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A Sinc–Galerkin Approximate Solution of the Reaction–Diffusion Process in an Immobilized Biocatalyst Pellet

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Abstract

In recent years, an increasing interest has focused on the use of Sinc methods as an essential tools for solving some singular problems arising in different areas of applied sciences. Due to the presence of singularity, these problems raise difficulties in obtaining their analytic or numerical solutions, and various schemes have been proposed to overcome these difficulties. However, among existing approaches, the Sinc methods are well-suited for handling singularity and have high performance on boundary value problems (BVPs) such as problems on unbounded domains or problems with endpoint singularities. In this work, in several geometries and kinetics, an implementation of the Sinc–Galerkin scheme is used to approximate effectiveness factor and concentration profile of key component when a single independent reaction takes place in a porous catalyst structure where enzymes are immobilized. A comparison between the proposed approximated solution and numerical solution reveals that the Sinc–Galerkin method (SGM), as demonstrated with examples, is reliable, accurate and its convergence rate is high.

1 Introduction

Recently, there is an interesting concern to estimate effectiveness factor (η) in bioengineering process where immobilized enzymes/cells are used as catalysts (hereafter called

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biocatalysts). Because of their excellent functionality, the immobilized biocatalysts have a great potential as industrial catalysts. Hence, many scientists and engineers have made numerical methods to estimate η for simulation of reaction–diffusion systems in industrial and commercial scales. In the present paper, we consider a reaction–diffusion process inside an inert permeable solid particle where the bacterial immobilization has been made inside it. At isothermal conditions, the steady regime of the reaction–diffusion process inside the catalyst porous structure is described by a singular BVP and governed by a dimensionless form as:

$$\frac{d}{dx}\left(x^m \frac{dy}{dx}\right) = \Phi^2 x^m R(y), \tag{1}$$

with the boundary conditions

$$\left.\frac{dy}{dx}\right|_{x=0} = 0, \quad \text{and} \quad y(x)\,|_{x=1} = 1. \tag{2}$$

Here, x is the spatial variable, y is the concentration of the key component, Φ is the Thiele modulus and m is the shape factor of the catalyst($m = 0$ for the slab and $m = 2$ for the sphere). The dimensionless reaction rate function $R(y)$ is normalized to be $R(1) = 1$. The effectiveness factor (η) is defined as the mean rate of reaction divided by the same rate of reaction evaluated at external conditions [10]:

$$\eta = \frac{m+1}{\Phi^2}\left.\frac{dy}{dx}\right|_{x=1}. \tag{3}$$

Also, in this paper the rate of reaction $R(y)$ appears in one of the following types:
(i) $R(y) = y^n$ (in slab geometry),
(ii) $R(y) = \frac{(1+\beta)y}{1+\beta y}$ (in spherical geometry),
(iii) $R(y) = \frac{(1+\beta)^2 y}{(1+\beta y)^2}$ (in slab geometry).
Several numerical approaches have been devised for solving a nonlinear BVP e.g., shooting technique, orthogonal collocation methods and finite differences methods are of the famous schemes among scientists and are well reflected in various books [2, 7, 8, 14, 32]. Moreover, a good account of work based on soft computing using Maple, Mathematica and Matlab, can be found in [35], [9] and [4], respectively.
Many investigations have been carried out in the literature, to establish approximate solutions of the above reaction–diffusion problem in some geometries, both in numeric and analytic manner [1, 11, 12, 15]. Li et al. [16] suggested a simple polynomial up to third degree to estimate η when chemical kinetics are well represented for a particular case of Michaelis–Menten model inside a spherical biocatalyst. They applied rate of reaction

of the type (ii) and the numerical results of their approach compared with a numerical shooting procedures similar to that described by Walas [33]. According to their numerical procedure, they were forced to impose the constraint $\beta \geq 0.75\Phi^2 - 1$. Moreover, the difference between the numerical solution (based on shooting technique) and the approximate solution of the reaction–diffusion process increases with increasing Φ^2 and decreasing β. According to their statement, the effectiveness factor of the biocatalyst particles may be estimated using the third-order approximate solution for some systems with low value of Φ^2 such as oxygen transport into natural mycelial pellets in submerged cultures. Gottifredi & Gonzo [10] manipulated analytically BVP's (1)-(2) into a convenient integral form and by the use of Polymath nonlinear algebraic equation routine [23] and through a Gaussian quadrature estimated effectiveness factor and concentration ($y(0)$), but in the slab geometry. They have also predicted the effectiveness factor in an asymptotic regime corresponding to large values of Φ for a particular case of Michaelis–Menten kinetics in a spherical pellet. However, according to our numerical results and in comparison with a robust shooting method [19], their asymptotic solutions are not sufficiently accurate. Recently, Danish et al. [5] applied an improved variant of Homotopy analysis method (HAM), known as the optimal HAM (OHAM), to approximate analytic solutions for η of the BVP's (1)-(2) when associated with the reaction rate of type (ii), but not for large values of Φ.

