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ORIGINAL

Solution of the non-isothermal reaction-diffusion equation in a spherical biocatalyst

Solución de la ecuación de reacción-difusión no isotérmica en un biocatalizador esférico

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ABSTRACT

This study develops a comprehensive mathematical model for substrate concentration in a spherical biocatalyst pellet under non-isothermal conditions, capturing the combined effects of heat and mass transfer along with reaction kinetics. Analytical solutions for the concentration profile and effectiveness factor are derived using the Taylor Series Method and validated against numerical simulations, revealing high accuracy and excellent agreement. The research further analyzes how dimensionless parameters, such as the Thiele modulus and Biot number, influence the effectiveness factor, emphasizing the effectiveness of the Taylor Series Method for modeling complex nonlinear bioreaction systems

Keywords: Non-Isothermal Reaction-Diffusion; Biocatalyst Pellet; Taylor Series Method; Effectiveness Factor; Thiele Modulus.

RESUMEN

Este estudio desarrolla un modelo matemático integral para la concentración de sustrato en un pellet esférico de biocatalizador en condiciones no isotérmicas, capturando los efectos combinados de la transferencia de calor y masa, junto con la cinética de la reacción. Las soluciones analíticas para el perfil de concentración y el factor de efectividad se derivan mediante el método de las series de Taylor y se validan con simulaciones numéricas, revelando una alta precisión y una excelente concordancia. La investigación analiza en profundidad cómo parámetros adimensionales, como el módulo de Thiele y el número de Biot, influyen en el factor de efectividad, destacando la eficacia del método de las series de Taylor para modelar sistemas complejos de biorreacción no lineales.

Palabras clave: Reacción-Difusión no Isotérmica; Pellet de Biocatalizador; Método de las Series de Taylor; Factor de Efectividad; Módulo de Thiele.

INTRODUCTION

Biocatalytic processes within porous spherical supports are widespread in chemical and biochemical industries. The design and optimization of these systems require a deep

understanding of the interplay between reaction kinetics, heat transfer, and mass transport. In particular, non-isothermal reaction-diffusion systems pose a significant challenge due to the non-linearity introduced by the temperature dependence of reaction rates.

The paper by Jamal and Khuri presented an analytical treatment of such systems using Green's Function and the Fixed-Point Iteration Method.[1] Complementing that, this thesis develops an alternative[2,3] analytical approach based on the Taylor Series Method (TSM) for the steady-state concentration profile.[4,5,6]

This method offers a direct and recursive means to evaluate concentration distributions. We derive expressions for concentration y(x), determine unknown constants using experimental data, and calculate the effectiveness factor η. The solutions are validated against numerical results, and the effects of key parameters on system behavior are discussed.[7,8]

Mathematical Model

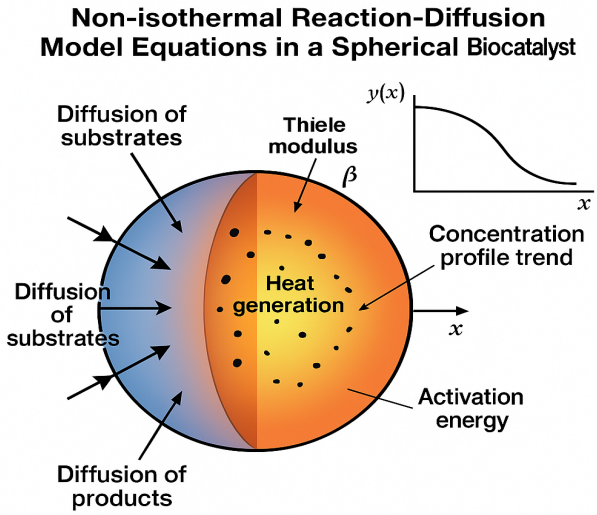


Figure 1. Substrate transport, heat diffusion, and reaction zone representation inside a spherical biocatalyst

Many chemical reactions take place inside a catalyst pellet, which is a porous material. Consider an inert permeable spherical solid particle. It is assumed that the biochemical reaction follows Michaelis–Menten kinetics. The application of mass balance for the substrate (A) over a thin spherical shell inside the biocatalyst yields the following model equation (2,3).

