\right] + \exp\left[-\frac{Pe(z+\xi)^2}{4t}\right]\right) - \frac{Pe}{2}\exp\left[\frac{Pe}{4}t + \frac{Pe}{2}(z+\xi)\right] \operatorname{erfc}\left[\sqrt{\frac{Pe}{4t}}(z+\xi) + \sqrt{\frac{Pe \cdot t}{4}}\right]\right\} \tag{12}$$

$$G_2(z, t-\tau) = \exp\left[-\left(\frac{Pe}{4} + Da\right)(t-\tau)\right] \left\{\frac{1}{\sqrt{\pi}}\sqrt{\frac{Pe}{4t}}\exp\left[-\frac{Pe \cdot z^2}{4(t-\tau)}\right] - \frac{Pe}{4}\exp\left[\frac{Pe}{2}z + \frac{Pe}{4}(t-\tau)\right] \operatorname{erfc}\left[z\sqrt{\frac{Pe}{4(t-\tau)}} + \sqrt{\frac{Pe(t-\tau)}{4}}\right]\right\} \tag{13}$$

and ξ, τ are dummy auxiliary variables for position and time, respectively.

METHODS FOR THE NUMERICAL EVALUATION

Computationally, the numerical evaluation of the analytical solutions for both models is unnecessarily involved and therefore extremely unattractive. As we see in the analytical solution of the finite model, Eq. (5), although the expression appears to be neat, the real task of evaluating a sufficient number (sometimes 3000) of eigenvalues consumes a great deal of computing time, depending on the values of *Pe* [Choe and Chang, 1995]. Furthermore, for the truncated model, the analytical solution Eq. (11) involves a complicated evaluation of the *erfc* function. Thus, a numerical evaluation of the analytical solutions of both models is not very practical.

A simple and straightforward shortcut to solve Eqs. (1)-(4) and Eqs. (7)-(10) numerically is by the Crank-Nicolson method [Mitchell and Griffiths, 1980]. For the finite model when the central difference for the spatial derivative with suitable space and time increments (Δz=0.005, Δt=0.005) is used, the dynamic solutions for $f(c)=Da \cdot c$, $g(z)=0$, and the unit step change in the inlet concentration, $h(t)=1$ ($t>0$), are obtained as solid lines shown in Fig. 1 for Pe=100 and Fig. 2 for Pe =1, each with Da=0.1 and 1. Solid lines in Fig. 3 show the effect of the values of Pe (Pe=100 and 0.1) when Da=0.1 for the finite model. This numerical approach is much more convenient than the evaluation of the analytical solution of Eq. (5) with the calculation of eigenvalues from the transcendental equation in Eq. (6).

Unlike the finite model, the truncated model as given above is not malleable to yield easy numerical solutions because of the boundary condition at infinity ($z\to\infty$). This situation, how-

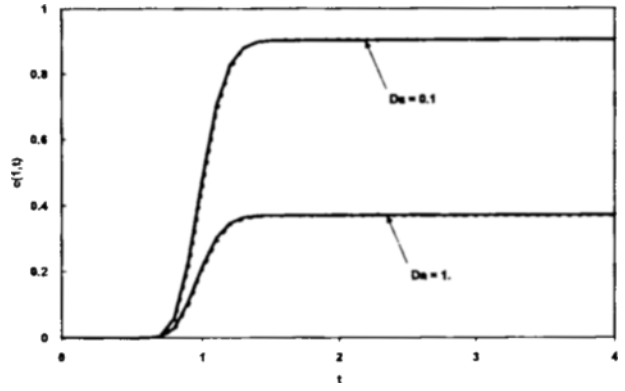

Fig. 1. The exit concentration response to the unit step change in the inlet concentration for Pe=100 with Da=0.1 and 1.
—: Finite model, ···: Truncated model

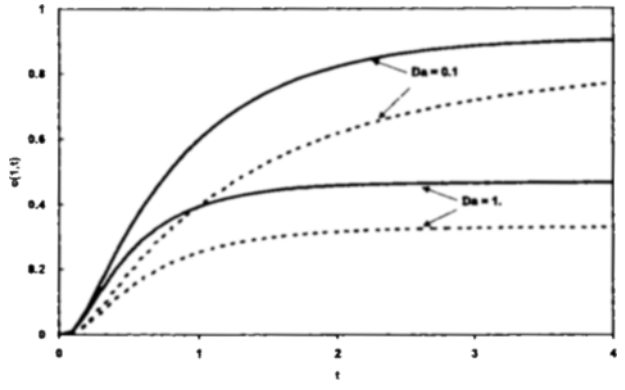

Fig. 2. The exit concentration response to the unit step change in the inlet concentration for Pe=1 with Da=0.1 and 1.
—: Finite model, ···: Truncated model

