

A mathematical study on reaction-diffusion model in biomedicine

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Abstract. The present investigation examines the Michaelis-Menten kinetics response diffusion problem in a planar, spherical, and cylindrical framework by employing a mathematical model. The substrate concentration is found to have straightforward outcomes with the Michaelis constant, modified Sherwood number, and Thiele modulus. The analytical approximation for the non-dimensional substrate concentration and unitless effectiveness factor are determined via the new approximate analytical methodology called Ananthaswamy - Sivasankari method for steady-state and homotopy perturbation method with Laplace transform method for non-steady state. Additionally, comparison between the analytical approximation and numerical simulation is provided with graphical illustration. There is a good correlation between the numerical results and the approximate analytical result.

Keywords: Mathematical modeling, Michaelis–Menten kinetics (M-MK), non-linear initial-boundary value problem, homotopy perturbation method, new approximate analytical method, numerical simulation.

AMS Subject Classification 2010: 35B20, 35C20, 35G31, 35J05, 35K57.

1 Introduction

One of the key domains of current research is the theory of non-linear processing. There are numerous non-linear applications in physics (hydrodynamics, plasmas, non-linear optics, non-linear electric

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circuits, and states of solid), general relativity, chemistry (chemical reactions), biology (oceans and atmosphere, animal dispersal), random media, as well as contemporary telecommunications in the interdisciplinary field of non-linear systems and coherent structures. Non-linear partial differential equations (PDEs), especially reaction-diffusion (R-D) equations, can describe a wide range of events in biology, physics, and chemistry. An enzyme is a material that a living specimen produces and that serves as a catalyst to initiate a particular biological reaction. Put differently, enzymes are proteins that aid in accelerating our bodies' chemical reactions, or metabolism. They degrade certain chemicals and construct others. Enzymes are found in all living things and are produced by our bodies automatically.

A biological organisation, usually an enzyme, that detects a particular analysis as well as a transducer that converts biomolecules into an electrical signal makes up biosensors, which are analytical instruments [32]. Because of their cheapness, simplicity, and great selectivity, these devices have been commonly utilised in industrial, medicinal, and environmental purposes [39]. A helpful tool for researching the accomplishments of biosensors of any type would be a mathematical model founded on R-D equations [7]. A non-linear variable in this class of R-D equations is linked to the enzymatic reactions recognised as the Michaelis–Menten Kinetics (M-MK) [29]. The M-MK model can be utilized to explain a number of physical, biological, and chemical phenomena [23]. Merchant [25] focused on the steady-state concentration of substrate in the biosensor response action at mixed enzyme kinetics. Indira [20] provided a mathematical framework based on catechol–polyphenol oxidase as a prototype electroenzymatic modeling system. In a one-dimensional (1-D) R-D cell, the cubic-autocatalysis involving M-MK was investigated by Merchant et al. [28].

With non-linear chemical kinetics, solving the steady-state R-D equation (R-DE) is a common challenge in theoretical and experimental biology. These issues occur in the overview of how substrates get into microbial cells [11, 23, 26], in transport through membranes, in the distribution of oxygen to breathing tissue [19, 31], in the preparation of substrate and product component balances for enzymes immobilised within particles [8, 13], and in the evaluation of any artificial kidney structure [22]. On account of the saturation, Michaelis-Menten (M-M), or Monod expressions employed to characterise substrate consumption, the issue is frequently well positioned as a two-point non-linear boundary-value problem (BVP) in these situations. The steady-state formulation of the equations controlling the interchange of substrates among vascular and extravascular sections divided by a barrier with limited, symmetrical substrate permeability was examined by Bucolo et al. [9].

The M-MK framework for oxygen delivery to heart tissue was covered by Napper et al. [30]. Anantha Jothi et al.'s [1] solved the M-MK problem semi-analytically via new homotopy perturbation technique (NHPM) for the two levels of the mathematical modeling of a biosensor. The model which was constructed on non-linear R-DE linked to enzymatic reactions for non M-MK and catalytic R-D processes in a catalyst slab, the spherical catalyst pellet, and porous catalysts, has been resolved approximate analytically by implementing novel approximate analytical techniques described in the investigation of Ananthaswamy et al. [5, 6]. In the studies of Vijayalakshmi et al. [37], the two specific models namely the spherical catalyst and the spherical biocatalyst, were resolved using the new approximate analytical method called Ananthaswamy-Sivasankari Method (ASM). In the work of Meenakshi et al. [27] and Seethalakshmi et al. [33], the typical Gray-Scott model for a cubic-autocatalytic reaction with linear decay linked with diffusion in a 1-D reactor and the mathematical representation relating to the deactivation of immobilised glucose under packed-bed reactors were resolved by applying the Akbari-Ganji's method (AGM). In the investigation, Subanya et al. [35] used the New Homotopy analysis method (NHAM) and the q-Homotopy analysis method (q-HAM) to compare the approximate analytical outcomes of immo-

bilised enzyme in porous planar, cylindrical, and spherical particles. Ananthaswamy et al. [2,4] discussed the mathematical model related to the cubic-autocatalytic process with M-M decay taken into consideration in 1-D R-D cell.

The Adomian decomposition methodology (ADM) was used in the work of Vijayalakshmi et al. [38] to address the model that was developed on non-linear R-DE including non-linear terms linked to enzymatic reactions of M-MK. Using an integral equation approach, Tosaka et al. [36] examined a mathematical framework regarding oxygen diffusion within a spherical cell containing Michaelis-Menten intake kinetics. M-MK was used by Maalmi et al. [24] to examine steady-state reactant diffusion with subsequent uptake at a tiny site of activity on an enormous macromolecule or cell. The cubic-autocatalysis in an 1-D R-D cell concerning M-MK was reported by Marchant et al. [28]. The M-M saturation type kinetics involving minimal diffusion in the axial and rapid diffusion in the transverse regions were used by Bucolo et al. [9] to analyse the removal of substrate from the extravascular compartment. Dang Do et al. [12] solved the R-D issue with M-MK in a general-shaped solid using an approximate analytical method combined with a finite integral transform. The fundamental susceptible-infected-recovered (SIR) epidemiological model using the M-M expression based on the interactions rate was presented by Chapwanya et al. [10].