In recent years there has been an increasing interest in the use of Sinc methods as an essential tools for solving some singular problems and those who have settled on unbounded domains [21, 22]. The Sinc method is a highly efficient numerical method developed by Frank Stenger, the pioneer of this field, people in his school and others [3, 17, 20, 30]. The books [13, 18, 28, 29] have provided excellent overviews of methods based on Sinc functions for solving ODEs, PDEs and IEs arising in applied sciences. See also [6, 24–27]. There are several advantages to using approximation based on Sinc numerical methods. It may readily handle the singularity, control the convergence of Sinc approximation solution in unbounded regions [21, 22] and has characterized by exponentially decaying errors [24]. The aim of this paper is to use a version of Sinc–Galerkin scheme with modified composite translated Sinc basis functions and three adjusting boundary polynomials to discritize (1)-(2). Our method consists of reducing the solution of singular BVP to a mild set of nonlinear algebraic equations.

2 A survey of some properties of the Sinc function

Let $\mathbb{C}$ denote the set of all complex numbers and for all $z \in \mathbb{C}$ define the sine cardinal or Sinc function by

$$sinc(z) \equiv \begin{cases} \frac{\sin(\pi z)}{\pi z} & \text{if } z \neq 0, \\ 1 & \text{if } z = 0. \end{cases} \tag{4}$$

For $h > 0$, and any integer k, the translated Sinc function with evenly spaced nodes is denoted $S(k,h)(z)$ and defined by

$$S(k,h)(z) \equiv sinc\left(\frac{z - kh}{h}\right).$$

The Sinc functions form an interpolatory set of functions, i.e.,

$$S(k,h)(jh) = \delta_{j,k} = \begin{cases} 1 & \text{if } j = k, \\ 0 & \text{if } j \neq k. \end{cases}$$

If f is a function defined on the real line $\mathbb{R}$ then the cardinal function of f, denoted $C(f,h)(z)$, is defined by

$$C(f,h)(z) \equiv \sum_{k=-\infty}^{\infty} f(kh) S(k,h)(z), \tag{5}$$

whenever the series in (5) converges. Obviously the cardinal function interpolates f at the points $\{kh\}_{k=-\infty}^{\infty}$. The series was addressed in [34] and analyzed in depth in [36]. The properties of cardinal expansion are derived in the infinite strip $\mathcal{D}_d$ of the complex w-plane, where for $d > 0$,

$$\mathcal{D}_d = \left\{ w = t + is \ : |s| < d \leq \frac{\pi}{2} \right\}.$$

Approximations can be constructed for infinite, semi-infinite and finite intervals (see, e.g., [28, pp. 65-70] and [31]). To construct approximations on the interval $(0,1)$, which is used in this paper, the eye-shaped domain in the z-plane

$$\mathcal{D}_E = \left\{ z = x + iy \ : \left| \arg\left(\frac{z}{1-z}\right) \right| < d \leq \frac{\pi}{2} \right\},$$

is mapped conformally onto the infinite strip $\mathcal{D}_d$ via

$$w = \phi(z) = \ln\left(\frac{z}{1-z}\right).$$

The basis functions on $(0,1)$ are taken to be the composite translated Sinc functions,

$$S_k(z) \equiv S(k,h) \circ \phi(z) = sinc\left(\frac{\phi(z)}{h} - k\right), \quad z \in \mathcal{D}_E. \tag{6}$$

The inverse map of $w = \phi(z)$ is

$$z = \phi^{-1}(w) = \frac{\exp(w)}{1 + \exp(w)}.$$

Thus, we may define the inverse images of the real line and the evenly spaced nodes $\{kh\}_{k=-\infty}^{k=\infty}$ as

$$\Gamma = \left\{\phi^{-1}(t) \in \mathcal{D}_E \,:\, -\infty < t < \infty\right\} = (0, 1),$$

and

$$x_k = \phi^{-1}(kh) = \frac{e^{kh}}{1 + e^{kh}}, \qquad k = 0, \pm 1, \pm 2, \ldots,$$

respectively.

