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Approximate Analytical Solution of Non-Linear Kinetic Equation in a Porous Pellet

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Abstract

A mathematical model for immobilized enzyme system in porous spherical particles was developed. This model contains a non-linear term related to reversible Micahlies-Menten kinetics. Analytical expression pertaining to the substrate concentration was reported for all possible values of Thiele module ϕ, parameters c_s and k. In this work, we report the theoretically evaluated steady-state concentration for immobilized enzyme systems in porous spherical particles for zero order, first order and second order reaction meacnisms. Herein we employ “Homotopy perturbation method” (HPM) to solve non-linear reaction /diffusion equation.

Keywords: Mathematical modelling, Non-linear equations, Homotopy perturbation method, Reaction/diffusion equation, Porous media.

Introduction

Non linear problems frequently arise in engineering, but many texts are oriented towards linear problems due to the difficulty of nonlinearity. In general, satisfactory results can be reached by using the first few terms of the approximate, series, solution. The Homotopy mehtod has been used to solve several mathematical problems in science and engineering, but there has been no reported application in chemical engineering to date.

The model for diffusion and reaction in fixed-bed reactor generates a typical differentiation equation in chemical engineering. Thiele [1] obtained the analytical solution for the first order reaction in 1939, and then Wheeler [2] and Aris [3], etc. discussed this problem in details in their books. However, most of their conclusions were based on the analytical solution for the irreversible reaction with the first reaction order. Several researchers, such as Satterfild [4], have considered solutions for the nonlinear model with nth order reaction, but approximate solutions were not derived. Finlayson [5] has applied many numerical methods to solve nonlinear models of fluid flow, heat transfer and chemical reactor by using pre-programmed computer packages. The difficulty in the solution of such problems occurs when there is a large change in reaction rate, where the method does not always converge and convergence may depend critically on the initial guess. A disadvantage of numeircal techniques is that they cannot give analytical expressions as solution.

A steady state heterogeneous model of fixed-bed reactor is described by partial differential equation (PDE) both for fluid and for catalyst pellet. The real difficulty in a solution is the reason why this model, despite its quite good accuracy, is not willingly used for modelling. The ordinary differential equation (ODE) based on average concentration in the pellet is usually called "an approximate model ". Various approximate models have been reported for diffusion and adsorption processes. They differ from one another with respect to accuracy and validity range. One can find more information e.g., in the papers by Goto and Hirose [6] (1993), and Zhang and Ritter (1997) [7]. To make use of approximate models idea for diffusion and chemical reaction processes other models should be developed. In a diffusion and reaction process fields, only a small number of equations that approximate a mass balance in the porous particle has been found (Kim, 1989 [8]; Goto & Hirose, 1993; Szukiewiez, 2000 [9]). Models reported so far in the literature concern only first-order reactions.

Recently, Miroslaw Szukiewicz and Roman Petrus [10] evaluated the effectiveness factor corresponding to the non-steady-state concentration of component observed at a porous pellet However, till date, to the best of our knowledge, there are no general analytical expressions that describe the concentration of component for all values of the Thiele modulus $\phi \subset [0,10]$ and the normalized parameters c_s and k have been reported. As a result, herein, we have deduced analytical expressions corresponding to the concentrations of component immobilized in a porous pellet. The purpose of this communication is to derive simple accurate polynomial expressions of concentration generated at a porous spherical particle using Homotopy perturbation method.

Mathematical formulation of the problem

The predict of diffusion and reaction rates in porous catalysts in an important problem in chemical engineering, indeed when the reaction rate depends on concentration in a nonlinear case. In this heterogeneous system, the system is constructed as simple diffusion using an effective diffusion coefficient. Steady state diffusion and reaction in a porous spherical particle can be described by [10]

$$\left(\frac{\partial^2 c}{\partial x^2} + \frac{2}{x}\frac{\partial c}{\partial x}\right) - \phi^2 R_A(c) = 0 \qquad (1)$$

where c is the concentration of component, ϕ is the Thiele module and $R_A(c)$ is the reaction rate. The boundary conditions are as follows.

$$c(x=0) = \text{extremum} = k \quad (2)$$

$$c(x=1) = c_s \quad (3)$$

Analytical approximate solution with three cases

Most of engineering problems, especially some diffusion and reaction equations are nonlinear, and in most cases it is difficult to solve them, especially analytically. Perturbation method is one the well-known methods to solve nonlinear problems, it is based on the existence of small/large parameters, the so-called perturbation quantity [27, 30].

