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Approximate analytical solutions for a mathematical model of a tubular packed-bed catalytic reactor using an Adomian decomposition method

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ABSTRACT

In this paper, a mathematical model of a tubular packed-bed catalytic reactor, which is modeled by a system of strongly nonlinear second-order partial differential equations with incompatible boundary conditions, will be solved. By properly using the boundary conditions and correctly choosing the solution search direction, approximate analytic solutions for the model can be obtained by the Adomian decomposition method. When the values of the dimensionless parameters in the system are assigned within a suitable range, the solutions describe objectively the distributions of the temperature and key reactant concentration in the reactor.

1. Introduction

For many years, classical partial differential equations or systems of equations arising from mathematics and physics have been very well known [1–6]. The solutions of these equations or systems are often existent and unique under the given initial and boundary conditions. However, the situation may be different in the applied sciences and engineering [7–9]. For instance, in catalytic and electrochemical engineering, certain problems which are modeled by second-order partial differential equations or systems of equations often involve boundary conditions matching one or both of the following descriptions: (i) the given boundary conditions in a coordinate direction are nonstandard [10]; (ii) the given boundary conditions in different coordinate directions are incompatible, meaning that the solutions of the equations or systems of equations cannot simultaneously satisfy all the given boundary conditions in different coordinate directions [8,9] exactly. In [10], the authors have pointed out that condition (i) cannot ensure the existence and uniqueness of the solutions for the model. As will be seen later, condition (ii) will give rise to a situation in which exact solutions for the model do not exist. In spite of this, it is still possible to search for rational and objective solutions for the model by properly using the given boundary conditions according to the degree of their effect on the objective solutions.

The mathematical model of the packed (or Fixed) bed catalytic reactor (PBCR) is a classical one in chemical reaction engineering [8,9], it is difficult to be solved numerically for a theoretical analysis due to its strong nonlinearity. Large numbers of catalytic reactions are exothermic reactions, which have been widely used in basic chemical and petrochemical industries [8], such as chemicals synthesis, hydrocarbon oxidation or hydrogenation, and coal to synthetic oil etc. Industrial PBCRs are usually in a cylindrical form, however, for highly exothermic gas–solid catalytic reactions the PBCR must be in a tubular form (TPBCR) because of its large area and short distance for heat transport and it can remove the reaction heat through the

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reactor wall in a timely manner to prevent the catalysts from overheating and losing activity [9, p. 136]. For such cases there is a need for a model which involves the resistance to heat and mass transfer in the radial direction, so as to predict a more detailed temperature and concentration pattern in the reactor.

Actual reaction processes in industrial reactors are very complex; hence reasonable simplification for modeling is necessary. A dimensionless model with universality is required for a theoretical analysis. Referred to the classic PBCR models in Ref. [8,9, p. 538, p. 134], a dimensionless TPBCR model which describes the distributions of the dimensionless temperature $\theta(r,z)$ and key reactant concentration $c_A(r,z)$ in the catalytic reactor is written as:

$$\begin{cases} \frac{\partial c_A}{\partial z} = \frac{\zeta}{Pe_m}\left(\frac{\partial^2 c_A}{\partial r^2} + \frac{1}{r}\frac{\partial c_A}{\partial r}\right) - Da_m \exp\left(-\frac{\varepsilon}{\theta}\right)c_A, \\ \frac{\partial \theta}{\partial z} = \frac{\zeta}{Pe_h}\left(\frac{\partial^2 \theta}{\partial r^2} + \frac{1}{r}\frac{\partial \theta}{\partial r}\right) + Da_h \exp\left(-\frac{\varepsilon}{\theta}\right)c_A, \end{cases} \tag{1}$$

where r and z are the dimensionless radial and axial distances respectively, ζ is the aspect ratio of the cylindrical reactor, $\zeta > 100$ was adopted for the tubular form in this model solution; Pe_m is the mass-transfer Peclet number, Pe_h is the heat-transfer Peclet number, Da_m is the mass-transfer Damköhler number, Da_h is the heat-transfer Damköhler number, ε is the dimensionless activation energy, and all of these are positive constants. A simpler kinetic expression for an irreversible reaction with first order was used for this dimensionless model $r(c,T) = k_0 \exp\left(-\frac{E_a}{R_g T}\right)c$,then it forms into the nonlinear term $N(c_A,\theta) = \exp\left(-\frac{\varepsilon}{\theta}\right)c_A$. It should be noted, there is a coefficient $\frac{1}{r}$ with a singularity[11] for the cylindrical (or tubular) geometry of the reactor.

