A Novel Study for A Model of Diffusion and Reaction in Porous Catalysts

U. Filobello-Nino, H. Vazquez-Leal *, V.M. Jimenez-Fernandez, D. Pereyra-Diaz,
C.E. Sampieri-Gonzalez. F.J. Gonzalez-Martinez, A.D. Contreras-Hernandez, O. Alvarez-Gasca,
B.E. Palma-Grayeb, J. Matias-Perez, L. Cuellar-Hernandez, J.E. Pretelin-Canela,
C. Hoyos-Reyes, L.J. Varela-Lara, J.L. Vazquez-Aguirre, L. Gil-Adalid.
Facultad de Instrumentación Electrónica, Universidad Veracruzana,
Circuito Gonzalo Aguirre Beltrán S/N, 9100,
Xalapa, Veracruz, México.

Abstract— **This work studies the nonlinear equation that models the diffusion and reaction in porous catalysts, which is of great importance in chemical engineering. The proposal is to obtain an approximate analytical expression that adequately describes the phenomenon considered. In order to find such approximation, we propose to use Laplace transform homotopy perturbation method (LT-HPM). It is observed in this analysis that the proposed solution is compact and easy to evaluate and involves polynomial functions of only five terms, which is ideal for practical applications. We find that the square residual error (S.R.E) of our solutions is in the range [10E-18, 10E-6] and this requires only fourth order approximation of the proposed method.**

Keywords— Homotopy perturbation metho; Laplace transform; nonlinear differential equations; porous catalysts diffusion and reaction.

I. INTRODUCTION

A relevant problem is the prediction of diffusion and reaction rates in porous catalysts, in the general case which the reaction rate depends nonlinearly on concentration [1]. Problems like the one mentioned, give rise to the search of solutions to nonlinear differential equations but unfortunately, solving this kind of equations is a difficult task. As a matter of fact, most of the times, it can only be get an approximate solution to such problems. With the end to approach various types of nonlinear problems, have been proposed several methods as an alternative to classical methods, such as variational approaches [2-5], tanh method [6], exp-function [7, 8], Adomian's decomposition method [1,9-14], parameter expansion [15], homotopy perturbation method [16-42], homotopy analysis method [43-45], and perturbation method [46,47] among others. Also, some exact solutions have been reported in [48].

Laplace Transform (LT) has been relevant in mathematics, both for its theoretical and practical interest, in particular because LT let to solve many problems in science and engineering, in a simpler way in comparison with other techniques [41,42,49]. The use of LT for nonlinear ordinary differential equations has focused on approximate solutions; reference [38] combined Homotopy Perturbation Method (HPM) and LT and denominated this method as LT-HPM, with the purpose to get precise solutions for these equations. Nevertheless, LT-HPM has been employed above all to solve problems with initial conditions [29,38,39]. For the above, this work presents LT-HPM method, in order to find approximate solutions for the second order nonlinear ordinary differential equation, that models a relevant problem in chemical engineering with, mixed boundary conditions [41,42].

Problems with boundary conditions on infinite intervals belong to problems on semi-infinite domains [29,40]; nevertheless, in this article we present a different approach to solve them.

II. HPM METHOD

With the purpose to understand how HPM works, we will present the following nonlinear problem [17,18]

$$A(u) - f(r) = 0, \qquad r \in \Omega, \tag{1}$$

which obeys the boundary conditions

$$B(u, \partial u / \partial n) = 0, \quad r \in \Gamma. \tag{2}$$

Where A symbolizes a differential operator, B is a boundary operator, $f(r)$ is a known function and Γ is the domain boundary for Ω. Besides A can be divided into two operators L and N, where L is linear and N nonlinear; in such a way that (1) can be expressed as follows

$$L(u) + N(u) - f(r) = 0. \tag{3}$$

In general terms, a homotopy is constructed in accordance with [17,18]

$$H(U,p) = (1-p)[L(U) - L(u_0)] + p[L(U) + N(U) - f(r)] = 0,$$
$$p \in [0,1], \quad r \in \Omega \tag{4}$$

or

$$H(U,p) = L(U) - L(u_0) + p[L(u_0) + N(U) - f(r)] = 0,$$
$$p \in [0,1], \quad r \in \Omega, \tag{5}$$

where p is known as homotopy parameter, with values within of interval 0 to 1, while u_0 approximates the solution of (3) regarding the boundary conditions of the problem.

