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The Approximate Analytical Solution of Non-Linear Equation for Simultaneous Internal Mass and Heat Diffusion Effects

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Abstract

For the first time a mathematical modelling of porous catalyst particles subject to both internal mass concentration gradients as well as temperature gradients, in endothermic or exothermic reactions has been reported. This model contains a non-linear mass balance equation which is related to rate expression. This paper presents an approximate analytical method (Modified Adomian decomposition method) to solve the non-linear differential equations for chemical kinetics with diffusion effects. A simple and closed form of expressions pertaining to substrate concentration and utilization factor is presented for all value of diffusion parameters. These analytical results are compared with numerical results and found to be in good agreement.

Keywords

Chemical and Biological Systems, Modified Adomian Decomposition Method, Nonlinear Reaction Diffusion, Porous Catalyst Particles, Mass and Diffusion Effect

1. Introduction

In many engineering and industrial applications, catalytic processes in chemical reactors are often considered to be very useful. This induces particular attention to the study of catalytic reactions at the single-particle level [1]. Moreover, the reaction behavior of porous catalyst particles had been studied over nearly a quarter of a century [2]-[4]. Majority of chemical reactions are accompanied by heat transfer effects; they either release or absorb

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heat. This can lead to appreciable increase (or decrease) of temperature toward the particle centre [5]-[7]. Since chemical reaction rates vary rapidly increase with temperature, this effect could radically change the behavior of the catalyst particles. Analysis of chemical kinetics with diffusion effects usually leads to solving strongly non-linear differential equations. Detailed reviews of mathematical models describing reactions in porous catalyst particle can be found in [8]. Assuming a flat geometry for the particle and that conductive heat transfer is negligible compared to convective heat transfer. The approximate behavior of the functional forms is sufficiently similar for various geometric forms [9] [10] so that the spherical particle is a approximation [11] [12] for most cases encountered, such as cylindrical pellets, or irregular granules. When the chemical reaction is accompanied by a heat effect, not only a mass concentration gradient, but also appreciable temperature gradients can exist within the particle. Weisz and Hicks [13] solved the non-linear mass balance equation using numerical method.

However, to the best of our knowledge, there was no rigorous analytical solution for the concentration of reactant of catalyst having been reported. The purpose of this communication is to derive simple analytical expression for concentration and utilization factor for all possible values of reaction/diffusion parameters using the modified Adomian decomposition method.

2. Mathematical Formulation of the Problem

The dimensionless mass transport equation of porous catalyst particle is [13]

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}+\frac{2}{x}\frac{\mathrm{d}y}{\mathrm{d}x}=\phi_0^2\, y\exp\left(\gamma\beta\frac{1-y}{1+\beta(1-y)}\right) \tag{1}$$

where

$$y=\frac{c}{c_0},\quad x=\frac{r}{R},\quad \phi_0=R\sqrt{\frac{k_0}{D}},\quad \beta=\frac{c_0HD}{KT_0}=\left(\frac{\Delta T}{T_0}\right)_{\max} \tag{2}$$

$$\Delta T=T-T_0=-\frac{HD}{K}(c_0-c),\quad \gamma=\frac{Q}{RT_0} \tag{3}$$

where y is the dimensionless concentration, x is the dimensionless radius of the spherical catalyst pellet, c is the dimensionless concentration of reactant, K is thermal conductivity, H is molar heat of reaction. The parameter γ expresses the sensitivity of the reaction rate to temperature; β is the maximum temperature variation $(\Delta T)_{\max}$ which could exist within the particle relative to the boundary temperature. The boundary conditions are

$$y(1)=1,\quad \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)_{x=0}=0 \tag{4}$$

The utilization factor (η) is given by

$$\eta=\frac{3}{\phi_0^2}\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)_{x=1} \tag{5}$$