$$D_e\left(\frac{d^2C_A}{dr^2}+\frac{2}{r}\frac{dC_A}{dr}\right)=\frac{r_mC_A}{(K_m+C_A)} \qquad (1)$$

Where; C_A is the concentration of substrate, D_e is the effective diffusivity, r is the radial distance, r_m is the maximum reaction rate, K_m is the Michaelis–Menten constant. The boundary conditions are:

$$\text{At } r=0,\ \frac{dC_A}{dr}=0 \text{ (center of catalyst)} \qquad (2)$$

At $r = R$, $C_A = C_{As}$(catalyst surface) (3)

Normalizing equation (1) using the following dimensionless variables.

$$y = \frac{C_A}{C_{AS}},\ x = \frac{r}{R},\ \phi = \sqrt{\frac{-r_{AS}R^2}{D_e D_{AS}}} = \sqrt{\frac{r_m R^2}{D_e K_m(1+\beta)}}\ ;\ \beta = \frac{C_{AS}}{K_m} \qquad (4)$$

Equation (4) gives the following dimensionless equation. We consider a steady-state, non-isothermal, nonlinear reaction–diffusion model in a spherical biocatalyst pellet. The dimensionless form of the governing equation for the normalized substrate concentration y(x) is given by:

$$y''(x) + \frac{2}{x}y'(x) - r(y) = 0,\ 0 \le x \le 1,\ \ r(y) = \phi^2 \frac{(1+\beta)y(x)}{1+\beta y(x)} \qquad (5)$$

Where *x* is the dimensionless radial coordinate, y(*x*) is the dimensionless concentration ϕ is the Thiele modulus, ß is a dimensionless activation energy parameter. The boundary conditions are given below:

$y'(0) = 0$ (6)
$y(1) = 1$ (7)

The effectiveness factor η for a spherical pellet is defined as:

$$\eta = \frac{3}{\phi^2}\frac{dy}{dx}|_{x=1}$$

Solution Methodology: Taylor Series Expansion

The nonlinear equation is analytically solved by expanding y(x):

$$y(x) = y(0) + \frac{y'(0)x}{1!} + \frac{y''(0)x^2}{2!} + \frac{y'''(0)x^3}{3!} + \frac{y'^v(0)x^4}{4!} + \frac{y^v(0)x^5}{5!} \qquad (8)$$

We obtain the solution of the normalized concentration y(*x*) as:

$$y(x) = k + \left(\phi^2 \frac{(1+\beta)k}{1+\beta k}\right)\left(\frac{1}{6}\right)x^2 \qquad (9)$$

To find k

By applying the boundary condition from Equation (5b) in (8) it becomes:

$$k + \left(\phi^2 \frac{(1+\beta)k}{1+\beta k}\right)\left(\frac{1}{6}\right) - 1 = 0 \qquad (10)$$

By using MAPLE, we can find the value of k by giving the experimental values for the unknown parameters ϕ, ß.

Effectiveness factor η for a spherical pellet

By applying the equation (9) in equation (6) the analytical expressions for the Effectiveness factor (η):

$$k + \left(\phi^2 \frac{(1+\beta)k}{1+\beta k}\right)\left(\frac{1}{6}\right) - 1 = 0 \qquad (10)$$

$$\eta = \left(\frac{3}{\phi^2}\right)\left(\left(\phi^2 \frac{(1+\beta)k}{1+\beta k}\right)\left(\frac{1}{3}\right)x\right)_{x=1} \qquad (11)$$

$$\eta = \left(\frac{(1+\beta)k}{1+\beta k}\right) \qquad (12)$$

By using MAPLE for equation. (9) We can find the value of '*k*'. Also, applying experimental values for β, in (11), we can find the Effectiveness factor η for a spherical pellet.

RESULTS AND DISCUSSION

The analytical expression for y(x) derived via the Taylor Series Method (TSM) has been evaluated and validated against numerical results across various values of the Thiele modulus ϕ and activation energy parameter ß. The following results and visual comparisons demonstrate the accuracy and applicability of the method.