Considering that solution for (4) or (5) is expressed in terms of p as

$$U = v_0 + v_1 p + v_2 p^2 + \ldots \tag{6}$$

Then, after substituting (6) into (5) and equating terms with identical powers of p, there can be evaluated the functions $v_0, v_1, v_2, \ldots$

Finally, considering the limit value $p \to 1$, a solution for (1) is obtained as follows

$$U = v_0 + v_1 + v_2 + v_3 ... \qquad (7)$$

III. LT-HPM METHOD

Next, it is shown how to employ the proposed method to calculate approximate solutions of Differential Equations such as (3) [29,38,39,41,42].

With this end, LT-HPM uses the same steps of basic HPM until (5); next it is applied LT on both sides of (5), to get

$$\Im\{L(U) - L(u_0) + p[L(u_0) + N(U) - f(r)]\} = 0. \qquad (8)$$

After employing the differential property of LT, it is obtained [49]

$$\begin{aligned} &s^n \Im\{U\} - s^{n-1}U(0) - s^{n-2}U'(0) - ... - U^{(n-1)}(0) = \\ &\Im\{L(u_0) - pL(u_0) + p[-N(U) + f(r)]\}, \end{aligned} \qquad (9)$$

or

$$\Im(U) = \left(\frac{1}{s^n}\right)\left\{\begin{matrix} s^{n-1}U(0) + s^{n-2}U'(0) + .. + U^{(n-1)}(0) \\ + \Im\{L(u_0) - pL(u_0) + p[-N(U) + f(r)]\} \end{matrix}\right\} \qquad (10)$$

After employing inverse Laplace transform to previous equation, we get

$$U = \Im^{-1}\left\{\left(\frac{1}{s^n}\right)\left\{\begin{matrix} s^{n-1}U(0) + s^{n-2}U'(0) + .. + U^{(n-1)}(0) \\ + \Im\{L(u_0) - pL(u_0) + p[-N(U) + f(r)]\} \end{matrix}\right\}\right\} \qquad (11)$$

If the solutions of (3) can be written as

$$U = \sum_{n=0}^{\infty} p^n v_n, \qquad (12)$$

then after substituting (12) into (11), yields in

$$\sum_{n=0}^{\infty} p^n v_n = \Im^{-1}\left\{\begin{matrix} \left(\frac{1}{s^n}\right)\{s^{n-1}U(0) + s^{n-2}U'(0) + .. + U^{(n-1)}(0)\} \\ + \left(\frac{1}{s^n}\right)\Im\left\{L(u_0) - pL(u_0) + p\left[-N(\sum_{n=0}^{\infty} p^n v_n) + f(r)\right]\right\} \end{matrix}\right\}. \qquad (13)$$

The comparison of coefficients with the same power of p results in

$$p^0 : v_0 = \Im^{-1}\left\{\left(\frac{1}{s^n}\right)\left(s^{n-1}U(0) + s^{n-2}U'(0) + .. + U^{(n-1)}(0)) + \Im\{L(u_0)\}\right)\right\},$$

$$p^1 : v_1 = \Im^{-1}\left\{\left(\frac{1}{s^n}\right)\left(\Im\{N(v_0) - L(u_0) + f(r)\}\right)\right\},$$

$$p^2 : v_2 = \Im^{-1}\left\{\left(\frac{1}{s^n}\right)\Im\{N(v_0, v_1)\}\right\},$$

$$p^3 : v_3 = \Im^{-1}\left\{\left(\frac{1}{s^n}\right)\Im\{N(v_0, v_1, v_2)\}\right\},$$

$$\vdots$$

$$p^j : v_j = \Im^{-1}\left\{\left(\frac{1}{s^n}\right)\Im\{N(v_0, v_1, v_2, ..., v_j)\}\right\},$$

$$\vdots$$

(14)

