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Exact analytical solution of a nonlinear reaction–diffusion model in porous catalysts

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ABSTRACT

In two papers published recently in Chemical Engineering Journal, [Y.P. Sun, S.B. Liu, S. Keith, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by decomposition method, Chem. Eng. J. 102 (2004) 1–10; S. Abbasbandy, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by means of the homotopy analysis method, Chem. Eng. J. 136 (2008) 144–150], a nonlinear model of diffusion and reaction in porous catalysts has been investigated by approximate analytical methods (the Adomian decomposition method, [Y.P. Sun, S.B. Liu, S. Keith, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by decomposition method, Chem. Eng. J. 102 (2004) 1–10] and the homotopy analysis method, [S. Abbasbandy, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by means of the homotopy analysis method, Chem. Eng. J. 136 (2008) 144–150], respectively). The present paper shows, however, that the model is exactly solvable in terms of Gauss' hypergeometric function. The exact solution is illustrated by specific examples. Several new physical features are reported and discussed in detail.

1. Introduction and problem formulation

The aim of the present paper is to give the exact analytical solutions of a nonlinear diffusion-reaction model investigated in the recent literature extensively by different approximation methods [1,2].

The model considered by Sun et al. [1] and Abbasbandy [2] describes the *steady* diffusion-reaction regime in a porous slab with plane boundaries at $X=0$ and $X=L$, respectively. The concentration distribution of the reactant, $C=C(X)$ satisfies the differential equation

$$D_e \frac{d^2C}{dX^2} - r(C) = 0 \tag{1}$$

where the reaction rate per unit volume r is a power law function of the concentration,

$$r = kC^n \tag{2}$$

The admitted range of the reaction order is $n \geq -1$. The boundary at $X=0$ is impermeable (vanishing mass flux) and that at $X=L$ is held at a constant concentration C_S,

$$D_e \left.\frac{dC}{dX}\right|_{X=0} = 0, \quad C|_{X=L} = C_S \tag{3}$$

In terms of the dimensionless variables

$$x = \frac{X}{L}, \quad c(x) = \frac{C(X)}{C_S} \tag{4}$$

the boundary value problems (1)–(3) is specified by equations

$$\frac{d^2c}{dx^2} - \phi^2 c^n = 0 \tag{5}$$

$$\left.\frac{dc}{dx}\right|_{x=0} = 0, \quad c|_{x=1} = 1 \tag{6}$$

where $\phi = (kL^2 C_S^{n-1}/D_e)^{1/2}$ denotes the Thiele modulus.

Approximate series solutions of the one-dimensional nonlinear boundary value problem (5), (6) have been given recently for different values of the parameters n and ϕ with the aid of Adomian's decomposition method and the homotopy analysis method by Sun et al. [1] and by Abbasbandy [2], respectively. The present paper gives the exact analytical solutions in terms of Gauss' hypergeometric function. For a comprehensive review of more general reaction diffusion problems in porous catalysis, see e.g. Ref. [3].

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Nomenclature

c	dimensionless concentration
C	concentration
C_S	prescribed concentration at $X = L$
D_e	effective diffusion coefficient
F	Gauss' hypergeometric function
k	reaction rate constant
K	integration constant
L	thickness of porous slab
m	$n + 1$
n	reaction order
q_M	mass flux at $X = L$
r	reaction rate per unit volume
u	variable of integration
x	dimensionless transversal coordinate
X	transversal coordinate
Greek symbols	
Γ	Euler's Gamma function
ϕ	$= (kL^2 C_S^{n-1}/D_e)^{1/2}$, Thiele modulus
Subscript/superscript	
Prime	differentiation with respect to x
0	at the boundary $x = 0$

2. The exact solution for $n > -1$

One easily sees that Eq. (5) admits the first integral

$$\frac{1}{2}\left(\frac{\mathrm{d}c}{\mathrm{d}x}\right)^2 - \frac{\phi^2}{m}c^m = K \tag{7}$$

where K is a constant of integration and $m = n + 1$. Eq. (7) holds for all $n \neq -1$. The case $n = -1$ will be discussed in Section 3.2.