Table 1. Comparison between the numerical and analytical results for y(x) for various values of ϕ for ß=1

	Numerical			TSM			Deviation		
x	ϕ=0,5	ϕ=1	ϕ=1,5	ϕ=0,5 k=0,9592	ϕ=1 k=0,8471	ϕ=1,5 k=0,6930	ϕ=0,5	ϕ=1	ϕ=1,5
0,1	0,9601	0,8474	0,6830	0,9596	0,8487	0,6961	0,0000	0,0000	0,0001
0,2	0,9609	0,8504	0,6891	0,9609	0,8534	0,7055	0,0000	0,0000	0,0001
0,3	0,9628	0,8576	0,7034	0,9630	0,8612	0,7212	0,0000	0,0000	0,0001
0,4	0,9656	0,8681	0,7245	0,9659	0,8721	0,7431	0,0000	0,0000	0,0001
0,5	0,9692	0,8818	0,7523	0,9696	0,8861	0,7713	0,0000	0,0000	0,0001
0,6	0,9737	0,8988	0,7869	0,9742	0,9033	0,8058	0,0000	0,0000	0,0001
0,7	0,9790	0,9190	0,8287	0,9796	0,9236	0,8465	0,0000	0,0000	0,0001
0,8	0,9852	0,9426	0,8779	0,9858	0,9470	0,8935	0,0000	0,0000	0,0001
0,9	0,9922	0,9696	0,9348	0,9929	0,9735	0,9467	0,0000	0,0000	0,0001
1,0	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	0,0000	0,0000	0,0000
Average Deviation							0,0000	0,0000	0,0001

Table 2. Comparison between the numerical and analytical results for y(x) for various values of ϕ for ß=2

	Numerical			TSM			Deviation		
x	ϕ=0,5	ϕ=1	ϕ=1,5	ϕ=0,5 k=0,9589	ϕ=1 k=0,8431	ϕ=1,5 k=0,6765	ϕ=0,5	ϕ=1	ϕ=1,5
0,1	0,9599	0,8445	0,6703	0,9593	0,8447	0,6798	0,0000	0,0000	0,0001
0,2	0,9607	0,8476	0,6767	0,9606	0,8495	0,6897	0,0000	0,0000	0,0001

0,3	0,9626	0,8550	0,6918	0,9627	0,8575	0,7062	0,0000	0,0000	0,0001
0,4	0,9654	0,8658	0,7141	0,9656	0,8687	0,7294	0,0000	0,0000	0,0001
0,5	0,9691	0,8798	0,7433	0,9694	0,8831	0,7591	0,0000	0,0000	0,0001
0,6	0,9736	0,8972	0,7797	0,9740	0,9007	0,7954	0,0000	0,0000	0,0001
0,7	0,9790	0,9178	0,8233	0,9795	0,9215	0,8383	0,0000	0,0000	0,0001
0,8	0,9851	0,9418	0,8743	0,9858	0,9455	0,8878	0,0000	0,0000	0,0001
0,9	0,9921	0,9692	0,9332	0,9929	0,9728	0,9439	0,0000	0,0000	0,0001
1,0	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	0,0000	0,0000	0,0000
Average Deviation							0,0000	0,0000	0,0001

Table 3. Comparison between the numerical and analytical results for y(x) for various values of ϕ for ß=3

	Numerical			TSM			Deviation		
x	ϕ=0,5	ϕ=1	ϕ=1,5	ϕ=0,5 k=0,9587	ϕ=1 k=0,8409	ϕ=1,5 k=0,6667	ϕ=0,5	ϕ=1	ϕ=1,5
0,1	0,9598	0,8430	0,6630	0,9592	0,8425	0,6701	0,0000	0,0000	0,0000
0,2	0,9606	0,8462	0,6696	0,9605	0,8474	0,6803	0,0000	0,0000	0,0001
0,3	0,9626	0,8536	0,6852	0,9626	0,8555	0,6973	0,0000	0,0000	0,0001
0,4	0,9654	0,8645	0,7082	0,9655	0,8668	0,7211	0,0000	0,0000	0,0001
0,5	0,9690	0,8788	0,7383	0,9693	0,8815	0,7517	0,0000	0,0000	0,0001
0,6	0,9736	0,8963	0,7756	0,9739	0,8993	0,7891	0,0000	0,0000	0,0001
0,7	0,9789	0,9172	0,8202	0,9794	0,9204	0,8333	0,0000	0,0000	0,0001
0,8	0,9851	0,9414	0,8724	0,9857	0,9448	0,8843	0,0000	0,0000	0,0001
0,9	0,9921	0,9690	0,9322	0,9929	0,9724	0,9421	0,0000	0,0000	0,0001
1,0	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	0,0000	0,0000	0,0000
Average Deviation							0,0000	0,0000	0,0001

