Analytical Exact and Approximate Solutions for Certain Diffusion Reactions

U. Filobello-Nino[1], M. A. Sandoval-Hernandez[2], O. Alvarez-Gasca[1], A.D. Contreras-Hernandez[1], C. Hoyos-Reyes[1], N. Carrillo-Ramon[1], J. Sanchez-Orea[1], L. Cuellar-Hernandez[1], J.M. Mendez-Perez[1], V.M. Jimenez-Fernandez[1], G.J. Morales-Alarcon[3], S.F. Hernandez-Machuca[1], F. Martinez-Barrios[4], M. Garcia-Lozano[2], A.J. Mota-Hernandez[2], N. Bagatella-Flores[5], H. Vazquez-Leal[1,*].

[1] Facultad de Instrumentación Electrónica, Universidad Veracruzana, Circuito Gonzalo Aguirre Beltrán S/N, Xalapa, 91000, Veracruz, México.

[2] Centro de Bachillerato Tecnológico industrial y de servicios No. 190, Av. 15 Col. Venustiano Carranza 2da Sección, Boca del Río, 94297, Veracruz, México.

[3] Instituto de Psicología y Educación, Universidad Veracruzana, Agustín Melgar 2, Col. 21 de Marzo, Xalapa, 91010 Veracruz, México.

[4] Centro de Bachillerato Tecnológico industrial y de servicios No. 268, Av. La Bamba, Geovillas del Puerto, Veracruz 91777, Veracruz, México.

[5] Facultad de Física, Universidad Veracruzana, Paseo No. 112. Desarrollo Habitacional Nuevo Xalapa, Xalapa, 91097, Veracruz, México.

***Abstract*:- This work presents the Taylor Series Method with shooting (STSM) with the purpose to find both approximate and exact solutions for the nonlinear problem that describes the steady state solutions of a highly nonlinear model of a coupled diffusion and nth-order chemical reaction in a spherical porous catalyst. After comparing STSM approximation with the exact solutions, we will conclude that the proposed solutions are besides of extremely handy, accurate (with relative error less than one percent in all the cases), therefore it follows that the proposed method is potentially an efficient tool to be used in practical applications instead of others cumbersome and complicated methods.**

I. INTRODUCTION

Most of the processes in nature are nonlinear, in such a way that, the mathematical models used with the purpose to get exact and approximate solutions do not always offer the required results. On the other hand, differential equations have shown to be an appropriate tool with the end to model complicated phenomena in nature.

Nature processes give rise to scientific problems and for the same reason the proposal of new methods with the purpose to obtain both exact and approximate solutions to the differential equations that govern these problems becomes compulsory. Given that the search for such solutions many times is a complicated task, it justifies the current research in this subject. Unlike the linear differential equations whose theory and solution methods can be found in many standard texts of differential equations [1] the case of nonlinear ordinary differential equations with exact solutions is less frequent [1]. One of the main contributions of this article is to show the potentiality of the proposed method in order to find both exact and approximate solutions with relative ease for the highly nonlinear problem that describes a coupled diffusion and nth-order chemical reaction in a spherical porous catalyst [2]. Given the great diversity of scientific problems, and their corresponding nonlinear differential equations to be solved, have been proposed several methods. Some of most employed in accordance with the literature are: tanh method [3], exp-function [4], Adomian's decomposition method [5, 6, 7, 8], parameter expansion [9], homotopy perturbation method (HPM) [10, 11, 12, 13, 14, 15, 16, 17,18], perturbation method [19, 20, 21,22, 23], modified Taylor series method [24], Homotopy Analysis Method [25], Variational iteration method [26, 27], among others.

The main goal of this work is to employ a version of Taylor Series Method with shooting (STSM) with the end to provide analytical solutions for the relevant highly nonlinear differential equation that describes the steady state solutions of a highly nonlinear model of a coupled diffusion and nth-order chemical reaction in a spherical porous catalyst [2]. As a matter of fact, the importance of the diffusion and reaction problems consists in their application in chemical and process engineering problems [28]. Respect to the process engineering field, diffusion and reaction problems arise above all in the heterogeneous catalysts by using porous structures where reaction could occur, other examples of technological interest are found in [28]. Next, we will see that STSM method is relatively easy to use and it is able to provide both, exact and analytical approximate solutions even for the case of nonlinear differential equations defined in closed intervals for which the most of the investigation works are essentially numeric. Traditionally, Taylor Series Method (TSM) is a known method which is given in terms of initial conditions for a proposed problem and it is not very employed at the moment to solve differential equations. As a matter of fact, one serious inconvenient of the problem to solve, is the presence of a singularity for $x = 0$; nevertheless, we will see that STSM method is indeed able to adequately handle it. In brief, the proposed method is given in the following terms. Given an ordinary differential equation, then like TSM, STSM proposes a Taylor series for the differential equation to solve, given that the goal is to solve a boundary value problem, then the successive derivatives of the differential equation to calculate the coefficients of the Series Taylor solution will be expressed in terms of an unknown initial condition. This quantity will be tried as a shooting constant which will be determinined requiring that the proposed series obey the other boundary condition. We will see that even, the mentioned method is able to find exact analytical solutions.

