Approximate solution for nonlinear model of the second and half order reactions in porous catalyst by decomposition method*

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Abstract The problem of the process of coupled diffusion and reaction in catalyst pellets is considered for the case of second and half order reactions. The Adomian decomposition method is used to solve the non-linear model. For the second, half and first order reactions, analytical approximate solutions are obtained. The variation of reactant concentration in the catalyst pellet and the effectiveness factors at $\phi < 10$ are determined and compared with those by the BAND's finite difference numerical method developed by Newman. At lower values of ϕ , the decomposition solution with 3 terms gives satisfactory agreement with the numerical solution; at higher values of ϕ , as the term number in the decomposition method is increased, an acceptable agreement between the two methods is achieved. In general, the solution with 6 terms gives a satisfactory agreement.

Keywords: Adomian decomposition method, nonlinear, analytical approximate solution, effectiveness factor.

Nonlinear problems that frequently arise in chemical engineering can be solved only by the numerical method. However, by using the numerical method, we can only obtain discontinuous values and not analyze it mathematically. Furthermore, the numerical method does not always converge when there is a large change in reaction rate. From the 1980s to the 1990s, Adomian^[1] had developed the decomposition method for solving the deterministic or stochastic differential equations. Cherrault^[2] proved the convergence of the solutions obtained with this method. In general, satisfactory result can be reached by the approximate solution that consists of the first few terms of the solution series. The Adomian decomposition method has been used to solve some mathematical problems in science and engineering^[3], but there has been no report of its application to chemical engineering so far.

The nonlinear problems in chemical reaction engineering come from the relationship between the reaction rate and kinetic parameters, such as concentration, temperature etc. In this paper, Adomian decomposition method is introduced as a new alternate one to solve the non-linear model of diffusion and reaction in porous catalysts.

1 The model of diffusion and reaction

The model for the process of coupled diffusion and reaction in the porous catalysts is a typical one in chemical reaction engineering. In general, a mass balance for per unit volume catalyst gives^[4]

$$\frac{\partial c'}{\partial t} = \nabla \cdot D_{e} \nabla c' + R(c'), \qquad (1)$$

where t is time, c' the chemical reactant concentration, R(c') the rate of reaction per unit volume, $D_{\rm e}$ the effective diffusion coefficient. For the porous slab catalyst pellet, the pellet is assumed to be infinite in both y and z directions, giving a large plane sheet with diffusion through the thickness of the sheet. At a steady state, we also assume that the variation of the concentrations in the y and z directions is negligible, so we have

$$\frac{d^2c'}{dx'^2} - \frac{R(c')}{D_c} = 0, (2)$$

where x' is diffusion distance. The boundary conditions are

$$x' = 0, -D_e \frac{dc'}{dx'} = 0,$$
 (3)

$$x' = l, \quad c' = c_0,$$
 (4)

where l is distance from pellet core. Eq. (2) is a boundary-value problem for ordinary differential equation. The reaction considered here is nth order irreversible reaction, i.e. $R(c') = kc'^n$, where k is re-

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action rate constant. In order to obtain a generalized solution under isothermal condition, dimensionless equations are derived by letting $x=\frac{x'}{l}$, $c=\frac{c'}{c_0}$, where x is dimensionless distance, c the dimensionless reactant concentration.

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

$$x = 0, \quad -D_e \frac{\mathrm{d}c}{\mathrm{d}x} = 0, \tag{6}$$

$$x = 1, \quad c = 1, \tag{7}$$

where the Thiele modulus $\phi = \frac{l^2kc_0^{n-1}}{D_e}$. The group

$$\frac{1}{kc_0^{n-1}}$$
 is a characteristic time for reaction, $\frac{l^2}{D_{\rm e}}$ a characteristic time for reaction,

acteristic time for diffusion. The Thiele modulus thus represents the ratio of the two characteristic times and measures the relative importance of diffusion and reaction in the coupled process.

In chemical reaction engineering the effectiveness factor of η is defined as the average reaction rate, i.e. with diffusion, divided by the reaction rate that is evaluated at the boundary condition (at x=1). For the planar catalyst, the effectiveness factor is given

$$\eta = \frac{1}{\phi^2} \frac{\left(\frac{\mathrm{d}c}{\mathrm{d}x}\right)_{x=1}}{R_{r=a}}.$$
 (8)

At lower values of ϕ (<0.5), $\eta \rightarrow 1$, which means that the rate of reaction is relatively uninfluenced by diffusion; at higher values of ϕ (>5), $\eta \rightarrow 1/\phi$, that the reactant concentration in the pore drops rapidly, that is, the rate of reaction is strongly influenced by diffusion.