3. Analytical Expression of the Concentration Using Modified Adomian Decomposition Method (MADM)

In the recent years, much attention is devoted to the application of the Adomian decomposition method to the solution of various scientific models [14]. The MADM yields, without linearization, perturbation, transformation or discretisation, an analytical solution in terms of a rapidly convergent infinite power series with easily computable terms. The decomposition method is simple and easy to use and produces reliable results with few iterations. The rate of convergence of modified Adomian decomposition method is higher than standard Adomian decomposition method [15]-[17]. Using this method (see Appendix A), we can obtain the analytical expression of concentration (see Appendix B), of the substrate as follows:

$$y(x)=1-\frac{\phi_0^2}{6}+\frac{7}{360}\phi_0^4(1-\gamma\beta)+\phi_0^2\left(\frac{1}{6}-\frac{\phi_0^2(1-\gamma\beta)}{36}\right)x^2+\frac{\phi_0^4(1-\gamma\beta)}{120}x^4 \tag{6}$$

Using Equations (5) and (6), we can obtain the effectiveness factor

$$\eta = 1 - \frac{\phi_0^2\left(1-\gamma\beta\right)}{15} \tag{7}$$

The Equation (6) and (7) represent the new and simple analytical expression of concentration of substrate and effectiveness factor provided

$$\frac{\phi_0^2}{6} - \frac{7}{360}\phi_0^2\left(1-\gamma\beta\right) < 1 \quad \text{and} \quad \frac{\phi_0^2\left(1-\gamma\beta\right)}{15} < 1 \tag{8}$$

4. Numerical Simulation

The diffusion Equation (1) for the boundary condition (Equation (4)) is also solved numerically. We have used the function pdex1 in MATLAB software to solve numerically the initial-boundary value problem for the nonlinear differential equation. This numerical solution is compared with our analytical results in **Figure 1** and **Figure 2**. Upon comparison, it gives a satisfactory agreement for all values of the dimensionless parameters γ, β and ϕ. The Matlab program is also given in Appendix *C*.

5. Discussion

The nonlinear system for coupled heat and mass transfer in a spherical non-isothermal catalyst pellet is solved analytically. The concentration of substrate depends on the following three factors γ, β and ϕ_0. γ is the activation energy parameter and β is the heat of reaction parameter which represents the ratio of the characteristic time of the enzymatic reaction to that of substrate diffusion.

Figure 1(a) and **Figure 1(b)** show the dimensionless concentration of substrate *y* for various dimensionless pellet raidus *x*. The concentrations were computed for various values of the dimensionless parameter. From **Figure 1(a)** and **Figure 1(b)**, it is evident that the value of concentration $y \approx 1$ when $x = 1$ and $\phi \le 0.5$ for all values of γ and β. The concentration differs significantly for all values of parameters γ and β. The value of the concentration *y* decreases when ϕ_0 increases.

The normalized numerical simulation of three dimensional substrate concentration *y* versus dimensionless pellet radius *x* is shown in **Figures 2(a)-(c)**. The time independent concentration *y* is represented in **Figures 2(a)-(c)**. For fixed value of $\beta = 0.1$, concentration $y(x)$ is slowly decreasing when ϕ is increasing. Then