The given boundary conditions are:

$$z = 0, \quad c_A(r,0) = 1, \tag{2}$$

$$z = 0, \quad \theta(r,0) = 1, \tag{3}$$

$$r = 0, \quad \frac{\partial c_A}{\partial r}(0,z) = 0, \tag{4}$$

$$r = 0, \quad \frac{\partial \theta}{\partial r}(0,z) = 0, \tag{5}$$

$$r = 1, \quad \frac{\partial c_A}{\partial r}(1,z) = 0, \tag{6}$$

$$r = 1, \quad \frac{\partial \theta}{\partial r}(1,z) = -Bi[\theta(1,z) - \theta_w], \tag{7}$$

where Bi is the heat transfer Boit number and θ_w is the dimensionless wall temperature.

Eqs. (1)–(7) constitute a dimensionless mathematical model for a packed-bed catalytic reactor. It should be noted that mathematically exact solutions for this model may not exist, meaning that there are no $c_A(r,z)$ and $\theta(r,z)$ which are continuous on the closed region $\{(r,z)|0 \leqslant r \leqslant 1, 0 \leqslant z \leqslant 1\}$ and satisfy exactly Eqs. (1)–(7) and whose second-order partial derivatives are continuous in the region $\{(r,z)|0 < r < 1, 0 < z < 1\}$. To find the most realistic possible distribution of the key reactant concentration and temperature in the reactor, the boundary conditions (2)–(7) need to be satisfied in varying degrees: some should be satisfied accurately, some should be satisfied approximately, and some are regarded only as reference conditions. When the first-order partial derivative of $c_A(r,z)$ is continuous on the closed region $\{(r,z)|0 \leqslant r \leqslant 1, 0 \leqslant z \leqslant 1\}$, the boundary condition (4) must be satisfied; otherwise, this will lead to $\frac{1}{r}\frac{\partial c_A}{\partial r} \to \infty (r \to 0^+)$ in the first equation of (1). In like manner, the boundary condition (5) must also be satisfied. In addition, the heat transfer on the boundary has a great impact on the variation of $c_A(r,z)$ and $\theta(r,z)$, so condition (7) should be satisfied. When the boundary conditions in the z-direction ((4), (5), and (7)) are satisfied, the conditions in the r-direction ((2), (3)) can be satisfied only approximately; otherwise, there may not exist solutions that fully satisfy these five boundary conditions because of their incompatibility. Condition (6) describing the boundary variation of $c_A(r,z)$ in a natural state can be regarded as a reference condition. Through the appropriate use of these boundary conditions, an approximate analytical solution for this model using the Adomian decomposition method will be sought, as described in the following discussion.

2. Theoretical derivation of approximate analytic solutions by ADM

In an operator form, the system of Eq. (1) can be written as:

$$\begin{cases} L_z c_A = \frac{\zeta}{Pe_m}(L_{rr}c_A + \frac{1}{r}L_r c_A) - Da_m c_A N(\theta), \\ L_z \theta = \frac{\zeta}{Pe_h}(L_{rr}\theta + \frac{1}{r}L_r \theta) + Da_h c_A N(\theta), \end{cases} \tag{8}$$

where L_z, L_r and L_{rr} are linear operators which are defined as $L_z = \frac{\partial}{\partial z}, L_r = \frac{\partial}{\partial r}$ and $L_{rr} = \frac{\partial}{\partial r^2}$ and $N(\theta)$ represents the strong non-linear function $\exp(-\frac{\varepsilon}{\theta})$.

To obtain solutions satisfying (4), (5), and (7), the r-direction is chosen as the solution search direction and the inverse operator L_{rr}^{-1} is defined as follows:

$$L_{rr}^{-1}(\cdot) = \int_1^r \left[\int_0^u (\cdot)dt\right]du. \tag{9}$$

Applying the inverse operator L_{rr}^{-1} to both sides of the first and second equation of (8) respectively yields:

$$c_A = \frac{Pe_m}{\zeta}L_{rr}^{-1}L_z c_A - L_{rr}^{-1}\left(\frac{1}{r}L_r c_A\right) + \frac{Pe_m Da_m}{\zeta}L_{rr}^{-1}[N(\theta)c_A] + A(z)r + B(z), \tag{10}$$