In the following, for our subsequent development, some required definitions and properties related to functions of the class $B(\mathcal{D}_E)$ are presented (For more details, see [18] and the references cited in).

Definition 2.1. *Let* $\mathrm{B}(\mathcal{D}_E)$ *be the class of functions* F *which are analytic in* $\mathcal{D}_E$ *and*

$$\int_{\phi^{-1}(t+L)} |F(z)dz| \,\to 0, \qquad \text{as } t \to \pm\infty,$$

where $L = \left\{iv \,:\, |v| < d \leq \frac{\pi}{2}\right\}$*, and on the boundary of* $\mathcal{D}_E$*, (denoted* $\partial\mathcal{D}_E$*), satisfy*

$$N(F) = \int_{\partial\mathcal{D}_E} |F(z)dz| \,< \infty.$$

Definition 2.2. *A function* $F \in \mathrm{B}(\mathcal{D}_E)$ *is said to decay exponentially with respect to the conformal mapping* ϕ *of* $\mathcal{D}_E$ *onto* $\mathcal{D}_d$ *if there exist positive constants* α*,* γ *and* K *so that*

$$|F(z)| \leq K \begin{cases} \exp(-\alpha\,|\phi(z)|), & \text{if } z \in \phi^{-1}\left((-\infty, 0)\right), \\ \exp(-\gamma\,|\phi(z)|), & \text{if } z \in \phi^{-1}\left([0, \infty)\right). \end{cases}$$

If the function $F \in B(\mathcal{D}_E)$ is decreasing exponentially, then the interpolation and quadrature formulas for $F(x)$ and $F(x)S_j(x)$ over $[0, 1]$ take the form

$$F(x) \cong \sum_{k=-M}^{N} F_k S_k(x), \tag{7}$$

$$\int_0^1 F(x)S_j(x)dx \cong h\frac{F(x_j)}{\phi'(x_j)}, \tag{8}$$

respectively and $F_k = F(x_k)$, and the mesh size is given by

$$h = \sqrt{\frac{\pi d}{\alpha M}}$$

where M is suitably chosen and

$$N = \left\llbracket \frac{\alpha}{\gamma} M + 1 \right\rrbracket,$$

($\llbracket x \rrbracket$ denotes the integer part of x).

For establishing our numerical scheme it is convenient to introduce the notation $\delta_{j,k}^{(p)}$ as

$$\delta_{j,k}^{(p)} = \frac{d^p}{d\phi^p} \left[S(j,h) \circ \phi(z) \right] \Big|_{z=x_k}, \quad p = 0,\, 1,\, 2,\, \ldots \ .$$

Hence for $p = 0, 1$ and 2 these quantities are as following

$$\delta_{j,k}^{(0)} = \begin{cases} 1 & \text{if } j = k, \\ 0 & \text{if } j \neq k, \end{cases}$$

$$\delta_{j,k}^{(1)} = \frac{1}{h} \begin{cases} 0 & \text{if } j = k, \\ \frac{(-1)^{k-j}}{k-j} & \text{if } j \neq k, \end{cases}$$

$$\delta_{j,k}^{(2)} = \frac{1}{h^2} \begin{cases} -\frac{\pi^2}{3} & \text{if } j = k, \\ \frac{-2(-1)^{k-j}}{(k-j)^2} & \text{if } j \neq k. \end{cases}$$

3 The formulation to approximate η and $y(x)$

For the boundary conditions (2), the Sinc basis functions $S_k(x)$ are not differentiable when x tends to 0. Thus, we use the nullifier function $\frac{1}{\phi'(x)}$ and modify the Sinc basis functions as $\frac{S_k(x)}{\phi'(x)}$. Now, the derivatives of the modified Sinc basis functions are defined and tend to zero as x approaches 0. Also, in the treatment of boundary conditions, a linear combination of the following boundary basis polynomials, which are obtained by Hermite interpolation at the nodes 0 and 1, must be added to Sinc expansion of numerical approximation to the solution of (1)-(2).

$$\varphi_1(x) = (2x+1)(1-x)^2, \quad \varphi_2(x) = x^2(3-2x), \quad \varphi_3(x) = x^2(x-1).$$

