



Point Solution Concept for Analysis of Reaction-Diffusion in Porous Catalysts

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Abstract

This study explores the application of the point solution concept in analyzing reaction-diffusion processes within porous catalysts, thus offering a novel perspective on this research area. Porous catalysts are of great significance in numerous industrial processes, and understanding the reaction-diffusion mechanisms inside them is crucial for optimizing catalytic performance. Existing methods, such as the homotopy perturbation method, can provide semi-analytical solutions for the entire solution domain; however, they are limited in their ability to accurately capture local behavior at a specific point. The present study proposes an approximate solution that is focused on achieving high accuracy at a specific point. The point solution method is applied to the mathematical equations describing porous catalyst systems and compared with traditional methods. The findings reveal that the point solution concept offers a comprehensive analysis of the impacts of critical parameters (e.g., the Thiele modulus, adsorption parameter, and reaction rate constant) on the reaction-diffusion process at specific points. This analysis unveils local variations and addresses the limitations of traditional methods. However, the application of this concept faces challenges, such as the complexity of porous catalyst systems and difficulties in choosing a good initial solution. Future research directions may include the development of more sophisticated point selection algorithms (AI-powered problem-solving technologies), the improvement of initial guess methods, and the integration with other technologies. This study contributes to a more profound understanding of the intricate systems of porous catalysts and provides a foundation for both theoretical research and practical applications.

Keywords: Porous catalysts; Reaction-diffusion Modeling; Pointwise Approximate Solution; Effectiveness factor; Thiele Modulus Analysis; Semi-Analytical Methods in Catalysis; Nonlinear Reaction-Diffusion Systems

1. Introduction

Porous catalysts are of fundamental importance in a multitude of industrial processes and have become indispensable in modern society. In the domain of environmental protection [1], they constitute pivotal components

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within catalytic converters. These converters utilize porous catalysts to transform harmful vehicle emissions, such as carbon monoxide, nitrogen oxides, and hydrocarbons, into less polluting substances, thereby ensuring the quality of the atmosphere. In the domain of power generation [2], porous catalysts play a pivotal role in enhancing the efficiency of fuel cells. The catalysts facilitate the conversion of chemical energy into electrical energy, a process that is crucial for the development of clean and sustainable energy sources. In the chemical industry [3], porous catalysts play a pivotal role in the synthesis of a wide range of products, including fundamental chemicals such as ammonia, a crucial component in fertilizers, and sophisticated pharmaceuticals that contribute to human health and well-being.

A comprehensive understanding of the reaction-diffusion mechanisms within porous catalysts is imperative for optimizing their performance [4-6]. In the course of research, a multitude of models have been proposed to describe these mechanisms. For instance, the fractal-fractional diffusion model [7] was introduced, where the fractional order is related to the porous medium's two-scale fractal dimensions [8-10]. This model has been demonstrated to facilitate enhanced capture of the intricate diffusion behaviour observed in porous materials [11]. Additionally, fractional diffusion models have been extensively studied within the mathematics community to account for the memory effect of the diffusion process [12].

Nevertheless, the accurate modelling of reaction-diffusion processes in porous catalysts is a challenging task. These catalysts possess a complex structure, characterized by pores that vary in size, shape, and connectivity. Furthermore, the chemical reactions occurring on their surfaces frequently exhibit non-linear kinetics. Conventionally, numerical simulations [13] and semi-analytical methods [14] have been the primary means of investigating these processes.

Numerical simulations have been shown to provide detailed information about the concentration distribution and reaction rates within the catalyst. However, these simulations are computationally expensive and require substantial computational resources. The accurate representation of the intricate geometry of porous catalysts in numerical models poses a significant challenge. Semi-analytical methods, such as the Akbari - Ganji method (AGM) [4], offer a more tractable way to obtain approximate solutions. The AGM has been successful in deriving analytical expressions for concentration profiles and effectiveness factors in porous catalysts. It can demonstrate how the concentration of reactants changes across the thickness of the catalyst. The modified Old Babylonian algorithm [15] and the AI-powered problem-solving process [16] are two promising candidates for this purpose. However, it should be noted that both numerical simulations and semi-analytical methods typically focus on obtaining global solutions that describe the overall behaviour of the system. Consequently, these approaches may not accurately capture the local behaviour at specific points within the catalyst. This local behaviour, which includes reaction rates and concentration gradients at the catalyst-fluid interface or at the centre of the catalyst particle, can significantly impact the overall conversion efficiency and catalytic performance.

