SERIES SOLUTIONS TO REACTION-DIFFUSION PROBLEMS IN CATALYTIC PELLETS WITH EXTERNAL MASS AND HEAT TRANSFER RESISTANCES

Boris Golman[1], Vsevolod V. Andreev[2], Piotr Skrzypacz[3]

[1]School of Engineering and Digital Sciences, Nazarbayev University, Kazakhstan, boris.golman@nu.edu.kz,
[2]Faculty of Energy and Electrical Engineering, Chuvash State University, Russia
[3]School of Sciences and Humanities, Nazarbayev University, Kazakhstan

XXIV International Conference on Chemical Reactors CHEMREACTOR-24
September 12 - 17, 2021

INTRODUCTION

The overall rate of many industrially important catalytic reactions depends not only on reaction kinetics but also on the rate of mass and heat transfer from the bulk phase to the outer surface of the catalyst pellet, and the rate of mass and heat diffusion in the pellet. Depending on the pellet morphology and kinetic, process and transport parameters, the reaction behavior in the pellet can be complex, including the formation of a so-called dead zone where no reaction takes place [1-3]. The numerical solution of the corresponding two-point boundary-value problems is a time-consuming and sometimes even challenging task. Thus, approximate solutions are desirable as they can be easily implemented in the overall reactor model.

The main goal of the present study is to derive the approximate solutions to the non-isothermal reaction-diffusion problems in the catalytic pellets for the case of arbitrary reaction kinetics, taking into account the presence of external mass and heat transfer resistances.

MATHEMATICAL MODEL

Consider the non-isothermal reaction of arbitrary kinetics $r\,(c,\theta)$ taking place in the catalyst pellet.

$$\frac{1}{x^s}\frac{d}{dx}\left(x^s\frac{dc(x)}{dx}\right) = \phi^2 r(c,\theta)$$

$$\frac{1}{x^s}\frac{d}{dx}\left(x^s\frac{d\theta(x)}{dx}\right) = -\phi^2\beta r(c,\theta)$$

B.C.: $\left.\frac{dc(x)}{dx}\right|_{x=0}=0,\quad \left.\frac{d\theta(x)}{dx}\right|_{x=0}=0$

$$1-c(1)=\frac{1}{Bi_m}\left.\frac{dc(x)}{dx}\right|_{x=1};\ 1-\theta(1)=\frac{1}{Bi_h}\left.\frac{d\theta(x)}{dx}\right|_{x=1}$$

Relationship between c and θ:

$$\theta(x)=1+\beta\left((1-c(1))\frac{Bi_m}{Bi_h}+c(1)-c(x)\right)$$

Using the above relationship:

$$r_1(c):=r(c,\theta)$$

SERIES SOLUTIONS

$$\frac{d^2c(x)}{dx^2}+\frac{s}{x}\frac{dc(x)}{dx}=\phi^2 r_1(c(x))$$

The Taylor approximation at x = 1:

$$c(x)\approx c(1)+(x-1)\frac{dc(x)}{dx}|_{x=1}+\frac{(x-1)^2}{2}\frac{d^2c(x)}{dx^2}|_{x=1}+\frac{(x-1)^3}{6}\frac{d^3c(x)}{dx^3}|_{x=1}+\frac{(x-1)^4}{24}\frac{d^4c(x)}{dx^4}|_{x=1}+\frac{(x-1)^5}{120}\frac{d^5c(x)}{dx^5}|_{x=1}+\frac{(x-1)^6}{720}\frac{d^6c(x)}{dx^6}|_{x=1}$$

The Taylor approximation at x = 0:

$$c(x)\approx c_0+\frac{\phi^2x^2}{2(1+s)}r_1(c_0)+\frac{\phi^4x^4}{8(1+s)(3+s)}r_1(c_0)\left.\frac{dr_1(c)}{dc}\right|_{x=0}+\frac{\phi^6x^6}{48(1+s)^2(5+s)}\left(r_1(c_0)\left.\frac{d^2r_1(c)}{dc^2}\right|_{x=0}+\frac{(1+s)}{(3+s)}\left(\left.\frac{dr_1(c)}{dc}\right|_{x=0}\right)^2\right)r_1(c_0),$$

where $c_0=c(0)$. Here, the odd derivatives are equal to zero.