2 The solution by the decomposition method

In general, a differential equation can be expressed as an operator equation,

$$\tilde{F}_{\mathcal{Y}} = g(x). \tag{9}$$

As the first step of decomposition, according to Adomian decomposition method, a deterministic nonlinear differential equation can be written as

$$\widetilde{F}y = Ly + L'y + Ny = g(x), \qquad (10)$$

where L is the highest order linear differential operator, L' the remainder of the linear operator, N the nonlinear operator of the function of y, and g(x) a forcing term. Operating Eq. (10) with L^{-1} , we have

$$L^{-1}Ly = L^{-1}g(x) - L^{-1}L'y - L^{-1}Ny$$
, (11)

where L^{-1} is an inverse operator and is a finite integral operator, simply symbolizes n-fold integration from 0 to x. For a second order differential equation

$$L = \frac{d^2}{dx^2}, \quad L^{-1} = \iint_0^x (g(x) - L'y - Ny) \cdot dx dx.$$
(12)

As the second step of decomposition, the solution of equation is expressed by a sum of partial solutions, the nonlinear term Ny is approached with Adomian polynomial, hence we have

$$y = \sum_{m=0}^{\infty} y_m, \quad Ny = f(y) = \sum_{m=0}^{\infty} A_m, \quad (13)$$

where A_m is the Adomian polynomial, m the term number of Adomian polynomial series. According to Adomian decomposition^[1], the expressions for A_0 , $A_1, A_2 \cdots A_m$ can be written as

$$A_{0} = h_{0}(y_{0}) = f(y_{0}),$$

$$A_{1} = h_{1}(y_{0})y_{1},$$

$$A_{2} = \frac{1}{2}[h_{2}(y_{0})y_{1}^{2} + 2h_{1}(y_{0})y_{2}],$$

$$\vdots$$

$$A_{m}$$

$$\vdots$$

where $h_m(y_0) = \left(\frac{d^m}{dc^m}\right) f(y)|_{y=y_0}$, f(y) is a non-linear function of y. Adomian partial solutions y_0 , y_1 , y_2 , y_m are

$$y_0 = \text{const},$$

 $y_1 = \phi^2 L^{-1} A_0,$
 $y_2 = \phi^2 L^{-1} A_1,$
 \vdots
 $y_m = \phi^2 L^{-1} A_{m-1},$
 \vdots

Thus the approximate solution of y with (m + 1) terms can be expressed as

$$y = \sum_{i=0}^{m} y_{i}$$

$$= y_{0} + \phi^{2} L^{-1} A_{0} + \phi^{2} L^{-1} A_{1} + \dots + \phi^{2} L^{-1} A_{m-1}.$$
(16)

For an *n*th order irreversible reaction, under the isothermal condition, we assume the effective diffusion coefficient D_e to be a constant, thus Adomian operator equation (5) can be written as

$$Lc = \phi^2 Nc. (17)$$

Operating with the inverse operation
$$L^{-1}$$
, we have $c = \phi^2 L^{-1} Nc$. (18)

According to the procedure above, Adomian polynomial A_m and partial solution c_m of Eq. (5) can be directly written as

$$A_{0} = c_{0}^{n};$$

$$c_{1} = \frac{1}{2!} \phi^{2} c_{0}^{n} x^{2},$$

$$A_{1} = \frac{1}{2!} \phi^{2} c_{0}^{2n-1} x^{2};$$

$$c_{2} = \frac{n}{4!} \phi^{4} c_{0}^{2n-1} x^{4},$$

$$A_{2} = \frac{4n^{2} - 3n}{4!} \phi^{4} c_{0}^{3n-2} x^{4};$$

$$c_{3} = \frac{4n^{2} - 3n}{6!} \phi^{6} c_{0}^{3n-2} x^{6},$$

$$A_{3} = \frac{34n^{3} - 63n^{2} + 30n}{6!} \phi^{6} c_{0}^{4n-3} x^{6};$$

$$c_{4} = \frac{34n^{3} - 63n^{2} + 30n}{8!} \phi^{8} c_{0}^{4n-3} x^{8},$$

$$A_{4} = \frac{496n^{4} - 1554n^{3} + 1689n^{2} - 630n}{8!} \phi^{8} c_{0}^{5n-4} x^{8};$$