The point solution concept [6] provides a novel perspective in this regard. The premise of the point solution concept is that, in certain instances, it is feasible to attain considerably higher accuracy at a specific point within the solution domain in comparison to other points. In the context of porous catalysts, this signifies that we can concentrate on acquiring highly precise information at specific points of interest, as opposed to pursuing a global solution that might diminish local variations.

The present study aims to explore the application of the point solution concept in analysing reaction-diffusion in porous catalysts. The proposed solution form is constrained to satisfy the boundary conditions, with a substantial weight placed at $x = 1$. This form is designed to greatly improve the accuracy at $x = 1$, which is a crucial point in many catalytic processes, such as the catalyst-fluid interface. By adapting the point solution method to the mathematical equations governing porous catalyst systems and comparing the results with traditional methods, we hope to gain new insights into the behaviour of porous catalysts. The potential benefits of this research include enhanced catalytic performance in various industrial applications, leading to more efficient and sustainable chemical processes.

2. Methods

In the study of porous catalysts, reaction-diffusion processes are commonly described by a nonlinear reaction-diffusion equation. For a porous catalyst with a reaction following the Langmuir-Hinshelwood-Hougen-Watson (LHHW) rate expression [17], the governing equation in its dimensional form is as follows [4]:

$$\frac{d^2w}{dx^2} + \frac{j}{x} \frac{dw}{dx} = \frac{k^2 w^m}{(1 + \lambda w)^n} \quad (1)$$

with the following boundary conditions:

$$w(1) = 1, w'(0) = 0 \quad (2)$$

where w is the dimensionless molar concentration, k is the Thiele module, j is the geometrical parameter for $j=0,1,2$ for flat, cylinder, and sphere, respectively. m and n are constants.

In practical applications, the dimensionless effectiveness factor defined below plays a key role:

$$\eta = \frac{(1+j)(1+\lambda)^n}{k^2} w'(1) \quad (3)$$

Equations (1) and (2) can be solved by various methods. Notable among these are the variational iteration method [18] and the homotopy perturbation method [19-21]. These methods offer alternative ways to solve the complex equations in porous catalyst research, complementing the traditional numerical simulations and semi-analytical methods. The selection of an appropriate method is contingent upon the specific requirements of the problem, including the desired level of accuracy, the complexity of the non-linearity, and the available computational resources. Existing methods, including the homotopy perturbation method, have made notable contributions by providing semi-analytical solutions that encompass the entire solution domain. These solutions offer a general understanding of the system's behaviour. However, they are not equipped to accurately capture the intricate local behaviour at specific points. To illustrate this point, consider a scenario where a reaction occurs predominantly at the catalyst-fluid interface. It is acknowledged that traditional methods may not be sufficiently equipped to accurately describe the rapid changes in concentration and reaction rates that occur at this critical interface. This inherent limitation can impede a comprehensive understanding of the catalytic process as a whole.

The point solution concept [6] is predicated on the attainment of highly precise solutions at specific points within the catalyst. The present study explores the potential of an approximate solution with high accuracy at $x=1$. To this end, the following assumption is made:

$$w(x) = 1 + x^2 \sum_{i=1}^N a_i (x-1)^i \quad (4)$$

where a_i ($i=1 \sim N$) are coefficients that need to be determined.

It is evident that the constraints specified by Equation (2) are satisfied at the boundaries of the domain under consideration. The boundary conditions are of paramount importance in determining the uniqueness and behaviour of the solution. When Eq. (4) satisfies these conditions, it is indicative of the mathematical model represented by Eq. (4) being consistent with the physical or mathematical requirements imposed by the boundary conditions.

The approximate solution of Eq. (4) gives a heavy weight at the point $x = 1$. This suggests that the approximate solution is designed or constructed in such a way that it emphasizes or focuses more on the value and behaviour at $x = 1$. This approach has the potential to significantly enhance the accuracy at $x = 1$. This enhancement in accuracy at $x = 1$ is of particular significance, as highlighted by Eq. (3).

In order to elucidate the solving process, we first consider the simplest case:

$$w(x) = 1 + a_1 x^2 (x-1) = 1 + a_1 (x^3 - x^2) \quad (5)$$

Differentiating Eq.(5) with respect to x twice results in:

$$w'(x) = a_1 (3x^2 - 2x) \quad (6)$$

$$w''(x) = a_1 (6x - 2) \quad (7)$$

Substituting w , w' , and w'' into the dimensionless reaction - diffusion equation results in the following one:

$$a_1(6x-2) + \frac{j}{x} a_1(3x^2-2x) = \frac{k^2 [1 + a_1 x^2 (x-1)]^m}{[1 + \lambda(1 + a_1 x^2 (x-1))]^n} \quad (8)$$

Evaluating this equation at $x=1$, we obtain:

$$4a_1 + ja_1 = \frac{k^2}{(1+\lambda)^n} \quad (9)$$

That is

$$a_1 = \frac{k^2}{(1+\lambda)^n(4+j)} \quad (10)$$

The dimensionless effectiveness factor is therefore obtained

$$\eta = \frac{(1+j)(1+\lambda)^n}{k^2} u'(1) = \frac{1+j}{4+j} \quad (11)$$

It should be noted that the results obtained after Eq. (11) may have relatively low accuracy due to the simple assumption of Eq. (5). The simplicity of the assumption made in Eq. (5) might not fully capture the complexity of the underlying physical or mathematical phenomena.