Considering the following values for the initial approximation: $U(0) = u_0 = \alpha_0, U'(0) = \alpha_1, .., U^{n-1}(0) = \alpha_{n-1}$; the exact solution is obtained in accordance with the following limit value $u = \lim_{p \to 1} U = v_0 + v_1 + v_2 + ...$

IV. PROBLEM FORMULATION

In accordance with [1,44], let us consider a coupled diffusion and reaction porous catalyst pellets. We will study the case where the reaction rate depends nonlinearly on concentration; in such a way that it is possible to envisage the system as a solid material with pores through which the reactants and products diffuse. For the sake of simplicity, the system is conceived as simple diffusion by employing an effective constant diffusion coefficient D_e.

The mass balance on a volume of the aforementioned medium is mathematically expressed by [1,44].

$$\frac{\partial Y}{\partial t} = D_e \nabla^2 Y - r(Y), \qquad (14)$$

where, Y is the chemical reactant concentration, $r(Y)$ the rate of reaction per unit volume, and t is the time.

Next [1,44,50], we will study the steady one dimensional case, $\frac{\partial Y}{\partial t} = 0$, in such a way that (14) is expressed as:

$$D_e \frac{d^2 Y}{dX^2} - r(Y) = 0, \qquad (15)$$

where X is the diffusion distance.

We will assume that the system is limited by plane boundaries at $X = 0$ and $X = L$, so that the side $X = 0$, is impermeable (vanishing mass flux) and that $X = L$ is held a constant concentration $Y = y_s$, therefore

$$\left(\frac{dY}{dX}\right)_{X=0} = 0, \qquad Y(L) = y_s, \qquad (16)$$

Next, we consider the case where the reaction rate per unit volume r, is given as a power law function of the concentration [1,44,50].

$$r = kY^n, \qquad (17)$$

in this equation n is called the reaction order and the constant k is a function of temperature (the admitted range of the reaction order is $n \geq -1$).

Finally, for a suitable solution, we express (15)-(17), in terms of the following dimensionless variables.

$$x = \frac{X}{L}, \quad y(x) = \frac{Y(X)}{y_s}, \qquad (18)$$

so that we get the following differential equation

$$y'' - m^2 y^n = 0, \qquad (19)$$

with boundary conditions

$$y'(0) = 0, \quad y(1) = 1. \qquad (20)$$

where prime denotes from here on, differentiation respect to x, and the Thiele modulus m is defined by

$$m = \left(kL^2 y_s^{n-1} / D_e\right)^{1/2}. \qquad (21)$$

Next, it is possible to express the boundary value problem (19)-(20) in terms of the initial value problem [45].

$$y'' - m^2 y^n = 0, \quad y(0) = A, \quad y'(0) = 0, \qquad (22)$$

liable to the additional condition $y(1) = 1$, besides A denotes the concentration of the reactant on the boundary at $x = 0$ and

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it is an unknown parameter to be determined as a part of the solution of the problem.

As a matter of fact, the problem as it is expressed in (22) will result particularly useful for application of LT-HPM algorithm. We will see that, this method is able to obtain very accurate and handy approximations. Also it calculates A, from the condition $y(1, A) = 1$.

V. APPLICATION OF LT-HPM TO OBTAIN HANDY SOLUTIONS FOR THE NONLINEAR CHEMICAL EQUATION UNDER STUDY

By convenience of this study, we will consider equivalently the system (22) , expressed in the most complete form

$$y'' - m^2 y^n = 0, \quad (n \geq -1), \qquad y(0) = A, \quad y'(0) = 0, \quad y(1) = 1. \tag{23}$$

Next, we will analyze the following representative case studies.