Table 4. Comparison between the numerical results and Taylor series solution for y(x) for various values of ß for ϕ =0,5

	Numerical			TSM			Deviation		
x	ß=1	ß=2	ß=3	ß=1 k=0,9592	ß=2 k=0,9589	ß=3 k=0,9587	ß=1	ß=2	ß=3
0,1	0,9601	0,9599	0,9598	0,9596	0,9593	0,9592	0,0000	0,0000	0,0000
0,2	0,9609	0,9607	0,9606	0,9609	0,9606	0,9605	0,0000	0,0000	0,0000
0,3	0,9628	0,9626	0,9626	0,9630	0,9627	0,9626	0,0000	0,0000	0,0000
0,4	0,9656	0,9654	0,9654	0,9659	0,9656	0,9655	0,0000	0,0000	0,0000
0,5	0,9692	0,9691	0,9690	0,9696	0,9694	0,9693	0,0000	0,0000	0,0000
0,6	0,9737	0,9736	0,9736	0,9742	0,9740	0,9739	0,0000	0,0000	0,0000
0,7	0,9790	0,9790	0,9789	0,9796	0,9795	0,9794	0,0000	0,0000	0,0000
0,8	0,9852	0,9851	0,9851	0,9858	0,9858	0,9857	0,0000	0,0000	0,0000
0,9	0,9922	0,9921	0,9921	0,9929	0,9929	0,9929	0,0000	0,0000	0,0000
1,0	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	0,0000	0,0000	0,0000
Average Deviation							0,0000	0,0000	0,0000

Table 5. Comparison between the numerical results and Taylor series solution for y(*x*) for various values of ß for ϕ =1

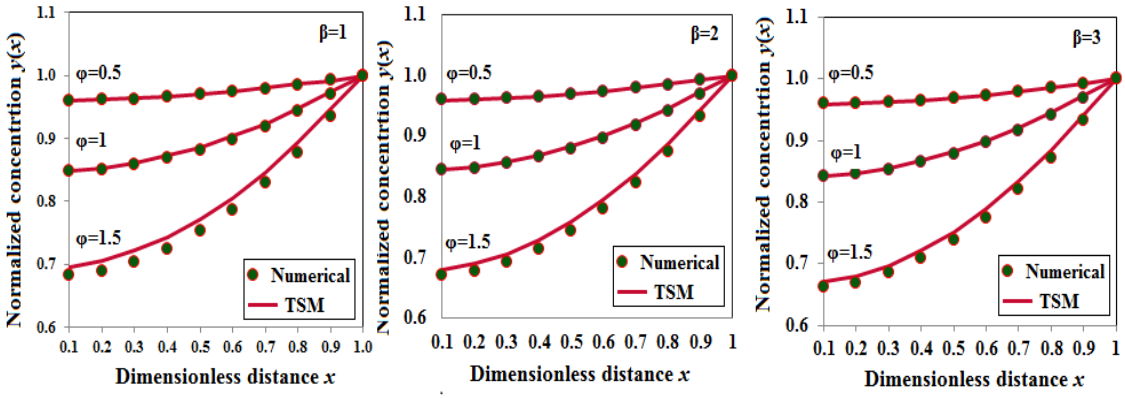
x	Numerical			TSM			Deviation		
	ß=0,5	ß=1	ß=10	ß=0,5 k=0,8508	ß=1 k=0,8471	ß=10 k=0,8362	ß=0,5	ß=1	ß=10
0,1	0,8500	0,8474	0,8399	0,8523	0,8487	0,8379	0,0000	0,0000	0,0000
0,2	0,8530	0,8504	0,8432	0,8569	0,8534	0,8429	0,0000	0,0000	0,0000
0,3	0,8600	0,8576	0,8508	0,8645	0,8612	0,8513	0,0000	0,0000	0,0000
0,4	0,8703	0,8681	0,8620	0,8751	0,8721	0,8630	0,0000	0,0000	0,0000
0,5	0,8837	0,8818	0,8766	0,8888	0,8861	0,8780	0,0000	0,0000	0,0000
0,6	0,9003	0,8988	0,8946	0,9056	0,9033	0,8964	0,0000	0,0000	0,0000
0,7	0,9202	0,9190	0,9159	0,9254	0,9236	0,9181	0,0000	0,0000	0,0000
0,8	0,9433	0,9426	0,9406	0,9482	0,9470	0,9432	0,0000	0,0000	0,0000
0,9	0,9699	0,9696	0,9686	0,9741	0,9735	0,9716	0,0000	0,0000	0,0000
1,0	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	0,0000	0,0000	0,0000
Average Deviation							0,0000	0,0000	0,0000