In order to improve the accuracy, we consider

$$w(x) = 1 + x^2 \{a_1(x-1) + a_2(x-1)^2\} = 1 + \{a_1(x^3 - x^2) + a_2(x^4 - 2x^3 + x^2)\} \quad (12)$$

Similarly, we have

$$w'(x) = a_1(3x^2 - 2x) + a_2(4x^3 - 6x^2 + 2x) \quad (13)$$

$$w''(x) = a_1(6x - 2) + a_2(12x^2 - 12x + 2) \quad (14)$$

Setting $x=1$ in Eqs.(13), (14) and (1), we have

$$w'(1) = a_1 \quad (15)$$

$$w''(1) = 4a_1 + 2a_2 \quad (16)$$

$$w''(1) + jw'(1) = \frac{k^2 w''(1)}{(1 + \lambda w(1))^n} \quad (17)$$

Further considering the boundary condition $w(1)=1$, we have

$$(4+j)a_1 + 2a_2 = \frac{k^2}{(1+\lambda)^n} \quad (18)$$

Differentiating Eq. (1) with respect to x results in:

$$\frac{d}{dx} \left[\frac{d^2 w}{dx^2} + \frac{j}{x} \frac{dw}{dx} \right] = \frac{d}{dx} \left[\frac{k^2 w^m}{(1+\lambda w)^n} \right] = \frac{k^2 m w^{m-1} (1+\lambda w)^n - n \lambda k^2 w^m (1+\lambda w)^{n-1}}{(1+\lambda w)^{2n}} \quad (19)$$

That results in

$$\begin{aligned} & \frac{d}{dx} \left[a_1(6x-2) + a_2(12x^2-12x+2) + \frac{j}{x} (a_1(3x^2-2x) + a_2(4x^3-6x^2+2x)) \right] \\ &= \frac{k^2 m w^{m-1} (1+\lambda w)^n - n \lambda k^2 w^m (1+\lambda w)^{n-1}}{(1+\lambda w)^{2n}} \end{aligned} \quad (20)$$

Evaluating this equation at $x=1$, we obtain:

$$6a_1 + 12a_2 + j(3a_1 + 2a_2) = \frac{k^2 m (1+\lambda)^n - n \lambda k^2 (1+\lambda)^{n-1}}{(1+\lambda)^{2n}} \quad (21)$$

or

$$(6+3j)a_1 + (12+2j)a_2 = \frac{k^2 m (1+\lambda)^n - n \lambda k^2 (1+\lambda)^{n-1}}{(1+\lambda)^{2n}} \quad (22)$$

Solving Eqs.(18) and (22) to find the values of the coefficients, we have

$$\begin{cases} a_1 = \frac{(6+j)A-B}{j^2+7j+18} \\ a_2 = -\frac{(3+6j)A-(4+j)B}{2(j^2+7j+18)} \end{cases} \quad (23)$$

where $A = \frac{k^2}{(1+\lambda)^n}$, $B = \frac{k^2 m (1+\lambda)^n - n \lambda k^2 (1+\lambda)^{n-1}}{(1+\lambda)^{2n}}$. Now the dimensionless effectiveness factor can be calculated as

$$\begin{aligned} \eta &= \frac{(1+j)(1+\lambda)^n}{k^2} w'(1) = \frac{(1+j)(1+\lambda)^n}{k^2} a_1 \\ &= \frac{(1+j)(1+\lambda)^n [(6+j)A+B]}{k^2(j^2+7j+18)} \\ &= \frac{(1+j)(1+\lambda)^n \left[(6+j) \frac{k^2}{(1+\lambda)^n} + \frac{k^2 m (1+\lambda)^n - n \lambda k^2 (1+\lambda)^{n-1}}{(1+\lambda)^{2n}} \right]}{k^2(j^2+7j+18)} \\ &= \frac{(1+j) [(6+j)(1+\lambda) + m - n \lambda k^2]}{(j^2+7j+18)(1+\lambda)} \end{aligned} \quad (24)$$