$$\theta = \frac{Pe_h}{\zeta}L_{rr}^{-1}L_z\theta - L_{rr}^{-1}\left(\frac{1}{r}L_r\theta\right) - \frac{Pe_h Da_h}{\zeta}L_{rr}^{-1}[N(\theta)c_A] + C(z)r + D(z), \tag{11}$$

where $A(z)$, $B(z)$, $C(z)$,and$D(z)$ are the undetermined functions. Performing the partial derivative operations with respect to r on both sides of (10) and using the boundary condition $r = 0, \frac{\partial c_A}{\partial r}(0,z) = 0$, the result is $A(z) = 0$. Then, letting $r = 1$, $0 \leqslant z \leqslant 1$ on both sides of (10), $c_A(1,z) = B(z)$, $0 \leqslant z \leqslant 1$. Similarly, according to (11) $C(z) = 0$, $0 \leqslant z \leqslant 1$ is obtained using the boundary condition $r = 0, \frac{\partial\theta}{\partial r}(0,z) = 0$ and $\theta(1,z) = D(z)$, $0 \leqslant z \leqslant 1$ is obtained by letting $r = 1$, $0 \leqslant z \leqslant 1$ on both sides of (11). Now Eqs. (10) and (11) can be rewritten as:

$$c_A = \frac{Pe_m}{\zeta}L_{rr}^{-1}L_z c_A - L_{rr}^{-1}\left(\frac{1}{r}L_r c_A\right) + \frac{Pe_m Da_m}{\zeta}L_{rr}^{-1}[N(\theta)c_A] + B(z), \tag{12}$$

$$\theta = \frac{Pe_h}{\zeta}L_{rr}^{-1}L_z\theta - L_{rr}^{-1}\left(\frac{1}{r}L_r\theta\right) - \frac{Pe_h Da_h}{\zeta}L_{rr}^{-1}[N(\theta)c_A] + D(z). \tag{13}$$

According to Adomian's decomposition method, the unknown functions $c_A(r,z)$ and $\theta(r,z)$ can be decomposed into the infinite series:

$$c_A(r,z) = \sum_{n=0}^{\infty} c_n(r,z), \tag{14}$$

$$\theta(r,z) = \sum_{n=0}^{\infty} \theta_n(r,z). \tag{15}$$

To implement the following recursive algorithm in the ADM, using the double decomposition method [12], we can also decompose $B(z)$ and $D(z)$ into infinite series:

$$B(z) = \sum_{n=0}^{\infty} b_n z^n, \tag{16}$$

$$D(z) = \sum_{n=0}^{\infty} d_n z^n, \tag{17}$$

where

$$b_0 = B(0) = c_A(1,0) = 1, \tag{18}$$

$$d_0 = D(0) = \theta(1,0) = 1. \tag{19}$$

The nonlinear function $N(\theta)$ can be decomposed into an infinite series of Adomian's polynomials

$$N(\theta) = \sum_{n=0}^{\infty} \overline{A_n}, \tag{20}$$

where the Adomian's polynomials $\overline{A_n}$ are generated according to the following formula [13]:

$$\overline{A_n}(\theta_0,\theta_1,\ldots,\theta_n) = \frac{1}{n!}\left[\frac{d^n}{d\lambda^n}N\left(\sum_{k=0}^{\infty}\lambda^k\theta_k\right)\right]_{\lambda=0} = \frac{1}{n!}\left[\frac{d^n}{d\lambda^n}N\left(\sum_{k=0}^{n}\lambda^k\theta_k\right)\right]_{\lambda=0}. \tag{21}$$

It is therefore possible to write:

$$\begin{aligned}
&\overline{A_0}(\theta_0) = \exp\left(-\frac{\varepsilon}{\theta_0}\right),\\
&\overline{A_1}(\theta_0,\theta_1) = \varepsilon\exp\left(-\frac{\varepsilon}{\theta_0}\right)\theta_1\theta_0^{-2},\\
&\overline{A_2}(\theta_0,\theta_1,\theta_2) = \frac{\varepsilon}{2}\exp\left(-\frac{\varepsilon}{\theta_0}\right)(2\theta_0^2\theta_2 - 2\theta_0\theta_1^2 + \varepsilon\theta_1^2)\theta_0^{-4},\\
&\ldots
\end{aligned} \tag{22}$$