The rest of this work is proposed in the following way. Section 2, provides the basic idea of STSM Method. Additionally Section 3 explains the antecedents for the nonlinear differential equation that describes the steady state solutions of a highly nonlinear model of a coupled diffusion and nth-order chemical reaction in a spherical porous catalyst, Section 4 presents the application of the proposed method, in the search for an approximate solution for the relevant problem above mentioned. Section 5 offers a discussion about the obtained solutions for this work. Finally, a brief conclusion of the relevant aspects of this article is given in Section 6.

II. ELEMENTS OF SHOOTING TAYLOR SERIES METHOD

Next, we will provide the basic theory of STSM.

We start assuming a nonlinear problem with the following form

$$u^{(n)} = N(u) - f(x), \qquad x \in \Omega, \tag{1}$$

with the boundary condition

$$B\left(u, \frac{\partial u}{\partial \eta}\right) = 0, \qquad x \in \Gamma. \tag{2}$$

In the above equations, n is the order of the differential equation (1), N represents a general operator; $f(x)$ denotes a known analytic function while B is a boundary operator, Γ as a matter of fact, is the boundary of the domain Ω, and $\partial u/\partial \eta$ is the differentiation along the normal drawn outwards from Ω.

Following the proposed method, we will get the successive derivatives of the differential equation to solve.

$$u^{(i)}(x_0), \qquad (i = 0,1, \dots), \tag{3}$$

in this expression x_0 denotes the expansion point.

The series solution for (1) can be expressed as

$$u_T = u(x_0) + \frac{u\prime(x_0)}{1!}(x - x_0)^1 + \frac{u\prime(x_0)}{2!}\ (x - x_0)^2 + \dots \quad x \in \Omega, \tag{4}$$

we note that derivatives $u^{(i)}(x_0)$, $(i = 0,1, \dots)$ are expressed in terms of one of the boundary conditions of (1).

With the purpose to get the coefficients of (4) $(u^{(i)}(x_0))$ $(i = 0,1, \dots)$, we just apply the condition $u_T(1) = 1$.

III. ANTECEDENTS FOR THE PROBLEM THAT DESCRIBES THE STEADY STATE SOLUTIONS OF A NONLINEAR MODEL OF A COUPLED DIFFUSION AND NTH-ORDER CHEMICAL REACTION IN A SPHERICAL POROUS CATALYST

The goal of the article is to provide exact and handy analytical approximate solutions for the problem of a highly nonlinear model of a coupled diffusion and nth-order chemical reaction in a spherical porous catalyst. As a matter of fact, [2] presented an approach for these problems for the case of exact solutions, while [29] obtained analytical approximate solutions by using Adomian decomposition method. This article will show that STSM method is able to provide both kinds of solutions for this complicated problem, by using essentially a single polynomial handy expression. Essentially, we will see that STSM solves an elementary algebraic equation by the proposed differential equation.

Assuming isothermal conditions, the differential equation that governs the steady regime of the nth-order reaction-diffusion process in the spherical geometric pellet is given by [27, 29]:

$$\frac{d^2c}{dr^2} + \frac{2}{r}\frac{dc}{dr} = \frac{k_v}{D_e}c^n, \tag{5}$$

where, c denotes the reactant concentration in pore of catalyst pellet, while D_e is the effective diffusion coefficient for reactant, r represents the distance from the pellet core and kv the reaction rate constant. The reaction order belongs to the range $n \geq 0$ and the boundary conditions are expressed for:

$$c(r = r_0) = c_s, \tag{6}$$

and

$$\left[\frac{dc}{dr}\right]_{r=0} = 0. \tag{7}$$

Expressing the boundary value problem (5)-(7) in terms of the dimensionless variables

$$x = \frac{r}{r_0}, \qquad y(x) = \frac{c(r)}{c_s}, \tag{8}$$

we get

$$\frac{d^2y}{dx^2} + \frac{2}{x}\frac{dy}{dx} = \phi^2 y^n, \tag{9}$$

$$y(1) = 1, \tag{10}$$

and

$$\left[\frac{dy}{dx}\right]_{x=0} = 0, \tag{11}$$

where $\phi = (k_v r_0^2 c_s^{n-1}/D_e)^{1/2}$ denotes the Thiele modulus.

