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A hybrid method of successive linearization method (SLM) and collocation method to steady regime of the reaction-diffusion equation

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This article presents a method based on combination of successive linearization method (SLM) and pseudo-spectral collocation method and then is applied on a nonlinear model of coupled diffusion and chemical reaction in a spherical catalyst pellet. It is obtained that this method can be used for nonlinear boundary value problems without difficulty because the nonlinear part of the equation becomes inactive by SLM and more, to treat the linear equation, even in the case of complicatedness, is straightforward by pseudo-spectral collocation method. Also, the results reveal the high efficiency with reliable accuracy of this hybrid method.

Keywords: successive linearization method; diffusion reaction equation; pseudo-spectral collocation method.

1. Introduction and the problem formulation

The steady regime of the reaction-diffusion process, at isothermal conditions, in the spherical geometric pellet is governed by [9]

$$D_e\left(\frac{d^2r}{dr^2}+\frac{2}{r}\frac{dc}{dr}\right)=k_vc^n, \tag{1}$$

where c is the reactant concentration in pore of catalyst pellet, D_e the effective diffusion coefficient for reactant, r the distance from the pellet core k_v is the reaction rate constant. The reaction order n in the above equation admits the range$[0,\infty]$. The boundary conditions at surface of catalyst and center of catalyst are assumed, respectively, as

$$c|_{r=r_0}=c_s, \tag{2}$$

$$\frac{dc}{dr}|_{r=0}=0. \tag{3}$$

By dimensionless variables

$$R=\frac{r}{r_0}, \qquad C\left(R\right)=\frac{c(r)}{c_s},$$

the boundary value problem (1)–(3) turns to

$$\frac{d^2C}{dR^2}+\frac{2}{R}\frac{dC}{dR}=\varphi^2C^n, \tag{4}$$

$$C|_{R=1}=1, \qquad \frac{dC}{dR}|_{R=0}=0, \tag{5}$$

where $\varphi=\left(\frac{k_vr_0^2c_s^{n-1}}{D_e}\right)^{\frac{1}{2}}$ denotes the Thiele modulus.

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The above problem is also of Lane-Emden type equation [14, 13, 5]. As a first step of the present approach in order to implement the method, we have to transform the governing Eqs. (4)-(5) from the physical region [0, 1] into the region [−1, 1] by using the mapping

$$R = \frac{x+1}{2}, \qquad -1 \le x \le 1.$$

By considering u (x) =C(2R−1) equation (4) is converted to the differential equation with boundary conditions on interval [−1, 1] i.e.

$$\frac{d^2u}{dx^2} + \frac{2}{x+1}\frac{du}{dx} = \frac{\varphi^2}{4}u^n, \tag{6}$$

$$u|_{x=1} = 1, \qquad \frac{du}{dx}|_{x=-1} = 0. \tag{7}$$

2. Successive linearization method (SLM)

The successive linearization method (SLM) firstly proposed by Motsa [12] is based on the assumption that the unknown functions u_n can be expanded as

$$u(x) = U_i(x) + \sum_{n=0}^{i-1} u_n(x), \tag{8}$$

where $U_i(x)$ are unknown functions and $u_n(x)$ are successive approximations whose solutions are obtained recursively, from solving the linear part of the equation that results from substituting (8) in the governing equations (6) using $u_0(x)$ as an initial approximation. The initial approximation is chosen in such a way that it satisfies the boundary conditions (7). A such initial approximation can be as

$$u_0(x) = 1. \tag{9}$$

The linearization technique is based on the assumption that $U_i(x)$ becomes increasingly smaller as i becomes large, that is

$$\lim_{i\to+\infty} U_i(x) = 0. \tag{10}$$

Substituting (8) in the governing equation (6), and using the Binomial theorem notation, gives

$$U_i'' + \frac{2}{x+1}U_i' - \frac{\varphi^2}{4}\sum_{s=0}^{n}\binom{n}{s}U_i^{n-s}\left[\sum_{k=0}^{i-1}u_k\right]^s = -\sum_{k=0}^{i-1}u_k'' - \frac{2}{x+1}\sum_{k=0}^{i-1}u_k'. \tag{11}$$

Starting from the initial approximation (9), the subsequent solutions for u_k, $k \ge 1$ are obtained by iteratively solving the linearized form of equations (11) which are given as

$$u_i'' + \frac{2}{x+1}u_i' - n\frac{\varphi^2}{4}a_{i-1}^{n-1}u_i = \phi_{i-1}(x), \tag{12}$$

$$u_i'(-1) = 0, \qquad u_i(1) = 0, \tag{13}$$

where

$$a_{i-1} = \sum_{k=0}^{i-1}u_k,$$

$$\phi_{i-1} = -\sum_{k=0}^{i-1}u_k'' - \frac{2}{x+1}\sum_{k=0}^{i-1}u_k' + \frac{\varphi^2}{4}\left(\sum_{k=0}^{i-1}u_k\right)^n.$$