Linear case

Case (i): For zero order reaction, the reaction term $R_A(c) = 1$. Analytical solution of equation (1) with the boundary conditions equations (2) and (3) using Modified Homotopy Perturbation method is

$$c(x) = k + \frac{\varphi^2 x^2}{2} - (c_s - k)(x \log x - x) - \frac{\varphi^2 x}{2} \quad (4)$$

Case (ii): The reaction term $R_A(c) = c$ for the first order reactions. In this case, solution of the equation (1) using Modified Homotopy perturbation method is

$$c(x) = (c_s - k)x + k - \varphi^2 x\left(\frac{c_s - k}{6} + \frac{k}{2}\right) + \varphi^2 \left(\frac{(c_s - k)x^3}{6} + \frac{kx^2}{2}\right) + (k - c_s)x \log x \quad (5)$$

Non linear case

(iii): When the reaction term $R_A(c) = c^2$ (second order reactions) the analytical solution of the equation (1) with the boundary conditions equations (2) and (3) using Homotopy perturbation method (Appendix-A) is

$$c(x) = \begin{array}{l} (c_s - k)x + k - \varphi^2\left(\frac{c_s^{\,2}}{12} + \frac{kc_s}{6} + \frac{k^2}{4}\right)x + (k - c_s)x \log x + \\ \varphi^2\left(\frac{(c_s - k)^2 x^4}{12} + \frac{k^2 x^2}{2} + \frac{kx^3 (c_s - k)}{3}\right) \end{array} \quad (6)$$

Case-(i).Figure-1

(a)

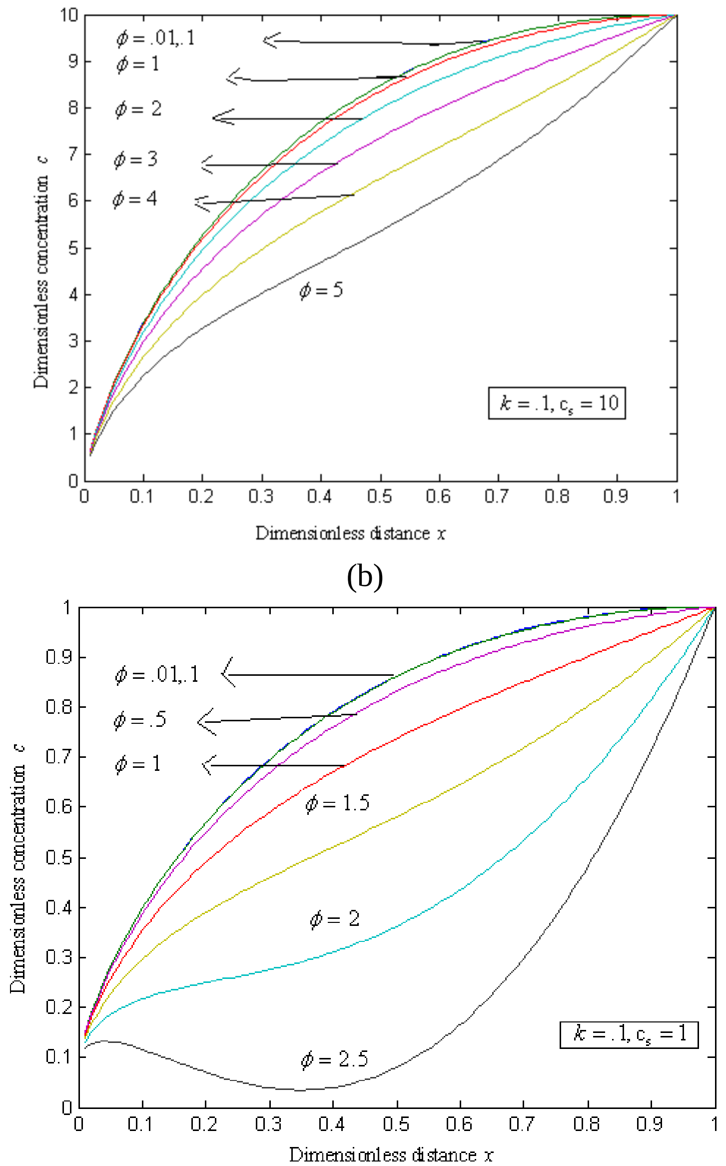
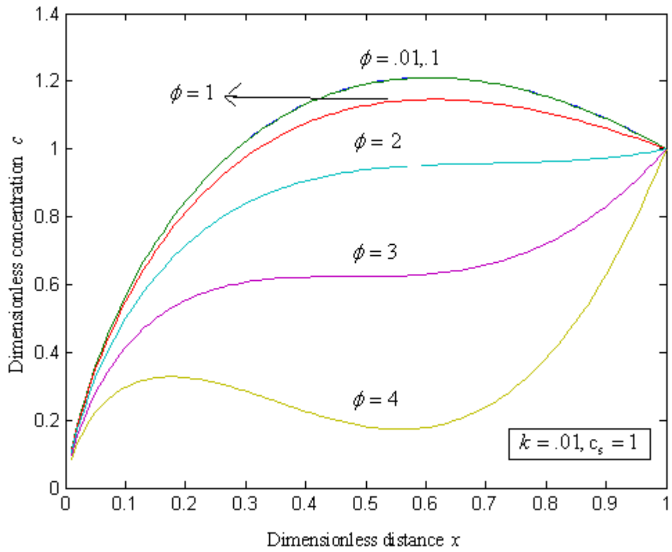