IV. APPLICATION OF STSM METHOD

Next, we will employ STSM method in order to find analytical approximate and exact solutions for the boundary value problem (9)-(11).

In accordance with STSM, first we propose the following Taylor approximation:

$$y(x) = y(0) + \frac{y''(0)}{2!}\ x^2 + \frac{y'''(0)}{3!}\ x^3 + \frac{y^{iv}(0)}{4!}\ x^4 + \cdots \tag{12}$$

where we have employed the initial condition (11).

We will rewrite (12) as follows

$$y(x) = \alpha + \frac{\beta}{2!}\ x^2 + \frac{\gamma}{3!}\ x^3 + \frac{\delta}{4!}\ x^4 \dots \tag{13}$$

after we have substituted the unknown initial conditions for some shooting constants.

We note the unknown initial conditions are calculated about $x = 0$, but at this point (9) has a singularity. With the end to avoid this problem, we multiply (9) by x and after we apply a derivative to the resulting equation to get

$$\frac{d^2y}{dx^2}+x\frac{d^3y}{dx^3}+2\frac{d^2y}{dx^2}=\phi^2y^n+n\phi^2xy^{n-1}\frac{dy}{dx}, \quad (14)$$

after evaluating (14) in $x=0$, we obtain:

$$\beta=\frac{\alpha^n}{3}\phi^2. \quad (15)$$

With the purpose to follow evaluating other shooting constants we differentiate (14):

$$4\frac{d^3y}{dx^3}+x\frac{d^4y}{dx^4}= 2n\phi^2y^{n-1}\frac{dy}{dx} +n\phi^2\left(y^{n-1}\frac{dy}{dx}+xy^{n-1}\frac{d^2y}{dx^2}+(n-1)xy^{n-2}\left(\frac{dy}{dx}\right)^2\right), \quad (16)$$

evaluating (16) in $x=0$, we obtain:

$$\gamma=0. \quad (17)$$

Continuing in this form, after differentiating (16) we get:

$$5\frac{d^4y}{dx^4}+x\frac{d^5y}{dx^5}= 2n\phi^2y^{n-1}\frac{d^2y}{dx^2}+2n\phi^2(n-1)y^{n-2}\left(\frac{dy}{dx}\right)^2 +n\phi^2\left(\begin{array}{c} y^{n-1}\frac{d^2y}{dx^2} \\ +x\left(y^{n-1}\frac{d^3y}{dx^3}+(n-1)y^{n-2}\left(\frac{dy}{dx}\right)\frac{d^2y}{dx^2}\right) \\ +(n-1)y^{n-2}\left(\frac{dy}{dx}\right)^2 \\ +x(n-1)\left(\begin{array}{c}(n-2)y^{n-3}\left(\frac{dy}{dx}\right)^3 \\ +2y^{n-2}\left(\frac{dy}{dx}\right)\frac{d^2y}{dx^2}\end{array}\right)\end{array}\right). \quad (18)$$

Next, we evaluate (19) in $x=0$, to get

$$\delta=\frac{5n\phi^2\alpha^{n-1}\beta}{3}. \quad (19)$$

Therefore, by substituting (15)-(19) into (13) we get

$$y(x)=\alpha+\frac{\alpha^n\phi^2}{6}\ x^2+\frac{n\phi^4\alpha^{2n-1}}{120}\ x^4. \quad (20)$$

We note the ease to obtain the approximate solution (20), which depends of arbitrary values of n and ϕ, besides it is clear that following this procedure we can easily add more terms to (20). We note that the procedure is based in elementary differentiations Nevertheless, we will show the effectiveness of (20) in order to model the proposed nonlinear problem.

V. CASE STUDIES

Case 1. $n=0$

Next, we will obtain an exact solution for this case.

We note that (20) can be simplified as:

$$y(x)=\alpha+\frac{\phi^2}{6}\ x^2, \quad (21)$$

applying the condition $y(1)=1$, we get

$$\alpha=1-\frac{\phi^2}{6}. \quad (22)$$

After substituting (22) into (21) we get

$$y(x)=1-\frac{\phi^2}{6}\ (1-x^2), \quad (23)$$

that is the exact solution for this problem [2].