Once each solution for u_k $(k \ge 1)$has been obtained, the approximate solution for $u(x)$ is obtained as

$$u(x) \approx \sum_{k=0}^{M}u_k(x), \tag{14}$$

where M is the order of SLM approximation. We remark that the coefficient parameters and the right hand side of equations (12) for i= 1, 2 , 3,. . ., are known (from previous iterations). Thus, equation (12) can easily be solved using analytical software such as Maple or Mathematica. As we know Symbolic computing manipulates algebraic expressions exactly, but it is unworkable for many applications since the space and time requirements tend to grow combinatorially, instead we can use numerical methods such as finite differences, finite elements, Runge-Kutta based shooting methods or collocation methods. In this work, equation (12) is solved using the Chebyshev spectral collocation method.

3. Pseudo-spectral collocation method

Chebyshev polynomials [15] are very useful as orthogonal polynomials on the interval $[-1,1]$ of the real line. These polynomials have very good properties in the approximation of functions so that appear frequently in several fields of mathematics, physics and engineering. Spectral collocation methods [3, 16] based on Chebyshev polynomials (also is called pseudo-spectral method) have been used to solve numerically differential equations by many authors (see for instance [1, 2, 4, 6, 7, 8, 10, 11]). This method is accomplished successfully by using Chebyshev polynomials approximation and generating approximations for the higher order derivatives through successive differentiation of the approximate solution.
The main advantage of spectral methods is their superior accuracy for problems whose solutions are sufficiently smooth functions. They converge fast compared to algebraic convergence rates for finite difference and finite element methods. In practice this means that good accuracy can be achieved with fairly coarse discretizations. This method is based on approximating the unknown functions by the Chebyshev interpolating polynomials in such a way that they are collocated at the Gauss-Lobatto points defined as

$$x_j = cos\frac{\pi j}{N}, \quad j = 0, 1, \ldots, N, \tag{15}$$

where N is the number of collocation points.
The unknown functions u_i are approximated as a truncated series of Chebyshev polynomials

$$u_i(x) \approx u_i^N(x) = \sum_{k=0}^{N} \tilde{u}_k T_k(x), \tag{16}$$

where $T_k$is the kth Chebyshev polynomial defined as

$$T_k(x) = cos\left(kcos^{-1}(x)\right), \tag{17}$$

and the discrete Chebyshev coefficients $\tilde{u}_k$ are determined by the forward discrete Chebyshev transform:

$$\tilde{u}_k = \frac{2}{c_k N} \sum_{j=0}^{N} \frac{1}{c_j} u_i(x_j) cos\frac{kj\pi}{N}, \tag{18}$$

where c_0=c_N and c_j= 1 for j= 1, 2, ..., N−1.
In Chebyshev pseudo-spectral method the numerical differentiation process performed as the matrix-vector product

$$u^{(l)} = D^{(l)} u, \tag{19}$$

where u is the vector of function values and $u^{(l)}$ is vector of approximate derivative values at the nodes $\{x_k\}$ and $D^{(l)}$ is the lth order Chebyshev differentiation matrix [16]. We express the entries of the Chebyshev differentiation matrix D as

$$\begin{aligned} D_{kj} &= \frac{c_j}{c_k} \frac{1}{2\ sin((k+j))\pi\ /((2N))sin((k-j)\pi/2N))}, \quad k \neq j, \\ D_{kk} &= -\frac{x_k}{2sin^2\left(\frac{k\pi}{N}\right)}, \quad k \neq 0, N, \\ D_{00} &= -D_{NN} = \frac{2N^2+1}{6}, \end{aligned} \tag{20}$$

where $c_k = (-1)^k$ for $k = 1,\ 2,\ \cdots,\ N-1$, and, $c_0 = \frac{1}{2}$, $c_N = \frac{(-1)^N}{2}$, also

$$D^{(l)} = (D)^l \quad l = 1, 2, \ldots.$$

When solving differential equations by pseudo-spectral method, the derivatives are approximated by the discrete derivative operators and linear two-point boundary value problem may thus be converted to a linear system.
By employing derivatives formulation (12), (13) transformed to the following expression

$$\sum_{k=0}^{N} D_{jk} u_i(x_k) + \frac{2}{x_k+1} \sum_{k=0}^{N} D_{jk} u_i(x_k) - n\frac{\varphi^2}{4} a_{i-1}^{m-1}(x_i) = \phi_{i-1}(x_k), \quad 1 \leq k \leq N-1. \tag{21}$$