$$\vdots$$

$$\vdots$$

$$(19)$$

3 Analytical approximate solutions

Let the approximate solution of c be $\theta_{m+1,n}$, $\theta_{m+1,n} = \sum_{0}^{m} c_m$, where m+1 is the term number of approximate solution, n the reaction order. We can now form successive approximations $\theta_{m+1,n} = \sum_{0}^{m} c_m$ as m increases. In this paper, we will first derive the approximate solution for linear case (the first order reaction) and compare it with its analytical solution, and then write the approximate solutions for the second and half order reactions. The analytical solutions of the equations by decomposition method will be compared with numerical solutions calculated by Newman's BAND program.

3.1 The linear case

For the first order reaction (n = 1), the equation of model is linear. According to Eq. (19), we have

$$\begin{cases} c_{m} = \frac{1}{(2m)!} \phi^{2m} c_{0} x^{2m}, \\ \sum_{m=1}^{\infty} c_{m} = c_{0} \left[1 + \sum_{m=1}^{\infty} \frac{1}{(2m)!} \phi^{2m} c_{0} x^{2m} \right] \\ = c_{0} \cosh(\phi_{x}). \end{cases}$$
(20)

Substituting the boundary condition Eqs. (6) and (7) into Eq. (20), we can obtain $c = \frac{\cosh(\phi x)}{\cosh(\phi)}$,

which is the analytical solution of the first order reaction.

3.2 The nonlinear case

The general approximate solutions for n th order reactions are

$$\theta_{m+1,n} = c_0 + c_1 + c_2 + \dots + c_m$$

$$= c_0 + \frac{1}{2!} \phi^2 c_0^n x^2 + \frac{n}{4!} \phi^4 c_0^{2n-1} x^4$$

$$+ \frac{4n^2 - 3n}{6!} \phi^6 c_0^{3n-2} x^6$$

$$+ \frac{34n^3 - 63n^2 + 30n}{8!} \phi^8 c_0^{4n-3} x^8$$

$$+ \frac{496n^4 - 1554n^3 + 1689n^2 - 630n}{10!} \phi^{10} c_0^{5n-4} x^{10}$$

$$+ \dots + c_m. \tag{21}$$

3.3 The approximate solution

3. 3. 1 The expressions of approximate solutions with 2 and 3 terms The formulas of solutions with 2 and 3 terms denoted as $\theta_{2,n}$ and $\theta_{3,n}$ respectively are obtained by taking the first two and three terms from Eq. (21). c_0 is an integration constant, obtained by letting Eq. (21) satisfy the condition x = 1, c = 1. c_0 and the approximate solution x = 1, $\theta_{m+1,n}$ with 2 and 3 terms for the second and half order reactions are shown in Tables 1 and 2.

Table 1. c_0 and the formulas of $\theta_{m+1,n}$ with 2 terms

n	c ₀	$\theta_{m+1, n}$
1	$c_0 = \left(1 + \frac{1}{2!}\phi^2\right)^{-1}$	$\theta_{2,1} = c_0 \left(1 + \frac{1}{2!} \phi^2 x^2 \right)$
2	$c_0 = \frac{\sqrt{1 + 2\phi^2} - 1}{\phi^2}$	$\theta_{2,2} = c_0 + \frac{1}{2!} \phi^2 c_0^2 x^2$
0.5	$c_0 = \frac{1}{16} (\sqrt{\phi^4 + 16} - \phi^2)^2$	$\theta_{2,0.5} = c_0 + \frac{1}{2!} \phi^2 c_0^{0.5} x^2$

Table 2. c_0 and the formulas of $\theta_{m+1,n}$ with 3 terms

n	c ₀	$\theta_{m+1, n}$
1	$c_0 = \left(1 + \frac{1}{2!} \phi^2 + \frac{1}{4!} \phi^4\right)^{-1}$	$\theta_{3,1} = c_0 \left(1 + \frac{1}{2!} \phi^2 x^2 + \frac{1}{4!} \phi^4 x^4 \right)$
2	$c_0 = \sqrt[3]{\frac{8}{\phi^6} + \frac{12}{\phi^4}} - \frac{2}{\phi^2}$	$\theta_{3,2} = c_0 + \frac{1}{2!} \phi^2 c_0^2 x^2 + \frac{2}{4!} \phi^4 c_0^3 x^4$
0.5	$c_0 = \left[\frac{1}{4} \left(\sqrt{\frac{2\phi^4}{3} + 16} - \phi^2 \right) \right]^2$	$\theta_{3,0.5} = c_0 + \frac{1}{2!} \phi^2 c_0^{0.5} x^2 + \frac{2}{4!} \phi^4 x^4$