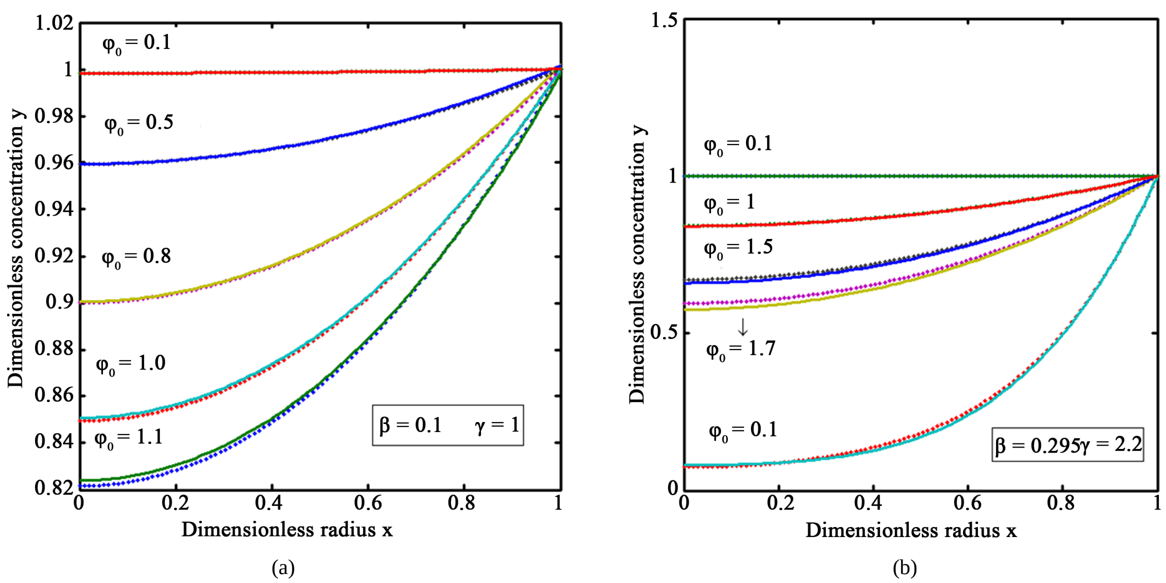
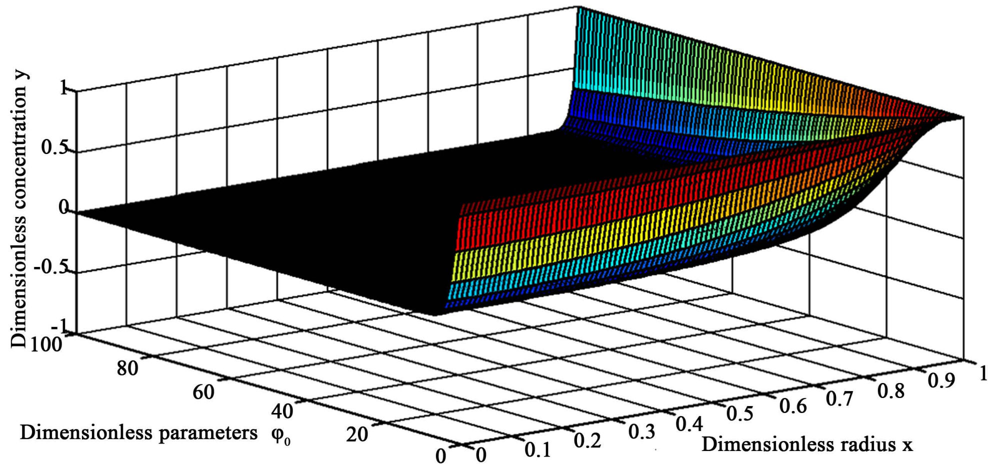
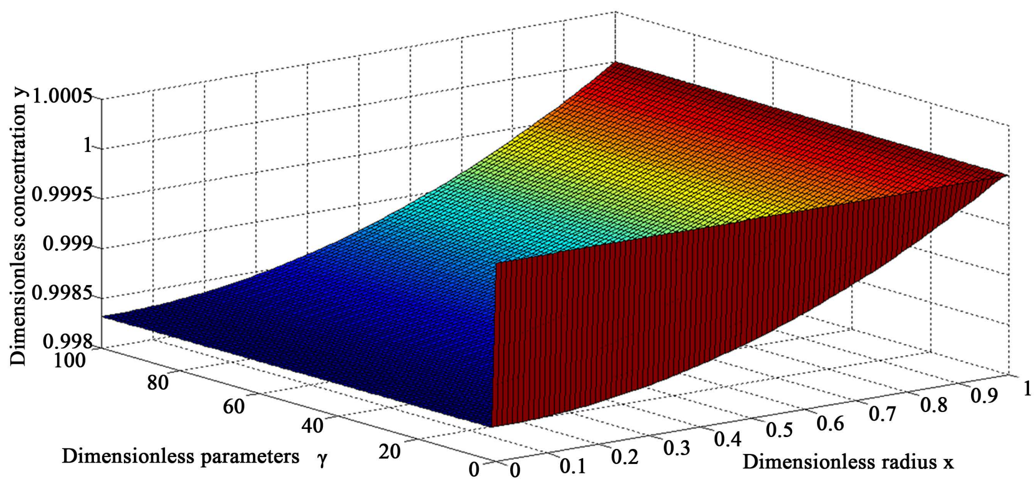