NAZARBAYEV UNIVERSITY

RESULTS

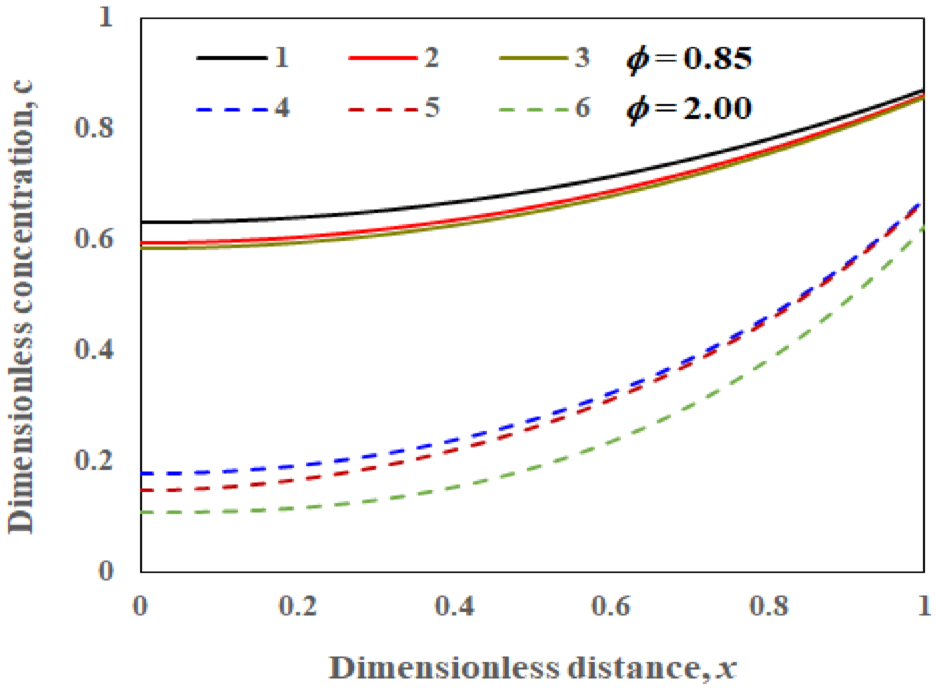

Fig 1: Approximate solutions. s=0, Bi_m=4, n=1:
1,4-exact isothermal; 2-Taylor series at x=0, isothermal;
3-Taylor series at x=0, non-isothermal β=0.07; γ=10; Bi_h=4;
5-Taylor series at x=1, isothermal;
6-Taylor series at x=1, non-isothermal.

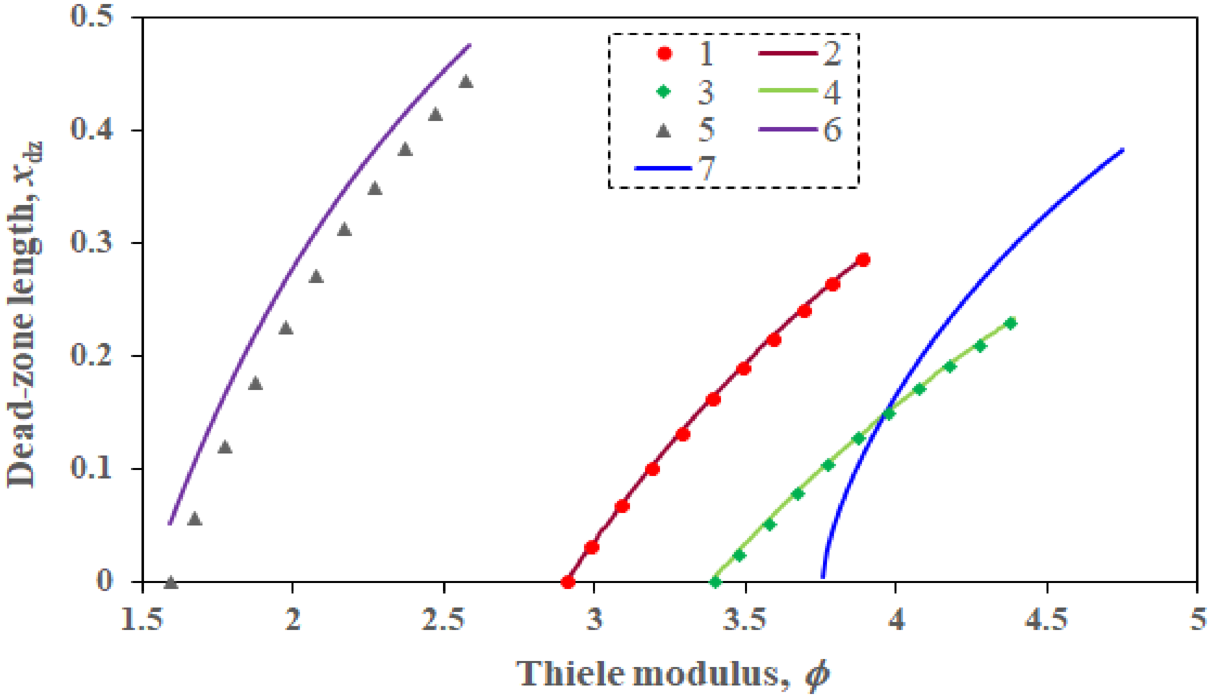

Fig 2: Effect of Thiele modulus on dead-zone length.
1-exact, 2-Taylor series, s=0, Bi_m=4, n=0.5;
3-exact, 4-Taylor series, s=0, Bi_m=4, n=0.2;
5-exact, 6-Taylor series, s=0, Bi_m=50, n=0.5;
7-Taylor series, s=2, Bi_m=4, n=0.5.