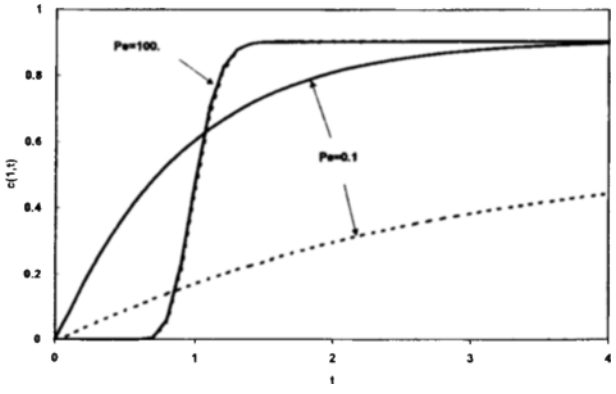

Fig. 3. The exit concentration response to the unit step change in the inlet concentration for *Da*=0.1 with *Pe*=100 and 0.1.
—: Finite model, ···: Truncated model

ever, can be alleviated by proposing the following coordinate transformation:

$$z = \frac{y}{2-y}, \quad (0 \le z \le \infty \Leftrightarrow 0 \le y \le 2). \tag{14}$$

This transformation not only eliminates the difficulty of the infinity boundary condition but also is amenable to the straightforward Crank-Nicolson method. With this transformation, Eqs. (7)-(10) become:

$$\frac{\partial c}{\partial t} = \frac{1}{Pe}\left[\frac{(2-y)^4}{4}\right]\frac{\partial^2 c}{\partial y^2} - \left[\frac{1}{Pe}\,\frac{(2-y)^3}{2} + \frac{(2-y)^2}{2}\right]\frac{\partial c}{\partial y} - f(c). \tag{15}$$

Initial condition: $c(y, 0)=g(y)$ (16)

Boundary conditions:

at the entrance (y=0) $$\frac{2}{Pe}\frac{\partial c}{\partial y} - c(0,t) = -h(t) \tag{17}$$

at the exit (y=2) $$\frac{1}{Pe}\frac{\partial c}{\partial y} = 0 \tag{18}$$

With this transformation, the truncated real reactor exit is now at y=1 which coincides conveniently with z=1. When the central difference for the spatial derivative with suitable space and time increments (Δz=0.005, Δt=0.005) is used, dynamic solutions for $f(c)=Da\cdot c$, g(z)=0, and a step change in the inlet concentration, h(t)=1 (t>0), are obtained as dotted lines shown in Fig. 1 for *Pe*=100 and Fig. 2 for *Pe*=1, with *Da*=0.1 and 1, respectively. Dotted lines in Fig. 3 show the effect of the values of *Pe* (*Pe*=100 and 0.1) when *Da*=0.1 for the truncated model.

Besides the Crank-Nicolson method, the method of lines [Schiesser, 1991] by means of a DSS/2 package [Schiesser, 1985] for double checking, produced the same solutions. For the method of lines, the Runge-Kutta-Niesse method was used for the time domain integration, the three point centered difference approximation was chosen for the second order spatial derivatives, and the four-point biased-upwind difference approximation was used for the first order spatial derivatives of both models [Choe et al., 1995].

RESULTS AND DISCUSSION

Figs. 1, 2 and 3 show the dynamic behavior for various values of *Pe* and *Da*, where we can compare the dynamic behavior of the two models. Solid lines are the solutions of the finite model and dotted lines are the solutions of the truncated model.

Figs. 1 and 2 show the dynamic behavior of the finite and the truncated models for *Pe*=100 and 1, respectively, with varying values of *Da* (*Da*=0.1 and 1). Fig. 1 shows that when the dispersion is not significant (*Pe*=100), the two models have almost identical dynamic behavior independent of the reaction rate (the values of *Da*). Fig. 2 shows that when the dispersion becomes significant (*Pe*=1), the dynamic behavior of the two models diverges from each other. We see the truncated model always gives lower dynamic concentration profiles than the finite model and their final steady states are different.

Fig. 3 shows the dynamic behavior when *Da*=0.1 with *Pe* =100 and 0.1. Again we see that for large values of *Pe* (*Pe*= 100) the dynamic behavior of the two models coincides. For smaller values of *Pe* (*Pe*=0.1), however, the difference in the dynamic behavior is significant.

The choice of the dynamic model depends on the circumstance of the problems posed and may be left to the discretion and judgment of the researcher, bearing in mind the difference in the dynamic behavior depends on the parameters. For example, when *Pe* is large, it makes no difference between the two models; when *Pe* is small, there is a significant difference in dynamic behavior between the two models.

The same technique above can be used for nonlinear reaction problems. The transformation proposed will alleviate the difficulty imposed by the boundary condition at infinity.

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NOMENCLATURE

c : the reactant concentration
Da : *Damköhler* number
f : the reaction rate term
g : the initial concentration distribution in the reactor
h : the feed concentration to the reactor at the inlet
Pe : *Péclet* number
y : transformed position for z
z : position
t : time
ξ : dummy auxiliary variable for position
τ : dummy auxiliary variable for time

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