Then $N(\theta)c_A$ can be represented in the form of an infinite series of Adomian's polynomials

$$N(\theta)c_A = \sum_{n=0}^{\infty} A_n, \tag{23}$$

where the A_n are determined by the following computation:

$$A_n(c_0, c_1, \ldots, c_n; \theta_0, \theta_1, \ldots, \theta_n) = \sum_{k=0}^{n} c_k \overline{A_{n-k}}. \tag{24}$$

According to (12), (13), (18), and (19), it is possible to choose the values of the zeroth components θ_0 and c_0 and to write recursive relations as follows:

$$\theta_0 = 1, \tag{25}$$

$$c_0 = 1, \tag{26}$$

$$c_n = \frac{Pe_m}{\zeta} L_{rr}^{-1} L_z c_{n-1} - L_{rr}^{-1}\left(\frac{1}{r} L_r c_{n-1}\right) + \frac{Pe_m Da_m}{\zeta} L_{rr}^{-1} A_{n-1} + b_n z^n, \tag{27}$$

$$\theta_n = \frac{Pe_h}{\zeta} L_{rr}^{-1} L_z \theta_{n-1} - L_{rr}^{-1}\left(\frac{1}{r} L_r \theta_{n-1}\right) - \frac{Pe_h Da_h}{\zeta} L_{rr}^{-1} A_{n-1} + d_n z^n, \tag{28}$$

where $n \geqslant 1$. For later numerical computation, assume the expressions

$$\begin{aligned}\overline{c_A} &= \overline{c_A}(r, z; \zeta, Pe_m, Da_m, Pe_h, Da_h, \varepsilon, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) \\ &= 1 + \sum_{n=1}^{7} c_n(r, z; \zeta, Pe_m, Da_m, Pe_h, Da_h, \varepsilon, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7)\end{aligned} \tag{29}$$

and

$$\begin{aligned}\overline{\theta} &= \overline{\theta}(r, z; \zeta, Pe_m, Da_m, Pe_h, Da_h, \varepsilon, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) \\ &= 1 + \sum_{n=1}^{7} \theta_n(r, z; \zeta, Pe_m, Da_m, Pe_h, Da_h, \varepsilon, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7),\end{aligned} \tag{30}$$

which denote the seven-term approximation to c and θ respectively. Given a set of values of the dimensionless parameters ζ, Pe_m, Da_m, Pe_h, Da_h, ε, Bi, and θ_w, Eqs. (29) and (30) can be rewritten as:

$$\begin{aligned}\overline{c_A} &= \overline{c_A}(r, z; \zeta, Pe_m, Da_m, Pe_h, Da_h, \varepsilon, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) = \overline{c_A}(r, z; b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) \\ &= 1 + \sum_{n=1}^{7} c_n(r, z; b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7),\end{aligned} \tag{31}$$

$$\begin{aligned}\overline{\theta} &= \overline{\theta}(r, z; \zeta, Pe_m, Da_m, Pe_h, Da_h, \varepsilon, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) = \overline{\theta}(r, z; b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) \\ &= 1 + \sum_{n=1}^{7} \theta_n(r, z; b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7).\end{aligned} \tag{32}$$

Substituting (32) into the mixed boundary condition (7) yields:

$$\sum_{n=1}^{7} \frac{\partial \theta_n}{\partial r}(1, z, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) - Bi\left[\theta_w - 1 - \sum_{n=1}^{7} \theta_n(1, z, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7)\right] = 0. \tag{33}$$

The left side of (33) is a polynomial of degree 7 in z, so (33) can be rewritten as:

$$\begin{aligned}P(z, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) = &\sum_{n=1}^{7} \frac{\partial \theta_n}{\partial r}(1, z, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) \\ &- Bi\left[\theta_w - 1 - \sum_{n=1}^{7} \theta_n(1, z, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7)\right] = 0.\end{aligned} \tag{34}$$

By comparing the coefficients of z on both sides of (34), a nonlinear system of algebraic equations can be obtained:

$$\begin{cases} P(0, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) = 0, \\ \frac{1}{n!}\frac{\partial^n P}{\partial z^n}(0, b_1, b_2, \ldots, b_7, d_1, d_2, \ldots, d_7) = 0 \quad (n = 1, 2, \ldots, 7). \end{cases} \tag{35}$$

To satisfy the boundary conditions (2) and (3) approximately, let

$$1+\sum_{n=1}^{7} c_n(r,0,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7)=1 \tag{36}$$

and

$$1+\sum_{n=1}^{7} \theta_n(r,0,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7)=1. \tag{37}$$