The above highlights the key steps, for higher order approximate solutions, we need to use the following equation to determine the coefficients in Eq. (4).

$$\frac{d^{(n)}}{dx^{(n)}} \left[\frac{d^2 w}{dx^2} + \frac{j}{x} \frac{dw}{dx} \right]_{x=1} = \frac{d^{(n)}}{dx^{(n)}} \left[\frac{k^2 w^m}{(1 + \lambda w)^n} \right]_{x=1}, n = 1 \sim N. \quad (25)$$

In this research, we have developed an approximate solution with a primary focus on achieving high accuracy at a particular point of interest. By applying the point solution method to the mathematical equations that govern porous catalyst systems, we have unearthed some significant findings. The point solution concept allows for a detailed and in-depth analysis of how key parameters, such as the Thiele modulus, adsorption parameter, and reaction rate constant, influence the reaction-diffusion process at specific points.

The point solution concept allows for a detailed analysis of how key parameters impact the reaction - diffusion process at specific points. Let's consider the Thiele modulus (k), the adsorption parameter (λ), and the reaction rate constant (n).

An increase in the Thiele modulus (k) generally indicates a higher diffusional resistance within the catalyst.

$$\frac{\partial \eta}{\partial k} < 0 \quad (26)$$

An increase in k leads to a more rapid decrease in effectiveness factor. This is because the slower diffusion caused by a higher k restricts the supply of reactants to the interior of the catalyst. At the same time, the effectiveness factor at these points also decreases, signifying a reduction in the catalytic efficiency.

The adsorption parameter (λ) plays a significant role in determining the amount of reactant adsorbed onto the catalyst surface.

$$\frac{\partial \eta}{\partial \lambda} < 0 \quad (27)$$

As λ increases, at points where the reaction is taking place, more reactant is adsorbed. This leads to an increase in the local reaction rate at these points, as observed from the point - solution - based analysis. However, if λ becomes too large, it can also cause saturation of the adsorption sites, and the reaction rate may no longer increase proportionally.

The reaction rate constant (n) directly affects the rate of the chemical reaction.

$$\frac{\partial \eta}{\partial n} = - \frac{(1+j)\lambda k^2}{(j^2 + 7j + 18)(1 + \lambda)} < 0 \quad (28)$$

With an increase in n , the reaction at specific points within the catalyst speeds up. The point solution concept shows that at points where the reaction is occurring, the concentration of reactants decreases more rapidly as n increases. This is because the reactants are consumed at a faster rate, and the diffusion process may not be able to replenish them quickly enough.

As an example, consider the case when $k=10$, $l=3$, $m=2$, $n=3$, and $j=2$, we have the following approximate solution

$$w(x) = 1 + x^2 \{ 0.358073(x-1) - 0.585938(x-1)^2 \} \quad (29)$$

Error! Reference source not found. shows a detailed comparison of the approximate solution derived from the point solution concept and the exact numerical solution. A striking discrepancy is evident at the boundary condition $x = 0$: the approximate solution yields $w(0) = 1$, stemming from the constraint that the assumed solution form satisfy the boundary condition $x = 1$. In contrast, the numerical solution yields $w(0) = 0.732833$, resulting in a relative error of 36.46%. This discrepancy underscores the trade-off between satisfying the boundary conditions and achieving global solution accuracy in the point solution approach.

Notably, the approximate solution's performance improves significantly near $x = 1$, a critical point in catalytic systems that often corresponds to the catalyst-fluid interface. At $x = 0.99$, the approximate solution yields $w(0.99) = 0.9964$, closely matching the numerical value of 0.9945 from Ref. [4], with a negligible relative error of only 0.19%.

This demonstrates the method's capability to achieve high local accuracy at the targeted point.

A more thorough examination of the solution's behaviour at $x = 1$ reveals a striking similarity between the tangents of the two curves depicted in Figure 1 at this specific point. This concurrence of tangents is of profound physical significance, as it pertains to the concentration gradient and reaction rate at the catalyst surface. These phenomena are mathematically encapsulated in Eq. (3). The congruence of the tangents signifies that the point solution effectively captures the local dynamics at $x = 1$, even in the presence of global discrepancies. This feature is of particular value when analysing critical parameters such as the Thiele modulus and adsorption effects, which dominate the behaviour at the catalyst-fluid interface.

In summary, while the point solution concept exhibits limitations in global accuracy, its ability to prioritize precision at specific points of interest—coupled with the faithful representation of local physical characteristics—validates its utility as a complementary approach to traditional global solution methods in porous catalyst research.