In order to illustrate our method we define

$$\mathcal{L}y = \frac{d^2y}{dx^2} + \frac{m}{x}\frac{dy}{dx}, \tag{9}$$

then, (1) is given by $\mathcal{L}y = \Phi^2 R(y)$. In the Sinc–Galerkin technique, the approximate solution for $y(x)$ in (1) subject to boundary condition (2) is presented by

$$y(x) \cong y_L(x) = Y(x) + u(x), \tag{10}$$

where

$$Y(x) = \sum_{k=-M}^{N} c_k \frac{S_k(x)}{\phi'(x)} = x(1-x) \sum_{k=-M}^{N} c_k S_k(x),$$

and $u(x)$ is a linear combination of $\varphi_i(x)$ $(1 \le i \le 3)$, based on boundary conditions (2), as follows:

$$u(x) = c_{_{-M-1}}\varphi_1(x) + \varphi_2(x) + c_{_{N+1}}\varphi_3(x).$$

The unknown coefficients $\{c_k\}_{k=-M-1}^{k=N+1}$ are determined by orthogonalizing the residual $\mathcal{L}y - \Phi^2 R(y)$ with respect to the Sinc basis functions $\{S_j(x)\}_{j=-M-1}^{j=N+1}$ in (6). The inner product is defined by

$$\langle f, g\rangle = \int_0^1 f(x)g(x)W(x)dx,$$

where $W(x)$ is a weight function given by

$$W(x) = \frac{1}{\sqrt{\phi'(x)}} = \sqrt{x(1-x)}.$$

According to boundary conditions (2) and the Sinc–Galerkin approach, we can discretize (1) to $L = N + M + 3$ nonlinear equations as follows:

$$\left\langle \mathcal{L}y_L - \Phi^2 R(y_L), S_j \right\rangle = 0, \qquad j = -M-1\,, \ldots,\, N+1, \tag{11}$$

Equations (11) can be equivalently written as

$$\langle \mathcal{L}Y, S_j\rangle + c_{_{-M-1}} \langle \mathcal{L}\varphi_1, S_j\rangle + \langle \mathcal{L}\varphi_2, S_j\rangle + c_{_{N+1}} \langle \mathcal{L}\varphi_3, S_j\rangle = \Phi^2 \langle R(y_L), S_j\rangle\,,$$

$$j = -M-1\,,\, \cdots\,,\, N+1. \tag{12}$$

Using (9), the inner product $\langle \mathcal{L}Y, S_j\rangle$ is given by

$$\int_0^1 \mathcal{L}Y(x)S_j(x)W(x)dx = \int_0^1 Y''(x)S_j(x)W(x)dx + \int_0^1 \frac{m}{x}Y'(x)S_j(x)W(x)dx. \tag{13}$$

Integration by parts to remove the derivatives from the dependent variable $Y(x)$ leads to the equality

$$\int_0^1 Y''(x)S_j(x)W(x)dx = B_T + \int_0^1 Y(x)\left(\frac{d^2}{d\phi^2}S_j(x) - \frac{1}{4}S_j(x)\right)\left(\frac{d\phi}{dx}\right)^{\frac{3}{2}}dx, \tag{14}$$

where the boundary term is

$$B_T = \left[Y'(x)S_j(x)W(x) - Y(x)\frac{d}{dx}\left(S_j(x)W(x)\right)\right]_{x=0}^{x=1} = 0. \tag{15}$$

Also, we have

$$\int_0^1 \frac{m}{x} Y'(x) S_j(x) W(x) dx = \int_0^1 Y(x) \left[\frac{m}{x^2 \phi'} S_j(x) - \frac{m}{x} \left(\frac{1-2x}{2} S_j(x) + \frac{dS_j(x)}{d\phi} \right) \right] \sqrt{\phi'} dx. \tag{16}$$

Applying the Sinc trapezoidal quadrature rule (8) to (14) and (16), we obtain

$$\langle \mathcal{L}Y, S_j \rangle = h \sum_{k=-M}^{N} c_k \frac{\delta_{j,k}^{(2)} - \frac{1}{4}\delta_{j,k}^{(0)}}{\sqrt{\phi'(x_k)}} - bh \sum_{k=-M}^{N} \frac{c_k}{\left(\phi'(x_k)\right)^{3/2}} \left[-\frac{\delta_{j,k}^{(0)}}{{x_k}^2 \phi'(x_k)} + \frac{(1-2x_k)\,\delta_{j,k}^{(0)} + 2\delta_{j,k}^{(1)}}{2x_k} \right].$$