Table 6. Comparison between the numerical results and Taylor series solution for y(*x*) for various values of ß for ϕ =1,5

X	Numerical			TSM			Deviation		
	ß=0,5	ß=1	ß=10	ß=0,5 k=0,7064	ß=1 k=0,6930	ß=10 k=0,6430	ß=0,5	ß=1	ß=10
0,1	0,6939	0,6830	0,6467	0,7094	0,6961	0,6467	0,0001	0,0001	0,0000
0,2	0,6997	0,6891	0,6538	0,7184	0,7055	0,6576	0,0001	0,0001	0,0000
0,3	0,7133	0,7034	0,6706	0,7333	0,7212	0,6758	0,0001	0,0001	0,0000
0,4	0,7334	0,7245	0,6951	0,7543	0,7431	0,7013	0,0002	0,0001	0,0000
0,5	0,7600	0,7523	0,7271	0,7813	0,7713	0,7341	0,0002	0,0001	0,0001
0,6	0,7932	0,7869	0,7666	0,8142	0,8058	0,7741	0,0002	0,0001	0,0001
0,7	0,8334	0,8287	0,8135	0,8532	0,8465	0,8215	0,0002	0,0001	0,0001
0,8	0,8810	0,8779	0,8681	0,8981	0,8935	0,8761	0,0002	0,0001	0,0001
0,9	0,9363	0,9348	0,9302	0,9490	0,9467	0,9380	0,0001	0,0001	0,0001
1,0	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	0,0000	0,0000	0,0000
Average Deviation							0,0001	0,0001	0,0000

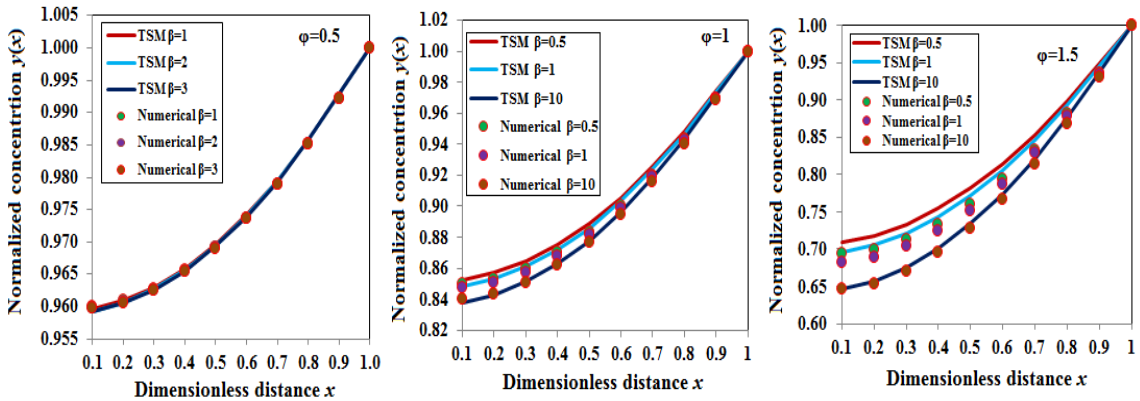
Comparison of Analytical and Numerical Solutions for Various ϕ