RESULTS

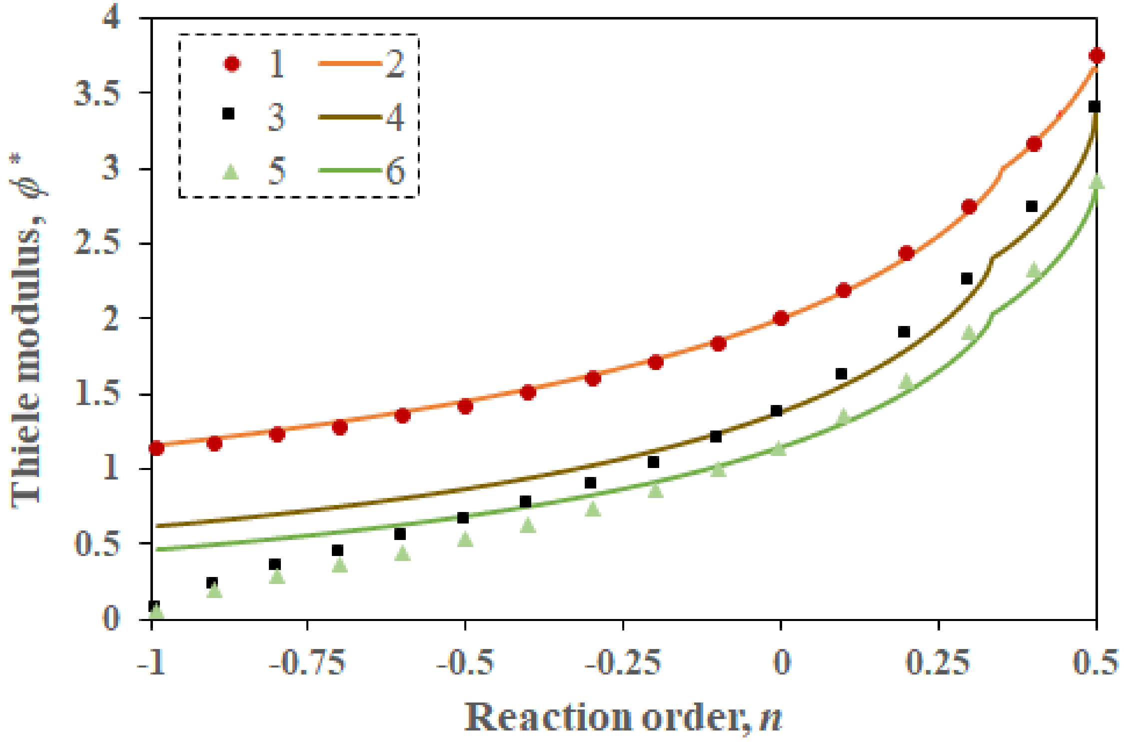

Fig 3: Variation of critical Thiele modulus with reaction order.

1-exact, 2-Taylor series, s=2, Bi_m=4;

3-exact, 4-Taylor series, s=0, Bi_m=50;

5-exact, 6-Taylor series, s=0, Bi_m=4.

DISCUSSION AND CONCLUSIONS

- The Taylor series approximation at $x = 1$ is more precise than the one at $x = 0$ for large values of Thiele modulus

  The deviation of the approximate solution by the Taylor series at x=1 from the exact one for the Thiele modulus ϕ = 2.00 is approximately the same as the deviation of the approximate solution by the Taylor series at x=0 from the exact one, but for a much smaller value of the Thiele modulus ϕ = 0.85, as illustrated in Fig.1. Similar results were obtained for non-isothermal case.

- The size of the dead zone x_{dz} and the critical Thiele modulus ϕ^* are determined with good accuracy using approximate formulas obtained by expanding solution in the Taylor series at $x = 1$.

  The results are illustrated in Figs.2 and 3.

- Consequently, the Taylor series approximations can be applied to analyze the effects of geometric, thermophysical, and physicochemical parameters on the non-isothermal reaction process in a porous catalyst granule for arbitrary reaction kinetics.

NAZARBAYEV UNIVERSITY

References

[1] B. Golman, V. V. Andreev, P. Skrzypacz. Dead-core solutions for slightly non-isothermal diffusion-reaction problems with power-law kinetics, Applied Mathematical Modelling 83 (2020) 576–589

[2] V.V. Andreev, P.Skrzypacz, B.Golman, The formation of dead zones in non-isothermal porous catalyst with temperature-dependent diffusion coefficient, International Journal of Chemical Kinetics, 59 (9), 711-722 (2019)

[3] P. Skrzypacz, V. V. Andreev, B. Golman. Dead-core and non-dead-core solutions to diffusion-reaction problems for catalyst pellets with external mass transfer, Chemical Engineering Journal, 385 (2020), 123927

Acknowledgements

This research was supported in part by a research grant 021220FD035 from Nazarbayev University.