



Computational Method for Reaction Diffusion-Model Arising in a Spherical Catalyst

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Abstract

In this paper, we consider Lane–Emden problems which have many applications in sciences. Mainly we focus on two special cases of Lane–Emden boundary value problems which models reaction–diffusion equations in a spherical catalyst and spherical biocatalyst. Here we propose a method to obtain approximate solution of these models. The main reason for using this technique is high accuracy and low computational cost compared to some other methods. Numerical results are shown using tables and figures. Accuracy of the computational method is shown by comparing numerical results by analytical methods.

Keywords Lane–Emden boundary value problem · Spherical catalyst · Spherical biocatalyst · Legendre scaling functions · Collocation method

Introduction

Lane–Emden type equation is a problem which has a singularity at the origin. In the neighbourhood of the singular point $t = 0$, the analytical solutions of this type of equation are always possible [1]. The Lane–Emden type equation is given as follows [2–6]:

$$x''(t) + \frac{\theta}{t}x'(t) + g(x(t)) = 0, \quad 0 \leq t \leq 1, \quad \theta > 0. \quad (1)$$

with

$$x'(0) = a_1 \text{ and } x(1) = a_2. \quad (2)$$

where $x(t)$ denote the unknown function on $[0, 1]$ and $x'(0)$ denote the derivative of $x(t)$ at time $t = 0$. a_1 and a_2 are constants.

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This equation describes many phenomena of chemistry, physics and astrophysics [7, 8]. This equation also shows variation of concentration or temperature in many field of chemistry, physics, bio-mathematics [9–11].

Spherical Catalyst Equation

In a spherical catalyst the chemical species dimensionless concentration is modelled by Lane–Emden boundary value problem and is given as [12, 13]:

$$x''(t) + \frac{2}{t}x'(t) - \rho^2x(t) \exp\left(\frac{\alpha\mu(1-x(t))}{1+\mu(1-x(t))}\right) = 0, \tag{3}$$

with

$$x'(0) = 0 \text{ and } x(1) = 1. \tag{4}$$

In above equation, x denote the concentration, t denote the dimensionless distance, μ denote the dimensionless activation energy, α denote the dimensionless heat of reaction and ρ denote the Thiele modulus [12, 13].

The following are the dimensionless parameters and variables,

$$t = \frac{r}{R}, \quad x = \frac{C_A}{C_{As}}, \quad \alpha = \frac{E}{R_gT_s}, \quad \mu = \frac{-(\Delta H)DC_{As}}{KT_s}, \quad \rho^2 = \frac{K_{ref}R^2}{D}.$$

The concentration of reactant A is denoted by C_A and C_{As} inside and on the surface of pellet respectively, effective diffusivity is denoted by D , E and ΔH represent activation energy and the heat of reaction respectively, K_{ref} represent the reaction constant, K represent the effective thermal conductivity, r represent the radial distance, R represent the radius of the catalytic pellet, R_g represent the universal gas constant and T_s represent the temperature at the surface.

The spherical pellet effectiveness factor τ is given as

$$\tau = \frac{3}{\rho^2} \left. \frac{dx}{dt} \right|_{t=1}.$$

Spherical Biocatalyst Equation

In a spherical biocatalyst the chemical species dimensionless concentration is modelled by Lane–Emden boundary value problem and is given as [14]:

$$x''(t) + \frac{2}{t}x'(t) - \rho^2\frac{(1+\mu)x(t)}{1+\mu x(t)} = 0, \tag{5}$$

with boundary conditions

$$\begin{aligned} x'(0) &= 0, \\ x(1) &= 1. \end{aligned} \tag{6}$$

The dimensionless parameters and variables are,

$$t = \frac{r}{R}, \quad x = \frac{C_A}{C_{As}}, \quad \mu = \frac{C_{As}}{K_m}, \quad \rho^2 = -\frac{r_{AS}R^2}{DD_{AS}}.$$

In this paper, we first consider a spherical catalytic pellet having a single reaction non-isothermally in it. In a spherical catalyst the chemical species concentration is modelled

by the Lane–Emden equation. We also study a spherical biocatalyst pellet having a single reaction non-isothermally in it.