Tables (1,2,3) and figures 2(a-c) show the concentration profiles for three values of ß = 1, 2, 3 as ϕ varies over 0,5, 1,0, 1,5, and 2. The observation that as ϕ increases, the substrate concentration at the center decreases due to stronger diffusion limitations. The Taylor Series results are in near-perfect agreement with numerical results, showing deviations of 0,0001 or less. This validates the efficiency of the TSM, especially for moderate nonlinearity.



(a) (b) (c)

Figure 2 (a-c). Comparison between the numerical and analytical results for y(*x*) for various values of ϕ for ß=1, 2, & 3



(a) (b) (c)

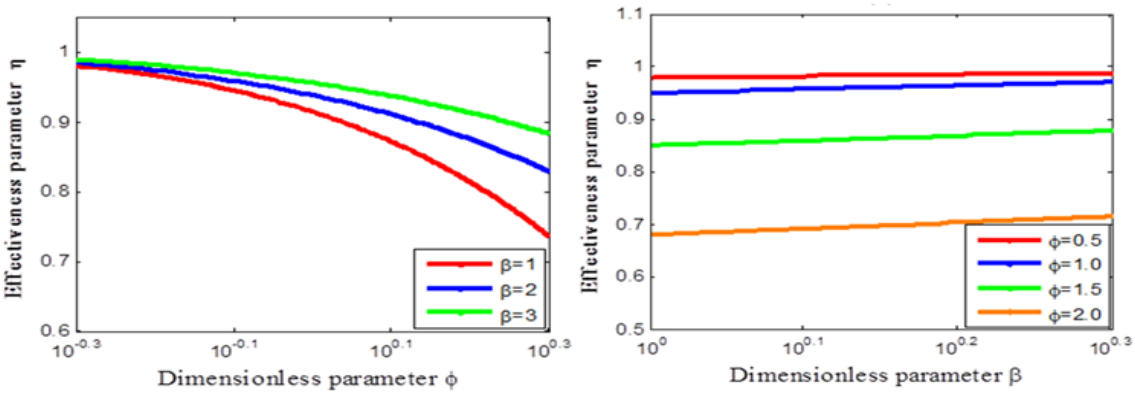
Figure 3 (a-c). Comparison between the numerical and analytical results for y(*x*) for various values of ß for ϕ =0,5, 1, & 1,5.

Effectiveness factor for a spherical pellet (η)

Table 7. Effectiveness factor (η) effectiveness factor (η) for various values of ß for ϕ=0,5, 1,1,5, 2, various values of ϕ for β=1, 2, 3

ß	ϕ	*k*	η	ϕ	ß	*k*	H
1	0,5	0,9592	0,9792		1	0,9592	0,9792
	1,0	0,8471	0,9172	0,5	2	0,9589	0,9859
	1,5	0,6930	0,8187		3	0,9587	0,9893
	2,0	0,5352	0,6972		1	0,8471	0,9172
2	0,5	0,9589	0,9859	1,0	2	0,8431	0,9416
	1,0	0,8431	0,9416		3	0,8409	0,9548
	1,5	0,6765	0,8625	1,5	1	0,6930	0,8187
	2,0	0,5000	0,7500		2	0,6765	0,8625

3	0,5	0,9587	0,9893		3	0,6667	0,8889
	1,0	0,8409	0,9548	2	1	0,5352	0,6972
	1,5	0,6667	0,8889		2	0,5000	0,7500
	2,0	0,4768	0,7847		3	0,4768	0,7847



(a) (b)

Figure 4 (a-b). Comparison between the numerical results and the analytical results for y(*x*) for ß = 1, 2, 3 as ϕ varies over 0,5, 1,0, 1,5, and 2

Comparison for Various ß at Fixed ϕ

Tables (4,5,6) and figures 3(a-c) analyze the effect of the thermal sensitivity ß at fixed ϕ = 0,5, 1,0, 1,5, and 2. The Observations that as ß increases, the exponential term becomes more sensitive, steepening the gradient near the surface. Even under strong non-linearity (e.g., ß = 10), the analytical solution shows excellent agreement with the numerical one. This demonstrates the robustness of the Taylor series approach for a wide parameter range.