The left sides of (36) and (37) are polynomials of degree 14 in r, so by comparing the coefficients of r on both sides of (36) and (37) respectively,

$$\begin{cases} \sum\limits_{n=1}^{7} c_n(0,0,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7)=0, \\ \frac{1}{k!}\sum\limits_{n=1}^{7} \frac{\partial^k c_n}{\partial r^k}(0,0,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7)=0 \quad (n=1,2,\ldots,14), \end{cases} \tag{38}$$

$$\begin{cases} \sum\limits_{n=1}^{7} \theta_n(0,0,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7)=0, \\ \frac{1}{k!}\sum\limits_{n=1}^{7} \frac{\partial^k \theta_n}{\partial r^k}(0,0,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7)=0 \quad (n=1,2,\ldots,14). \end{cases} \tag{39}$$

By solving the systems of Eqs. (35), (38), and (39), it is possible to obtain all valves of $b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7$ which satisfy (35) exactly and satisfy (38) and (39) approximately. Finally, setting

$$\overline{c_A}(r,z)=\overline{c_A}(r,z,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7) \tag{40}$$

and

$$\overline{\theta_A}(r,z)=\overline{\theta_A}(r,z,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7), \tag{41}$$

leads to approximate analytic solutions of $c_A(r,z)$ and $\theta(r,z)$.

3. Concrete expressions and graphs of approximate analytic solutions

As in [10], MATLAB is used as a tool for symbolic and numerical operations, and relative data for a tubular fixed-bed catalytic reactor (TFBCR) [8] have been chosen as the basis for determining the values of the dimensionless parameters in the model.

Assigning a set of values for the dimensionless parameters ζ, Pe_m, Da_m, Pe_h, Da_h, ε and Bi e.g. $\zeta = 155.2$, $Pe_m = 282.46$, $Da_m = 109.89$, $Pe_h = 248.3$, $Da_h = 75$, $\varepsilon = 9$, and $Bi = 1.5$, and substituting these values into (31) and (32) respectively yields:

$$\overline{c_A}(r,z,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7)=1+0.123r^2+b_1z+\sum_{n=2}^{7} c_n(r,z,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7) \tag{42}$$

and

$$\overline{\theta_A}(r,z,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7)=1-0.0074r^2+d_1z+\sum_{n=2}^{7} \theta_n(r,z,b_1,b_2,\ldots,b_7,d_1,d_2,\ldots,d_7), \tag{43}$$

According to the definition of a partial derivative and the boundary condition (3),

$$\frac{\partial\theta}{\partial r}(1,0)=\lim_{\Delta r\to 0^-}\frac{\theta(1+\Delta r,0)-\theta(1,0)}{\Delta r}=0. \tag{44}$$

Combining the mixed boundary condition (7) and the results obtained above in (19) and (44) yields $\theta_w = 1$; otherwise, boundary condition (3) in the r-direction and condition (7) in the z-direction will be clearly incompatible.

After all the parameter values have been determined, a search is conducted for a solution of Eq. (35) near the initial point

$$(b_1,b_2,b_3,b_4,b_5,b_6,b_7,d_1,d_2,d_3,d_4,d_5,d_6,d_7)=(-0.3,-0.2,-0.1,0,0,0,0,0.3,0.2,0.1,0,0,0,0), \tag{45}$$

using the MATLAB function fsolve () to find the solution

$$\begin{aligned}(b_1,b_2,b_3,b_4,b_5,b_6,b_7,d_1,d_2,d_3,d_4,d_5,d_6,d_7)=(&-0.3006,-0.0822,-0.0591,0.0450,0.0385,0.0253,0.0,\\ &0.2264,0.1205,0.0613,-0.0119,-0.0035,0.0007,0.0).\end{aligned} \tag{46}$$

Substituting (46) into the left-hand side of the first equation of (38) yields −0.2107. Evidently, (46) cannot satisfy approximately the system of Eq. (38). A search for a solution of the system of equations composed by the system of Eq. (35) and the first equation of (38) near the initial point (45) yields:

$$(b_1, b_2, b_3, b_4, b_5, b_6, b_7, d_1, d_2, d_3, d_4, d_5, d_6, d_7) = (-0.3024, -0.0996, -0.0375, 0.0398, 0.0354, 0.0234, 0.0, 0.2287, 0.1204, 0.0620, -0.0120, -0.0035, 0.0007, 0.0). \quad (47)$$