Furthermore, according to (8), the inner products $\langle f, S_j \rangle$ and $\langle \mathcal{L}\varphi_i, S_j \rangle \, (1 \le i \le 3)$ are approximated by

$$\left\langle \Phi^2 R(y_L), S_j \right\rangle = \frac{h \Phi^2 R(y_L(x_j))}{\left(\phi'(x_j)\right)^{3/2}}, \tag{17}$$

and

$$\langle \mathcal{L}\varphi_i, S_j \rangle = \frac{h \left[\varphi_i''(x_j) + \frac{m}{x_j} \varphi_i'(x_j) \right]}{\left(\phi'(x_j)\right)^{3/2}}, \tag{18}$$

respectively, where $y_L(x_j)$ can be replaced by

$$y_L(x_j) = \begin{cases} u(x_j) + \frac{c_j}{\phi'(x_j)} & \text{if } j = -M, \ldots, N, \\ u(x_j) & \text{if } j = -M-1, N+1. \end{cases} \tag{19}$$

By substituting (13)-(19) into (12) and rearranging the sums, we convert the BVPs (1)-(2) into a set of L nonlinear algebraic equations as follows:

$$\sum_{k=-M}^{N} \frac{c_k}{\left(\phi'(x_k)\right)^{3/2}} \left[m \left(\frac{1}{x_k^2 \phi'(x_k)} - \frac{1-2x_k}{2x_k} \right) \delta_{j,k}^{(0)} - \frac{m}{x_k} \delta_{j,k}^{(1)} + \phi'(x_k) \delta_{j,k}^{(2)} \right] + c_{-M-1} \frac{\mathcal{L}\varphi_1(x_j)}{\left(\phi'(x_j)\right)^{3/2}}$$

$$+ \frac{\mathcal{L}\varphi_2(x_j)}{\left(\phi'(x_j)\right)^{3/2}} + c_{N+1} \frac{\mathcal{L}\varphi_3(x_j)}{\left(\phi'(x_j)\right)^{3/2}} = \frac{\Phi^2 R(y_L(x_j))}{\left(\phi'(x_j)\right)^{3/2}},$$

$$j = -M-1, \cdots, N+1. \tag{20}$$

The system (20) can be solved for the unknown coefficients $c_j \ (-M-1 \le j \le N+1)$ by applying an iterative method, like the Newton's method, consequently, $y(x)$ given in (10) can be estimated.

We end this section by giving a lemma which obtains two approximate representation corresponding to η and $y(0)$.

Lemma 3.1. *Let $y(x)$ be the solution of BVPs (1)-(2) approximated by the Sinc–Galerkin method, then the Sinc–Galerkin solutions of effectiveness factor and dimensionless concentration of the key reactant at the center of catalyst are respectively as follows:*

$$\eta = \frac{m+1}{\Phi^2} c_{N+1}, \quad y(0) = c_{-M-1}, \tag{21}$$

where m denotes the shape factor of the catalyst.

Proof. It is enough to use the asymptotic behavior of $Y(x)$ and $Y'(x)$ near 0 and 1, respectively as follows:

$$Y(0) = Y'(1) = 0.$$

□

4 Numerical results and discussion

In this section, we approximate effectiveness factor and concentration profile inside a bio-catalyst particle of slab or spherical geometry to clarify the accuracy and efficiency of our method for different values of Φ and β. Throughout this section, we choose heuristically $\alpha = 1$, $\gamma = 1$ and $d = \pi/2$ which leads to $h = \pi/\sqrt{2M}$. Also the Sinc–Galerkin solution of (1)-(2) will be compared very favorably with the numerical solution obtained by a robust shooting technique [19]. By generating the `shoot` routine, a Maple implementation of shooting method, Meade et al. [19] handled numerical solutions of a class of two-point BVPs similar to that of (1)-(2). Our numerical experiments are implemented in Maple 15 programming. The programs are executed on a Notebook System with 2.0 GHz Intel Core 2 Duo processor with 2 GB 533 MHz DDR2 SDRAM.

Before starting this section, we refer the reader to the fact that Li et al. [16] introduced definition of the dimensionless rate of reaction and Thiele modulus in a different way and by comparison we find that

$$\Phi_{Li}^2 = \frac{1+\beta}{9}\Phi^2,$$

where the subscript Li denotes Li et al. [16] definition for the specific case of a Michaelis–Menten kinetic expression. Moreover, the subscripts N, Li, GG and SG on η or $y(0)$, which are subsequently used, stand for Numerical, Li et al., Gottifredi & Gonzo and Sinc–Galerkin, respectively.