One of the most well-known and straightforward framework for the non-linear R-D process is M-MK [29]. It is expressed in the form of an equation that links substrate concentration to reaction velocity in a system where substrate S combines to an enzyme E reversibly to create an enzyme-substrate complex ES , which subsequently undergoes an irreversible reaction to produce a product P and regenerates the free enzyme E . Here is a systematic representation of this model by Izadi et al. [21]:



In the scheme mentioned above, k_{on} is the bimolecular relationships rate constant of the binding between the enzyme and the substrate, k_{off} is the uni-molecular rate constant of the ES complex splitting to form free enzyme and substrate again, and k_{cat} is the uni-molecular rate constant of the ES complex dissolving to produce free enzyme and product P . The following is the Michaelis-Menten equation (M-ME) for this system:

$$v = \frac{d[P]}{dt} = \frac{V_{max}[S]}{K_M + [S]}. \quad (2)$$

Here, V_{max} stands for the highest velocity the system can reach at the highest (saturating) substrate concentrations. When the substrate concentration is 50% of the V_{max} , the reaction velocity is known as the Michaelis constant K_M (also written as K_S alternately). The substrate S concentration is denoted by $[S]$. For over a century, the rate at which products are formed in enzymatic processes has been estimated via the M-ME. The impact of enzyme-substrate disassociation on enzymatic processes at the single-molecule level was mathematically examined by Shlomi et al. [34].

In the prior work Izadi et al. [21] treated immobilised catalysts of M-MK numerically under steady-state by employing the quasilinearization method (QLM) – Chatterjea polynomials (ChPs) matrix collocation, which lacks the analytical framework of the model. In order to fill the gap, we have presented this study by developing a comprehensive semi-analytical framework for the immobilised catalysts of M-MK equations by using the ASM. The application of ASM not only provides convergent closed-form solutions for the concentrations even in a single iteration but also offers analytical reference solutions that serve as standards for subsequent research.

The main objective of this work is to produce semi-analytical results for the non-dimensional substrate concentration by using a novel ASM for steady-state and homotopy perturbation method with Laplace transform for non-steady state. Finally, both the semi-analytical expressions and the numerical simulation are compared and graphically represented. The effects of several kinds of parameters, including the Thiele modulus for non-dimensional concentration, the dimensionless Michaelis constant, and the modified Sherwood number, were highlighted. Additionally, the dimensionless current's graphical representation is exhibited.

2 Mathematical formulation of the problem

An enzymatic process that takes place isothermally inside a porous support particle is going to be examined. It is assumed that the particle's shape has enough symmetry to allow the composition to change at any point in space based on just one spatial variable (e.g. spherical enzyme and slab support). The following represents the non-dimensional balance of materials of substrate species within the porous support [21]:

$$\frac{\partial M}{\partial t} = \frac{1}{\chi^S} \frac{\partial}{\partial \chi} \left(\chi^S \frac{\partial M}{\partial \chi} \right) - \frac{2h^2 M}{\beta + M}, \quad (3)$$

where the following is a description of the dimensionless parameters [21]:

$$h = L \sqrt{\frac{V_m}{2DS_0}}, \quad M = \frac{S}{S_0}, \quad \beta = \frac{K_M}{S_0}. \quad (4)$$

The immobilised catalyst's shape is $S = 0, 1, 2$ described by the exponent using slab planar, cylindrical and spherical, respectively.

The initial and boundary requirements that apply to Eq. (3) are

$$\text{At } t = 0, \quad M = 0, \quad (5)$$

$$\text{At } \chi = 0, \quad \frac{\partial M}{\partial \chi} = 0 \quad (\text{symmetry condition}), \quad (6)$$

$$\text{At } \chi = 1, \quad \frac{\partial M}{\partial \chi} = S_h(1 - M), \quad (7)$$

where $S_h = \left(\frac{k_m L}{D} \right)$ denotes the modified Sherwood number and k_m represents the mass-transfer coefficient. In mathematical modeling of porous catalysts, the symmetry boundary condition is usually, Neumann boundary condition applied at the center or axis of a particle (planar, cylindrical, or spherical) where the concentration profile is expected to be symmetric.

The following notation can be used to express Eq. (3) for the enzyme support of slab.

In this instance, Eq. (3) was reduced to the dimensionless type under non-steady state shown below:

Case 1: Planar particle ($S = 0$)

$$\frac{\partial M}{\partial t} = \frac{\partial^2 M}{\partial \chi^2} - \frac{2h^2 M}{\beta + M}. \quad (8)$$

Case 2: Cylindrical particle ($S = 1$)

$$\frac{\partial M}{\partial t} = \frac{\partial^2 M}{\partial \chi^2} + \frac{1}{\chi} \frac{\partial M}{\partial \chi} - \frac{2h^2 M}{\beta + M}. \quad (9)$$

Case 3: Cylindrical particle ($S = 2$)

$$\frac{\partial M}{\partial t} = \frac{\partial^2 M}{\partial \chi^2} + \frac{2}{\chi} \frac{\partial M}{\partial \chi} - \frac{2h^2 M}{\beta + M}. \quad (10)$$

The Effectiveness factor under non-steady state is represented by

$$Ef = \eta - \frac{(1 + \beta)}{2h^2} \left[\frac{\partial M}{\partial \chi} \right]_{\chi=1}. \quad (11)$$

The respective boundary requirements are stated in Eqs. (5) - (7).

In this instance, Eq. (3) was reduced to the dimensionless type under steady-state shown below:

Case 1: Planar particle ($S = 0$)

$$\frac{d^2 M}{d\chi^2} - \frac{2h^2 M}{\beta + M} = 0. \quad (12)$$

Case 2: Cylindrical particle ($S = 1$)

$$\frac{d^2 M}{d\chi^2} + \frac{1}{\chi} \frac{dM}{d\chi} - \frac{2h^2 M}{\beta + M} = 0. \quad (13)$$

Case 3: Cylindrical particle ($S = 2$)

$$\frac{d^2 M}{d\chi^2} + \frac{2}{\chi} \frac{dM}{d\chi} - \frac{2h^2 M}{\beta + M} = 0. \quad (14)$$

The respective boundary requirements are stated in Eqs. (6) – (7).