A. *Case studies 1 and 2*

Reaction order $n = 2$,

Thiele modulus $m = 0.3$ and $m = 0.6$.

After identifying

$$L(y) = y''(x), \tag{24}$$

$$N(y) = -m^2 y^2, \tag{25}$$

we propose the following homotopy equation

$$(1-p)(y'' - y_0'') + p\left[y'' - m^2 y^2\right] = 0, \tag{26}$$

or

$$y'' = y_0'' + p\left[-y_0'' + m^2 y^2\right]. \tag{27}$$

Applying LT to (27) we obtain

$$\Im(y'') = \Im\left\{y_0'' + p\left[-y_0'' + m^2 y^2\right]\right\}. \tag{28}$$

Next, in accordance with [49], we rewrite (28) as follows

$$s^2 Y(s) - sy(0) - y'(0) = \Im\left(y_0'' + p\left(-y_0'' + m^2 y^2\right)\right), \tag{29}$$

where $Y(s) = \Im(y(x))$.

Taking into account that $y'(0) = 0$, it is possible to rewrite (29) as

$$s^2 Y(s) - sA = \Im\left(y_0'' + p\left(-y_0'' + m^2 y^2\right)\right), \tag{30}$$

where $A = y(0)$.

After solving for $Y(s)$ and applying $\Im^{-1}$ we get

$$y(x) = \Im^{-1}\left\{\frac{A}{s} + \frac{1}{s^2}\left(\Im\left(y_0'' + p\left(-y_0'' + m^2 y^2\right)\right)\right)\right\}. \tag{31}$$

In according with the propose method, we will assume that the solution for (23) is expressed as

$$y(x) = \sum_{n=0}^{\infty} p^n v_n, \tag{32}$$

Next, we will choose

$$v_0(x) = A, \tag{33}$$

as the first approximation for the solution of (23) that fulfills the condition $y'(0) = 0$.

Substituting (32) and (33) into (31), we obtain

$$\sum_{n=0}^{\infty} p^n v_n = \Im^{-1}\left\{\frac{A}{s} + \frac{1}{s^2}\Im\left(y_0'' + p\left(-y_0'' + m^2\left(v_0 + pv_1 + p^2 v_2 + ..\right)^2\right)\right)\right\} \tag{34}$$

After equating terms with the same powers of p, it is obtained

$$p^0 : v_0(x) = \Im^{-1}\left\{\frac{A}{s}\right\}, \tag{35}$$

$$p^1 : v_1(x) = m^2 \Im^{-1}\left\{\left(\frac{1}{s^2}\right)\Im\left(v_0^2\right)\right\}, \tag{36}$$

$$p^2 : v_2(x) = m^2 \Im^{-1}\left\{\left(\frac{1}{s^2}\right)\Im\left(2v_0 v_1\right)\right\}, \tag{37}$$

$$p^3 : v_3(x) = m^2 \Im^{-1}\left\{\left(\frac{1}{s^2}\right)\Im\left(v_1^2 + 2v_0 v_2\right)\right\}, \tag{38}$$

$$p^4 : v_4(x) = m^2 \Im^{-1}\left\{\left(\frac{1}{s^2}\right)\Im\left(2v_0 v_3 + 2v_1 v_2\right)\right\}, \tag{39}$$

The solutions for $v_0(x),\ v_1(x),\ v_2(x), ..$ are

$$p^0 : v_0(x) = A, \tag{40}$$

$$p^1 : v_1(x) = \frac{m^2 A^2 x^2}{2}, \tag{41}$$

$$p^2 : v_2(x) = \frac{m^4 A^3}{12} x^4, \tag{42}$$

$$p^3 : v_3(x) = \frac{m^6 A^4}{72} x^6, \tag{43}$$

$$p^4 : v_4(x) = \frac{m^8 A^5}{504} x^8, \tag{44}$$

$$\vdots$$

By substituting solutions (40)-(44) into (32) results in a fourth order approximation

$$y(x) = A + \frac{m^2 A^2 x^2}{2} + \frac{m^4 A^3}{12} x^4 + \frac{m^6 A^4}{72} x^6 + \frac{m^8 A^5}{504} x^8. \tag{45}$$

Next, we will consider separately the cases of Thiele modulus $m = 0.3$ and $m = 0.6$.

