Journal of the Taiwan Institute of Chemical Engineers 48 (2015) 49–55

Contents lists available at ScienceDirect

Journal of the Taiwan Institute of Chemical Engineers

journal homepage: www.elsevier.com/locate/jtice

Multiplicity results and closed-form solution for catalytic reaction in a flat particle

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ARTICLE INFO

Article history:
Received 19 July 2014
Received in revised form 6 October 2014
Accepted 19 October 2014
Available online 24 December 2014

Keywords:
Exact analytic solutions
Catalytic reaction
Flat particle
Multiple solutions

ABSTRACT

Assume a flat geometry for the particle and that conductive heat transfer is negligible compared to convective heat transfer in the study of heat and mass transfer for a catalytic reaction within a porous catalyst flat particle. This article shows the governing differential equation, which is the direct result of a material and energy balance, is exactly solvable and furthermore, gives exact analytical solution in the implicit form for further physical interpretation. A full discussion is given and, it is also revealed that the problem may admit unique, dual or even more triple solutions depending on the values of Thiele modulus and other parameters of the model.

1. Preliminaries and problem formulation

Simultaneous mass and heat transfer inside a porous catalyst particle have been widely studied [1–6]. Differential mass and enthalpy balances, describing simultaneous heat and mass transfer within porous catalyst particle can be written in the form [2]

$$\frac{d^2y}{dx^2}+\frac{a}{x}\frac{dy}{dx}=\phi^2 f(y)\exp\left[-\gamma\left(\frac{1}{\tau}-1\right)\right], \tag{1}$$

$$\frac{d^2\tau}{dx^2}+\frac{a}{x}\frac{d\tau}{dx}=-\beta\phi^2 f(y)\exp\left[-\gamma\left(\frac{1}{\tau}-1\right)\right], \tag{2}$$

with boundary conditions

$$x=0:\frac{dy}{dx}=\frac{d\tau}{dx}=0, \tag{3}$$

$$x=1:y+\frac{1}{Nu_M}\frac{dy}{dx}=1,\quad \tau+\frac{1}{Nu_H}\frac{d\tau}{dx}=1. \tag{4}$$

In Eqs. (1) and (2) a geometry of the particle is defined by means of the value of parameter a ($a=0$ for flat plate particle, $a=1$ for cylindrical particle and $a=2$ for spherical particle). Parameters y, β and ϕ represent dimensionless energy of activation, a parameter describing heat evolution and Thiele's modulus, respectively, Nu_M and Nu_H denote Sherwood and Nusselt numbers and $f(y)$ represents a reaction rate expression.

In Ref. [2], the basic features of the solution space (such as multiple solutions, the corresponding parameter ranges in which they occur, detailed numerical results and examples, *etc.*) have also been reported by Hlaváček et al. (1968). In this paper, we are interested in extracting exact solution of the problem (1)–(4) and then discussing about the multiplicity of solutions when the flat plate particle is $a=0$ and the reaction rate expression is in the form of $f(y)=y$. We will discuss the problem in two cases separately: (1) $Nu_M=Nu_H$ and then (2) $Nu_M\neq Nu_H$.

2. The exact analytical solution for the case $Nu_M = Nu_H$

Eqs. (1) and (2) can be simplified in the case, where $Nu_M=Nu_H=Nu$. By combining (1) and (2) we then obtain [2]

$$\frac{d^2\tau}{dx^2}+\frac{a}{x}\frac{d\tau}{dx}+\beta\left(\frac{d^2y}{dx^2}+\frac{a}{x}\frac{dy}{dx}\right)=0, \tag{5}$$

which can be rewritten in the form

$$\frac{d^2}{dx^2}(\tau+\beta y)+\frac{a}{x}\frac{d}{dx}(\tau+\beta y)=0. \tag{6}$$

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http://dx.doi.org/10.1016/j.jtice.2014.10.023
1876-1070/

If we denote

$$g = \tau + \beta y, \tag{7}$$

then we conclude $g'(x) = C_1 x^{-a}$ from (6) where C_1 is constant. Therefore, conditions (3) yield $C_1 = 0$, then

$$g = \text{const}. \tag{8}$$

Making use of boundary condition (4) we obtain

$$\beta\left(y + \frac{1}{Nu}\frac{\mathrm{d}y}{\mathrm{d}x}\right) + \left(\tau + \frac{1}{Nu}\frac{\mathrm{d}\tau}{\mathrm{d}x}\right) = g + Nu\frac{\mathrm{d}g}{\mathrm{d}x} = \beta + 1, \tag{9}$$

and thus

$$g = \beta + 1, \tag{10}$$

therefore

$$\tau = 1 + \beta(1 - y). \tag{11}$$

Substituting (11) into (1) we obtain the material balance in the form

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + \frac{a}{x}\frac{\mathrm{d}y}{\mathrm{d}x} = \phi^2 f(y)\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right], \tag{12}$$

with boundary conditions

$$x = 0:\ \frac{\mathrm{d}y}{\mathrm{d}x} = 0, \tag{13}$$

$$x = 1:\ y + \frac{1}{Nu}\frac{\mathrm{d}y}{\mathrm{d}x} = 1. \tag{14}$$

As mentioned previously, we will consider the case flat plate particle ($a = 0$) and deal with the reaction rate expression in the form of $f(y) = y$. In this case, reaction rate is proportional to the expression [2]

$$r \approx y\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right]. \tag{15}$$

