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Classical Perturbation Method for the Solution of a Model of Diffusion and Reaction

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Abstract

In this paper, we employ perturbation method (PM) to solve nonlinear problems. As case study PM is employed to obtain approximate solutions for the nonlinear differential equation that models the diffusion and reaction in porous catalysts. We find that the square residual error (S.R.E) of our solutions is in the range and this requires only the third order approximation of PM, which shows the effectiveness of the method.

Keywords: Perturbation Method; Nonlinear Differential Equations; Porous Catalysts, Diffusion and Reaction.

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1. Introduction

A relevant problem in chemical engineering is the prediction of diffusion and reaction rates in porous catalysts, in the general case which the reaction rate depends nonlinearly on concentration [24,29]. Therefore, it is important to search for accurate approximate solutions to the equations describing these phenomena. However, it is well known that nonlinear differential equations that describe them are difficult to solve. The perturbation method (PM) is a well established method; it is among the pioneer techniques to approach various kinds of nonlinear problems. Although the method appeared in the early 19th century, the application of a perturbation procedure to solve nonlinear differential equations was performed later on that century. The most significant efforts were focused above all on celestial mechanics, fluid mechanics, and aerodynamics [1,28]. In a broad sense, the method proposes to express a nonlinear differential equation in terms of one linear part and other nonlinear. The nonlinear part is considered as a small perturbation through a small parameter (the perturbation parameter ε). The assumption that the nonlinear part is small compared to the linear is something restrictive. To remedy the above, other alternatives have been proposed: variational approaches [5-7], tanh method [8], exp-function [9,10], Adomian's decomposition method [11,12], parameter expansion [13], homotopy perturbation method [3,4,14,15,17-20,22,23], homotopy analysis method [16], homotopy asymptotic method [2], among others. Although the PM method provides in general, better results for small perturbation parameters $\varepsilon << 1$ we will see that our approximation, besides to be handy, have a good accuracy, even for relatively large values of the perturbation parameter [21, 26, 27], which extends the usefulness of PM method to cases less restricted.

The rest of the work is organized as follows. In Section 2, we introduce the basic idea of the PM method. For Section 3, we provide an application of the PM method, by solving the differential equation that models the diffusion and reaction in porous catalysts. Section 4 discusses the main results obtained. Finally, a brief conclusion is given in Section 5.

2. Basic idea of perturbation method

Let the differential equation of one dimensional nonlinear system be in the form

$$L(x) + \varepsilon N(x) = 0, \tag{1}$$

where we assume that x is a function of one variable $x = x(t)$, $L(x)$ is a linear operator which, in general, contains derivatives in terms of t, $N(x)$ is a nonlinear operator, and ε is a small parameter [21,26,27].

Considering the nonlinear term in (1) to be a small perturbation and assuming that the solution for (1) can be written as a power series in the small parameter ε.

$$x(t) = x_0(t) + \varepsilon x_1(t) + \varepsilon^2 x_2(t) + \ldots \tag{2}$$

Substituting (2) into (1) and equating terms having identical powers of ε, we obtain a number of differential equations that can be integrated, recursively, to find the values for the functions: $x_0(t)$, $x_1(t)$, $x_2(t)$ …

3. Application of PM to obtain handy approximate solutions for the nonlinear chemical equation under study.

The objective of this section is employ PM, in order to search for handy approximate solutions for the nonlinear problem of diffusion and reaction in porous catalysts.

We will consider the case where the reaction rate can depend nonlinearly on concentration, so that we can conceive the system under study as a solid material with pores through which the reactants and products diffuse [24,25,29].

In terms of dimensionless variables, the above problem is expressed in terms of the following nonlinear boundary value problem with mixed boundary conditions.

$$y'' - m^2 y^n = 0 \qquad (n \geq -1) \qquad y'(0) = 0, \qquad y(1) = 1, \tag{3}$$

where prime denotes from here on, differentiation respect to x, m denotes the Thiele modulus, and n is known as the reaction order [24, 25].

In accordance with PM method, we identifying terms:

$$L(y) = y''(x), \tag{4}$$

$$N(y) = -m^2 y^2, \tag{5}$$

In order to obtain an approximate analytical solution for nonlinear problem (3), after identifying $\varepsilon = m^2$ with the PM parameter, we assume a solution for (3) in the form

$$y(x) = y_0(x) + \varepsilon y_1(x) + \varepsilon^2 y_2(x) + \varepsilon^3 y_3(x) + \varepsilon^4 y_4(x) + \ldots, \qquad \text{(see (2))}. \tag{6}$$

Equating the terms with identical powers of ε it can be solved for $y_0(x)$, $y_1(x)$, $y_2(x)$,…

and so on. Later it will be seen that, a very good handy result is obtained, by keeping just up to third order approximation.

We will consider the following cases study:

Case study A $\quad n = 2, \quad m = 0.3$ and $m = 0.5$,

Case study B $\quad n = 3, \quad m = 0.3$ and $m = 0.5$.