The solutions for the spherical catalyst and spherical biocatalyst models can be obtained using many methods. In [15], authors solved these models using analytical method. Danish et al. [16], used OHAM to solve these models analytically. The author in [12] used the variational iteration method to find the analytical solutions of these spherical catalyst and spherical biocatalyst models. Recently, Singh in [17], proposed the OHAM to solve analytically these models. In [18], a numerical treatment using third order approximation was used to solve these models. Saadatmandi et al. [14], solved these models numerically. In present paper, we suggest an algorithm with the use of Legendre scaling functions (LSFs) and the collocation method to solve these models. In this method, first unknown function is approximated using finite dimensional approximations. By use of this approximations the spherical catalyst and spherical biocatalyst models are converted into a system of algebraic equations. By collocating these equations we obtain the approximate solution of these models. This method has many applications in differential equations [19–31]. Numerical results are demonstrated using figures and tables. Results are also compared with some recently developed analytical method.

Preliminaries and operational matrix

Here we describe some basic definitions. The LSFs. in one dimension are defined by

$$\epsilon_k(t) = \begin{cases} \sqrt{2k+1} S_k(2t-1), & \text{for } 0 \leq t < 1, \\ 0, & \text{otherwise.} \end{cases} \tag{7}$$

where $S_k(t)$ is Legendre polynomials of order k on the interval $[-1, 1]$, and given by;

$$S_k(t) = \sum_{k=0}^i (-1)^{i+k} \frac{(i+k)!}{(i-k)! (k!)^2} t^k. \tag{8}$$

The collections $\{\epsilon_k(t)\}$ form an orthonormal basis for $L^2[0, 1]$. The k th degree LSF is given by

$$\epsilon_k(t) = (2k+1)^{\frac{1}{2}} \sum_{k=0}^i (-1)^{i+k} \frac{(i+k)!}{(i-k)! (k!)^2} t^k. \tag{9}$$

A function $f \in L^2[0, 1]$, with bounded second derivatives can be approximated as,

$$f(t) = \lim_{n \rightarrow \infty} \sum_{k=0}^n c_k \epsilon_k(t), \tag{10}$$

where $c_k = \langle f(t), \epsilon_k(t) \rangle$

Equation (10), for finite dimension is written as,

$$f \cong \sum_{k=0}^m c_k \epsilon_k(t) = C^T \Pi_m(t), \tag{11}$$

where C and $\Pi_m(t)$ are $(m+1) \times 1$ vectors and given by

$$C = [c_0, c_1, \dots, c_m]^T \text{ and } \Pi_m(t) = [\epsilon_0, \epsilon_1, \dots, \epsilon_m]^T. \tag{12}$$

Theorem 1 Let $\Pi_m(t) = [\epsilon_0, \epsilon_1, \dots, \epsilon_m]^T$, and consider q be a positive integer then

$$I^q \epsilon_i(t) = I^{(q)} \Pi_m(t), \tag{13}$$

where $I^{(q)} = (u(i, j))$, is $(m + 1) \times (m + 1)$ matrix of integral operator whose entries are given by

$$u(i, j) = (2i + 1)^{1/2} (2j + 1)^{1/2} \sum_{k=0}^i \sum_{l=0}^j (-1)^{i+j+k+l} \frac{(i + k)! (j + l)!}{(i - k)! (j - l)! (k!) (l!)^2 (q + k + 1 + 1)(q + k)!}. \tag{14}$$

Proof Pl. see [19, 24].

Outline of Method

Here, we will derive method for the solution of fractional reaction–diffusion equations in a spherical catalyst and spherical biocatalyst. First, we consider the initial value problem with an undetermined constant in the determination of boundary value problem. i.e.

$$x''(t) + \frac{2}{t} x'(t) - \rho^2 x(t) \exp\left(\frac{\alpha\mu(1 - x(t))}{1 + \mu(1 - x(t))}\right) = 0, \tag{15}$$

$$x''(t) + \frac{2}{t} x'(t) - \rho^2 \frac{(1 + \mu)x(t)}{1 + \mu x(t)} = 0, \tag{16}$$

with initial and boundary conditions

$$x(0) = \beta, x'(0) = 0 \text{ and } x(1) = 1, \tag{17}$$

where $x(0) = \beta$, represents an undetermined constant.

Taking the following approximation:

$$x''(t) = C^T \Pi_n(t). \tag{18}$$

Integrating Eq. (18), we obtain

$$x'(t) = C^T I^{(1)} \Pi_n(t) + A^T \Pi_n(t), \tag{19}$$

where $I^{(1)}$, is an operational matrix of integration of order 1.