Reaction rate will increase in the direction of increasing temperature (or decreasing concentration) if:

$$\frac{\mathrm{d}r}{\mathrm{d}y} < 0. \tag{16}$$

On differentiating (15) condition (16) takes the form

$$1 - \frac{\gamma\beta y}{[1+\beta(1-y)]^2} < 0. \tag{17}$$

Let us assume that (16) holds, in a limiting case, at least at the point $x = 1$; then for $Nu \to \infty$ (*i.e.* for $y(1) = 1$) we have $\gamma\beta > 1$. Finally, by denoting $\lambda = \phi^2$, the problem is

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - \lambda y\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right] = 0, \tag{18}$$

$$\frac{\mathrm{d}y}{\mathrm{d}x}(0) = 0, \quad y(1) = 1. \tag{19}$$

Youdong Lin et al. [7] have considered the problem (18) and (19) and solved numerically by the so-called interval analysis method. They obtained three approximate solutions in their testing example in the case $\lambda = 0.1$ ($\gamma = 20$ and $\beta = 0.4$). Ford and Pennline [5] have proved the existence and uniqueness of the solution for some domains of the parameters of the model. In Ref. [6] Kumar and Singh have applied Modified Adomian Decomposition Method (MADM) to obtain approximative analytical solutions. Our work is motivated by two factors. The first is to show the mentioned problem is exactly solvable and more, to give exact analytical solution in the implicit form for further physical interpretation. The second one, which is the result of the first one, is to show the problem can have more than one stationary solution. It is obtained two critical values namely λ_1 and λ_2 for which the problem admits dual solutions and more, the problem admits triple solutions in the inside of the interval $\lambda_1 < \lambda < \lambda_2$ and unique solution in the outside of the interval.

Consider the generalization of Eqs. (18) and (19) which comes from (12) to (14) *i.e.*

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - \lambda y\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right] = 0, \tag{20}$$

$$\frac{\mathrm{d}y}{\mathrm{d}x}(0) = 0, \quad y(1) + \frac{1}{Nu}\frac{\mathrm{d}y}{\mathrm{d}x}(1) = 1, \tag{21}$$

the problem (20) and (21) is the same as (18) and (19) when $Nu \to \infty$. By transformation $u = \mathrm{d}y/\mathrm{d}x$, we have

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = \frac{\mathrm{d}u}{\mathrm{d}x} = \frac{\mathrm{d}u}{\mathrm{d}y}\frac{\mathrm{d}y}{\mathrm{d}x} = u\frac{\mathrm{d}u}{\mathrm{d}y}. \tag{22}$$

So, Eq. (20) is converted to the following:

$$u\frac{\mathrm{d}u}{\mathrm{d}y} = \lambda y\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right], \tag{23}$$

which is the first order ordinary differential equation of separable type so, by integration and replacing u by $\mathrm{d}y/\mathrm{d}x$, we conclude

$$\frac{1}{2}\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2 = \frac{\lambda e^{\gamma}(\beta y e^{\gamma/(\beta(y-1)-1)}(\gamma + \beta y) - \gamma(2\beta + \gamma + 2)\,\mathrm{ExpIntegralEi}(\gamma/((y-1)\beta - 1)))}{2\beta^2} - \frac{\lambda(\beta+1)(\beta+\gamma+1)e^{\gamma((1/(\beta(y-1)-1))+1)}}{2\beta^2} + C, \tag{24}$$

where C is the integral constant and ExpIntegralEi is second exponential integral function which is defined by

$$\mathrm{ExpIntegralEi}(z) = -\int_{-z}^{+\infty}\frac{\exp(-t)}{t}\mathrm{d}t. \tag{25}$$

Using the first boundary condition (21), Eq. (24) gives

$$C = -\frac{\lambda e^{\gamma}(\beta y_0 e^{\gamma/(\beta(y_0-1)-1)}(\gamma + \beta y_0) - \gamma(2\beta + \gamma + 2)\,\mathrm{ExpIntegralEi}(\gamma/(\beta(y_0-1)-1)))}{2\beta^2} + \frac{\lambda(\beta+1)(\beta+\gamma+1)e^{\gamma(1/(\beta(y_0-1)-1)+1)}}{2\beta^2}, \tag{26}$$

where $y_0 = y(0)$ is unknown concentration of the reactant at ($x = 0$) which will be obtained later by the help of second boundary condition (21). Setting above equation into (24) and then, by