Case study A

The procedure mentioned above for these values, results in the following differential equations

$$\varepsilon^0)\ y_0'' = 0, \qquad y_0'(0) = 0, \quad y_0(1) = 1, \tag{7}$$

$$\varepsilon^1)\ y_1'' - y_0^2 = 0, \qquad y_1'(0) = 0, \quad y_1(1) = 0, \tag{8}$$

$$\varepsilon^2)\ y_2'' - 2y_0 y_1 = 0, \qquad y_2'(0) = 0, \quad y_2(1) = 0, \tag{9}$$

$$\varepsilon^3)\ y_3'' - y_1^2 - 2y_0 y_2 = 0, \qquad y_3'(0) = 0, \quad y_3(1) = 0, \tag{10}$$

…

and so on.

Thus, after solving the above differential equations, we get

$$y_0(x) = 1, \tag{11}$$

$$y_1(x) = \frac{x^2}{2} - \frac{1}{2}, \tag{12}$$

$$y_2(x) = \frac{x^4}{12} - \frac{x^2}{2} + \frac{5}{12}, \tag{13}$$

$$y_3(x) = \frac{x^6}{72} - \frac{x^4}{8} + \frac{13x^2}{24} - \frac{31}{72}, \tag{14}$$

...

By substituting (11)-(14) into (6) we obtain a third order approximation for the solution of (3).

On the other hand, employing the values $m = 0.3$ and $m = 0.5$ we obtain respectively the following handy approximate solutions as follows.

$$y(x) = 0.9580611250 + 0.041344875x^2 + 0.000583875x^4 + 0.0000101250x^6 \tag{15}$$

$$y(x) = 0.8943142361 + 0.1022135417x^2 + 0.003255208333x^4 + 0.0002170138889x^6 \tag{16}$$

Case study B

Following the explained procedure, we get

$$\varepsilon^0)\ y_0'' = 0, \qquad y_0'(0) = 0, \quad y_0(1) = 1, \tag{17}$$

$$\varepsilon^1)\ y_1'' - y_0^3 = 0, \qquad y_1'(0) = 0, \quad y_1(1) = 0, \tag{18}$$

$$\varepsilon^2)\ y_2'' - 3y_0^{\,2}y_1 = 0, \qquad y_2'(0) = 0, \quad y_2(1) = 0, \tag{19}$$

$$\varepsilon^3)\ y_3'' - 3y_0y_1^2 - 3y_0^{\,2}y_2 = 0, \quad y_3'(0) = 0, \quad y_3(1) = 0, \tag{20}$$

…

and so on.

After solving the elementary differential equations (17)-(20), we obtain

$$y_0(x) = 1, \tag{21}$$

$$y_1(x) = \frac{x^2}{2} - \frac{1}{2}, \tag{22}$$

$$y_2(x) = \frac{x^4}{8} - \frac{3x^2}{2} + \frac{11}{8}, \tag{23}$$

$$y_3(x) = \frac{3x^6}{80} - \frac{x^4}{2} + \frac{39x^2}{16} - \frac{79}{40}, \tag{24}$$

...

By substituting (21)-(24) into (6) we obtain a third order approximation for the solution of (3).

Next, we propose once again the values $m = 0.3$ and $m = 0.5$, to obtain the following handy approximate solutions.

$$y(x) = 0.964697725 + 0.0346269375x^2 + 0.000648x^4 + 0.0000273375x^6 \tag{25}$$

$$y(x) = 0.930078125 + 0.0693359375x^2 + 0.0005859375x^6 \tag{26}$$

4. Discussion

The fact that PM depends on a parameter which is assumed small, suggests that the method is limited. In this work, the PM method has been applied to the important problem of finding an approximate solution for the nonlinear differential equation with mixed boundary conditions that models the diffusion and reaction in porous catalysts. This equation is relevant due to its applications in the design and operation of catalytic reactors [24]. The PM method provides in general, better results for small perturbation parameters $\varepsilon << 1$, (see (1)) and when are included the most number of terms from (2). To be precise, ε is a parameter of smallness, that measure how greater is the contribution of linear term $L(x)$ than the one of $N(x)$ in (1). In order to show the accuracy of our solutions (15), (16), (25), and (26) (see Figure1 and Figure 2) we propose calculate their square residual error (S.R.E) defined as $\int_a^b R^2\left(u(t)\right)dt$, where a and b are two values depending on the given problem (for our case study $a = 0$ and $b = 1$), while the residual is defined by the relation $R\left(\bar{u}(t)\right) = L\left(\bar{u}(t)\right) + \varepsilon N\left(\bar{u}(t)\right)$, where $\bar{u}(t)$ is an approximate solution to (1) [2]. The resulting values for the case study A: $n = 2$; $m = 0.3$ and $m = 0.5$ were respectively of $2.991002066 \times 10^{-9}$ and 0.000009385188717 while for the second case B, $n = 3$; $m = 0.3$ and $m = 0.5$ we got the values 0.0001390320968 and 0.005677464758, which confirm the accuracy of PM. If more accuracy for our solutions is required, it is possible to keep higher orders, following the PM algorithm (see section 2).

