DEAD-CORE SOLUTIONS TO FAST DIFFUSION EQUATION FOR CATALYTIC PELLETS WITH EXTERNAL MASS TRANSFER RESISTANCE

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

[1]School of Sciences and Humanities, Nazarbayev University, Kazakhstan

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

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

INTRODUCTION

We present semi-analytic approaches for solving two-point boundary value diffusion-reaction problems for catalytic pellets in the case of power-law reaction kinetics with fractional exponent and fast diffusion by considering the presence of external mass resistance. We extend our analytic approach [1,2,3] to the model problems with non-linear diffusion. The dimensionless steady-state mass balance for a single *n*-th order chemical reaction and diffusion in the catalytic pellets of planar geometry is given by

$$\frac{d^2}{dx^2}\left(c^m\right) - \phi^2 c_+^n = 0$$

where m stands for the diffusion exponent and ϕ denotes the Thiele modulus. We consider the physical solutions that satisfy

$$\frac{dc^m}{dx}(1) = Bi_m(1-c(1)), \qquad \frac{dc^m}{dx}(0) = 0.$$

For certain combinations of the pellet size, effective diffusivity, mass transfer coefficient, bulk reactant concentration, reaction order and reaction rate constant, the diffusion exponent the dead zone can be formed close to the pellet center. We study the effects of process parameters on the concentration profiles and formation of dead zones.

Dead-core solution for pellets of planar geometry

Substituting $c^m = v$, the mass balance equation reads as follows

$$\frac{d^2}{dx^2}(v) = \phi^2 v^{\frac{n}{m}} \quad \text{and} \quad \frac{d}{dx}v(1) = Bi_m\left(1 - v^{\frac{1}{m}}(1)\right)$$

Then, the dead-core solution is given by

$$v(x) = \begin{cases} \left(\sqrt{\dfrac{\phi^2\left(1-\frac{n}{m}\right)^2}{2\left(1+\frac{n}{m}\right)}}(x - x_{dz})\right)^{\frac{2}{\left(1-\frac{n}{m}\right)}}, & \text{for } x > x_{dz} \\ 0, & \text{for } 0 \le x \le x_{dz} \end{cases}$$

Dead-core solution for pellets of planar geometry

Using the mass transfer condition at the pellet external boundary, we obtain the following equation for the length of the dead-zone

$$\left(\frac{2}{1-\frac{n}{m}}\right)\left(\frac{\phi^2(1-\frac{n}{m})^2}{2(1+\frac{n}{m})}\right)^{\frac{1}{1-\frac{n}{m}}}(1-x_{dz}))^{\frac{1+\frac{n}{m}}{1-\frac{n}{m}}} = Bi_m\left(1-\left(\sqrt{\frac{\phi^2(1-\frac{n}{m})^2}{2(1+\frac{n}{m})}}(1-x_{dz})\right)^{\frac{2}{m-n}}\right)$$

Setting $x_{dz}=0$ implies that the critical Thiele modulus is implicitely determined by

$$\left(\frac{2}{Bi_m(1-\frac{n}{m})}\right)\left(\frac{\phi^2(1-\frac{n}{m})^2}{2(1+\frac{n}{m})}\right)^{\frac{1}{1-\frac{n}{m}}} - \left(\frac{\phi^2(1-\frac{n}{m})^2}{2(1+\frac{n}{m})}\right)^{\frac{1}{m-n}} = 1$$

Critical Thiele Modulus in the case of negligible external mass resistance ($\boldsymbol{Bi_m} \to \infty$)

Critical Thiele modulus

$$\phi_{crt}(m,n) = \frac{\sqrt{2\left(\frac{n}{m}+1\right)}}{1-\frac{n}{m}}$$

Dead-core solution

$$v(x) = \left(\frac{x - x_{dz}}{1 - x_{dz}}\right)^{\frac{2}{1-\frac{n}{m}}}$$

$$\Downarrow$$

$$c(x) = \left(v(x)\right)^{\frac{1}{m}} = \left(\frac{x - x_{dz}}{1 - x_{dz}}\right)^{\frac{2}{m-n}}$$

Dead-zone length

$$x_{dz} = 1 - \sqrt{\frac{2\left(1+\frac{n}{m}\right)}{\phi^2\left(1-\frac{n}{m}\right)^2}} > 1 - \sqrt{\frac{2(1+n)}{\phi^2(1-n)^2}}$$