With the purpose to find A, we require that (45) satisfies $y(1, A) = 1$, for $m = 0.3$, so that we obtain

$$A = 0.958090536681. \tag{46}$$

In the same way for $m = 0.6$, we get

$$A = 0.859724737059. \tag{47}$$

Substituting (46) into (45), we obtain

$$\begin{aligned} y(x) = {} & 0.958090536681 + 0.0413071864415x^2 \\ & + 0.000593640366398x^4 + 0.00000853141825856x^6 \\ & + 1.05092628403 \times 10^{-7} x^8. \end{aligned} \tag{48}$$

On the other hand, by substituting (47) into (45), we get

$$\begin{aligned} y(x) = {} & 0.859724737059 + 0.133042792232x^2 \\ & + 0.00686281077415x^4 + 0.000354007691298x^6 \\ & + 0.0000156522429935x^8. \end{aligned} \tag{49}$$

B. *Case studies 3 and 4*

Next we will study the cases

Reaction order $n=-1$,

Thiele modulus $m=0.3$ and $m=0.6$.

In this case we identify from (23)

$$L(y)=y''(x), \tag{50}$$

$$N(y)=-m^2y^{-1}, \tag{51}$$

Next, we propose

$$(1-p)(y''-y''_0)+p\left[y''-m^2y^{-1}\right]=0, \tag{52}$$

or

$$y''=y''_0+p\left[-y''_0+m^2y^{-1}\right]. \tag{53}$$

Applying L.T. to (53)

$$\Im(y'')=\Im\left\{y''_0+p\left[-y''_0+m^2y^{-1}\right]\right\}.$$

Using the differential property of LT

$$s^2Y(s)-sy(0)-y'(0)=\Im\left(y''_0+p\left(-y''_0+m^2y^{-1}\right)\right), \tag{54}$$

where $Y(s)=\Im(y(x))$.

From condition $y'(0)=0$, (54) is simplified as

$$s^2Y(s)-sA=\Im\left(y''_0+p\left(-y''_0+m^2y^{-1}\right)\right), \tag{55}$$

with $A=y(0)$.

After solving for $Y(s)$ and applying $\Im^{-1}$ we get

$$y(x)=\Im^{-1}\left\{\frac{A}{s}+\frac{1}{s^2}\left(\Im\left(y''_0+p\left(-y''_0+m^2y^{-1}\right)\right)\right)\right\}. \tag{56}$$

Next, we will assume that

$$y(x)=\sum_{n=0}^{\infty}p^nv_n, \tag{57}$$

and

$$v_0(x)=A. \tag{58}$$

After substituting (58), (57) into (56)

$$\sum_{n=0}^{\infty}p^nv_n=$$

$$\Im^{-1}\left\{\frac{A}{s}+\frac{1}{s^2}\Im\left(y''_0+p\left(-y''_0+m^2\left(v_0+pv_1+p^2v_2+..\right)^{-1}\right)\right)\right\} \tag{59}$$

Equating terms with the same powers of p terms we get

$$p^0: v_0(x)=\Im^{-1}\left\{\frac{A}{s}\right\}, \tag{60}$$

$$p^1: v_1(x)=m^2\Im^{-1}\left\{\left(\frac{1}{s^2}\right)\Im\left(v_0^{-1}\right)\right\}, \tag{61}$$

$$p^2: v_2(x)=m^2\Im^{-1}\left\{\left(\frac{1}{s^2}\right)\Im\left(\frac{-v_1}{A^2}\right)\right\}, \tag{62}$$

$$p^3: v_3(x)=m^2\Im^{-1}\left\{\left(\frac{1}{s^2}\right)\Im\left(\frac{v_1^2}{A^3}-\frac{v_2}{A^2}\right)\right\}, \tag{63}$$

$$p^4: v_4(x)=m^2\Im^{-1}\left\{\left(\frac{1}{s^2}\right)\Im\left(-\frac{v_3}{A^2}+\frac{2v_1v_2}{A^3}-\frac{v_1^3}{A^4}\right)\right\} \tag{64}$$