Figure 1: Influence of Thiele modulus ϕ on the concentration c obtained from the equation

(4). The curve is plotted for some fixed values of k and c_s (a) $k=.1, c_s=10$, (b) $k=.1, c_s=1$

Case-(ii). Figure-2

(a)



(b)

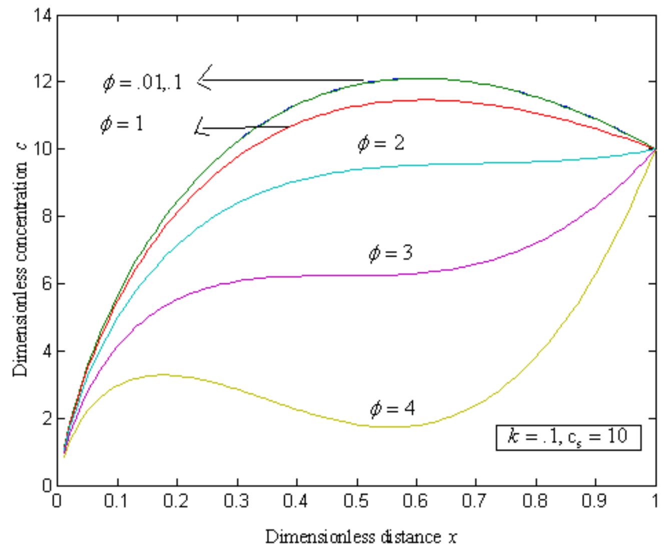
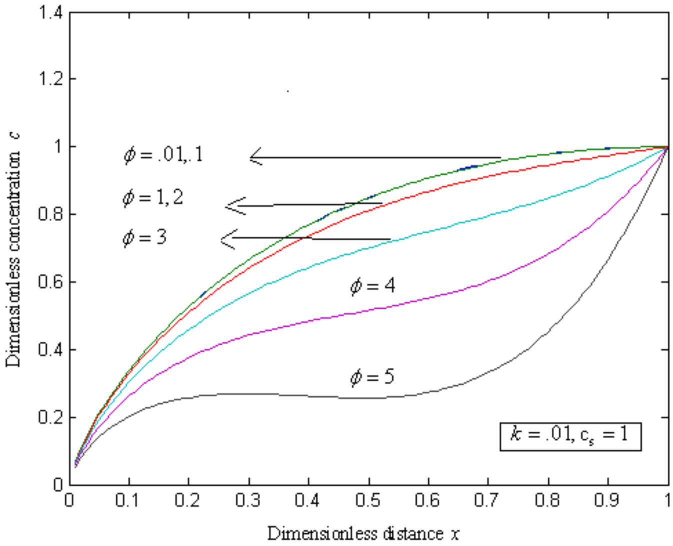


Figure 2: Influence of Thiele modulus ϕ on the concentration c obtained from the equation