Figures 1 and 2 illustrate the computed dimensionless concentration profiles of a Michaelis–Menten model with the reaction rate of type (ii) by using Sinc–Galerkin method for different values of Φ and β ($\Phi = 2$, $\beta = 1$; $\Phi = 5$, $\beta = 20$). The numerically obtained profiles [19] and those obtained by Li et al. [16] and Danish et al. [5] have also been shown in these figures. The figures tell us the SG solutions are in good agreement with those obtained numerically or by OHAM. Moreover, despite restrictions imposed by Li et al. [16] on the values of Φ and β, their third-order approximate solution is not as good as SG solution.

Table 1 provides a comparison among the numerical solutions of effectiveness factor and

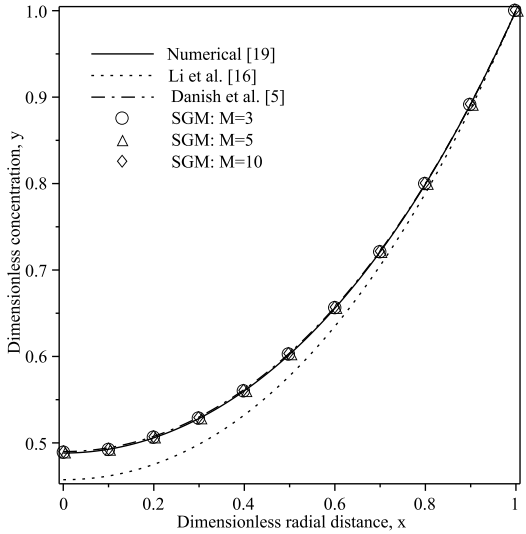

Figure 1: Substrate concentration distribution inside the biocatalyst particle when $\Phi = 2$ and $\beta = 1$.

approximate results obtained by Li et al. [16], Gottifredi & Gonzo [10] and SGM for the above mentioned Michaelis–Menten model. The results of this table show that Li et al. [16] approach is unstable for large values of Φ and η_{Li} reach a constant value, around 0.5, almost independently of Φ and β values. The Gottifredi & Gonzo solution is in an asymptotic regime and its relative error is in the range 1.87–11.75%. In contrast, the relative error between the SG approximate solution and the numerical solution is not more than 0.15%, which indicate our approximate solution provides an efficient and reasonable method to evaluate the effectiveness factor of desired reaction–diffusion problem for large values of Φ. However, for higher values of Φ, one may consider larger values of M.

We examine our method for a nth order irreversible power-law kinetic expression of type (i) in a slab pellet. For different values of n and Φ, tables 2 and 3 show that the values of η and $y(0)$ by using SG method, GG method and the numerical (eventual exact) method. Besides, according to table 3, by increasing M, the deviations among Sinc–Galerkin and numerical solutions of η and $y(0)$ are significantly decreased.

Tables 4 and 5 compare the approximated dimensionless concentration profile $y(x)$ in-

Table 1: Comparison of the numerical and approximated values of effectiveness factor (η) obtained by Sinc–Galerkin method (with $M = 15$) and the other two methods

$\beta = 2$				
	Φ_{Li}	15	20	30
	Li et al. [16]	0.5053	0.5030	0.5014
	Gottifredi & Gonzo [10]	0.1343	0.1007	0.0671
	SGM	0.1292	0.0978	0.0658
	Numerical	0.1293	0.0979	0.0659
	Li et al.	290.80	413.79	660.97
% Error*	Gottifredi & Gonzo	3.87	2.87	1.84
	SGM	0.08	0.10	0.15
$\beta = 6$				
	Φ_{Li}	10	20	30
	Li et al. [16]	0.5250	0.5063	0.5027
	Gottifredi & Gonzo [10]	0.3322	0.1661	0.1108
	SGM	0.3044	0.1590	0.1076
	Numerical	0.3043	0.1592	0.1077
	Li et al.	72.53	218.03	366.76
% Error	Gottifredi & Gonzo	9.17	4.33	2.88
	SGM	0.03	0.13	0.09
$\beta = 10$				
	Φ_{Li}	10	20	30
	Li et al. [16]	0.5383	0.5096	0.5043
	Gottifredi & Gonzo [10]	0.4289	0.2144	0.1430
	SGM	0.3838	0.2030	0.1378
	Numerical	0.3838	0.2033	0.1380
	Li et al.	40.26	150.66	265.43
% Error	Gottifredi & Gonzo	11.75	5.46	3.62
	SGM	0.00	0.15	0.14

*%Error= $|(\eta_{Numerical} - \eta_{Computed})/\eta_{Numerical}| \times 100$.