3.3.2 The approximate solution with more than 4 terms c_0 in the approximate solution with less than 4 terms can be analytically obtained by applying the boundary condition^[5]. Those in the approximate solutions with more than 4 terms have to be calculated with a numerical method. The approximate solution with 6 terms is written as

$$\theta_{6,1} = c_0 \left(1 + \frac{1}{2!} \phi^2 x^2 + \frac{1}{4!} \phi^4 x^4 + \frac{1}{6!} \phi^6 x^6 + \frac{1}{8!} \phi^8 x^8 + \frac{1}{10!} \phi^{10} x^{10} \right), \qquad (22)$$

$$\theta_{6,2} = c_0 + \frac{1}{2!} \phi^2 c_0^2 x^2 + \frac{2}{4!} \phi^4 c_0^3 x^4 + \frac{10}{6!} \phi^6 c_0^4 x^6 + \frac{80}{8!} \phi^8 c_0^5 x^8 + \frac{1000}{10!} \phi^{10} c_0^6 x^{10}, \qquad (23)$$

$$\theta_{6,0.5} = c_0 + \frac{1}{2!} \phi^2 c_0^{0.5} x^2 + \frac{1}{2 \times 4!} \phi^4 c_0^0 x^4 - \frac{1}{2 \times 6!} \phi^6 c_0^{-0.5} x^6 + \frac{7}{2 \times 8!} \phi^8 c_0^{-1} x^8 - \frac{56}{10!} \phi^{10} c_0^{-1.5} x^{10}. \qquad (24)$$

3.4 Effectiveness factors of the catalyst

The general solution of the effectiveness factor for nth order reaction can be obtained from Eqs. (8) and (21), that is

$$\eta_{m+1, n} = \frac{1}{\phi^{2}} \left(\frac{\mathrm{d}\theta_{m+1, n}}{\mathrm{d}x} \right)_{x=1} \\
= c_{0}^{n} + \frac{n}{3!} \phi^{2} c_{0}^{2n-1} + \frac{4n^{2} - 3n}{5!} \phi^{4} c_{0}^{3n-2} \\
+ \frac{34n^{3} - 63n^{2} + 30n}{7!} \phi^{6} c_{0}^{4n-3} \\
+ \frac{496n^{4} - 1554n^{3} + 1689n^{2} - 630n}{9!} \phi^{8} c_{0}^{5n-4} \\
+ \cdots + \frac{1}{\phi^{2}} \left(\frac{\mathrm{d}c_{m}}{\mathrm{d}x} \right)_{x=1}.$$
(25)

Eq. (25) shows that the number of terms in the solution of effectiveness factor is one less than that of the dimensionless concentration solution.

For the first order reaction (n = 1), the approximate solution $\eta_{3,1}$ of the effectiveness factor with 3 terms is

$$\eta_{3,1} = c_0 + \frac{1}{3!} \phi^2 c_0 = \left(1 + \frac{1}{2!} \phi^2 + \frac{1}{4!} \phi^4 \right)^{-1} \left(1 + \frac{1}{3!} \phi^2 \right).$$
(26)

For the second order reaction
$$(n = 2)$$

$$\eta_{3,2} = \left(\sqrt[3]{\frac{8}{\phi^6} + \frac{12}{\phi^4}} - \frac{2}{\phi^2} \right)^2 + \frac{\phi^2}{3} \left(\sqrt[3]{\frac{8}{\phi^6} + \frac{12}{\phi^4}} - \frac{2}{\phi^2} \right)^3.$$
(27)

For the half order reaction (n = 0.5) $\eta_{3,0.5} = \frac{1}{4} \left(\sqrt{\frac{2\phi^4}{3} + 16} - \phi^2 \right) + \frac{\phi^4}{12}.$ (28)

Similarly, the approximate solutions of the effectiveness factor with 4, 5, 6 terms for the 1, 2 and 0.5 order reactions can be obtained with Eq. (25).