Effectiveness Factor Analysis

Table (7) and figure 4(a-b) present the effectiveness factor η for various combinations of ϕ and ß. For a fixed ß, increasing ϕ decreases η due to higher internal diffusion resistance, and for a fixed ϕ, increasing ß increases η, reflecting enhanced reaction rates from thermal sensitivity. These findings highlight the importance of optimizing transport and reaction parameters.

Accuracy and Practical Implications

The average deviations between numerical and analytical solutions are minimal (mostly 0,0001 or less), confirming the high fidelity of TSM. Low-order Taylor expansions can reliably model the system for engineering applications. This provides a fast, accurate alternative to computationally intensive simulations in catalyst design.

CONCLUSIONS

This analytical investigation addresses a non-isothermal, nonlinear reaction–diffusion system within a spherical biocatalyst pellet. The Taylor Series Method provides an accurate, recursive solution for the dimensionless concentration profile, $y(x)$, and the effectiveness factor, η, a vital metric for catalytic performance. Analytical results align closely with numerical solutions across various Thiele modulus (ϕ) and Biot number (β) values, underscoring the precision and reliability

of TSM for these problems. Insights into the effects of these parameters offer valuable guidance for optimizing reactor design, demonstrating that the Taylor Series Method offers a practical and computationally efficient approach to analyzing complex nonlinear systems.

Nomenclature

ϕ Thiele Modulus None.
η Effectiveness factor None.
ß Dimensionless heat of reaction None.
x=r/R, y=$C_{A/}C_{AS}$.
C_A Concentration of reactant A inside the pellet.
C_{AS} Concentration of reactant A at the pellet surface.
R Radius of spherical catalytic pellet.
r Distance along the radial direction of the catalytic pellet.
r_A Arrhenius reaction rate.
D_e Effective diffusivity inside the catalytic pellet.
D_{AS} Effective diffusivity at the surface of the catalytic pellet.
K_m Michaelis–Menten constant.

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ANNEXES

Appendix A: Taylor Series Method Summary

The solution of the normalized concentration y(x) using the Taylor series method is as follows. The non-linear differential equation is given as follows:

$$y''(x) + \frac{2}{x}y'(x) - r(y) = 0,\ 0 \le x \le 1, \qquad (13)$$

$$r(y) = \phi^2 \frac{(1+\beta)y(x)}{1+\beta y(x)}$$

The boundary conditions are given below:

$$y'(0) = 0 \qquad (14)$$
$$y(1) = 1 \qquad (15)$$

The effectiveness factor η for a spherical pellet is defined as:

$$\eta = \frac{3}{\phi^2}\frac{dy}{dx}|_{x=1} \qquad (16)$$

We assume that the solution of equation (13). y(*x*), can be expanded in a Maclaurin series:

$$y(x) = y(0) + \frac{y'(0)x}{1!} + \frac{y''(0)x^2}{2!} + \frac{y'''(0)x^3}{3!} + \frac{y'^v(0)x^4}{4!} + \frac{y^v(0)x^5}{5!} \qquad (17)$$

To determine the value of the derivatives at *x*=0 we rewrite equation (13), as:

$$y"(x) = -\frac{2}{x}y'(x) + r(y) \qquad (18)$$

Assuming r(y) is sufficiently differentiable we may then evaluate derivatives of y(*x*) recursively giving:

$$y'''(x) = \frac{-2}{x}y''(x) + \frac{2}{x^2}y'(x) + r'(y)y'(x) \qquad (19)$$
$$y'^v(x) = \frac{-2}{x}y'''(x) + \frac{4}{x^2}y''(x) - \frac{4}{x^3}y'(x) + r'(y)y''(x) + r''(y)y'(x)^2 \qquad (20)$$
$$y^v(x) = \frac{-2}{x}y'^v(x) + \frac{6}{x^2}y'''(x) - \frac{12}{x^3}y''(x) + \frac{12}{x^4}y'(x) + r'(y)y'''(x) + 3r''(y)y'(x)y''(x) + r'''(y)y'(x)^3 \qquad (21)$$