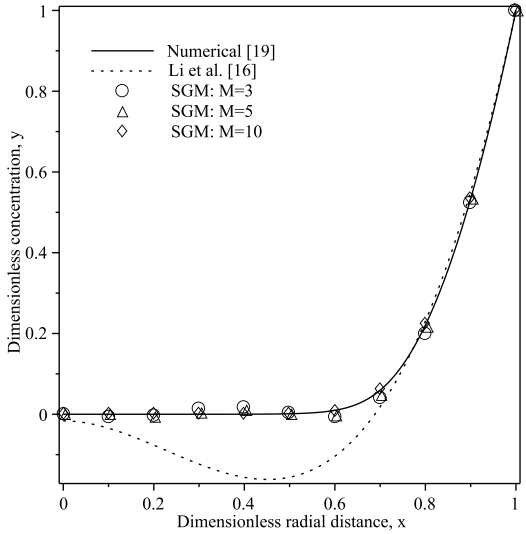

Figure 2: Substrate concentration distribution inside the biocatalyst particle when $\Phi = 5$ and $\beta = 20$.

side a slab biocatalyst pellet with Langmuir-Hinshelwood reaction kinetics of form (iii) with those computed by Gottifredi & Gonzo and numerically for $\beta = 2$ and $\Phi = 1$ and 2. According to tabular values of x, in the vicinity of center of particle and with the increase in Φ, the deviation between y_N and y_{GG} is increased, while the Sinc–Galerkin approximation of $y(x)$ obtained with low computational effort, is in good agreement with corresponding numerical solution, even for x near origin. It should be emphasized that for this special rate expression, $R'(1) < 0$ when $\beta > 1$, and therefore in the internal of pellet $R(x) > R(1)$. Also the apparent reaction order is negative and for different values of β and Φ, the corresponding η values can be greater than one. In tables 6 and 7, the predictive solutions of η based on SG and GG schemes are reported for different values of β and $\Phi(\beta = 1.5, 2$ and Φ in the range $0 < \Phi \leq 3)$. The final two tables show that η_{GG} is in fair agreement with our prediction and numerical solution. Due to exponentially decaying error property, our computed solutions are moderately low-cost and have small or negligible deviations from numerical values.

Table 2: Numerical and approximated values of η and $y(0)$ for different values of Φ, for a power–law kinetic, $R(y) = y^n$

Φ	$y_N(0)$	η_N	$y_{GG}(0)$	η_{GG}	$y_{SG}(0)$	η_{SG}
0.30	0.955837	0.985135	0.955003	0.984997	0.955837	0.985133
0.60	0.833046	0.942157	0.825258	0.940426	0.833047	0.942151
1.00	0.594446	0.849847	0.561278	0.842379	0.594457	0.849832
1.50	0.294290	0.7056815	0.241401	0.693524	0.294327	0.705661
2.00	0.099525	0.568214	0.055594	0.559991	0.099584	0.568195
2.30	0.040594	0.499986	0.011926	0.495205	0.040657	0.499968
2.40	0.028442	0.479970	0.003490	0.476152	0.0285057	0.479952

$n = 0.5$, $M = 10$, slab geometry.

Table 3: Numerical and approximated values of η and $y(0)$ for different values of Φ, for a power–law kinetic, $R(y) = y^n$

Φ	$y_N(0)$	η_N	$y_{GG}(0)$	η_{GG}	$y_{SG}(0)$		η_{SG}	
					$M = 10$	$M = 20$	$M = 10$	$M = 20$
0.30	0.958091	0.944810	0.956191	0.944864	0.958091	0.958091	0.944893	0.944899
0.60	0.859724	0.821647	0.848380	0.821505	0.859729	0.859725	0.821627	0.821645
0.80	0.784878	0.733492	0.765435	0.757971	0.784889	0.784878	0.733463	0.733490
1.00	0.712256	0.652516	0.685360	0.652817	0.712278	0.712258	0.652481	0.652513
1.50	0.557912	0.494815	0.519498	0.496152	0.557969	0.557916	0.494766	0.494811
2.00	0.443723	0.390008	0.401616	0.391828	0.443826	0.443730	0.389948	0.390003
3.00	0.297419	0.268561	0.247755	0.269944	0.297627	0.297433	0.268485	0.268555
4.00	0.212590	0.203141	0.137781	0.203829	0.212914	0.212613	0.203052	0.203134

$n = 2$, slab geometry.