(5). The curve is plotted for some fixed values of k and c_s. (a) $k = .01, c_s = 1$ (b) $k = .1, c_s = 10$

Case-(iii).Figure-3

(a)



(b)

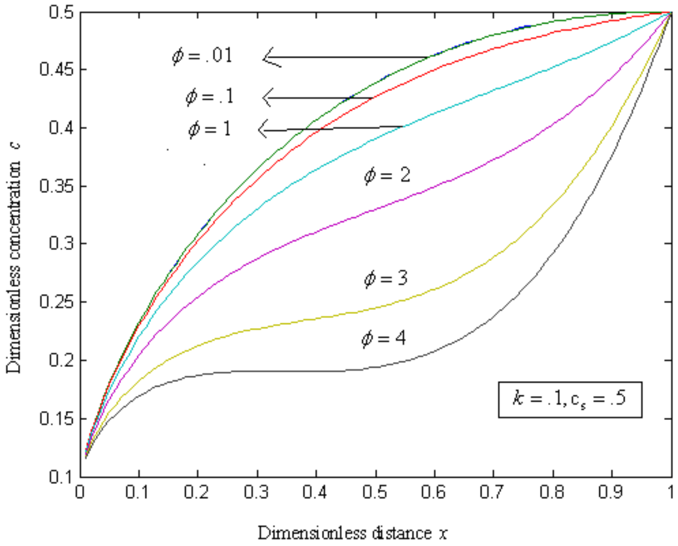
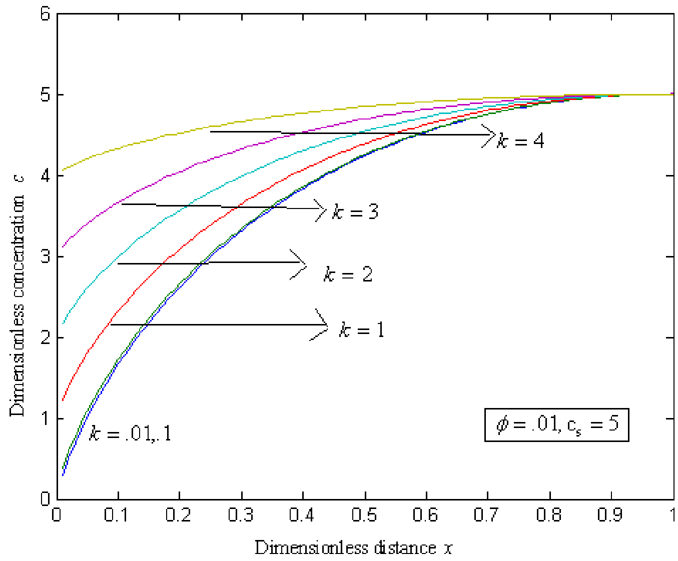


Figure 3: Influence of Thiele modulus ϕ on the concentration c obtained from the equation

(6). The curve is plotted for some fixed values of k and c_s. (a) $k = .01, c_s = 1$
(b) $k = .1, c_s = .5$

Figure: 4



From fig.4, it is clear that when k increases, the concentration c increases.

Discussion

The equations (4) to (6) represents the new analytical expressions of concentrations c for zero, first and second order reactions. The kinetic response of a porous pellet depends on the concentration of component A. The concentration of component depends on the following three factors ϕ, c_s, and k. Thiele modulus ϕ represents the ratio of the characteristic time of the enzymatic reaction to that of component diffusion. The variation in the Thiele modulus ϕ can be achieved by varying either the thickness of the enzyme layer or the amount of enzyme immobilized in the porous pellet. The Thiele modulus ϕ is indicative of the competition between the diffusion and reaction in the enzyme layer. When ϕ is small, the kinetics dominate and the uptake of component is kinetically controlled. Under these conditions, the concentration of component profile across the porous pellet is essentially uniform. The overall kinetics is governed by the total amount of active enzyme. Diffusion limitations are the principal determining factor when Thiele modulus is large.

Fig. 1 to 3 represents the normalized steady state concentration c versus dimensionless distance x for different values of the dimensionless parameter ϕ. From the figure it is inferred that the value of the concentration c increases when the value of ϕ decreases. Fig.4 represents the concentration versus the dimensionless distance x for various values of k. From this figure it is observed that the concentration increases when the constant k increases.