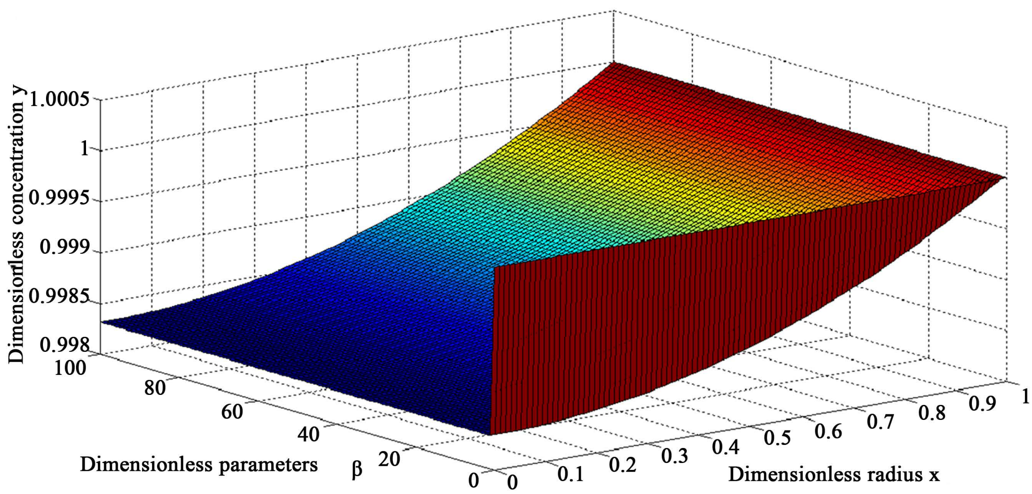
Figure 1. Plot of dimensionless concentration *y* versus dimensionless pellet radius *x*. The concentrations were computed for various values of the dimensionless parameter ϕ when (a) $\beta = 0.1, \gamma = 1$ (b) $\beta = 0.295, \gamma = 2.2$. The curves are plotted using Equation (6). (—) denotes the analytical results and (▪▪▪) denotes the numerical simulations.



(a)



(b)



(c)

Figure 2. The normalized dimensionless concentration y versus dimensionless pellet radius x and dimensionless parameters ϕ_0, γ and β calculated using Equation (6). The plot was constructed for the values of (a) $\beta = 0.1, \gamma = 0.1$, (b) $\phi = 0.1, \beta = 0.1$ and (c) $\phi = 0.1, \gamma = 0.1$.

the concentration of $y(x)=1$ when $x=1$ and also for all values of ϕ_0, γ and β. From these figure, it should be noted that the value of the concentration of substrate decreases for all values of γ. From this Figures, it is apparent that the value of the concentration of substrate increases when the values of β increases.

The variation in effectiveness factor for various values of γ, β and ϕ_0 using Equation (7) is shown in **Figure 3** and **Figure 4**. From **Figure 3**, it is evident that the effectiveness factor increases with the increasing value of the dimensionless parameter γ. From **Figure 4**, it is also observed that the effectiveness factor increases with the increasing value of the dimensionless parameter β.

6. Conclusion

In this work, we have discussed the mathematical model of catalyst particle in a porous medium through which reactants diffuses. We have obtained the approximate analytical expression for the steady state concentration of substrate for all values of γ and β in a packed bed reactor using the modified Adomian decomposition method. A satisfactory agreement with the numerical result is noted. Moreover, we have also presented a closed form expression for the utilization factor. The proposed model can be used to solve the nonlinear convective mass and heat diffusion problems.