The Effectiveness factor under steady-state is given by

$$Ef = \eta = \frac{(1 + \beta)}{2h^2} \left[\frac{dM}{d\chi} \right]_{\chi=1}. \quad (15)$$

3 Approximate analytical expressions

Numerous scientific and technical domains are greatly impacted by differential equations (DEs), both linear and non-linear, which can be utilised to depict a broad variety of responses. Several non-linear ordinary differential equations (ODEs) of the second-order do not have sufficient semi-analytical results. The homotopy analysis technique (HAM) [2], variational iteration method (VIM) [5], new homotopy perturbation approach (NHPM) [1], Akbari-Ganji's technique [27], new homotopy analysis approach (NHAM) [35], q-homotopy analysis technique [35] and new approximate analytical methodology [5, 6, 37] these are the few approximate analytical techniques for accurately resolving second-order ODEs in non-linear.

3.1 Approximate analytical expressions for Eqs. (12) – (14) under steady state

The second-order non-linear ODEs are predicted using an efficient methodology entitled the ASM [5, 6, 37]. This approach is capable of helping to deal with DEs that are linear or non-linear. Additionally, this approach is readily adaptable to various non-linear problems, including boundary value issues in the biological, chemical, and physical sciences, especially those involving M-MK problems. Furthermore, the proposed new method can be used to tackle the boundary and initial value problems. It is possible to establish higher-order boundary conditions for the DE and its derivatives. This method is a non-iterative method which does not required iterative steps as compared to the HAM, HPM, and VIM. Also, it provides the approximate analytical solution even in a single iteration, which is closer to an exact solution.

The approximate analytical solution for Eq. (11) by employing the ASM for case 1: the planar particle $S = 0$ fulfils the boundary condition is as follows:

$$M(\chi) = le^{a\chi} + me^{-a\chi}. \quad (16)$$

$$\frac{dM}{d\chi} = ale^{a\chi} - ame^{-a\chi}. \quad (17)$$

By utilizing the boundary condition Eqs. (6) – (7) in Eqs. (16) – (17), we get the parameters values l & m as follows:

$$l = m, \quad m = \frac{S_h}{a(e^a - e^{-a}) + S_h(e^a + e^{-a})}. \quad (18)$$

As a result, Eq. (16), becomes

$$M(\chi) = \frac{S_h(e^{a\chi} + e^{-a\chi})}{a(e^a - e^{-a}) + S_h(e^a + e^{-a})}. \quad (19)$$

Now, by simplifying and applying Eq. (19) to Eq. (12), we obtain

$$\frac{S_h a^2 (e^{a\chi} + e^{-a\chi})}{a(e^a - e^{-a}) + S_h(e^a + e^{-a})} - \frac{2h^2 \left[\frac{S_h(e^{a\chi} + e^{-a\chi})}{a(e^a - e^{-a}) + S_h(e^a + e^{-a})} \right]}{\beta + \left[\frac{S_h(e^{a\chi} + e^{-a\chi})}{a(e^a - e^{-a}) + S_h(e^a + e^{-a})} \right]} = 0. \quad (20)$$

Moreover, by setting $\chi = 1$, Eq. (20) becomes

$$\frac{S_h a^2 (e^a + e^{-a})}{a(e^a - e^{-a}) + S_h(e^a + e^{-a})} - \frac{2h^2}{\beta + 1} = 0. \quad (21)$$

Equation (21) can be solved to yield the parameter value a .

Hence an approximate analytical outcomes of Eq. (12) is attained as follows:

$$M(\chi) = \frac{S_h(e^{a\chi} + e^{-a\chi})}{a(e^a - e^{-a}) + S_h(e^a + e^{-a})} = \frac{S_h \cosh(a\chi)}{a \sinh(a) + S_h \cosh(a)}. \quad (22)$$

The following is the effectiveness factor for case 1: planar particle ($S = 0$):

$$\eta = \left(\frac{1 + \beta}{2h^2} \right) \left(\frac{S_h(e^a - e^{-a})}{a(e^a - e^{-a}) + S_h(e^a + e^{-a})} \right). \quad (23)$$

where a is derived from Eq. (21).

Similarly, the approximate analytical answer by applying ASM for case 2: cylindrical particle ($S = 1$) of Eq. (13) that meets the boundary condition which is stated in Eqs. (6) - (7) is as follows:

$$M(\chi) = \frac{S_h(e^{b\chi} + e^{-b\chi})}{b(e^b - e^{-b}) + S_h(e^b + e^{-b})} = \frac{S_h \cosh(b\chi)}{b \sinh(b) + S_h \cosh(b)}. \quad (24)$$

The following is the effectiveness factor for case 2: cylindrical particle ($S = 1$):

$$\eta = \left(\frac{1 + \beta}{2h^2} \right) \left(\frac{S_h(e^b - e^{-b})}{b(e^b - e^{-b}) + S_h(e^b + e^{-b})} \right). \quad (25)$$

The approximate analytical solution via the ASM for case 3: spherical particle ($S = 2$) of Eq. (14) that meets the boundary condition which is stated in Eqs. (6) - (7) is as follows:

$$M(\chi) = \frac{S_h(e^{m\chi} + e^{-m\chi})}{m(e^m - e^{-m}) + S_h(e^m + e^{-m})} = \frac{S_h \cosh(m\chi)}{m \sinh(m) + S_h \cosh(m)}. \quad (26)$$

The following is the effectiveness factor for case 3: spherical particle ($S = 2$):

$$\eta = \left(\frac{1 + \beta}{2h^2} \right) \left(\frac{S_h(e^m - e^{-m})}{m(e^m - e^{-m}) + S_h(e^m + e^{-m})} \right). \quad (27)$$