Integrating Eq. (19), we obtain

$$x(t) = C^T I^{(2)} \Pi_n(t) + A^T I^{(1)} \Pi_n(t) + B^T \Pi_n(t), \tag{20}$$

where

$$x'(0) = A^T \Pi_n(t) \text{ and } x(0) = B^T \Pi_n(t). \tag{21}$$

Further, taking

$$1 = D^T \Pi_n(t). \tag{22}$$

Mathematical Model of Spherical Catalyst Equation

Grouping Eqs. (15), (17)–(22), we get

$$C^T \Pi_n(t) + \frac{2}{t} (C^T I^{(1)} + A^T) \Pi_n(t) - \rho^2 (C^T I^{(2)} + A^T I^{(1)} + B^T) \Pi_n(t) \exp \left(\frac{\alpha \mu (D^T - (C^T I^{(2)} + A^T I^{(1)} + B^T)) \Pi_n(t)}{(D^T + \mu (D^T - (C^T I^{(2)} + A^T I^{(1)} + B^T))) \Pi_n(t)} \right) = 0. \tag{23}$$

The residual for Eq. (23), is given as

$$R_n(t) = C^T \Pi_n(t) + \frac{2}{t} (C^T I^{(1)} + A^T) \Pi_n(t) - \rho^2 (C^T I^{(2)} + A^T I^{(1)} + B^T) \Pi_n(t) \exp \left(\frac{\alpha \mu (D^T - (C^T I^{(2)} + A^T I^{(1)} + B^T)) \Pi_n(t)}{(D^T + \mu (D^T - (C^T I^{(2)} + A^T I^{(1)} + B^T))) \Pi_n(t)} \right). \tag{24}$$

Since the residual has $n + 1$, unknowns therefore collocating Eq. (24), at n points given by $t_i = \frac{i}{n}, i = 1, 2, \dots, n$.

$$R_n(t_i) = C^T \Pi_n(t_i) + \frac{2}{t_i} (C^T I^{(1)} + A^T) \Pi_n(t_i) - \rho^2 (C^T I^{(2)} + A^T I^{(1)} + B^T) \Pi_n(t_i) \exp \left(\frac{\alpha \mu (D^T - (C^T I^{(2)} + A^T I^{(1)} + B^T)) \Pi_n(t_i)}{(D^T + \mu (D^T - (C^T I^{(2)} + A^T I^{(1)} + B^T))) \Pi_n(t_i)} \right). \tag{25}$$

Further, using approximation in boundary condition

$$(C^T I^{(2)} + A^T I^{(1)} + B^T) \Pi_n(1) = 1. \tag{26}$$

From Eqs. (25) and (26), we get a system of $n + 1$ equations whose solution gives the unknowns in the approximations. Using this in the Eq. (20), we get solution for spherical catalyst model.

Mathematical Model of Spherical Biocatalyst Equation

Grouping Eqs. (16), (17)–(22), we get

$$C^T \Pi_n(t) + \frac{2}{t} (C^T I^{(1)} + A^T) \Pi_n(t) - \rho^2 \frac{(1 + \mu)(C^T I^{(2)} + A^T I^{(1)} + B^T) \Pi_n(t)}{(D^T + \mu(C^T I^{(2)} + A^T I^{(1)} + B^T)) \Pi_n(t)} = 0. \tag{27}$$

The residual for Eq. (27), is given as

$$R_n(t) = C^T \Pi_n(t) + \frac{2}{t} (C^T I^{(1)} + A^T) \Pi_n(t) - \rho^2 \frac{(1 + \mu)(C^T I^{(2)} + A^T I^{(1)} + B^T) \Pi_n(t)}{(D^T + \mu(C^T I^{(2)} + A^T I^{(1)} + B^T)) \Pi_n(t)}. \tag{28}$$

Since the residual has $n + 1$, unknowns therefore collocating Eq. (28), at n points given by $t_i = \frac{i}{n}, i = 1, 2, \dots, n$.

$$R_n(t_i) = C^T \Pi_n(t_i) + \frac{2}{t_i} (C^T I^{(1)} + A^T) \Pi_n(t_i) - \rho^2 \frac{(1 + \mu)(C^T I^{(2)} + A^T I^{(1)} + B^T) \Pi_n(t_i)}{(D^T + \mu(C^T I^{(2)} + A^T I^{(1)} + B^T)) \Pi_n(t_i)}. \tag{29}$$