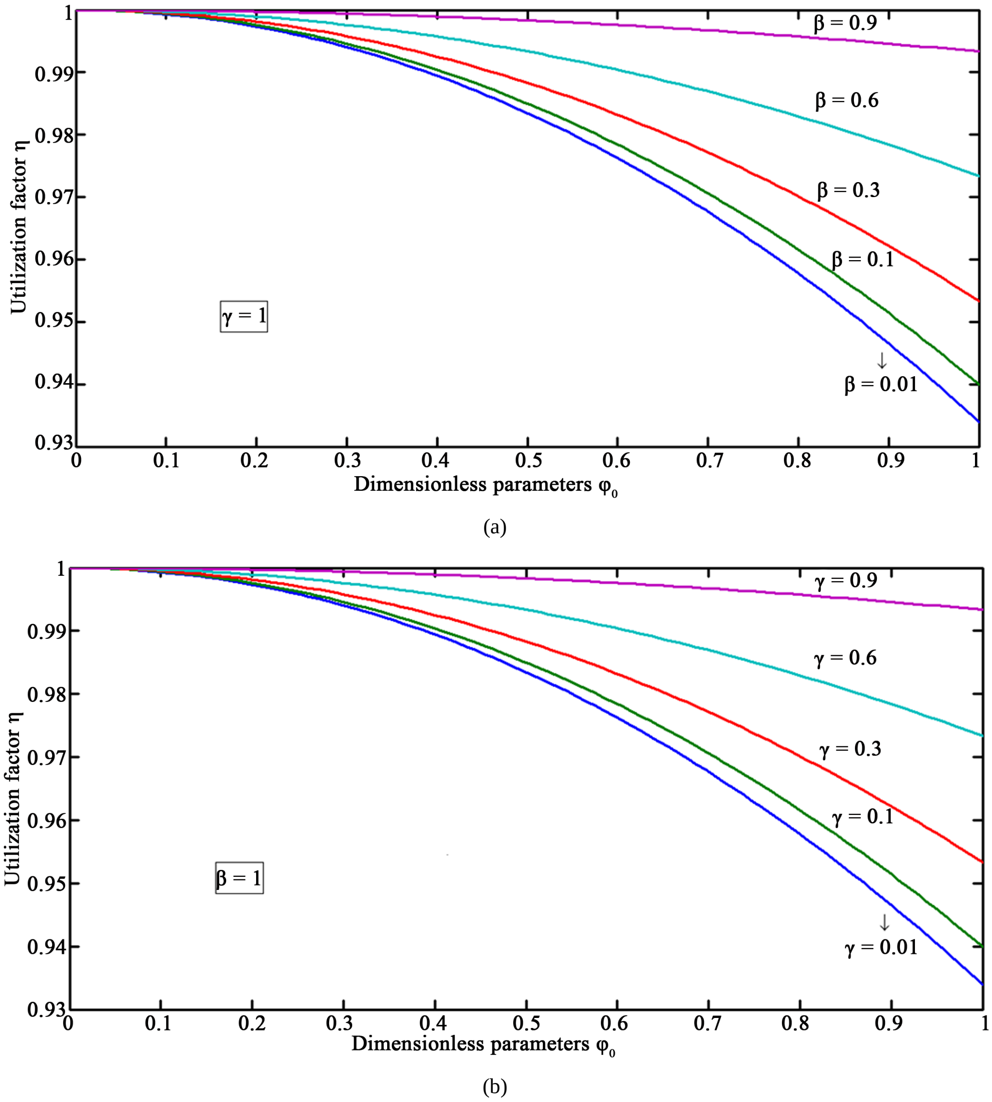


Figure 3. Plot of the utilization factor η versus dimensionless parameter ϕ_0 for various values of (a) β and (b) γ.

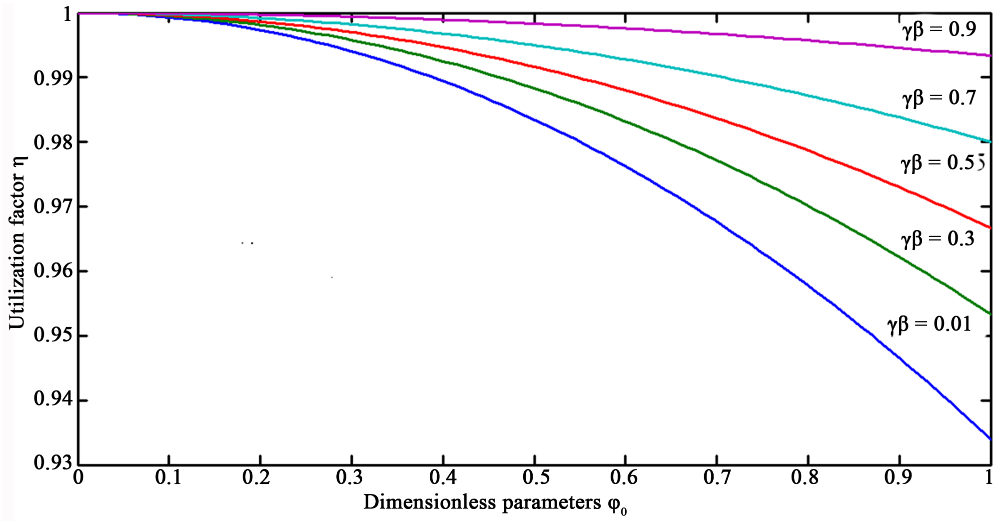


Figure 4. Plot of the utilization factor η versus dimensionless parameter ϕ_0 for various values of $\gamma\beta$.