3.2 Approximate analytical expressions for the Eqs. (8) - (10) under non-steady state

The HPM emerged by Ji-huan He [14–18] to yield approximation analytical results. An incredibly straightforward and effective method for obtaining an approximate analytical response with respect to linear and non-linear differential equations is HPM. The HPM has been successfully applied to a variety of boundary and initial value issues. The perturbation strategy is thought to have a small number of parameters. Since there are many non-linear scenarios, the semi-analytical formulas generated by perturbation techniques might be suitable for very small values of minor parameters. In many cases, perturbation answers are just as successful when the scientific system's parameters are low. Since there are no standards for the existence of minor parameters, the approximation is unable to completely depend upon. Therefore, simultaneously analytical and experimental verification of the accuracy of the approximation are crucial. HPM has recently been suggested as a possible remedy to these challenges. He [17] uses a unique approach based on the homotopy perturbation strategy to resolve differential equations in non-linear by the zeroth iteration. Adopting the homotopy perturbation approach and the Laplace transform technique [3, 4], we acquired the time-dependent solutions to the Eqs. (8) - (10).

The homotopy for the governing Eq. (8) is constructed as

$$(1-r) \left[\frac{\partial M}{\partial t} - \frac{\partial^2 M}{\partial \chi^2} + \frac{2h^2 M}{\beta + M} \right] + r \left[\frac{\partial M}{\partial t} - \frac{\partial^2 M}{\partial \chi^2} + \frac{2h^2 M}{\beta + M} \right] = 0. \quad (28)$$

Equation (28) has an approximate response that is

$$M = M_0 + rM_1 + r^2M_2 + \dots \quad (29)$$

By putting Eq. (29) in Eq. (28) and comparing the coefficients of r^0 , we attained

$$r^0 : \frac{\partial M}{\partial t} - \frac{\partial^2 M}{\partial \chi^2} + \frac{2h^2 M}{\beta + M} = 0. \quad (30)$$

The initial and boundary requirements are

$$\text{At } t = 0, M_i = 0, i = 0, 1, 2, 3, \dots, \quad (31)$$

$$\text{At } \chi = 0, \frac{\partial M_i}{\partial \chi} = 0, i = 0, 1, 2, 3, \dots, \quad (32)$$

$$\text{At } \chi = 1, \frac{\partial M_0}{\partial \chi} = S_h(1 - M), \frac{\partial M_i}{\partial \chi} = 0, i = 1, 2, 3, \dots. \quad (33)$$

Taking Laplace transform for Eqs. (30) - (33) as follows:

$$r^0 : \frac{\partial \bar{M}}{\partial t} - \frac{\partial^2 \bar{M}}{\partial \chi^2} + \frac{2h^2 \bar{M}}{\beta + \bar{M}} = 0, \quad (34)$$

$$\text{At } t = 0, \bar{M}_i = 0, i = 0, 1, 2, 3, \dots, \quad (35)$$

$$\text{At } \chi = 0, \frac{\partial \bar{M}_i}{\partial \chi} = 0, i = 0, 1, 2, 3, \dots, \quad (36)$$

$$\text{At } \chi = 1, \frac{\partial \bar{M}_0}{\partial \chi} = S_h(1 - M), \frac{\partial \bar{M}_i}{\partial \chi} = 0, i = 0, 1, 2, 3, \dots. \quad (37)$$

Next, using the newly proposed approximate analytical outcomes stated in Eq. (22) in Eq. (34), we were able to

$$\bar{M}(\chi) = \frac{S_h \cosh(a\chi)}{a \sinh(a) + S_h \cosh(a)}. \quad (38)$$

With the complex inversion formula, let us now solve Eq. (38).

To do this, we must assess the $\text{Res} \left[\frac{S_h \cosh(s+a)\chi}{s(a \sinh(s+a) + S_h \cosh(s+a))} \right]$.

Identification of the poles for \bar{M}_0 , we observe that a pole is present at $s = 0$ and the equation's solution yields an infinitely many poles $\sinh(s+a) + \cosh(s+a) = 0$. (i.e.,) there are infinite number of poles at $s_p = -a - \frac{(2p+1)^2 \pi^2}{4}$ and $s_p = -a - p^2 \pi^2$ where $p = 0, 1, 2, 3, \dots$

Therefore, we observe that

$$\begin{aligned} L^{-1} = & \text{Res} \left[\frac{S_h \cosh(s+a)\chi}{s(a \sinh(s+a) + S_h \cosh(s+a))} \right]_{s=0} \\ & + \text{Res} \left[\frac{S_h \cosh(s+a)\chi}{s(a(\sinh(s+a)) + S_h(\cosh(s+a)))} \right]_{s=s_p}. \end{aligned} \quad (39)$$

In Eq. (39), the first residue is provided by

$$\begin{aligned} & \text{Res} \left[\frac{S_h \cosh(s+a)\chi}{s(s \sinh(s+a) + S_h \cosh(s+a))} \right]_{s=0} \\ & = \lim_{s \rightarrow 0} \left[\frac{(s-0)e^{st} S_h \cosh(s+a)\chi}{s(a \sinh(s+a) + S_h \cosh(s+a))} \right], \end{aligned} \quad (40)$$

$$= \frac{S_h \cosh(a\chi)}{a \sinh(a) + S_h \cosh(a)}. \quad (41)$$

In Eq. (39), the second residue is supplied by

$$\begin{aligned} & \text{Res} \left[\frac{S_h \cosh(s+a)\chi}{s(s \sinh(s+a) + S_h \cosh(s+a))} \right]_{s=s_p} \\ &= \lim_{s \rightarrow s_p} \left[\frac{e^{st} S_h \cosh(s+a)\chi}{\frac{d}{ds}(s(a \sinh(s+a) + S_h \cosh(s+a)))} \right], \end{aligned} \quad (42)$$

$$\begin{aligned} &= \sum_{p=0}^{\infty} \frac{(-1)^{p+1} (2p+1) \pi \cos(\frac{2p+1}{2} \pi \chi) e^{-(a^2 + \frac{(2p+1)^2 \pi^2}{4})t}}{a^2 + \frac{(2p+1)^2 \pi^2}{4}} \\ &+ \sum_{p=0}^{\infty} \frac{-2(-1)^p (p\pi) \cos(p\pi \chi) e^{-(p^2 \pi^2 + a^2)t}}{p^2 \pi^2 + a^2}. \end{aligned} \quad (43)$$