Further, using approximation in boundary condition

$$(C^T I^{(2)} + A^T I^{(1)} + B^T) \Pi_n(1) = 1. \tag{30}$$

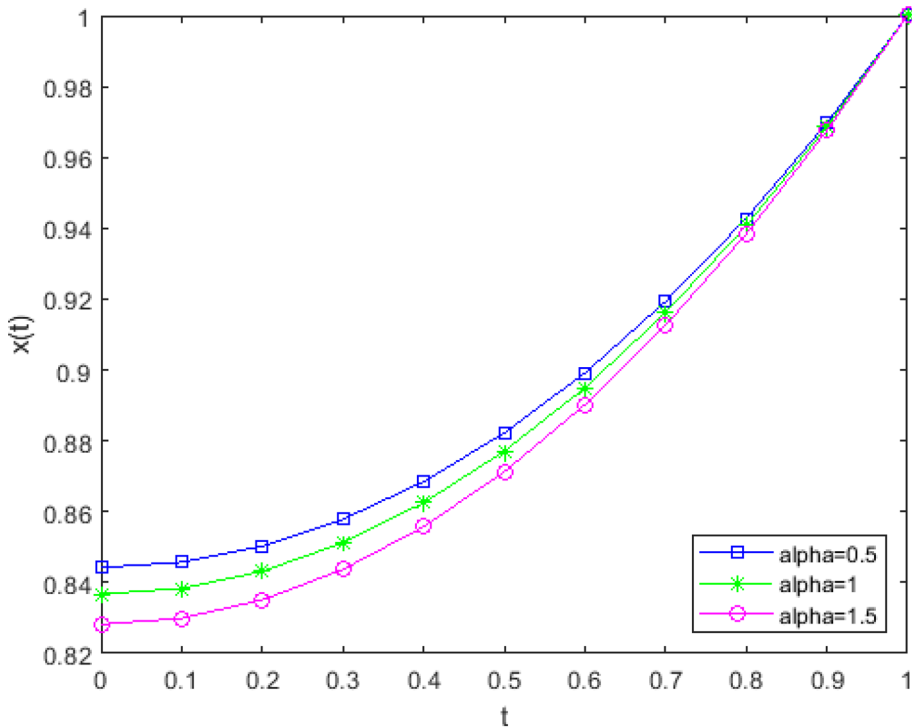


Fig. 1 Effect of dimensionless heat of reaction on the concentration $x(t; \alpha, \mu, \rho)$ at different choices of alpha (α)

From Eqs. (29) and (30), we get a system of $n + 1$ equations whose solution gives the unknowns in the approximations. Using this in the Eq. (20), we get solution for spherical biocatalyst model.

Numerical Simulation and Discussion

Here, we show the numerical simulation for our proposed method. We compare our numerical results with some analytical techniques in literature. The concentration depends on the μ , α and ρ . Here, we show how the concentration $x(t)$ is effected by these parameters.

Numerical Simulation for Spherical Catalyst Model

We show the numerical simulation results for spherical catalyst model by varying its parameters. In Fig. 1, we have shown the effect of dimensionless heat of reaction by varying α on the concentration $x(t; \alpha, \mu, \rho)$ by fixing the value of dimensionless activation energy ($\mu = 1$) and Thiele modulus ($\rho = 1$).

From Fig. 1, it is clear that concentration varies continuously with increasing of α . In Fig. 2, we have shown the effect of Thiele modulus by varying ρ on the concentration $x(t; \alpha, \mu, \rho)$ by fixing the value $\mu = 1$ and $\alpha = 1$. From Fig. 2, we can see that concentration varies constantly with increasing of ρ .