4 Discussion

The reactant concentration in the catalyst pellet and the effectiveness factors as a function of reaction order and Thiele modulus have been calculated by using the decomposition solution and compared with the numerical solution by Newman's BAND program^[6,7]. The BAND program has been proven to be very effective for solving non-linear problems of diffusion and reaction in electrochemical systems^[7].

4.1 Distribution of reactant concentration

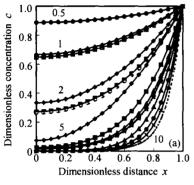
Fig. 1 shows the variation of reactant dimensionless concentration in the catalyst slab for different reaction orders as a function of Thiele modulus.

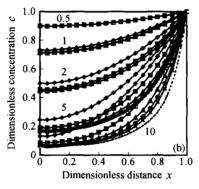
For the first order reaction, Fig. 1(a) presents the typical trend of variation of concentration. The error between the analytical and numerical results for all data is within 0.0001. The values predicted by decomposition method are in agreement with those by the analytical solution. At a lower value of $\phi(<1)$, the maximum error is only 0.0188, the relative error is 2.68%, the decomposition solution with 2 terms is good enough. Furthermore, the solution with 3 terms is overlapped with analytical solution. At a higher value of ϕ (≥ 5), diffusion strongly influences the rate of reaction, a large error arises, however, with the increase in the number of terms in decomposition solution, a reasonable agreement with the numerical solution is achieved. As the number of terms reaches 6, the de-composition solution yields satisfactory agreement with the analytical solution, for example, at $\phi = 5$, the maximum error is 0.0026, relative error is 0.427%.

Fig. 1(b) and (c) show the variation of concentration for the second and half order reactions respectively. In the case of these reactions, there is no analytical solution to the non-linear model, so comparisons with a numerical method can only be done. For the second order reaction, there is a good agreement (the overlapping of the two curves shown in Fig. 1 (b)) between the decomposition solution with 3 terms and numerical one at $\phi = 1.0$. With the increasing in Thiele modulus, the difference between the two solutions increases. In the case of $\phi > 5$, the solution with 6 terms is required to achieve reasonable agreement, for example, at $\phi = 5$, the maximum difference is 0.0168, the relative difference is 3.32%. For a half order reaction, shown as Fig. 1(c), the so-

lution of the decomposition method gives a good a-greement with the numerical solution at lower values of Thiele modulus ($\phi \leq 1$); at higher values of ϕ , either the 3 terms or 4 terms solution gives acceptable agreement with the numerical method. For example, at $\phi = 2$, the maximum difference between the two solutions is 0.0288, and the relative difference is 6.01%. In the case of $\phi > 2$, since the property of the problem to the 0.5th order reaction is so particular that the numerical solution of finite difference does

not easily converge and the decomposition solution is not stable. As shown in Fig. 1(c), there is a phenomenon that the curves of the solutions with 3 and 4 terms are at two sides of that of the numerical solution, the curve of 4 terms solution is above, but that of 3 terms solution is under. In the case of the number of terms m+1>4, the unsteadiness of the solution of the decomposition method is more obvious. As ϕ increases up to 2.5, neither the numerical nor decomposition solution is convergent.





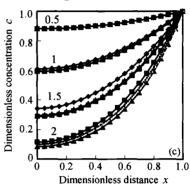


Fig. 1. Variation of dimensionless concentration as a function of Thiele modulus \$\phi\$. (a) 1st order reaction; (b) 2nd order reaction; (c) 0.5th order reaction. \$\phi\$ 2 terms, \$\mathbb{\Bar{a}}\$ 3 terms, \$\mathbb{\A}\$ 4 terms, \$\mathbb{\Omega}\$ 5 terms, \$\mathbb{\Omega}\$ - - numerical solution.

It is known that c_0 is the value of c at x=0, where the boundary condition is $\frac{\mathrm{d}x}{\mathrm{d}c}=0$. For the coupled process of diffusion-reaction, all of the formulas of particular solutions are obtained if the c_0 is known. It is obvious that, the stronger the non-linearity of the problem is, the more terms in decomposition solution will be needed and that the non-linearity of this kind of problem depends on the values of parameter ϕ and reaction order.

4.2 Relationship of effectiveness factor with \$\phi\$

Effectiveness factor is an important concept in chemical reaction engineering. Fig. 2 shows the variation of effectiveness factor for the first, second and half order reactions as a function of Thiele modulus. Clearly, all of the curves show the trend of a decrease in effectiveness factor as Thiele modulus increases.