The approximate analytical response of Eq. (8) for case 1: the planar particle $S = 0$ is obtained by combining Eqs. (41) and (43), as follows:

$$\begin{aligned} M(\chi) &= \frac{S_h \cosh(a\chi)}{a \sinh(a) + S_h \cosh(a)} \\ &+ \sum_{p=0}^{\infty} \frac{(-1)^{p+1} (2p+1) \pi \cos(\frac{2n+1}{2} \pi \chi) e^{-(a^2 + \frac{(2p+1)^2 \pi^2}{4})t}}{a^2 + \frac{(2p+1)^2 \pi^2}{4}} \\ &- \sum_{p=0}^{\infty} \frac{2(-1)^p (p\pi) \cos(p\pi \chi) e^{-(p^2 \pi^2 + a^2)t}}{p^2 \pi^2 + a^2}. \end{aligned} \quad (44)$$

The effectiveness factor of Eq. (11) for case 1: the planar particle ($S = 0$) is attained as follows:

$$\eta = \frac{(1+\beta)}{2h^2} \left[\frac{S_h a \cosh(a)}{a \sinh(a) + S_h \cosh(a)} + \sum_{p=0}^{\infty} \frac{\frac{(2p+1)^2 \pi^2}{2} e^{-(a^2 + \frac{(2p+1)^2 \pi^2}{4})t}}{a^2 + \frac{(2p+1)^2 \pi^2}{4}} \right]. \quad (45)$$

where a is derived from Eq. (21).

In a similar manner, we may solve Eqs. (9) and (10).

The approximate analytical outcomes of the Eq. (9) for case 2: the cylindrical particle $S = 1$ as follows:

$$\begin{aligned} M(\chi) &= \frac{S_h \cosh(b\chi)}{b \sinh(b) + S_h \cosh(b)} \\ &+ \sum_{p=0}^{\infty} \frac{(-1)^{p+1} (2n+1) \pi \cos(\frac{2p+1}{2} \pi \chi) e^{-(b^2 + \frac{(2p+1)^2 \pi^2}{4})t}}{b^2 + \frac{(2p+1)^2 \pi^2}{4}} \\ &- \sum_{p=0}^{\infty} \frac{2(-1)^p (p\pi) \cos(p\pi \chi) e^{-(p^2 \pi^2 + b^2)t}}{p^2 \pi^2 + b^2}. \end{aligned} \quad (46)$$

The effectiveness factor of Eq. (11) for case 2: the cylindrical particle ($S = 1$) is attained as follows:

$$\eta = \frac{(1+\beta)}{2h^2} \left[\frac{S_h b \cosh(b)}{b \sinh(b) + S_h \cosh(b)} + \sum_{p=0}^{\infty} \frac{\frac{(2p+1)^2 \pi^2}{2} e^{-(b^2 + \frac{(2p+1)^2 \pi^2}{4})t}}{b^2 + \frac{(2p+1)^2 \pi^2}{4}} \right]. \quad (47)$$

The approximate analytical results of the Eq. (10) for case 3: the spherical particle $S = 2$ as follows:

$$M(\chi) = \frac{S_h \cosh(m\chi)}{m \sinh(m) + S_h \cosh(m)} + \sum_{p=0}^{\infty} \frac{(-1)^{p+1} (2p+1) \pi \cos(\frac{2p+1}{2} \pi \chi) e^{-(m^2 + \frac{(2p+1)^2 \pi^2}{4})t}}{m^2 + \frac{(2p+1)^2 \pi^2}{4}} - \sum_{p=0}^{\infty} \frac{2(-1)^p (p\pi) \cos(p\pi \chi) e^{-(p^2 \pi^2 + m^2)t}}{p^2 \pi^2 + m^2}. \quad (48)$$

The effectiveness factor of Eq. (11) for case 3: the spherical particle ($S = 2$) is attained as follows:

$$\eta = \frac{(1 + \beta)}{2h^2} \left[\frac{S_h m \cosh(m)}{m \sinh(m) + S_h \cosh(m)} + \sum_{p=0}^{\infty} \frac{\frac{(2p+1)^2 \pi^2}{2} e^{-(a^2 + \frac{(2p+1)^2 \pi^2}{4})t}}{m^2 + \frac{(2p+1)^2 \pi^2}{4}} \right]. \quad (49)$$

4 Numerical simulation

By employing the ASM, the approximate analytical solutions for the non-dimensional substrate concentration under steady-state as well as the approximate analytical expressions for the dimensionless concentration for substrate under non-steady state through homotopy perturbation strategy with Laplace transform have been obtained. Our approximate analytical results for non-linear DEs can be validated with numerical simulation [1,2]. MATLAB programming is given in Appendix B. The numerical simulation generated by MATLAB and the derived semi-analytical equation are presented in Figures 1 – 3 and Figs.5 – 7.

5 Results and discussions

The performance and accuracy of the suggested semi-analytical approach are assessed in this section by presenting and analysing the results that were obtained. Non-dimensional concentration for planar, cylindrical and spherical particle are attained utilizing the new approximate analytical method namely ASM is contrasted with numerical simulation calculated with the pedpe solver in MATLAB. Excellent agreement is shown in the comparisons based on Eqs. (22), (24) and (26) for time-independent, Eqs. (44), (46) and (48) for time dependent confirming the validity of the semi-analytical technique. A thorough analysis of the computational results is provided in the discussion that follows.

For non-dimensional concentration of planar particle: Equations (22) and (44) are used to illustrate the non-dimensional concentration $M(\chi)$ versus dimensionless distance χ for planar particles in Fig.1 under time-independent and Fig.5 under time-dependent. As the non-dimensional michaelis constant β and modified sherwood number S_h increase, consequently the dimensionless concentration likewise increases, as witnessed in Figs.1 and 5.