…

The solution for equations (60)-(64) yields in

$$p^0: v_0(x)=A, \tag{65}$$

$$p^1: v_1(x)=\frac{m^2x^2}{2A}, \tag{66}$$

$$p^2: v_2(x)=-\frac{m^4}{24A^3}x^4, \tag{67}$$

$$p^3: v_3(x)=\frac{m^6x^6}{144A^5}, \tag{68}$$

$$p^4: v_4(x)=-\frac{25m^8x^8}{8064A^7}, \tag{69}$$

…

and so on.

By substituting (65)-(69) into (57) we obtain a handy eight order approximation

$$y(x)=A+\frac{m^2x^2}{2A}-\frac{m^4}{24A^3}x^4+\frac{m^6}{144A^5}x^6-\frac{25m^8}{8064A^7}x^8. \tag{70}$$

We will consider separately the cases of Thiele modulus $m=0.3$ and $m=0.6$.

To calculate the value of A, we solve the algebraic equation $y(1)=1$ from (70), and use $m=0.3$ so that we obtain

$$A=0.953172744786 \tag{71}$$

In the same way for $m=0.6$, we get

$$A=0.779378540012. \tag{72}$$

Substituting (71) into (70), we obtain

$$\begin{aligned}y(x)&=0.953172744786+0.0472107498314x^2\\&-0.000389725596578x^4+0.00000643438374400x^6\\&-2.03404017857\times10^{-7}x^8.\end{aligned} \tag{73}$$

After substituting (72) into (70), we obtain

$$\begin{aligned}y(x)&=0.779378540012+0.230953241281x^2\\&-0.0114063955916x^4+0.00112668572799x^6\\&-0.0000520714285714x^8.\end{aligned} \tag{74}$$

C. *Case studies 5 and 6*

Reaction order $n=1/2$,

Thiele modulus $m=0.3$ and $m=0.6$.

In this case, from (23)

$$L(y)=y''(x). \tag{75}$$

$$N(y)=-m^2y^{1/2}, \tag{76}$$

Since a similar procedure is followed to the previous cases, we only present the relevant results

In this case we obtain the following handy eight order approximation.

$$y(x)=A+\frac{m^2\sqrt{A}x^2}{2}+\frac{m^4}{48}x^4-\frac{m^6}{1440\sqrt{A}}x^6+\frac{m^8}{11520A}x^8. \tag{77}$$

Case $m=0.3$

$$A=0.955836657231. \tag{78}$$

By substituting (78) into (77) results in

$$y(x) = 0.955836657231 + 0.0439951046242x^2 + 0.00016875x^4 - 5.17813292968\times10^{-7}x^6 + 5.95845791947\times10^{-9}x^8. \quad (79)$$

Case $m = 0.6$.

$$A = 0.833045373527. \quad (80)$$

After substituting (80) into (77), we get

$$y(x) = 0.833045373527 + 0.164288374824x^2 + 0.0027x^4 - 0.0000354985555505x^6 + 0.00000175020478636x^8. \quad (81)$$