The first boundary condition (6) and Eq. (7) give for the integration constant K the value

$$K = -\frac{\phi^2}{m}c_0^m \tag{8}$$

where $c_0 = c(0)$ denotes the (yet unknown) concentration of the reactant at the impermeable boundary of the porous slab, and represents one of the quantities of main engineering interest of the problem. Thus, Eq. (7) becomes

$$\left(\frac{\mathrm{d}c}{\mathrm{d}x}\right)^2 = \frac{2\phi^2}{m}(c^m - c_0^m) \tag{9}$$

and yields

$$x = \frac{1}{\phi}\left(\frac{m}{2c_0^{m-2}}\right)^{1/2}\int_1^{c/c_0}\frac{\mathrm{d}u}{\sqrt{u^m - 1}} \quad (m \neq 0) \tag{10}$$

Using the software package of *Mathematica*®, the integral in Eq. (10) can be expressed in terms of Gauss' hypergeometric function $F \equiv {}_2F_1(a,b;\, c;\, z)$ as follows:

$$\int_1^u \frac{\mathrm{d}u}{\sqrt{u^m - 1}} = \frac{2}{2-m}\left[u^{1-m/2}F\left(\frac{1}{2}-\frac{1}{m}, \frac{1}{2};\; \frac{3}{2}-\frac{1}{m};\; u^{-m}\right) - F\left(\frac{1}{2}-\frac{1}{m}, \frac{1}{2};\; \frac{3}{2}-\frac{1}{m};\; 1\right)\right] \tag{11}$$

For a comprehensive description of the hypergeometric function F, see e.g. [4], Chap. 15. With the aid of Eqs. (15.3.6) and (15.1.8) of Ref. [4], Eq. (11) can be transcribed into form

$$\int_1^u \frac{\mathrm{d}u}{\sqrt{u^m - 1}} = \frac{2}{m}u^{1-m}(u^m - 1)^{1/2}F\left(1, 1-\frac{1}{m};\; \frac{3}{2};\; 1 - u^{-m}\right) \tag{12}$$

and thus, the exact solution of the problem is obtained in the implicit form

$$x = \frac{1}{\phi}\left(\frac{2}{mc_0^{m-2}}\right)^{1/2}\left(\frac{c}{c_0}\right)^{1-m}\left[\left(\frac{c}{c_0}\right)^m - 1\right]^{1/2} \times F\left(1, 1-\frac{1}{m};\; \frac{3}{2};\; 1 - \left(\frac{c}{c_0}\right)^{-m}\right) \tag{13}$$

Now, the concentration c_0 at the impermeable boundary of the porous slab can be determined from the exact solution (13) and the second boundary condition (6) as solution of the transcendental equation

$$\frac{1}{\phi}\left[\frac{2}{m}(1 - c_0^m)\right]^{1/2}F\left(1, 1-\frac{1}{m};\; \frac{3}{2};\; 1 - c_0^m\right) = 1 \tag{14}$$

In addition to c_0, a further quantity of engineering interest of the present problem is the mass flux

$$q_M = -D_e\left.\frac{\mathrm{d}C}{\mathrm{d}X}\right|_{X=L} = -\frac{D_e C_S}{L}\left.\frac{\mathrm{d}c}{\mathrm{d}x}\right|_{x=1} \tag{15}$$

through the boundary $X = L$ where the constant concentration C_S was prescribed. This *ingoing* mass flux is necessary in order to maintain the *steady* reaction regime during the consumption of the reactant in the chemical reaction. The dimensionless concentration gradient $\mathrm{d}c/\mathrm{d}x|_{x=1} \equiv c'(1)$ occurring in Eq. (15) is obtained by differentiation of Eq. (13) in the form

$$c'(1) = \frac{(m/2)^{1/2}\phi}{\begin{gathered}\left(m + 2(1-m)(1-c_0^m)/2(1-c_0^m)^{1/2}F\right)(1, 1-1/m;\; 3/2;\; 1-c_0^m)\\ +(2(1-m)/3)c_0^m(1-c_0^m)^{1/2}F(2, 2-1/m;\; 5/2;\; 1-c_0^m)\end{gathered}} \tag{16}$$

The equivalent expression of $c'(1)$,

$$c'(1) = \left[1 - m + \frac{m}{2(1-c_0^m)} + \frac{2(1-m)}{3\phi}c_0^m\left[\frac{2}{m}(1-c_0^m)\right]^{1/2} \times F\left(2, 2-\frac{1}{m};\; \frac{5}{2};\; 1-c_0^m\right)\right]^{-1} \tag{17}$$

results from Eqs. (14) and (16) easily. From geometrical point of view, the value of $c'(1)$ represents the slope of the dimensionless concentration profile $c = c(x)$ at the boundary $x = 1$.

3. Discussion

The main advantage of the exact analytical solution (13) consists of the facts that (i) the mathematical properties of the hypergeometric function F are well established (see e.g. Ref. [4]) and (ii) today, well-performing commercial computer software is available both for symbolical and numerical calculations involving the function F (in the present paper throughout Wolfram's *Mathematica*® has been used). This circumstance facilitates both the analytical and numerical investigation of the concentration distribution $c = c(x)$ substantially (without to be confronted with the convergence problems arising in approximation methods). In the following, the features of the solution $c = c(x)$ will be examined for positive and negative values of the reaction order in the range $n \geq -1$.