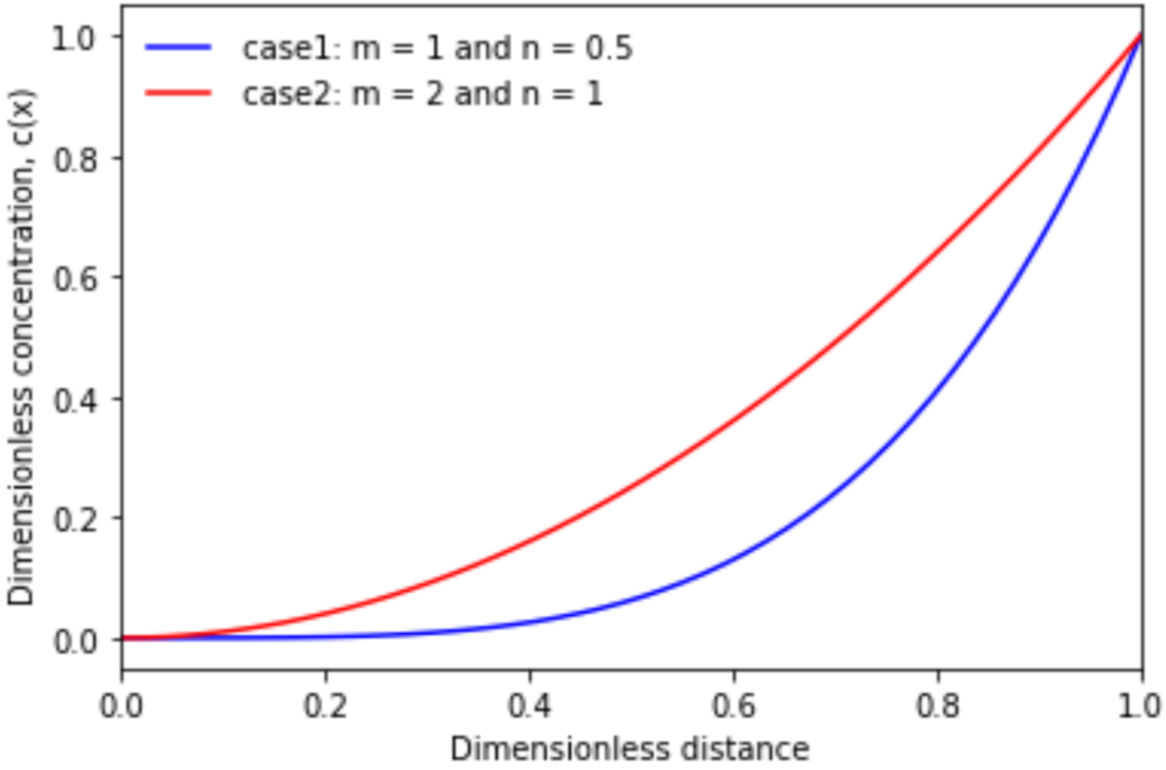
Critical solution

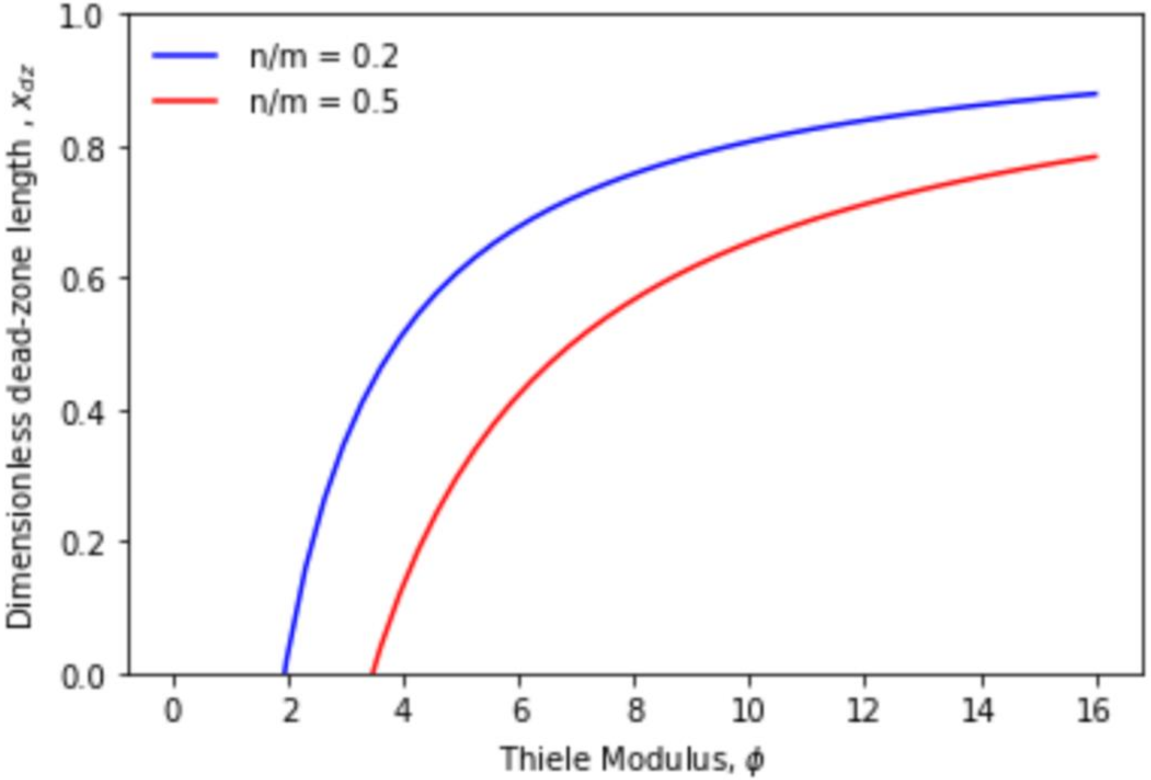
$$c(x) = \left(v_{crt}(x)\right)^{\frac{1}{m}} = x^{\frac{2}{m-n}}$$

In the case of m=1 the obtained results coincide with those from our previous works.

NAZARBAYEV UNIVERSITY

Numerical illustrations





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 090118FD5347 from Nazarbayev University.