Also, we should add two other equations for imposing boundary condition to the above system. So we obtain

$$A_{i-1} U_i = \phi_{i-1},$$

in which A_{i-1} is a $(N+1)\times(N+1)$ square matrix and U_{i-1} and ϕ_{i-1} are a $(N+1)\times 1$ column vectors defined by

$$U_i = [u_i(x_0), u_i(x_1), \ldots, u_i(x_{N-1}), u_i(x_N)],$$

$$\phi_{i-1} = [\emptyset_{i-1}(x_0), \emptyset_{i-1}(x_1), \ldots, \emptyset_{i-1}(x_{N-1}), \emptyset_{i-1}(x_N)],$$

$$A_{i-1} = D^2 + diag\left(\frac{1}{x+1}\right) D - n\frac{\varphi^2}{4} diag(a_{i-1}^{m-1}(x)).$$

Now by solving this linear system we obtain the unknown $u_i(x_k)$, $k = 0,\ 1, \ldots N$.

Table 1. Comparison of approximate and exact value of C(0) **with collocation points** N=32 **when** n=1

φ	$C(0)$(approximate)	exact
0.25	0.989658790825327	0.989658790825502
0.5	0.959517375667612	0.959517375667470
0.75	0.912057326419731	0.912057326420212
1	0.850918128239655	0.850918128239323
2	0.551441129543725	0.551441129543566
3	0.299464709006526	0.299464709006468
4	0.146574281303474	0.146574281303462

Table 2. Comparison of approximate and exact value of C(0) **with collocation points** N=32 **when** n=5

φ	M=2	M=3	M=4	M=5	exact
0.25	0.989945449808219	0.989945449806960	0.989945449806962	0.989945449806969	0.989945449807005
0.5	0.963433054176965	0.963433044002271	0.963433044002275	0.963433044002269	0.963433044002285
0.75	0.927902917900584	0.927901798730157	0.927901798729865	0.927901798729868	0.927901798729866
1	0.889564303037429	0.889543617670041	0.889543617524158	0.889543617524154	0.889543617524132
2	0.758042014143261	0.754152071340470	0.754141435351016	0.754141435281835	0.754141435281767
3	0.684973146416467	0.659657874464967	0.658983343027451	0.658982963292719	0.658982963293183
4	0.654865634924277	0.596254737275574	0.591040504100040	0.591012026803125	0.591012026071536

4. Numerical results

In this section, we show the accuracy and fast convergence of the hybrid method of the SLM and pseudo-spectral collocation method by comparing the exact analytical solution for some cases of reaction order n and Thiele modulus'. In the case n=1, the problem (4) is linear boundary differential equation which has exact analytical solution. We apply Chebyshev pseudo-spectral collocation method by considering N = 32 for obtaining numerical approximation of C(0) for some case of ' as given in Table 1. In this case, also solutions have been plotted for some Thiele modulus' in Figure 1. We have provided Table 2 and Figure 2 for $n = 5$ as well. Tables 3 and 4 in addition Figures 3 and 4 are given for those reaction orders and Thiele modulus for which the problem (4)-(5) does not have known exact solution.

Remark 1 *All results presented in this section can be compared to those exact solutions given by Ref. [9].*

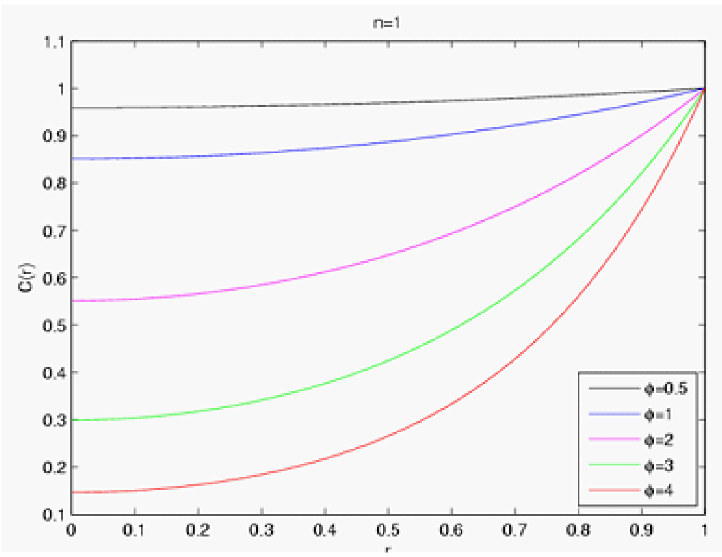

Figure 1. Approximate solutions of the problem (4)-(5) with collocation points N=32