Where:

$$r(y) = \phi^2 \frac{(1+\beta)y(x)}{1+\beta y(x)}, r'(y) = \frac{dr(y)}{dx}, r''(y) = \frac{d^2r(y)}{dx^2}, r'''(y) = \frac{d^3r(y)}{dx^3} \qquad (22)$$

We now evaluate:

$$y''(0), y'''(0), y'^{v}(0), y^{v}(0) \qquad (23)$$

by substituting *x*=0 into. Furthermore, we can impose the boundary condition y' (0)=0 to give:

$$y'(0) = 0, \qquad (24)$$

$$y"(0) = r(y_0), \qquad (25)$$

$$y'''(0) = \frac{-2}{x}y"(0) = \frac{-2}{x}r(y_0), \qquad (26)$$

$$y'^{v}(0) = \frac{-2}{x}y'''(0) + \frac{4}{x^2}y''(0) + r'(y_0)y''(0) = \frac{8}{x^2}r(y_0) + [r'(y_0)]r(y_0), \qquad (27)$$

$$y^{v}(0) = \frac{-2}{x}y'^{v}(0) + \frac{6}{x^2}y'''(0) - \frac{12}{x^3}y''(0) + r'^{(y_0)y'''(0)} = \frac{-40}{x^3}r(y_0) \qquad (28)$$

By using equation. (10)-(14), we obtain the solution of the normalized concentration y(*x*) as:

$$y(x) = y_0 + \frac{r(y_0)x^2}{2!} + \frac{\frac{-2}{x}r(y_0)x^3}{3!} + \frac{\left(\frac{8}{x^2}r(y_0)+[r'(y_0)]r(y_0)\right)x^4}{4!} + \frac{\left(\frac{-40}{x^3}r(y_0)\right)x^5}{5!} + \cdots \qquad (29)$$

Where y_0 is the unknown value y(0).
Let:

$$y_0 = k$$

$$r(y) = \phi^2\frac{(1+\beta)y(x)}{1+\beta y(x)} \qquad (30)$$

$$r'(y) = \frac{dr(y)}{dx} = (1+\beta)\phi^2\left[\frac{(1+\beta y(x))y'(x)-y(x)\beta y'(x)}{(1+\beta y(x))^2}\right] = \phi^2\frac{(1+\beta)y'(x)}{(1+\beta y(x))^2} \qquad (31)$$

$$r(y_0) = \phi^2\frac{(1+\beta)k}{1+\beta k} \text{ and } r'(y_0) = \phi^2\frac{(1+\beta)y'(0)}{(1+\beta k)^2} = 0 \qquad (32)$$

By using equation (30) We obtain the solution of the normalized concentration y(*x*) as:

$$y(x) = k + \left(\phi^2\frac{(1+\beta)k}{1+\beta k}\right)\left(\frac{1}{6}\right)x^2 \qquad (33)$$

To find k:
By applying the boundary condition from (31) it becomes

$$k + \left(\phi^2\frac{(1+\beta)k}{1+\beta k}\right)\left(\frac{1}{6}\right) - 1 = 0 \qquad (34)$$

By using MAPLE We can find the value of *k* by giving the experimental values for the unknown parameters ϕ, β.

Effectiveness factor η for a spherical pellet

By applying the equation (30) the analytical expressions for the Effectiveness factor (η):

$$\eta = \left(\frac{3}{\phi^2}\right)\left(\left(\phi^2 \frac{(1+\beta)k}{1+\beta k}\right)\left(\frac{1}{3}\right)x\right)_{x=1} \qquad (35)$$

$$\eta = \left(\frac{(1+\beta)k}{1+\beta k}\right) \quad (36)$$

By using MAPLE We can find the value of '*k*'. Also, applying experimental values for β, in (16), we can find the Effectiveness factor η for a spherical pellet.