For non-dimensional concentration of cylindrical particle: Equations (24) and (46) is used to illustrate the non-dimensional concentration $M(\chi)$ versus dimensionless distance χ for cylindrical particles in Fig.2 under time-independent and Fig.6 under time-dependent. As the non-dimensional michaelis

constant β increases, consequently the dimensionless concentration likewise increases, as witnessed in Fig.2. Fig.6 displays how the dimensionless concentration drops as the thiele modulus h values rise.

For non-dimensional concentration of spherical particle: By employing Eqs. (26) and (48) for spherical particles, Fig.3 for time-independent and Fig.7 for time-dependent demonstrate the dimensionless concentration $M(\chi)$ against non-dimensional distance χ . Fig.7 reveal that when the modified sherwood number S_h are elevated, so does an associated dimensionless concentration. Fig.3 highlights how the dimensionless concentration drops as the thiele modulus h values rise.

For effectiveness factor: The effectiveness factor with different dimensionless parameters is portrayed in Fig.4 under steady – state by implementing Eq. (24) for cylindrical particle. It displays that the effectiveness factor η with the non-dimensional michaelis constant β . From this, it shows that when the thiele modulus h enhanced, the efficacy factor drops. Fig.8 under non-steady state implementing eqn. (48) for spherical particles. It interlines that the effectiveness factor η against thiele modulus h . From this, we noted that the amount of modified sherwood number S_h get enhances then the effectiveness factor falls.

For error analysis: The contrast for the previous work (QLM-ChPs method) with the present work under steady-state and numerical simulation with the approximate analytical method under non-steady state for the fixed quantities of the parameters is displayed in Table 1. This table indicates that the average absolute error percentage for the concentrations is 0.01, and 0.0006 (approximately), which shows that the method's accuracy. This demonstrates that the solutions are convergent, accurate, and reliable in a single iteration, providing a solid foundation for the parametric and chemical analysis presented. It is clear from analysing the figures and tables that the ASM regularly offers a better approximation with the previous work and simulation within the specified time interval. Nevertheless, even with a short time span, ASM successfully captures this behaviour. This led us to conclude that the ASM yields an approximation with greater precision than the numerical simulation and the previous work.

6 Conclusion

In the case of the non-dimensional material balance for the species of substrate within the porous support, the new approximation analytical technique was used to resolve semi-analytically. By implementing ASM as well as homotopy perturbation technique with laplace transform, the approximate analytical results of the non-dimensional concentration under steady-state, non-steady state and effectiveness factor were determined. Numerical simulation was then used to compare our approximate analytical findings. The ASM and homotopy perturbation method yields significantly more accurate results that are comparable to the numerical simulation's output. By comparing ASM results with numerical simulations, this study highlights the ASMs ability in addressing non-linear BVPs in a single iteration and confirms the validity of the proposed approach. The study concluded that ASM is a robust and efficient tool for analysing non-linear electrochemical systems. This work underlined the power of approximate analytical expressions, allowing explicit insights and broad generalizations, and hence enriching our understanding of the MMK process. The ASMs significance resides in its potential to unravel porous catalyst determined by the MM equations and engineering applications. With the aid of the approximate analytical solution, the researchers should be able to visualise how various parameters affect concentration.

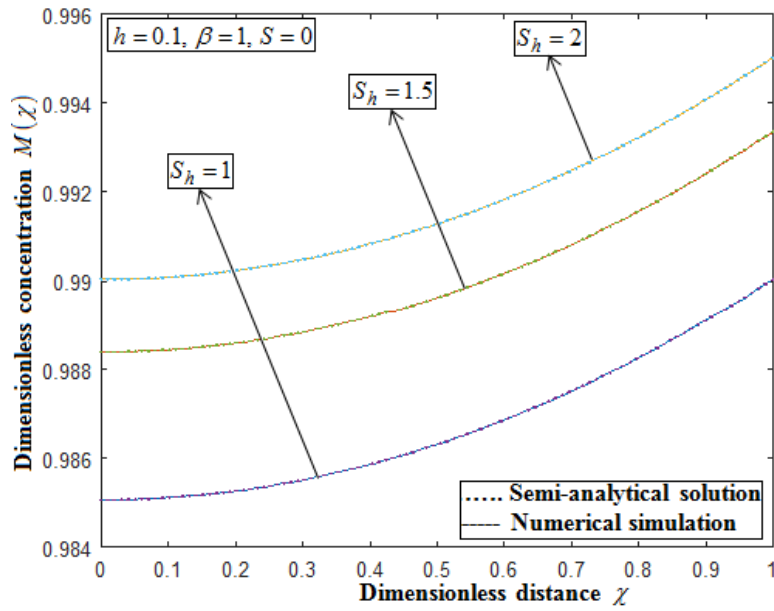


Figure 1: Effect of modified sherwood number S_h for planar particle for time-independent

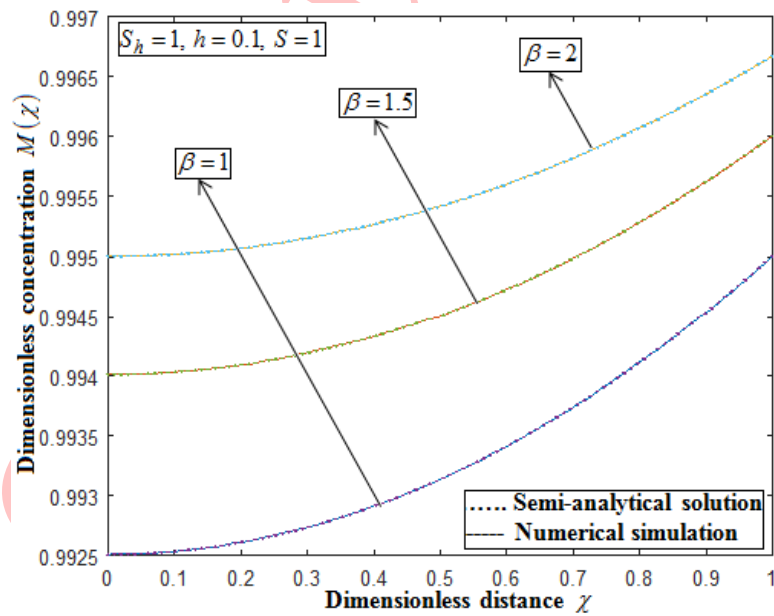


Figure 2: Impact for non-dimensional michaelis constant β for cylindrical particle for time-independent