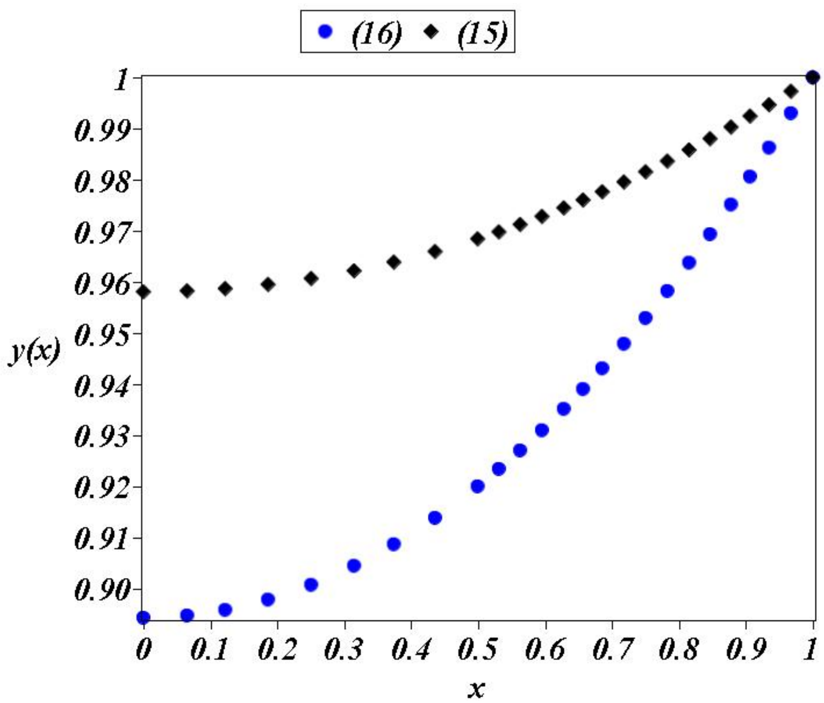

Figure 1: Proposed solutions of (3); (15), (16) for cases study: $n = 2$; $m = 0.3$ and $m = 0.5$.

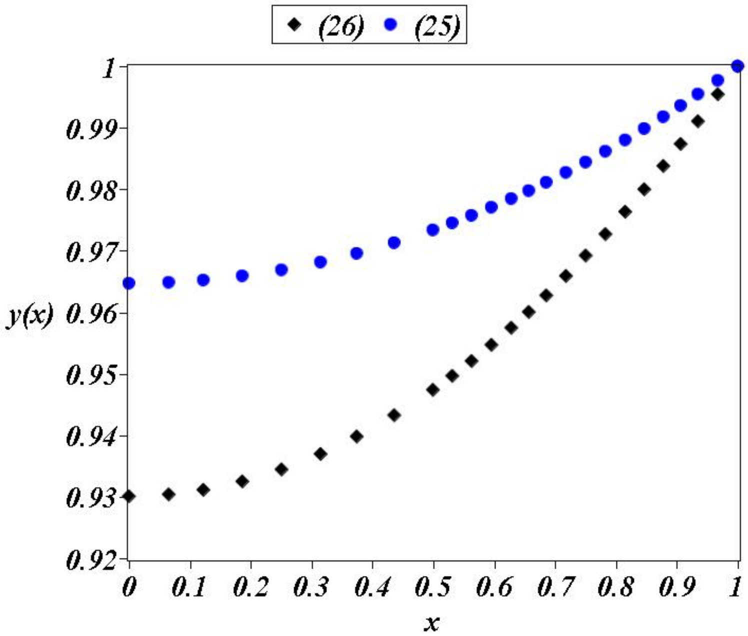

Figure 2: Proposed solutions of (3); (25), (26) for cases study: $n = 3$; $m = 0.3$ and $m = 0.5$.

Finally, it is worth mentioning that this problem has been studied for others authors, but using more complicated methods than PM. Thus, for instance, [24] found an approximate solution for (3), by using of Adomian decomposition method for some values of n and m . It is well known that Adomian is a powerful tool, but the process of obtaining its polynomial solutions is not straightforward for practical applications, the above differs considerably from PM, which is based on the solution of elementary differential equations (see (7)-(10) and (17)-(20)).

5. Conclusions

In this study, PM was presented to construct analytical approximate solutions for the nonlinear problem of diffusion and reaction in porous catalysts modeled by (3), in the form of rapidly convergent series. The success of the method for this case has to be considered as a possibility to apply it in other nonlinear problems, instead of using other sophisticated and difficult methods. From the values of square residual error (S.R.E) of the proposed solutions, it is deduced that they have good precision.

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