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# NUMERICAL SOLUTION OF A NONLINEAR BOUNDARY VALUE PROBLEM IN CATALYST PORES USING FINITE DIFFERENCE METHOD AND MATLAB FSOLVE

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**Abstract**

This study presents a robust numerical framework for solving nonlinear boundary value problems (BVPs) in catalytic pores by combining the finite difference method (FDM) with MATLAB's fsolve solver. The governing nonlinear diffusion–reaction equation is discretized using central finite differences, and the resulting system of nonlinear algebraic equations is iteratively solved with fsolve. Concentration profiles were investigated across a wide range of Thiele modulus values and reaction orders, and the predictions were compared against analytical solutions available in the literature. The results demonstrate excellent agreement with analytical benchmarks, confirming the accuracy and stability of the proposed approach. For zeroth-order kinetics, reactant depletion occurs rapidly at relatively low Thiele modulus values, whereas first-order kinetics require significantly higher Thiele modulus values for complete consumption. These findings highlight the dominant role of pore-scale transport limitations in catalyst performance. Beyond validation, the methodology provides a flexible computational platform that can be readily extended to more complex scenarios, including variable diffusivities, multidimensional geometries, and higher-order reaction mechanisms. The integration of FDM with iterative solvers such as fsolve thus offers an adaptable and efficient tool for advancing catalyst design and optimization in heterogeneous reaction engineering.

**Keywords:** Catalyst Pore, Boundary Value Problem, Finite Difference Method, MATLAB, Fsolve, Nonlinear Differential Equation.

## INTRODUCTION

Boundary value problems (BVPs) play a central role in mathematical modeling of physical and chemical engineering systems, particularly in processes involving heat transfer, mass transfer, and heterogeneous reactions. Unlike initial value problems, where conditions are specified at a single point, BVPs impose constraints at two or more boundary locations, making them inherently more challenging to solve. Analytical solutions to nonlinear BVPs are often unavailable, which necessitates the development of reliable numerical methods. Moreover, the flexibility of the numerical scheme allows for straightforward extension to more complex geometries, variable diffusivities, and higher-order reactions. The accuracy and stability of the method make it a suitable tool for

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catalyst pore modeling [1],[2] in industrial applications. In the context of catalytic processes, the transport and reaction of species inside catalyst pores significantly influence overall reaction efficiency. Accurately predicting concentration profiles within pores is therefore essential for catalyst design and optimization. The finite difference method (FDM) provides a straightforward discretization scheme for converting governing differential equations into algebraic systems, which can then be solved numerically. When combined with iterative solvers such as MATLAB's fsolve, this approach offers a robust and flexible tool for tackling nonlinear BVPs [3], [4] in chemical reaction engineering. This study focuses on applying FDM in conjunction with fsolve to solve the nonlinear diffusion–reaction equation in a cylindrical catalyst pore. By examining concentration profiles under varying Thiele modulus values and reaction orders, the work demonstrates the effectiveness of the numerical approach and validates its results against analytical solutions [5] from the literature.

### Problem Definition

The governing differential equation for the diffusion of species A and its reaction on the surface of a cylindrical pore (such as in a solid catalyst), under the assumption that the reactant diffuses only in the axial direction (x) and undergoes an nth-order reaction, can be expressed as:

$$D_A \frac{d^2 C_A}{dx^2} = k C_A^n \qquad 0 \leq x \leq 1 \tag{1}$$

at x = 0, the concentration of the reactant A is held at a constant concentration Cs,

$$C_A|_{x=0} = C_s \tag{2}$$

The boundary at x = L is impermeable (vanishing mass flux).

$$\left.\frac{dC_A}{dx}\right|_{x=L} = 0 \tag{3}$$

### NUMERICAL METHODOLOGY

Rearrangement of eq. (1) gives,

$$\frac{d^2 C_A}{dx^2} = \alpha^2 C_A^n$$

$$\alpha = \sqrt{\frac{k}{D_A}}$$

Where α is known as the Thiele modulus. The domain x ∈ [0,1] is discretized using N+2 nodes. The first derivative is approximated by central finite differences:

$$\frac{dC_A}{dx} = \frac{C_A{}^{(i+1)} - C_A{}^{(i-1)}}{2\Delta x} \tag{4}$$

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While central finite differences formula for the second derivative is:

$$\frac{d^2C_A}{dx^2} = \frac{{C_A}^{(i+1)} - 2{C_A}^{(i)} + {C_A}^{(i-1)}}{(\Delta x)^2} \tag{5}$$