Conclusions

The time independent linear and non-linear reaction/diffusion equation has been formulated and solved analytically. An approximate analytical expression for the concentrations in porous spherical particle under steady state conditions for various reaction order are obtained by using the Homotopy perturbation method. The primary result of this work is simple approximate calculation of concentration for all possible values of sparameters. This method can be easily extended to find the solution of all other non-linear reaction diffusion equations in porous cylindrical particle for various complex boundary conditions.

References

[1] Thiele, E.W, 1939, " Relation between catalytic activity and size of particle", Ind. Eng. Chem. 31, 916-920.
[2] Wheeler, A., 1955, Reaction rate and selectivity in catalyst pores, catalysis 2 105-165.
[3] Aris, R., 1975, Mathematical Theory of Diffusion and Reaction in Permeable Catalyst, Oxford University Press, London.
[4] Satterfild G.Ns., 1973, Mass Transfer in Heterogeneous Catalysis, MIT Press, Cambridge.
[5] Finalayson, B. A., 1980, Nonlinear Analysis inChemical Engineering, McGraw-Hill, New York.
[6] Goto, M., & Hirose.T., 1993, " Approximate rate equation for intraparticle diffusion with or Without Reaction ", Chemical Engineering Science, 48(10), 1912-1915.
[7] Zhang, R., & Ritter, J.A., 1997, " New approximate model for nonlinear adsorption and diffusion in a single particle", Chemical Engineering Science, 52(18), 3161-3172.
[8] Kim, D.H., 1989, "Linear driving force formulas for diffusion and reaction in porous catalysts" A.I.Ch.E. Journal, 35, 343-346.
[9] Szukiewies, M.K., 2000, " New approximate model for diffusison and reaction in a porous catalyst", A. I. Ch.E. Journal 46, 661-665.
[10] Miroslaw Szukiewiez, Roman Petrus, 2004, "Approximate model for diffusion and reaction in a Porous pellet and an effectiveness factor", Chemical Engineering Sciences 59, 479-483.
[11] Cole, J. D., 1968, Perturbation methods in applied mathematics, Blaisdell Publishing Company, Waltham, Massachusetts.
[12] Nayfeh, A. H., 2000, Perturbation Methods, John Wiley and Sons, New York.
[13] Szukiewies, M.K., 2002, " An approximate model for diffusion and reaction in a porous pellet" Chemical Engineering Sciences, 57, 1451-1457.
[14] Szukiewies, M.K., 2001, " Approximate model for diffusion and reaction in a porous catalyst With mass-transfer resistances", A.I.Ch.E. Journal 47, 2131-2135.

[15] Ghori, Q. K., Ahmed, M., Siddiqui, A. M., 2007, "Application of Homotopy perturbation method to squeezing flow of a Newtonian fluid", *International Journal of Nonlinear Science and Numerical Simulation,* Vol. 8(2), pp. 179-184.
[16] Ozis, T., Yildirim, A., 2007, "A comparative study of He's homotopy perturbation method fordetermining frequency-amplitude relation of a nonlinear oscillater with discontinuities", *International Journal of Nonlinear Science and Numerical Simulation,* Vol. 8(2), pp. 243-248.
[17] Li, S. J., and Liu, Y. X., 2006, "An improved approach to nonlinear dynamical system identification using PID neural networks", *International Journal of Nonlinear Science and Numerical Simulation,* Vol. 7(2), pp. 177-182.
[18] Mousa, M. M., Ragab, S. F., 2008, "Application of the Homotopy Perturbation Method to Linear and Nonlinear Schrödinger Equations", *Zeitschrift fur Naturforschung,* Vol. 63, pp. 140-144.
[19] He, J. H., 1999, "Homotopy perturbation technique", *Computer Methods in Applied Mechanics and Engineering,* Vol. 178, pp. 257-262.
[20] He, J. H., 2003, "Homotopy perturbation method: a new nonlinear analytical Technique", *Applied Mathematics and Computation,* Vol. 135, pp. 73-79.
[21] He, J. H., 2003, "A simple perturbation approach to Blasius equation", *Applied Mathematics and Computation,* Vol. 140, pp. 217-222.
[22] He, J. H., 2006, "Homotopy perturbation method for solving boundary value problems", *Physics Letter A*, Vol. 350, pp. 87-88.
[23] He, J. H., "Some asymptotic methods for strongly nonlinear equations, " *International Journal of Modern Physics B*, Vol. 20, no. 10, pp. 1141-1199.
[24] Eswari, A., Rajendran, L., 2010, "Analytical solution of steady state current at a micro Disk biosensor", *Journal of Electroanalytical Chemistry,* Vol. 641, pp. 35-44.
[25] Meena, A., Rajendran, L., 2010, "Mathematical modeling of amperometric and Potentiometric biosensors and system of non-linear equations-Homotopy perturbation approach", *Journal of Electroanalytical Chemistry,* Vol. 644, pp. 50-59.
[26] Yan-Ping Sun, Shi-Bin Liu, Scott Keith, 2004, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by the decomposition method, Chemical Engineering Journal 102, 1-10.
[27] Abbasbandy, S., 2008, "Approximate solution for the nonlinear model of diffusion and reaction in Porous catalysts by means of the homotopy analysis method", Chemical Engineering Journal 136, 144-150.
[28] Adomian, G., 1994, Solving Frontier Problems of Physics: The Decomposition Method, Kluwer Academic Publishers, Dordrecht.
[29] Karmishin, A. V., Zhukov, A. I., Kolosov, V. G., 1990, Methods of Dynamics Calculation and Testing for Thin- Walled Structures, Mashinostroyenie, Moscow.
[30] Lyapunov, A. M, 1992, General Problem on Stability of Motion (English translation), Taylor and Francis, London.