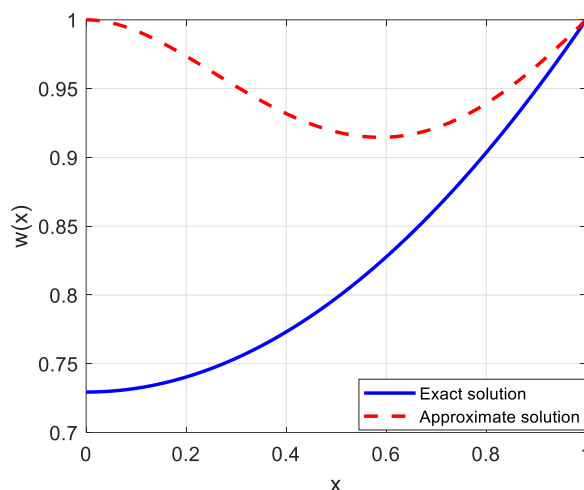


Fig 1: Approximate solution vs. exact solution

Nonetheless, the application of the point solution concept is not without its challenges. The complexity of porous catalyst systems is a major hurdle. Porous catalysts possess a highly irregular pore structure, with pores varying widely in size, shape, and connectivity. Additionally, factors such as pore size distribution, tortuosity, and surface - to - volume ratio all interact in complex ways, making it extremely difficult to incorporate all these aspects into the point solution framework. Another significant challenge lies in the selection of a suitable initial solution. A poor initial guess can lead to inaccurate results, and finding an appropriate starting point requires a deep understanding of the system and often relies on trial - and - error methods.

Looking ahead, future research can be pursued in several promising directions. One area of focus could be the development of more advanced point - selection algorithms, leveraging state-of-the-art AI-powered problem-solving technologies. These algorithms could analyse the structure of the catalyst, the nature of the reactants, and the reaction conditions to identify the most critical points for analysis. This would significantly enhance the efficiency and accuracy of the point solution concept. Another direction could be the improvement of initial - guess methods. By drawing on prior knowledge from similar catalyst systems or using data - driven approaches, we can develop more informed initial guesses, reducing the uncertainty in the solution process. Additionally, integrating the point solution concept with other advanced technologies, such as micro - tomography for visualizing the pore structure or in - situ spectroscopy for monitoring reaction intermediates, could lead to a more comprehensive and accurate understanding of porous catalyst behaviour.

3. Conclusion

This study has investigated the application of the point solution concept for analysing reaction-diffusion processes in porous catalysts, presenting a novel approach to a research area of significant industrial importance. The findings contribute to a more in-depth understanding of these intricate systems and have far-reaching implications for both theoretical knowledge and practical applications.

The point solution concept offers a distinct advantage by enabling highly accurate analysis at specific points within porous catalysts. This is in contrast to traditional methods such as the Akbari-Ganji method (AGM) and numerical simulations. The AGM provides global semi-analytical solutions, which may overlook local variations,

while numerical simulations, despite offering comprehensive results, can be computationally intensive. By focusing on local behaviour, the point solution concept fills a crucial gap, allowing for a more detailed examination of concentration profiles and reaction rates at critical points. This has exposed local variations that were previously obscured by global averaging, thereby enhancing our understanding of the underlying processes.

The application of the point solution concept has facilitated the analysis of key parameters, including the Thiele modulus, adsorption parameter, and reaction rate constant. This analysis has yielded valuable insights into the individual impacts of these parameters on the reaction-diffusion process at specific points. For instance, an increase in the Thiele modulus was found to lead to a more rapid decrease in the effectiveness factor due to increased diffusional resistance. In addition, changes in the adsorption parameter affected the amount of reactant adsorbed and, consequently, the local reaction rate. This detailed understanding can serve as a guiding principle in the design of more efficient porous catalysts. By optimizing catalyst formulations based on how these parameters influence the local effectiveness factor, it becomes possible to enhance overall catalytic performance, leading to more efficient and sustainable chemical processes across various industries.

However, it is imperative to acknowledge the constraints imposed by the point solution concept. The inherent complexity of porous catalyst systems poses a significant challenge. The irregular pore structures of these catalysts, in conjunction with parameters such as size distribution, tortuosity, and surface-to-volume ratio, complicate the incorporation of all pertinent aspects within the framework of the point solution concept. The necessity of simplifying assumptions is acknowledged; however, it is recognized that such assumptions can introduce inaccuracies. Furthermore, the selection of appropriate analysis points is not straightforward, as it requires a deep understanding of the catalytic process and the underlying mechanisms. The accuracy of the point-solution calculations is contingent on the availability of accurate initial estimates, a task that is often challenging to accomplish.

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