VI. DISCUSSION

This article introduced LT-HPM in order to get handy accurate approximate solutions for the problem with mixed boundary conditions that describes the problem of the diffusion and reaction in porous catalysts. Such as it is explained in [1], the understanding of this process it turns out relevant for the chemical engineer due to its applications in the design and operation of catalytic reactors. It should be mentioned that this problem has been successfully attacked for several authors. Thus, [1] found an approximate solution for (23), by using the Adomian decomposition method for some values of n order and Thiele modulus m. Although Adomian is a powerful tool, the process of obtaining its polynomial solutions are not straightforward for practical applications. On the other hand [44] showed the application of homotopy analysis method HAM, to get the approximate solution of the nonlinear model (23), for the cases of $n = 0.5, 2,$ and $4,$ for several values of m. Although in general HAM is very accurate, its expressions use to be long and cumbersome, as to be used in practical applications thus, [44] proposed approximations of 6th, 15th, 20th, 35th, and 50th order. What is more, [50] went beyond, this article showed that, this model is exactly solvable in terms of Gauss hypergeometric function. The main advantage of this paper is that the hypergeometric function is well known, although its study it is not elementary. [45] employed HAM to investigate in all detail the case $n = -1.$ The solutions obtained are very long, and correspond to 30 th and 50 th order approximations of HAM, even though this paper obtained multiple solutions for this case. Unlike of the above studies, the goal of this article is to show the manner of getting handy approximate solutions for nonlinear problems like (23), through the use of LT-HPM. In fact, Figure (1), Figure (2), and Figure (3) show the accuracy of LT-HPM for the problem under study.

In more precise terms, Figure 1 compares the numerical solution of (23) for cases study: $n = 2$, $m = 0.3$ and $n = 2$, $m = 0.6$ and approximations (48) and (49). Although the mentioned figure, shows the high accuracy of the proposed solutions, it was verified by evaluating the square residual error (S.R.E) of (48) and (49) given by $\int_a^b R^2\left(u(t)\right)dt$, where a and b are two values depending on the given problem, the residual is defined by $R\left(\bar{u}(t)\right) = L\left(\bar{u}(t)\right) + N\left(\bar{u}(t)\right) - f(t)$, and $\bar{u}(t)$ is an approximate solution to (3) [16]. The resulting values were respectively of $7.75287785167\times10^{-16}$ and $2.37672485412\times10^{-10}$, which confirms the high accuracy of LT-HPM. Figure 2, compare numerical solution of (23) for $n = -1$, $m = 0.3$ and $n = -1$, $m = 0.6$ with (73) and (74) for the same values. We note that the figures appear indeed overlapping, while the S.R.E of (73) and (74) are of $6.10465343999\times10^{-10}$, and 0.00000335024984825. Finally, the cases $n = 0.5$, $m = 0.3$ and $n = 0.5$, $m = 0.6$, are shown in Figure 3, and the corresponding S.R.E for approximations (79) and (81) are scarcely of $4.29941296548\times10^{-18}$ and $5.79207356623\times10^{-12}$ respectively.

It is clear from the above discussion that LT-HPM describes a highly accurate way for solving, the nonlinear problem (23). On the other hand, is worth to note that our proposed solutions (48), (49), (73), (74), (79) and (81) are short and simple polynomial functions, ideal for practical applications. In all the cases considered we keep the order of approximation as four. If more accuracy for solutions is even required, one can go on with higher orders in a straightforward fashion, following LT-HPM algorithm.

Our results $y(x)$, indicate the concentration under steady conditions. From definition of Thiele modulus m (21), we identify the quantity $1/LKy_s^{n-1}$ as a characteristic property for reaction, and D_e/L as a characteristic property for diffusion [1,44]. Therefore, the bigger the value of m, the bigger in proportion the diffusion respect to reaction phenomena and viceversa. From values of S.R.E one deduce that LT-HPM is more accurate for the cases, where the diffusion is relatively less important than reaction for a given value of n, that is for small values of m. Figure 1, Figure 2, and Figure 3, explain the above, noting that the curves with larger value of m present a major curvature than those, with smaller values, and for the same reason, they are more complicated to model. The simplicity and accuracy of the proposed method indicates that, unlike other methods, our solutions keep the nature of the studied phenomena and on the other hand, the reliability of the obtained results for the initially unknown values of the concentration of the reactant A.