Table 4: Concentration profile for different values of x for $R(y) = \frac{(1+\beta)^2 y}{(1+\beta y)^2}$

x	y_N [19]	y_{SG}	y_{GG}
0.0	0.4425	0.4425	0.427
0.1310	0.4522	0.4521	——
0.2360	0.4738	0.4737	0.584
0.3396	0.5072	0.5072	0.609
0.5341	0.6027	0.6026	0.679
0.7949	0.7965	0.7965	0.829
0.8987	0.8941	0.8941	0.909
0.9467	0.9430	0.9429	0.9504

$\beta = 2$, $M = 5$, $\Phi = 1$, slab pellet.

Table 5: Concentration profile for different values of x for $R(y) = \frac{(1+\beta)^2 y}{(1+\beta y)^2}$

x	y_N [19]	y_{SG}	y_{GG}
0.0	0.0173	0.0176	0.0131
0.111	0.0210	0.0212	——
0.222	0.0335	0.0337	——
0.334	0.0598	0.0594	0.208
0.511	0.1500	0.1501	0.298
0.659	0.2998	0.3004	0.417
0.786	0.5005	0.5006	0.569
0.882	0.7000	0.7000	0.729
0.963	0.8997	0.8997	0.905

$\beta = 2$, $M = 5$, $\Phi = 2$, slab pellet.

Table 6: Numerical and approximated values of η and $y(0)$ for different values of Φ, for Langmuir–Hinshelwood type, $R(y) = \frac{(1+\beta)^2 y}{(1+\beta y)^2}$

Φ	$y_N(0)$ [19]	η_N [19]	$y_{SG}(0)$	η_{SG}	$y_{GG}(0)$	η_{GG}
0.141	0.9900	1.0013	0.9900	1.0013	0.99	1.0013
0.443	0.9003	1.0125	0.9003	1.0125	0.90	1.0086
0.623	0.8228	1.0231	0.8004	1.0231	0.80	1.0090
0.877	0.6006	1.0336	0.6006	1.0336	0.60	0.9900
1.215	0.2959	0.9823	0.2959	0.9823	0.30	0.9150
1.361	0.1993	0.9243	0.1993	0.9244	0.20	0.8680
1.660	0.0874	0.7893	0.0874	0.7893	0.10	0.7640
1.870	0.0500	0.7060	0.0500	0.7060	0.05	0.6940
2.111	0.0267	0.6272	0.0267	0.6272	0.02	0.6230

$\beta = 1.5$, $M = 10$, slab geometry.

Table 7: Numerical and approximated values of η and $y(0)$ for different values of Φ, for Langmuir–Hinshelwood type, $R(y) = \frac{(1+\beta)^2 y}{(1+\beta y)^2}$

Φ	$y_N(0)$ [19]	η_N [19]	$y_{SG}(0)$	η_{SG}	$y_{GG}(0)$	η_{GG}
0.20	0.9799	1.0045	0.9799	1.0044	0.979	1.0014
0.40	0.9182	1.0181	0.9182	1.0181	0.914	1.0038
0.60	0.8107	1.0414	0.8107	1.0414	0.802	1.0029
1.00	0.4425	1.0972	0.4425	1.0972	0.427	0.9669
1.40	0.1196	0.9708	0.1196	0.9708	0.111	0.8690
2.00	0.0173	0.6966	0.0173	0.6967	0.013	0.6815
3.00	8.417e-04	0.4647	1.045e-03	0.4649	3.47e-04	0.4645

$\beta = 2$, $M = 10$, slab geometry.

5 Conclusion

The present work exhibits the reliability of the Sinc–Galerkin method with its new boundary treatment to solve the two point singular BVPs that arise frequently in mathematical model of diffusion and reaction in porous catalyst. The method was applied to calculate effectiveness factor of power–law kinetics and Langmuir–Hinshelwood rate expressions in slab and spherical geometries. Approximated results are in close agreement with numerical/exact solutions even for small and large values of Φ and unlike some existing approaches [11,37], our method has a high performance to predict effectiveness factor in those cases where the apparent reaction order is negative and $\eta > 1$.

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