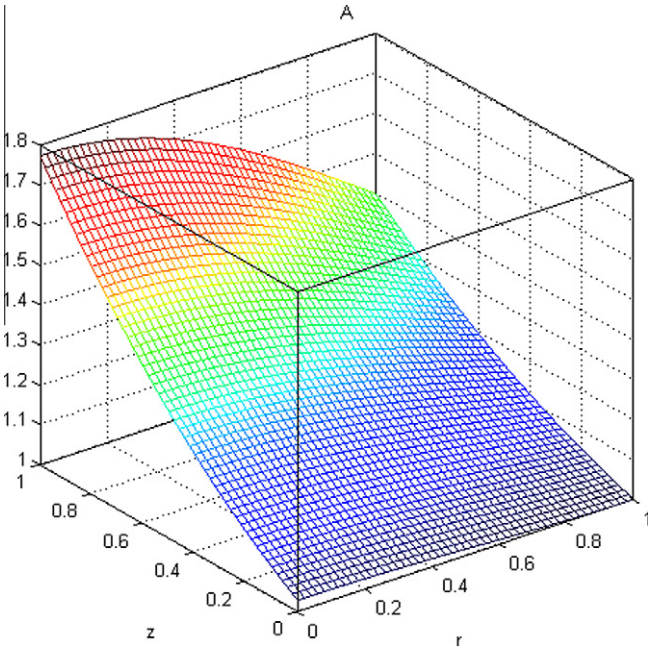

Fig. A. Distribution of dimensionless temperature $\theta(r,z)$.

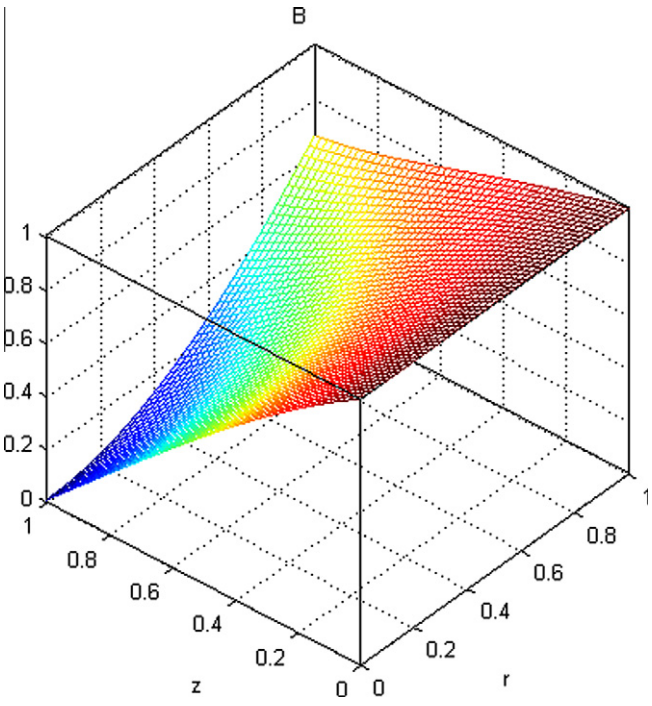

Fig. B. Distribution of dimensionless key reactant concentration $c_A(r,z)$.

Substituting (47) into the left-hand side of every equation of systems (38) and (39) yields a maximum absolute value of 0.0572. It can therefore be concluded that (47) is not only the solution of (35), but also an approximate solution of (38) and (39). Substituting (47) into (42) and (43) respectively yields an expression for the approximate analytic solutions $c_A(r,z)$ and $\theta(r,z)$. These expressions are very long, so their values are plotted in Figs. A and B.

The TPBCR model aims to determine the coupled influence of various transport and kinetics parameters and to show how they influence the operating performance of the reactor. The predicted dimensionless temperature and concentration (conversion rate of reaction) distributions will provide a theoretical basis for designing and optimizing the TFBCR. For instance, the design would be directed towards avoiding eventual detrimental over temperatures in the axis of the reactor.

4. Conclusion

Second-order partial differential equations or systems of equations with incompatible boundary conditions often appear in engineering problems. When exact solutions for this type of problems do not exist, solutions satisfying the given boundary conditions to various degrees according to the degree of impact of these conditions on the objective solutions can be sought, so that rational solutions can be obtained. The Adomian decomposition method provides approximate analytic solutions which can satisfy the given conditions to various degrees. This method can also be applied to similar problems involving higher-order partial differential equations or systems of equations.

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