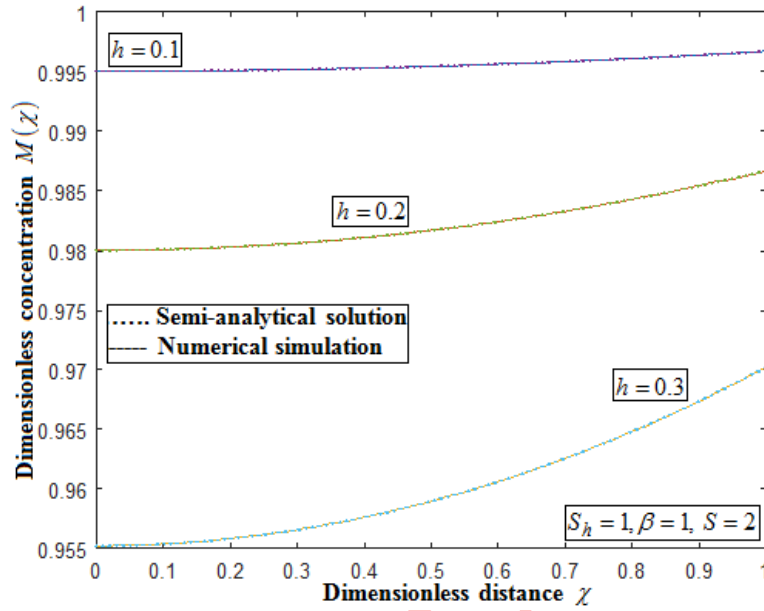


Figure 3: Effect for thiele modulus h for spherical particle for time-independent

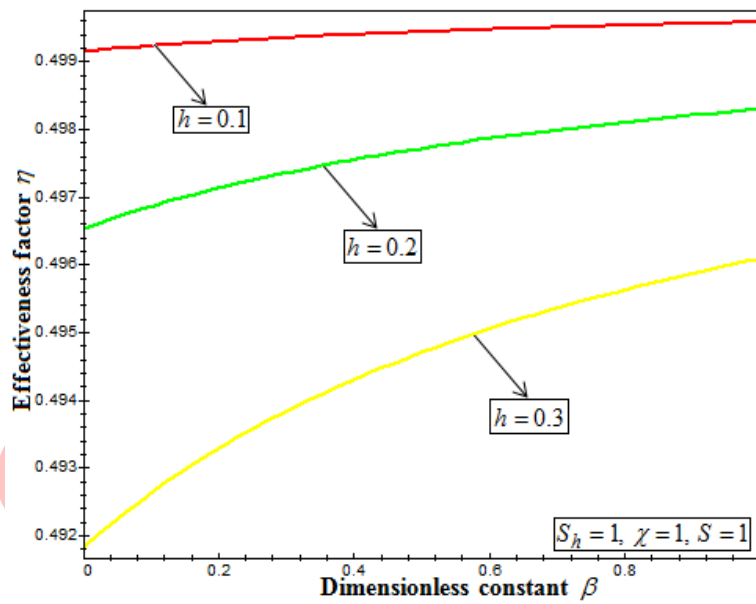


Figure 4: Curves for thiele modulus h in effectiveness factor for cylindrical particle for time-independent

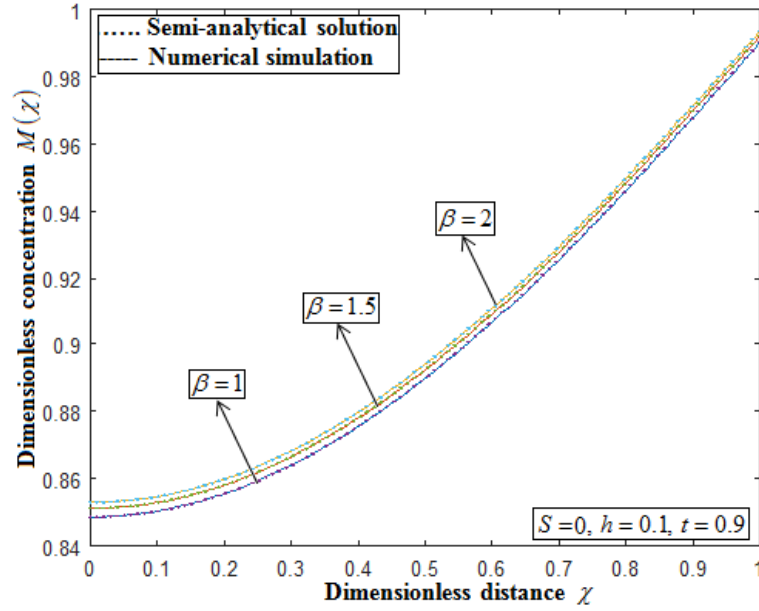


Figure 5: Impact of non-dimensional Michaelis constant β for planar particle for time-dependent

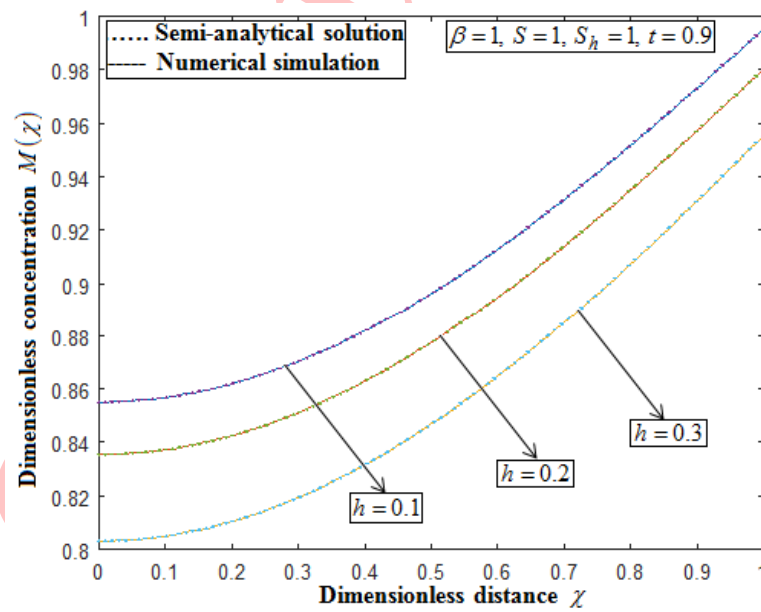


Figure 6: Influence of Thiele modulus h for cylindrical particle for time-dependent

