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A second-order approximate solution of the reaction–diffusion process in spherical porous catalyst

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Abstract
The model for coupled diffusion and nth-order reaction in spherical catalyst pellet was solved using second-order polynomial model. The approximate solution is also validated by comparing the results with data from exact solution. Approximate solution was in good agreement for describing the reactant concentration distribution inside the particles for lower Φ. The results have indicated that the method proposed here could be of value for a quick estimation of reactant distribution and effectiveness factor of some systems with lower Φ such as oxygen transport into natural mycelial pellets in submerged cultures.

Keywords: Second-order approximate solution, Diffusion–reaction, Modeling, Effectiveness factor.

Introduction

An approximate solution to a differential equation in the form of an analytic expression can be found by the some methods such as method of series (power series, trigonometric series, and so on). Termination of the process after a finite number of steps yields an approximate solution. If a solution is represented by means of an infinite series, a finite portion of the series can be taken as the approximate solution [1, 2].

Approximate methods are often applied, even when an analytical solution is at hand, owing to the complexity of the exact solution. For example, when an eigenvalue expression requires trial–error solutions in terms of a parameter then the numerical works require to successfully using the analytical solution may become more intractable than a full numerical solution would have been. If this is the case, solving the problem directly by approximate techniques is attractive since it may be less tending to human error than the analytical counterpart [3].

Linear approximation methods are useful to characterize certain aspects of the dynamic properties of complicated models. First-order approximations provide adequate answers to questions such as local existence and determinacy of equilibrium and the size of the second moments of endogenous variables [4].

Diffusion and conduction in disordered media have received a lot of interest [5]. In general, satisfactory results can be reached by using the few terms of the approximate, series, solution [6]. The model for coupled diffusion and reaction in porous catalyst pellets generates a typical differential equation in chemical engineering. Thiele [7] obtained the analytical solution for the first order reaction in 1939, and then Wheeler [8] and Aris [9], etc. discussed this problem in details in their books. However, most of their conclusions were based on the analytical solution for the irreversible reaction with the first reaction order [10].

The main goal of the present paper is to give approximate solution of nth-order reaction which represents the case of the mathematical model in a spherical porous catalyst.

Problem formulation

At isothermal conditions, the steady regime of the nth-order reaction-diffusion process in the spherical geometric pellet is governed by dimensionless form, with the independent variable having the domain from 0 to 1.

By defining the following nondimensional variables and parameters [11]:

$$y = \frac{C}{C_s} \qquad x = \frac{r}{R} \tag{1}$$

The mass balance equation and the boundary conditions take the following clean form:

$$\frac{d^2y}{d^2x} + \frac{2}{x}\frac{dy}{dx} - \phi^2 y^n = 0 \tag{2}$$

$$x = 0 \qquad \frac{dy}{dx} = 0 \tag{3}$$

$$x = 1 \qquad y = 1 \tag{4}$$

$$\phi = \left(\frac{kR^2 C_s^{\,n-1}}{D_e}\right)^{\frac{1}{2}} \tag{5}$$

where Φ denotes the Thiele modulus. Cs is the reactant concentration in surface of catalyst pellet, De the effective diffusion coefficient for reactant, and k the reaction rate constant.

The quantities of physical interest are the concentration in the center of catalyst

$$x=0 \qquad y=Y_0 \tag{6}$$

Also, in the theory of chemical reaction engineering in spherical geometry, the effectiveness factor is defined as [11, 12].