Finally, future investigations of LT-HPM should follow the aim of [45], where the authors obtained multiple solutions of (23), for the case n= - 1.

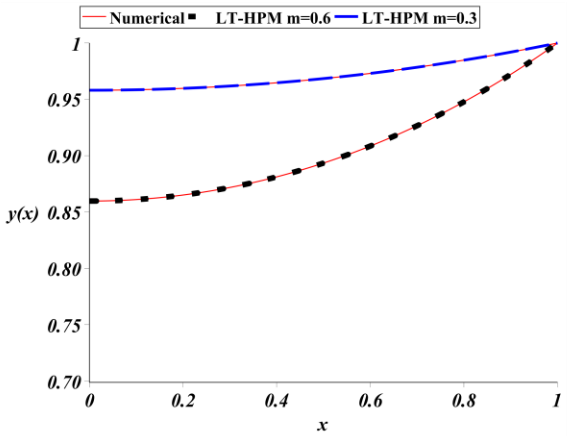

Figure 1 Comparison between numerical solution of (23) for cases study: $n = 2$, $m = 0.3$ and $n = 2$, $m = 0.6$ and LT-HPM approximations (48) and (49).

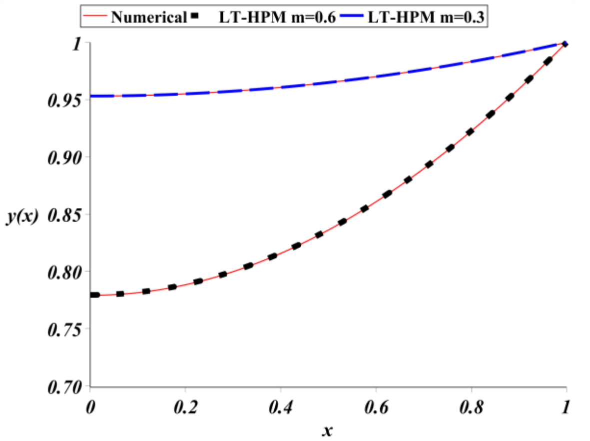

Figure 2 Comparison between numerical solution of (23) for cases study: $n = -1$, $m = 0.3$ and $n = -1$, $m = 0.6$ and LT-HPM approximations (73) and (74).

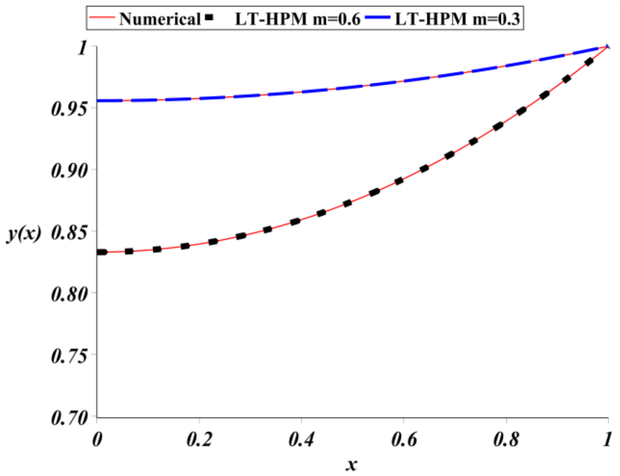

Figure 3 Comparison between numerical solution of (23) for cases study: $n = 0.5$, $m = 0.3$ and $n = 0.5$, $m = 0.6$ and LT-HPM approximations (79) and (81).

VII. CONCLUSION

From this study we conclude that LT-HPM is a useful tool to get accurate and handy solutions for the considered problem, which describes the phenomenon of the diffusion and reaction in porous catalyst. One of the highlights of this work lies in the practical and precise solutions obtained by LT-HPM compared to other methods, like HAM and Adomian Decomposition Method. We emphasize that one advantage of LT-HPM is that it does not require to solve several recurrence differential equations like other perturbative methods. Finally it is clear that the proposed methodology can be applied equally to other nonlinear problems, especially to heat diffusion problems.

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