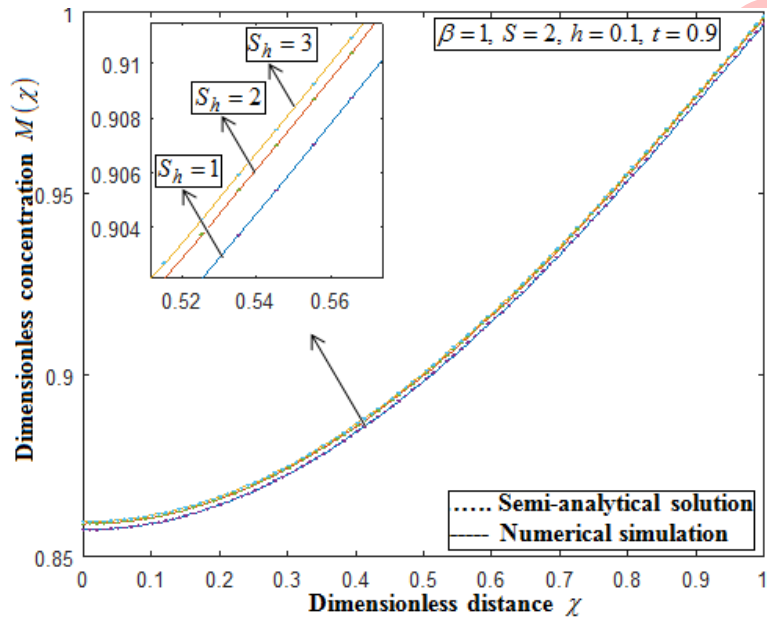


Figure 7: Curves for modified sherwood number S_h for spherical particle for time-dependent

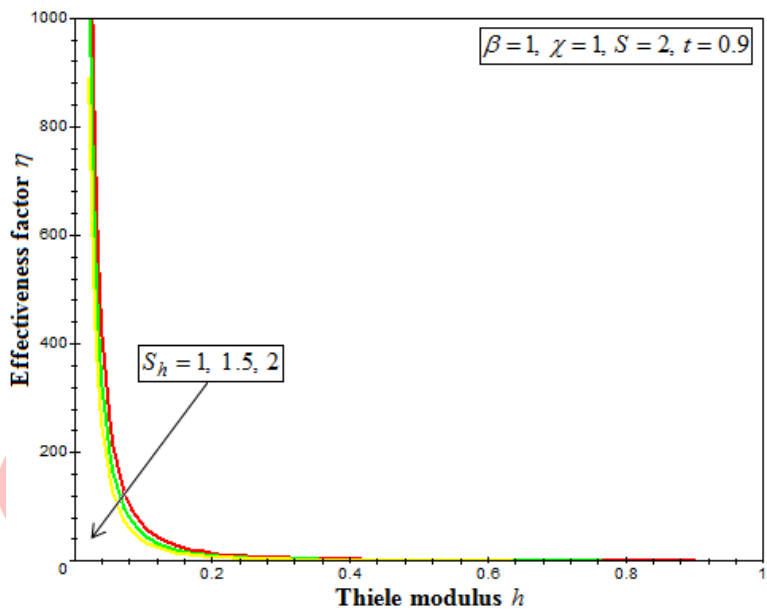


Figure 8: Variance of sherwood number S_h for spherical particle

Table 1: Comparison of our approximate analytical solutions with previous work (QLM-ChPs method) [21] under steady-state by using Eq.(26) and numerical simulation with our approximate analytical expressions under non-steady state by using Eq.(48) for fixed values of $h = 0.1$, $\beta = 1$, $S_h = 1$

χ	Steady-state			Non-Steady state		
	Previous work [21]	Present work (26)	Error %	Numerical Simulation	Present work (48)	Error %
0	0.99501	0.99500	0.001	0.99500	0.99500	0.000
0.2	0.99507	0.99506	0.001	0.99505	0.99506	0.001
0.4	0.99527	0.99526	0.001	0.99525	0.99526	0.001
0.6	0.99561	0.99560	0.001	0.99560	0.99560	0.000
0.8	0.99607	0.99606	0.001	0.99605	0.99606	0.001
1	0.99667	0.99666	0.001	0.99665	0.99666	0.001
Absolute average error %			0.001	0.0006		

7 Appendices

Appendix A: Nomenclature

Symbol	Meaning
M	Non-dimensional concentration
S	Substrate concentration
S_0	Bulk-substrate concentration
K_M	Michaelis constant
D	Effective diffusivity inside the particle
V_M	Maximum reaction rate
χ	Dimensionless distance
L	Half length of the particle
h	Thiele modulus
β	Non-dimensional michaelis constant
S_h	Modified Sherwood numberr
η	Effectiveness factor

Appendix B: MATLAB Programming for the Eq. (10)

```
functionpdepe
m = 2;
```

```

x = linspace(0,1);
t = linspace(0,1);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:, :, 1);
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distancex')
ylabel('u1(x,2)')
function[c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = DuDx;
h = 0.1;
alpha = 1;
M = -2 * h^2 * u(1)/(alpha + u(1));
s = M;
functionu0 = pdex4ic(x);
u0 = 1;
function[pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
S = 1;
pl = 0;
ql = 1;
pr = -S * (1 - ur);
qr = 1;

```

Conflict of interests

The authors declare that there is no conflict of interests.

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