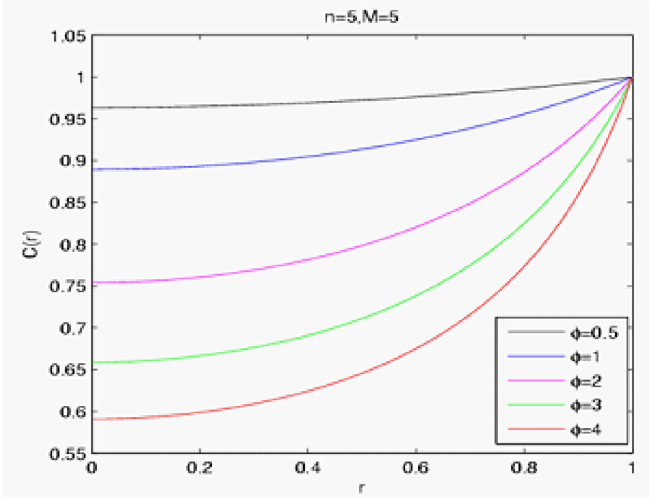

Figure 2. Approximate solutions of the problem (4)-(5) with collocation points N=32

Table 3. Comparison of approximate and exact value of C(0) **with collocation points** N=32

n	φ	M=2	M=3	M=4	M=5
2	0.25	0.989732675889290	0.989732675889287	0.989732675889291	0.989732675889289
2	0.75	0.916923510940118	0.916923507252235	0.916923507252238	0.916923507252240
2	1	0.863972286330311	0.863972161422443	0.863972161422451	0.863972161422447
2	2	0.639027322041255	0.638867666886289	0.638867662832321	0.638867662832325
2	3	0.468399301624146	0.465182082036108	0.465178999236353	0.465178999233939

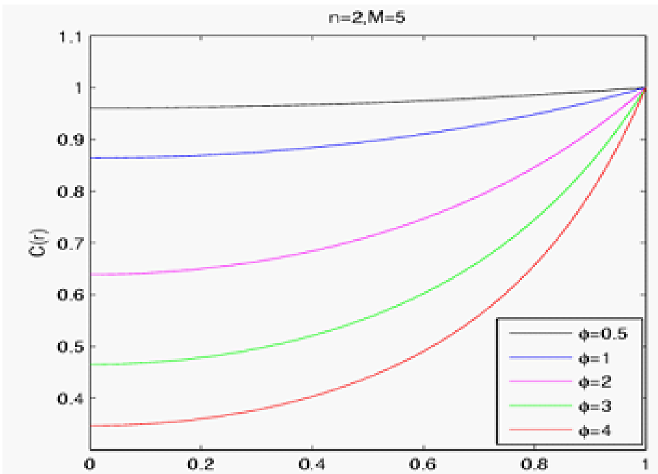

Figure 3. Approximate solutions of the problem (4)-(5) with collocation points N=32

5. Conclusion

In this paper, we have presented a method based on successive linearization method (SLM) and pseudo-spectral collocation method for obtaining the solution of the problem of diffusion reaction in spherical porous catalyst. We have shown that the SLM is a robust and reliable technique for obtaining semi-analytical solutions of nonlinear differential equations especially when it is combined by a numerical powerful method like pseudo-spectral collocation method.

Table 4. Comparison of approximate and exact value of C(0) **with collocation points** N=32

n	φ	M=2	M=3	M=4	M=5
3	0.25	0.989805045304709	0.989805045304675	0.989805045304669	0.989805045304662
3	0.75	0.921087819199368	0.921087754515380	0.921087754515377	0.921087754515377
3	1	0.874219088111702	0.874217370592920	0.874217370592531	0.874217370592532
3	2	0.692126882350104	0.691197300016726	0.691197011571961	0.691197011571934
3	3	0.567061374762437	0.556239841566273	0.556176486852542	0.556176485019289

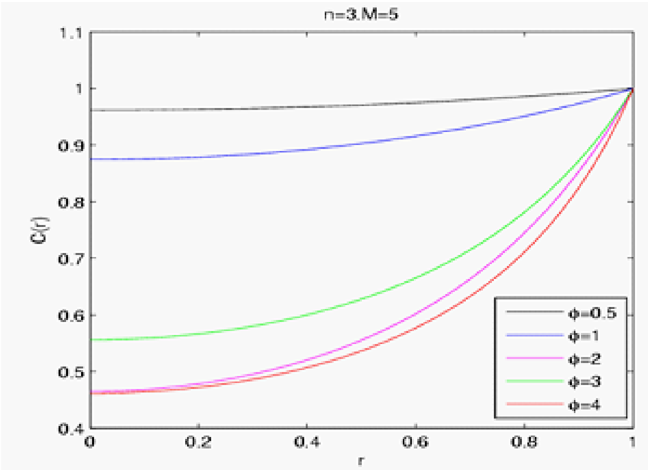

Figure 4. Approximate solutions of the problem (4)-(5) with collocation points N=32

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