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Appendix A. Basic Concept of Modified Adomian Decomposition Method [16]

Consider the nonlinear differential equation in the form

$$y'' + \frac{2n}{x} y' + \frac{n(n-1)}{x^2} y + F(x,y) = g(x); \ \ n \geq 0 \tag{A.1}$$

with initial condition

$$y(0) = A, \ y'(0) = B \tag{A.2}$$

where $F(x,y)$ is a real function, $g(x)$ is the given function and A and B are constants. The differential operation is proposed as follows [17]

$$L = x^{-n} \frac{\mathrm{d}^2}{\mathrm{d}x^2} x^n y \tag{A.3}$$

So, the problem (A.1) can be written as,

$$Ly = g(x) - F(x,y). \tag{A.4}$$

The inverse operator L^{-1} is therefore considered a two-fold integral operator, as below.

$$L^{-1}(.) = x^{-n} \int_0^x \int_0^x x^n (.) \mathrm{d}x \mathrm{d}x \tag{A.5}$$

Applying L^{-1} of (A.5) to the first three terms $y'' + \frac{2n}{x} y' + \frac{n(n-1)}{x^2} y$ of Equation (A.1) we find

$$\begin{aligned} L^{-1}\left(y'' + \frac{2n}{x} y' + \frac{n(n-1)}{x^2} y \right) &= x^{-n} \int_0^x \int_0^x x^n \left(y'' + \frac{2n}{x} y' + \frac{n(n-1)}{x^2} y \right) \mathrm{d}x \mathrm{d}x \\ &= x^{-n} \int_0^x \left(x^n y' + n x^{n-1} y \right) \mathrm{d}x = y - y(0) \end{aligned} \tag{A.6}$$

By operating L^{-1} on (A.4), we have

$$y(x) = A + L^{-1} g(x) - L^{-1} F(x,y) \tag{A.7}$$

The Adomian decomposition method introduce the solution $y(x)$ and the nonlinear function $F(x,y)$ by infinity series

$$y(x) = \sum_{n=0}^{\infty} y_n(x), \tag{A.8}$$

$$F(x,y) = \sum_{n=0}^{\infty} A_n \tag{A.9}$$

where the components $y_n(x)$ of the solution $y(x)$ will be determined recurrently and the Adomian polynomials A_n of $F(x,y)$ are evaluated [22, 23, 25] using the formula

$$A_n(x) = \frac{1}{n!} \frac{\mathrm{d}^n}{\mathrm{d}\lambda^n} N\left(\sum_{n=0}^{\infty} \left(\lambda^n y_n \right) \right) \Bigg|_{\lambda=0} \tag{A.10}$$

By substituting (A.8) and (A.9) into (A.7),

$$\sum_{n=0}^{\infty} y_n(x) = A + L^{-1} g(x) - L^{-1} \sum_{n=0}^{\infty} A_n \tag{A.11}$$

Through using the Adomian decomposition method, the components $y_n(x)$ can be determined as

$$\begin{aligned} y_0(x) &= A + L^{-1} g(x) \\ y_{n+1}(x) &= -L^{-1}(A_n), \ n \geq 0 \end{aligned} \tag{A.12}$$

which gives

$$\begin{aligned} y_0(x) &= A + L^{-1}g(x) \\ y_1(x) &= -L^{-1}(A_0) \\ y_2(x) &= -L^{-1}(A_1) \\ y_3(x) &= -L^{-1}(A_2) \\ &\cdots \end{aligned} \tag{A.13}$$

From (A.9) and (A.12), we can determine the components $y_n(x)$, and hence the series solution of $y(x)$ in (A.7) can be immediately obtained.