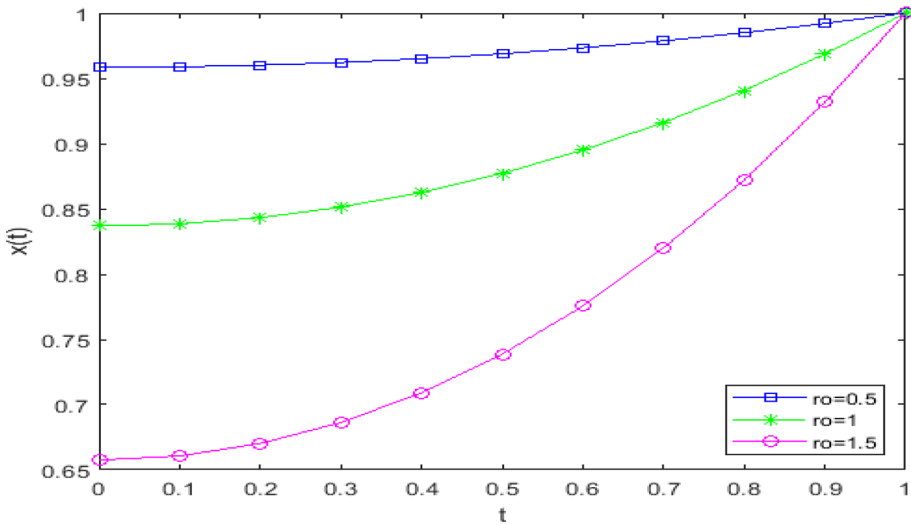


Fig. 2 Effect of Thiele modulus on the concentration $x(t; \alpha, \mu, \rho)$ at different choices of rho (ρ)

Table 1 Comparison of numerical results for different values of dimensionless heat of reaction (α)

t	Used technique ($\alpha = 0.5$)	Technique in [17] ($\alpha = 0.5$)	Used technique ($\alpha = 1$)	Technique in [17] ($\alpha = 1$)	Used technique ($\alpha = 1.5$)	Technique in [17] ($\alpha = 1.5$)
0.0	0.8442594	0.8442594	0.8367615	0.8367615	0.8282279	0.8282279
0.1	0.8457656	0.8457651	0.8383651	0.8383666	0.8299455	0.8299479
0.2	0.8502895	0.8502888	0.8431844	0.8431860	0.8351059	0.8351091
0.3	0.8578510	0.8578503	0.8512303	0.8512320	0.8437109	0.8437143
0.4	0.8684827	0.8684820	0.8625224	0.8625242	0.8557637	0.8557671
0.5	0.8822295	0.8822289	0.8770865	0.8770882	0.8712661	0.8712694
0.6	0.8991479	0.8991473	0.8949523	0.8949537	0.8902154	0.8902182
0.7	0.9193047	0.9193043	0.9161509	0.9161520	0.9125997	0.9126020
0.8	0.9427761	0.9427758	0.9407117	0.9407124	0.9383935	0.9383950
0.9	0.9696453	0.9696451	0.9686576	0.9686579	0.9675510	0.9675518
1.0	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000

In Table 1, results are compared for different values of α by fixing the value of dimensionless activation energy ($\mu = 1$) and Thiele modulus ($\rho = 1$).

In Table 2, results are compared for different values of ρ by fixing the value $\mu = 1$ and $\alpha = 1$.

From Tables 1 and 2, we observe that our results are accurate and have good agreement with method in [17]. In Table 3, we have listed, the value of effectiveness factor for different values of parameters.

From Table 3, it is clear that effectiveness factor is increasing with the increase of dimensionless heat of reaction α and it decrease with the increase of Thiele modulus (ρ).

In Table 4, results are compared with variational iteration method [12].

Table 2 Comparison of numerical results for different values of Thiele modulus (ρ)

t	Used technique ($\rho = 0.5$)	Technique in [17] ($\rho = 0.5$)	Used technique ($\rho = 1$)	Technique in [17] ($\rho = 1$)	Used technique ($\rho = 1.5$)	Technique in [17] ($\rho = 1.5$)
0.0	0.9583911	0.9583911	0.8367785	0.8367785	0.6575456	0.6575456
0.1	0.9588068	0.9588068	0.8383702	0.8383832	0.6606348	0.6607732
0.2	0.9600537	0.9600537	0.8431862	0.8432014	0.6701998	0.6703284
0.3	0.9621321	0.9621321	0.8512314	0.8512456	0.6864292	0.6864317
0.4	0.9650424	0.9650424	0.8625229	0.8625355	0.7090615	0.7092056
0.5	0.9687850	0.9687850	0.8770871	0.8770971	0.7387347	0.7388698
0.6	0.9733604	0.9733604	0.8949525	0.8949603	0.7755713	0.7756891
0.7	0.9787692	0.9787692	0.9161509	0.9161564	0.8198630	0.8199543
0.8	0.9850118	0.9850118	0.9407119	0.9407150	0.8718951	0.8719526
0.9	0.9920887	0.9920887	0.9686573	0.9686591	0.9318945	0.9319237
1.0	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000