Appendix A

We construct the Homotopy as follows

$$(1-p)\left[\frac{d^2c}{dx^2}\right]+p\left[\frac{d^2c}{dx^2}+\frac{2}{x}\frac{dc}{dc}-\phi^2c^2\right]=0 \tag{A1}$$

The approximate analytical solution of (4) is

$$c = c_0 + pc_1 + p^2c_2 + ... \tag{A2}$$

The initial approximations is as follows

$$c_0(0) = k \text{ and } c_{0,x}(1) = c_s \tag{A3}$$
$$c_i(0) = 0 \text{ and } c_{i,x}(1) = 0,\ i = 1,2$$

Substituting eqn. (6) into equation (5) we have

$$(1-p)\left[\frac{d^2\left(c_0+pc_1+p^2c_2+......\right)}{dx^2}\right]$$
$$+p\begin{bmatrix}\dfrac{d^2\left(c_0+pc_1+.....\right)}{dx^2}+\dfrac{2}{x}\dfrac{d\left(c_0+pc_1+....\right)}{dx}\\ -\varphi^2\left(c_0+pc_1+p^2c_2+......\right)\end{bmatrix}=0 \quad (9)$$

(A5)

Comparing the coefficients of like powers of p in equation (9) we get

$$p^0 : \frac{d^2c_0}{dx^2}=0 \tag{A5}$$

$$p^1 : \frac{d^2c_1}{dx^2}+\frac{2}{x}\frac{dc_0}{dx}-\phi^2c_0^{\ 2} = 0 \tag{A6}$$

Solving the equations (10) and (11), we can find the following results:

$$c_0(x)=(c_s-k)x+k \tag{A7}$$

$$c_1(x)=-\varphi^2\left(\frac{c_s^{\ 2}}{12}+\frac{kc_s}{6}+\frac{k^2}{4}\right)x+(k-c_s)x\log x$$
$$+\varphi^2\left(\frac{(c_s-k)^2x^4}{12}+\frac{k^2x^2}{2}+\frac{kx^3(c_s-k)}{3}\right)$$

(A8)

According to HPM, we can conclude that

$$c=\lim_{p\to 1}c(x)=c_0+c_1+....$$

$$= (c_s - k)x + k - \varphi^2\left(\frac{c_s^{\,2}}{12} + \frac{kc_s}{6} + \frac{k^2}{4}\right)x + (k - c_s)x\log x + \varphi^2$$

$$\left(\frac{(c_s - k)^2 x^4}{12} + \frac{k^2x^2}{2} + \frac{kx^3(c_s - k)}{3}\right) \qquad \text{(A9)}$$

Notation

c	Concentration of component A
c_s	Surface concentration of component A
R_A	Reaction rate
x	Position in pellet
ϕ	Thiele modulus
k	Extremum value