Replacing the second derivative in equation (1) by the formula from equation (5) yields,

$$C^{(i-1)} - 2C^{(i)} - \Delta x^2 \alpha^2 C^{(i)n} + C^{(i+1)} = 0 \tag{6}$$

As the second condition (eq. 3) is assigned for the far end of the catalyst pore (e.g., x = L or n = n), Replacing the first derivative in equation (3) by the formula from equation (4) for the last node yields,

$${C_A}^{(n+1)} = {C_A}^{(n-1)} \tag{7}$$

By applying eq. (6) for equally spaced (n-1) number of nodes along the pore length and with combination of eq. (7) for the nth node (last node), a nonlinear system of n equations is obtained, and then solved by MATLAB's fsolve [6] solver.

### MATLAB fsolve

fsolve solves systems of nonlinear equations of several variables. x = fsolve (FUN, X0) starts at the matrix X0 and tries to solve the equations in FUN. FUN accepts input x and returns a vector (matrix) of equation values F evaluated at x [6].

### MATLAB Code

The MATLAB implementation is structured into two components. The first is the main script file, which incorporates the solver syntax, the initial estimates of the reactant concentration at each discretized node, and the output commands. The second component is an M-function file, which defines the nonlinear system of equations within a for-loop to accommodate a large number of discretization points. The M-function subroutine is invoked by the main script, and the nonlinear equations are solved iteratively using the *fsolve* routine until convergence is achieve

## RESULTS AND DISCUSSIONS

The numerical results obtained using the MATLAB *fsolve* solver were validated against the analytical exact solution [7], demonstrating complete agreement. At α = 0, the concentration profile remained constant at unity, extending from the surface concentration to the pore end. For all reaction orders n ≥ 0, (Figure 2 and Figure 3) increasing values of the Thiele modulus led to a more pronounced concentration decay from the pore mouth concentration $C_S$ along the pore length. For the zeroth-order reaction (Figure 1), the concentration dropped to zero within the pore when the Thiele modulus reached its maximum value (α = 1.4), indicating a reaction rate significantly higher than the rate of diffusion. In contrast, for the first-order case (Figure 2), the Thiele modulus had to be more than four times larger to drive the concentration to zero at the pore outlet. At high α values, the reactant was almost entirely consumed near the pore mouth, resulting in a

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negligible effectiveness factor. Conversely, when α = 0, the concentration profile remained uniform throughout the pore length, corresponding to purely diffusive transport in the absence of reaction.

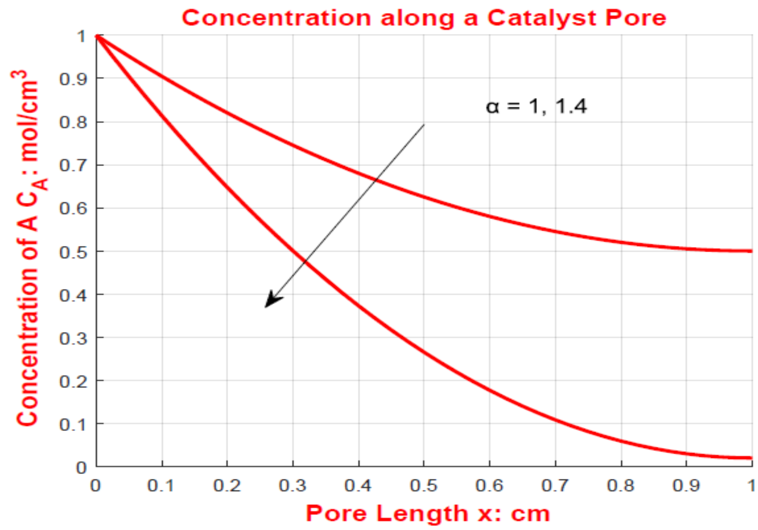


**Figure 1: Concentration along a catalyst Pore for zero-order reaction**

At high α values in both cases, the reactant is consumed predominantly near the pore entrance, resulting in a negligible effectiveness factor. These results align well with theoretical predictions from mass transport and reaction engineering principles [1], [2], confirming the robustness of the finite difference approach combined with fsolve. In contrast, for the first and second order reaction, the concentration profile decays more gradually, requiring α values greater than 5 to achieve negligible concentration at the pore end. This indicates that for first and second order kinetics, diffusion is relatively more significant compared to the zeroth-order case.