Table 3 Comparison of effectiveness factor for different values of parameters

β	α	ρ	μ	Effectiveness factor present method	Effectiveness factor method in [17]
0.8442594	0.5	1	1	0.963812	0.963818
0.8367615	1.0	1	1	0.991217	0.991210
0.8282279	1.5	1	1	1.02187	1.02184
0.9583911	1	0.5	1	0.999411	0.999413
0.8367785	1	1.0	1	0.991296	0.991167
0.6575456	1	1.5	1	0.962358	0.961743

Table 4 Comparison of numerical results at $\alpha = 1, \mu = 1$ and for different values of Thiele modulus (ρ)

t	Used technique ($\rho = 0.5$)	Technique in [12] ($\rho = 0.5$)	Used technique ($\rho = 1.5$)	Technique in [12] ($\rho = 1.5$)
0.0	0.9554170	0.9554170	0.6471921	0.6471921
0.1	0.9569721	0.9558604	0.6543974	0.6503923
0.2	0.9591596	0.9571910	0.6672786	0.6600325
0.3	0.9616089	0.9594096	0.6846433	0.6762321
0.4	0.9647015	0.9625176	0.7080187	0.6991897
0.5	0.9685565	0.9665172	0.7380499	0.7291836
0.6	0.9732026	0.9714109	0.7751042	0.7665715
0.7	0.9786649	0.9772020	0.8195569	0.8117906
0.8	0.9849475	0.9838942	0.8717037	0.8653577
0.9	0.9920524	0.9914918	0.9317848	0.9278689
1.0	1.0000000	1.0000000	1.0000000	1.0000000

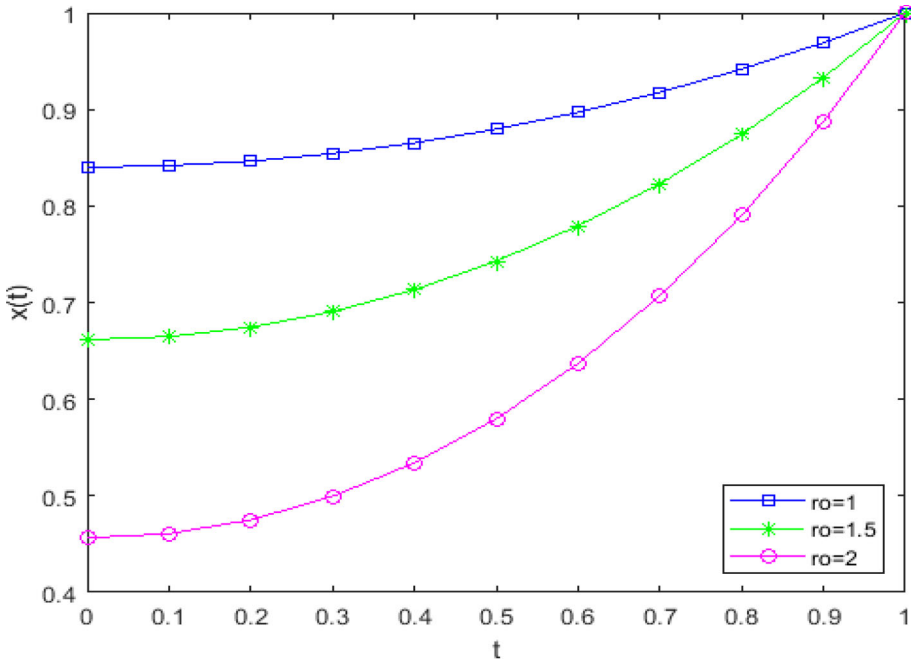


Fig. 3 Effect of Thiele modulus on the concentration $x(t; \mu, \rho)$ at different choices of rho (ρ)