Case 2. $n=1,\ \ \phi=2$

In accordance with [2] this case possesses an exact solution.

Nevertheless, STSM will obtain a precise analytical approximate solution for this case:

After substituting $n=1$ and $\phi=2$ into (20) we get:

$$y(x)=\alpha+\frac{2\alpha}{3}x^2+\frac{2\alpha}{15}x^4. \quad (24)$$

In accordance with the proposed method, in order to determinate α we substitute (24) into the condition $y(1)=1$ to get an algebraic equation, whose solution is given by

$$\alpha=0.5555. \quad (25)$$

Therefore, substituting (25) into (24) we get

$$y(x)=0.5555+0.37037037\ x^2+0.0740740\ x^4. \quad (26)$$

We note the handiness of (26).

Next, we compare the precision of (26) with the exact solution [2] for some values of x, in order to know the reliability of (26).

Table 1: Comparison between (26) and exact solution for (9)-(11) using $n=1, \phi=2$.

x	Exact	STSM (26)	Relative error using (26)
0	0.5510	0.5555	0.81%
0.2	0.5660	0.5704	0.79%
0.4	0.6121	0.6167	0.74%
0.6	0.6933	0.6984	0.74%
0.8	0.8187	0.8228	0.5054%
1.0	0.4796933928	0.4700209520	0%

We note that the relative error committed by using (26) is scarcely less than one percent.

Case 3. $n=5,\ \ \phi=1.$

This case possesses an exact solution [2].

We will see that STSM method will provide a handy precise analytical approximate solution for this case:

Substituting $n=5$ and $\phi=1$ into (20) yields

$$y(x)=\alpha+\frac{\alpha^5}{6}\ x^2+\frac{\alpha^9}{24}\ x^4. \quad (27)$$

Again, to calculate α we use the condition $y(1)=1$ in order to obtain an equation

$$\alpha+\frac{\alpha^5}{6}+\frac{\alpha^9}{24}=1, \quad (28)$$

the solution of (28) is given by

$$\alpha=0.8914. \quad (29)$$

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After substituting (29) into (27) we get a handy solution

$$y(x) = 0.8914 + 0.0938\ x^2 + 0.0148\ x^4. \quad (30)$$

Next, we will show again the precision of the proposed approximation (30) comparing it with the exact solution [2].

Table 2: Comparison between (26) and exact solution for (9)-(11) using $n = 5, \phi = 1$.

x	Exact	STSM (30)	Relative error using (30)
0	0.88950	0.89140	0.20%
0.2	0.89932	0.89517	0.21%
0.4	0.90477	0.90678	0.22%
0.6	0.92497	0.92708	0.22%
0.8	0.95565	0.95749	0.19%
1.0	1	1	0%

From Table 2 we see that the relative error committed by using (26) is scarcely of two tenths of one percent.

Case 4. $n = 3/2, \quad \phi = 1.$

In accordance with [2], this case does not correspond to an exact solution. We will see that the proposed method provides a handy approximation with good precision.

Substituting $n = 3/2$ and $\phi = 1$ into (20) yields in the following approximation.

$$y(x) = \alpha + \frac{\alpha^{3/2}}{6}\ x^2 + \frac{\alpha^2}{80}\ x^4. \quad (31)$$

After applying the boundary condition $y(1) = 1$, we get from (31) the algebraic equation

$$\alpha + \frac{\alpha^{3/2}}{6} + \frac{\alpha^2}{80} = 1, \quad (32)$$

the solution of (32) is given by

$$\alpha = 0.8582. \quad (33)$$

After substituting (33) into (31) we get a handy accurate solution

$$y(x) = 0.8582 + 0.1325\ x^2 + 0.0092x^4. \quad (34)$$

We will show the precision of (34) comparing it with the numerical solution.

Table 3: Comparison between (34) and numerical solution for (9)-(11) using $n = 3/2, \phi = 1$.

x	Exact	STSM (34)	Relative error using (34)
0	0.8579	0.8582	0.034%
0.2	0.8632	0.8635	0.036%
0.4	0.8793	0.8796	0.038%
0.6	0.9067	0.9070	0.033%
0.8	0.9465	0.9467	0.021%
1.0	1	1	0%

From Table 3 we see that the relative error committed by using (34) is about three hundredths of one percent.

Case 5. $n = 2, \ \phi = 1.$

In accordance with [2], this case does not possess an exact solution.

Next, we will get a handy precise analytical approximate solution for this case.