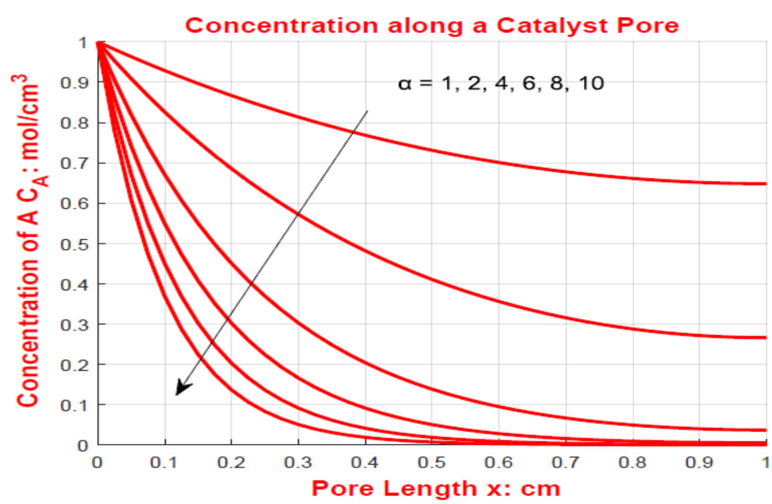


**Figure 2: Concentration along a catalyst Pore for first-order reaction**

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The numerical results obtained using MATLAB's fsolve [3] solver demonstrated excellent agreement with the analytical solution reported in literature, thereby validating the computational approach.

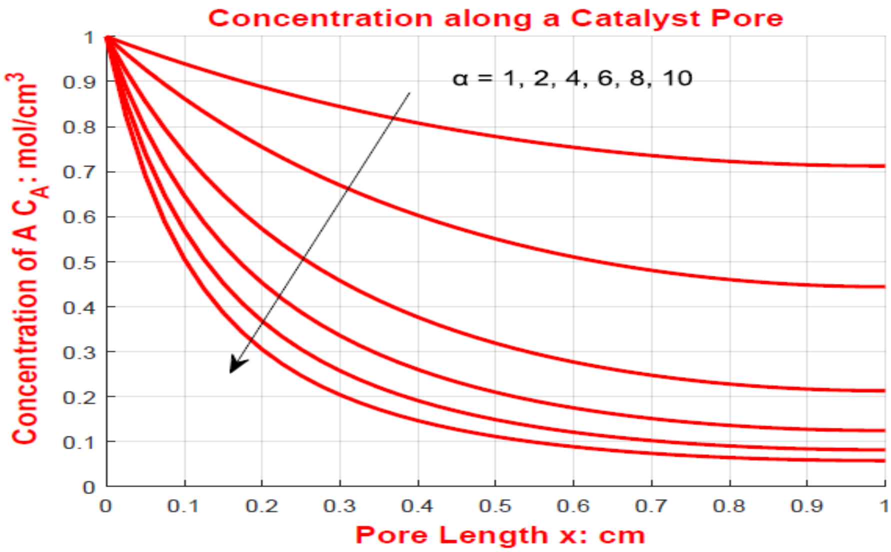


**Figure 3: Concentration along a catalyst Pore for for second-order reaction**

## CONCLUSION

This work demonstrated the successful application of the finite difference method coupled with MATLAB's fsolve solver to obtain numerical solutions of a nonlinear boundary value problem in a cylindrical catalyst pore. The method showed excellent agreement with analytical solutions, confirming its accuracy and reliability.

The analysis revealed that the Thiele modulus strongly governs the interplay between diffusion and reaction, with higher values leading to sharper concentration gradients and negligible effectiveness factors. Beyond validating the approach for zeroth, first and second order kinetics, the flexibility of the methodology highlights its potential for extension to more complex scenarios, including higher-order reactions, variable diffusivities, and multidimensional geometries. These features make the approach a valuable computational tool for both academic research and industrial catalyst design.

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