Table 5 Comparison of numerical results for different values of Thiele modulus (ρ)

t	Used technique ($\rho = 1$)	Technique in [17] ($\rho = 1$)	Used technique ($\rho = 1.5$)	Technique in [17] ($\rho = 1.5$)	Used technique ($\rho = 2$)	Technique in [17] ($\rho = 2$)
0.0	0.8401441	0.8401441	0.6614868	0.6614868	0.4564643	0.4564643
0.1	0.8417115	0.8417117	0.6646777	0.6646917	0.4608336	0.4612215
0.2	0.8464182	0.8464184	0.6743143	0.6743302	0.4751546	0.4755901
0.3	0.8542757	0.8542759	0.6904600	0.6904739	0.4994820	0.4998553
0.4	0.8653033	0.8653035	0.7132276	0.7132390	0.5341764	0.5344752
0.5	0.8795277	0.8795279	0.7427755	0.7427837	0.5798510	0.5800566
0.6	0.8969826	0.8969828	0.7792974	0.7793031	0.6371888	0.6373242
0.7	0.9177083	0.9177084	0.8230199	0.8230235	0.7070042	0.7070867
0.8	0.9417511	0.9417512	0.8741952	0.8741969	0.7901669	0.7902033
0.9	0.9691627	0.9691628	0.9330933	0.9330944	0.8875264	0.8875513
1.0	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000

From Table 4, it clear that our proposed method has good agreement with variational iteration method [12].

Table 6 Comparison of effectiveness factor for different values of parameters

β	ρ	μ	Effectiveness factor used technique	Effectiveness factor technique in [17]
0.8401441	1	2	0.977095	0.977095
0.6614868	1.5	2	0.946801	0.946738
0.4564643	2	2	0.902908	0.902501

Numerical Simulation for Spherical Biocatalyst Model

We show the numerical simulation results for spherical biocatalyst model by varying its parameters. In Fig. 3, we have shown the effect of Thiele modulus by varying ρ on the concentration $x(t; \mu, \rho)$ by fixing the values of dimensionless activation energy ($\mu = 2$). From Fig. 3, it is clear that concentration varies continuously with increasing of ρ .

In Table 5, we have compared results by method in [17] for different values of ρ by fixing the value of dimensionless activation energy ($\mu = 2$). From Table 5, we observe that our results are accurate and show good agreement with method in [17].

In Table 6, we have listed, the value of effectiveness factor for different values of parameters. From Table 6, it is clear that effectiveness factor decreases with the increasing of Thiele modulus (ρ).

Conclusions

In this paper, we have studied the diffusion of reactants in an idealized spherical catalytic pellet and spherical biocatalyst pellet. We have also computed the behaviour of concentration at the spherical origin $t = 0$ of the pellets. We have converted spherical catalyst and spherical biocatalyst model into a system of algebraic equations. Desired accuracy is achieved only for few basis number elements. Proposed computational method is accurate and handy for computation purpose.

Declarations

Conflict of interest The authors declare that they have no competing interests.

References

1. Davis, H.T.: Introduction to Nonlinear Differential and Integral Equations. Dover, New York (1962)
2. Lane, J.H.: On theoretical temperature of the sun under the hypothesis of a gaseous mass maintaining its internal heat and depending on the laws of gases known to terrestrial experiment. Am. J. Sci. Arts Ser. **50**(2), 57–74 (1870)
3. Van Gorder, R.A.: Exact first integrals for a Lane–Emden equation of the second kind modeling a thermal explosion in a rectangular slab. New Astron. **16**(8), 492–497 (2011)
4. Singh, H.: An efficient computational method for the approximate solution of nonlinear Lane–Emden type equations arising in astrophysics. Astrophys. Space Sci. **363**(4), 363–371 (2018)
5. Rach, R., Duan, J.S., Wazwaz, A.M.: On the solution of non-isothermal reaction–diffusion model equations in a spherical catalyst by the modified Adomian method. Chem. Eng. Commun. **202**(8), 1081–1088 (2015)