Appendix B: General Solution of Equation (1) Using the Adomian Decomposition Method

In this appendix, we derive the general solution of nonlinear Equation (1) by using the Adomian decomposition method. We write the Equation (1) in the operator form,

$$L(y) = \phi_0^2 y \exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right] \tag{B.1}$$

where $L = x^{-1}\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}x$. Applying the inverse operator $L^{-1}(.) = x^{-1}\int_0^x\int_0^x x(.)\mathrm{d}x\mathrm{d}x$ on both sides of Eqn. (B.1) yields

$$y(x) = Ax + B + \phi_0^2 L^{-1}\left(y\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right]\right) \tag{B.2}$$

where A and B are the constants of integration. We let,

$$y(x) = \sum_{n=0}^{\infty} y_n(x) \tag{B.3}$$

and

$$N[y(x)] = \sum_{n=0}^{\infty} A_n \tag{B.4}$$

where

$$N[y(x)] = \left(y\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right]\right) \tag{B.5}$$

In view of Equations (B. 3 - B. 5), Equation (B. 2) gives

$$\sum_{n=0}^{\infty} y_n(x) = Ax + B + \phi_0^2 L^{-1}\sum_{n=0}^{\infty} A_n \tag{B.6}$$

We identify the zeroth component as

$$y_0(x) = Ax + B \tag{B.7}$$

Using the boundary condition (4) we get,

$$y_0 = 1 \tag{B.8}$$

and the remaining components can be obtained using the recurrence relation

$$y_{n+1}(x) = \phi_0^2 L^{-1}A_n,\ n \ge 0 \tag{B.9}$$

where A_n are the Adomian polynomials of $y_1, y_2, \cdots, y_n$. We can obtain the first few A_n as follows:

$$A_0 = N(y_0) = 1 \tag{B.10}$$

$$A_1 = \frac{\mathrm{d}}{\mathrm{d}\lambda}\left[N\left(y_0 + \lambda y_1\right)\right] = \frac{\phi_0^2}{6}(1-\gamma\beta)\left(x^2-1\right) \tag{B.11}$$

The remaining polynomials can be generated easily, and so,

$$y_1 = \frac{\phi_0^2}{6}(1-\gamma\beta)\left(x^2-1\right) \tag{B.12}$$

$$y_2 = \frac{7\phi_0^4(1-\gamma\beta)}{360} + \phi_0^4(1-\gamma\beta)\left(\frac{x^4}{120} - \frac{x^2}{36}\right) \tag{B.13}$$

Adding (B. 8), (B. 12) and (B. 13) we get the Equation (6) in the text.

Appendix C: The Matlab Program to Find the Numerical Solution of Equation (1)

```
function pdex1
m = 2;
x = linspace(0,1);
t = linspace(0,100);
sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
u = sol(:,:,1);
surf(x,t,u)
title('Numerical solution computed with 20 mesh points.')
xlabel('Distance x')
ylabel('Time t')
figure
plot(x,u(end,:))
title('Solution at t = 2')
xlabel('Distance x')
ylabel('u(x,2)')
% --------------------------------------------------------------
function [c,f,s] = pdex1pde(x,t,u,DuDx)
c = 1;
f = DuDx;
Q=1;
B=1.5;
r=1;
s =-(Q^2)*u*exp(r*B*(1-u)/(1+B*(1-u)));
% --------------------------------------------------------------
function u0 = pdex1ic(x)
u0 = 1;
% --------------------------------------------------------------
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t)
pl = 0;
ql = 1;
pr = ur-1;
qr = 0;
```

Nomenclature

C_{A} Concentration of reactant A inside the catalyst pellet (mole/cm^3)
$C_{\mathrm{A,s}}$ Concentration of reactant A at the surface of catalyst pellet (mole/cm^3)
D_ε Effective diffusivity inside the catalyst pellet (cm^2·s^{-1})

E Activation energy ($kJ \cdot mol^{-1}$)
r_A Arrhenius reaction rate (s^{-1})
R_g Universal gas constant (8.3145 $J \cdot k^{-1} \cdot mol^{-1}$)
T Temperature inside the catalyst pellet (K)
T_{ref} Reference temperature (K)
T_s Temperature at the surface of catalyst pellet (K)
x Dimensionless radius of the spherical catalyst pellet (none)
y Dimensionless concentration along radial direction of catalyst pellet (none)

Greek Symbols

β Dimensionless heat reaction
γ Dimensionless activation energy
η Effectiveness factor
ϕ Thiele modulus