Substituting $n = 2$ and $\phi = 1$ into (20) yields in the following approximation.

$$y(x) = \alpha + \frac{\alpha^2}{6}x^2 + \frac{\alpha^3}{60}\ x^4. \quad (35)$$

After applying the boundary condition $y(1) = 1$, we get the algebraic equation

$$\alpha + \frac{\alpha^2}{6} + \frac{\alpha^3}{60} = 1. \quad (36)$$

The solution of (36) is given by

$$\alpha = 0.8646. \quad (37)$$

The obtaining of (37) results again in the solution of the proposed problem for the values $n = 2$, $\phi = 1$. After substituting (37) into (35) we get a handy accurate solution

$$y(x) = 0.8646 + 0.12458\ x^2 + 0.01077x^4. \quad (38)$$

We will show the precision of (38) comparing it with the numerical solution.

Table 4: Comparison between (38) and numerical solution for (9)-(11) using $n = 2, \phi = 1$.

x	Exact	STSM (38)	Relative error using (38)
0	0.8640	0.8646	0.069%
0.2	0.8689	0.8696	0.080%
0.4	0.8841	0.8848	0.080%
0.6	0.9101	0.9108	0.082%
0.8	0.9482	0.9487	0.057%
1.0	1	1	0%

From Table 4 we see that the relative error committed by using (38) is about between five hundredths and eight hundredths of one percent.

VI. DISCUSSION

In this work STSM was employed with the purpose to find both, exact and analytical approximate solutions for the rather complicated nonlinear ordinary differential equation which describes the problem of a nonlinear model of a coupled diffusion and nth-order chemical reaction in a spherical porous catalyst. We note that (9) has a singularity in $x = 0$, we noted that STSM is much appropriate to handle this difficulty. The rearrangement of the equation and the systematic increasing of the order of the differential equation to solve, demonstrated its efficiency with the purpose to handle the aforementioned singularity. As a matter of fact, as result of this procedure based in just differentiations, we proposed, with little effort, to provide the general handy solution (20), which depends in principle of arbitrary values of the reaction order n, and the Thiele modulus ϕ. In this step, the proposed procedure is very simple, for given values of n and ϕ we apply the right boundary condition $y(1) = 1$ in order to get an algebraic equation from the proposed solution, to determine the unknown initial condition α whose solution provides the sought analytical approximate or the exact solution.

As a matter of fact, we provide five case studies in order to show the potentiality of the proposed method. The first case study proposed the reaction order $n = 0$. STSM got the correct exact solution for this problem [2]. For the case studies 2 and 3, we obtained handy precise analytical approximate solutions. In accordance with [2] these problems, which derives from the values $n = 1$, $\phi = 2$ and $n = 5$, $\phi = 1$ correspond to exact solutions. It is notable from Tables 1 and 2 that the relative error committed by using approximations (26) and (30) for these cases are scarcely less than one percent and two tenths of one percent respectively. Finally, Cases 4 and 5 correspond to non-exact solutions [2]. Nevertheless from Tables 3 and 4 we deduce that the relative error committed by using our approximations (34) and (38) for this case are about three hundredths and eight hundredths of one percent respectively. Therefore, our expressions for the proposed problem are not only precise but we emphasize that they are short polynomial expressions of only three terms. Besides, it is very important to emphasize that, it is possible to improve the accuracy of our STSM approximations by keeping more terms in expansion (20).

VII. CONCLUSIONS

This work presented STSM with the end to provide both, exact and analytical approximate solutions for the nonlinear problem that describes the complicated nonlinear ordinary differential equation which describes the problem of a nonlinear model of a coupled diffusion and nth-order chemical reaction in a spherical porous catalyst. Despite of the fact that (9) has a singularity in $x = 0$, STSM was able to handle it adequately with the end to get handy analytical solutions for this important problem. The method basically works calculating derivatives of several orders and expresses the solution of a differential equation in terms of the solution of one or more algebraic equations. The comparison with other methods of the literature [2] shows the convenience of employing STSM as a practical tool with the purpose to obtain accurate solutions for boundary value problems instead of using other more sophisticated and cumbersome procedures. As a matter of fact [29] employed Adomian decomposition method with the end to get analytical approximate solutions for the problem (9)-(11). Nevertheless, Adomian decomposition method requires to calculate the so denominated Adomian coefficients in order to linearize the nonlinear term and uses the concept of operator and inverse operator. As a consequence, from article [29], we noted that the employed procedure by using Adomian method is clearly more complex than the one proposed for this work. Thus, we emphasize that the use of the Taylor series is many times an adequate method to obtain handy analytical approximate solutions, and should be employed more frequently.

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