6. Singh, H., Srivastava, H.M., Kumar, D.: A reliable algorithm for the approximate solution of the non-linear Lane–Emden type equations arising in astrophysics. *Numer. Methods Partial Differ. Equ.* **34**(5), 1524–1555 (2018)
7. Chandrasekhar, S.: *Introduction to Study of Stellar Structure*. Dover, New York (1967)
8. Horedt, G.P.: *Polytropes: Applications in Astrophysics and Related Fields*. Kluwer Academic Publishers, Dordrecht (2004)
9. Duan, J.-S., Rach, R., Wazwaz, A.M.: Steady-state concentrations of carbon dioxide absorbed into phenylglycidyl ether solutions by the Adomian decomposition method. *J. Math. Chem.* **53**(4), 1054–1067 (2015)
10. Wazwaz, A.M.: The variational iteration method for solving new fourth-order Emden–Fowler type equations. *Chem. Eng. Commun.* **202**(11), 1425–1437 (2015)
11. Wazwaz, A.M.: Solving systems of fourth-order Emden–Fowler type equations by the variational iteration method. *Chem. Eng. Commun.* **203**(8), 1081–1092 (2016)
12. Wazwaz, A.M.: Solving the non-isothermal reaction–diffusion model equations in a spherical catalyst by the variational iteration method. *Chem. Phys. Lett.* **679**, 132–136 (2017)
13. Rach, R., Duan, J.-S., Wazwaz, A.M.: Solving coupled Lane–Emden boundary value problems in catalytic diffusion reactions by the Adomian decomposition method. *J. Math. Chem.* **52**(1), 255–267 (2014)
14. Saadatmandi, A., Nafar, N., Toufighi, S.P.: Numerical study on the reaction cum diffusion process in a spherical biocatalyst. *Iran. J. Math. Chem.* **5**(1), 47–61 (2014)
15. Sevukaperumal, S., Rajendran, L.: Analytical solution of the concentration of species using modified Adomian decomposition method. *Int. J. Math. Arch.* **4**(6), 107–117 (2013)
16. Danish, M., Kumar, S., Kumar, S.: OHAM solution of a singular BVP of reaction cum diffusion in a biocatalyst. *Int. J. Appl. Math.* **41**(3), 223–227 (2011)
17. Singh, R.: Optimal homotopy analysis method for the non-isothermal reaction–diffusion model equations in a spherical catalyst. *J. Math. Chem.* **56**(9), 2579–2590 (2018)
18. Li, X., Chen, X.D., Chen, N.: A third order approximate solution of the reaction diffusion process in an immobilized biocatalyst particle. *Biochem. Eng. J.* **17**, 65–69 (2004)
19. Singh, H.: A new numerical algorithm for fractional model of Bloch equation in nuclear magnetic resonance. *Alex. Eng. J.* **55**, 2863–2869 (2016)
20. Singh, H.: Operational matrix approach for approximate solution of fractional model of Bloch equation. *J. King Saud Univ. Sci.* **29**(2), 235–240 (2017)
21. Petráš, I.: Modeling and numerical analysis of fractional-order Bloch equations. *Comput. Math. Appl.* **61**, 341–356 (2011)
22. Singh, H., Sahoo, M.R., Singh, O.P.: Numerical method based on Galerkin approximation for the fractional advection–dispersion equation. *Int. J. Appl. Comput. Math.* **3**(3), 2171–2187 (2016)
23. Wu, J.L.: A wavelet operational method for solving fractional partial differential equations numerically. *Appl. Math. Comput.* **214**, 31–40 (2009)
24. Singh, H., Srivastava, H.M., Kumar, D.: A reliable numerical algorithm for the fractional vibration equation. *Chaos Solitons Fractals* **103**, 131–138 (2017)
25. Tohidi, E., Bhrawy, A.H., Erfani, K.: A collocation method based on Bernoulli operational matrix for numerical solution of generalized pantograph equation. *Appl. Math. Model.* **37**, 4283–4294 (2013)
26. Singh, H., Srivastava, H.M.: Numerical simulation for fractional-order Bloch equation arising in nuclear magnetic resonance by using the Jacobi polynomials. *Appl. Sci.* **10**(8), 2850 (2020)
27. Singh, C.S., Singh, H., Singh, V.K., Singh, O.P.: Fractional order operational matrix methods for fractional singular integro-differential equation. *Appl. Math. Modell.* **40**, 10705–10718 (2016)
28. Singh, H., Srivastava, H.M.: Jacobi collocation method for the approximate solution of some fractional-order Riccati differential equations with variable coefficients. *Phys. A* **523**, 1130–1149 (2019)
29. Singh, C.S., Singh, H., Singh, S., Kumar, D.: An efficient computational method for solving system of nonlinear generalized Abel integral equations arising in astrophysics. *Phys. A* **525**, 0–8 (2019)
30. Singh, H., Pandey, R.K., Baleanu, D.: Stable numerical approach for fractional delay differential equations. *Few-Body Syst.* **58**, 156 (2017)
31. Singh, H., Singh, C.S.: Stable numerical solutions of fractional partial differential equations using Legendre scaling functions operational matrix. *Ain Shams Eng. J.* **9**, 717–725 (2018)