For the first order reaction (Fig. 2 (a)), at lower values of $\phi(<2)$, any decomposition solution gives satisfactory agreement with the numerical solution. When ϕ is above 2.5, only the solutions with more terms (for example, m=5) get acceptable agreement with the numerical one. For instance, when $\phi=5$, the decomposition solution with 6 terms has a difference of 0.0020, and the relative difference is only 1.02%.

For the second order reaction (Fig. 2 (b)), only one approximate analytical solution is known so far, which is obtained by one-term orthogonal collocation OC^[7]. As can be seen, the agreement between this approximate analytical solution with both the numerical one of finite difference and decomposition one is poor. At lower values of $\phi(\leq 2)$, comparing the performance of the orthogonal collocation solution with that of the decomposition one, the former is better; however, at higher values of $\phi(\geqslant 5)$, the latter is better. The difference between the decomposition solution with 3 terms and the numerical solution is equivalent to that of orthogonal collocation one and numerical one. For example, at $\phi = 5$, the difference between the decomposition solution and the numerical solution is 0.0695, while that of the solution by oneterm orthogonal collocation and the numerical one is 0.0646. With increasing in the number of terms in decomposition solution, the values of the effectiveness factor predicted by decomposition solution approach those calculated by numerical one. As the term number reaches 6, at $\phi = 5$, comparing the decomposition solution with the numerical one, the difference between the two is 0.0011 and the relative difference is 0.644%.

Fig. 2(c) shows effectiveness factor of the half order reaction. At lower values of $\phi(\leq 1.5)$, the de-

composition solution with 3 or 4 terms gives satisfactory agreement with the numerical solution. Comparing the 3 terms decomposition solution with the nu-

merical one, the maximum difference is 0.0154 and the relative difference is 1.60%; as $\phi \ge 2$, the two solutions are unstable, even not convergent.

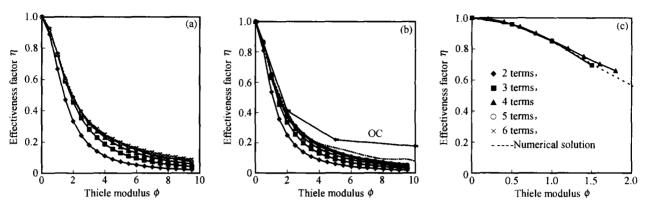


Fig. 2. Variation of effectiveness factor as a function of Thiele modulus. (a) 1st order reaction; (b) 2nd order reaction; (c) 0.5th order reaction

The effectiveness factors of the 2nd and 0.5th order reactions have their own nonlinear properties. As shown in Fig. 2 (b), there is a phenomenon that the five curves of effectiveness factor by decomposition solution for 2nd order reaction are under that of numerical one, that is, the solution of effectiveness factor by the decomposition method approaches the numerical one from lower value direction. However in Fig. 2 (c), the curve of the 3 terms decomposition solution is above that of the numerical solution, but the curve of the 4 terms decomposition solution appears under it. In the case of Thiele modulus above 2, the decomposition solution with 3 terms is unstable, this is not shown in Fig. 2 (c).

In this paper, the effectiveness factor is calculated by using the concentration gradient value at x=1, where the boundary condition is c=1, so the error of the concentration derivative at this end point is maximum, and the difference between the decomposition solution and the numerical one is maximum too. If the effectiveness factor is calculated by the integral method, as shown in Eq. (29), the difference could have been reduced.

$$\eta = \frac{\int_0^1 \theta_{m+1, n}^n dx}{R_{x=1}} = \int_0^1 \theta_{m+1, n}^n dx.$$
 (29)

The value calculated by Eq. (29) is relative to the integral area under the curves in Fig. 1. This will be discussed in another paper.

5 Conclusions

The Adomian decomposition method has been

successfully used to solve the nonlinear model of the second and half order reactions for a coupled diffusionreaction process in a catalyst pellet. For the simple nonlinear differential equation, an approximate analytical solution, which can give continuous values of dimensionless concentration and effectiveness factor, can be obtained by the decomposition method. At lower values of ϕ , the formula of the decomposition solution with 3 terms is easy to derive and yields a satisfactory agreement with the numerical solution; at higher values of ϕ , the reasonable agreement between the numerical solution and the decomposition one is achieved as the number of terms in the decomposition method increases, for instance, m = 5. Once the decomposition solution is unstable, the numerical one by finite difference method is not easily convergent; in this case, the accuracy is difficult to be judged.

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