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On the exact results of a non-linear model arising in catalytic reaction in a flat particle with power kinetics reaction rate

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ABSTRACT

The latest study of a model of heat and mass transfer for a catalytic reaction within a porous catalyst flat particle (Journal of the Taiwan Institute of Chemical Engineers 48 (2015) 49–55 [7]) shows that this model can be exactly solved when the reaction rate is taken linear term as $f(y)=y$, where y is heat within porous catalyst particle. In this paper, the mentioned model is revisited by considering the power kinetics nth order reaction rate instead of a linear reaction term. It is shown that the problem is still exactly tractable. Furthermore, it is revealed that previous results can be recovered from this exactly solvable generalization case. It is also proved that the problem might have multiple stationary solutions (unique, dual and triple solutions) depending on the values of the parameters of the model.

1. Introduction

The model of simultaneous mass and heat transfer within a porous catalyst particle [1–7] is governed by the following system of non-linear differential equations:

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

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

with boundary conditions

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

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

In Eqs. (1)–(2) the geometry of a particle is defined in terms of the value of parameter a ($a=0$ for a flat plate particle, $a=1$ for a cylindrical particle and $a=2$ for a spherical particle) and γ is the parameter describing energy of activation. β and ϕ represent the parameters of heat evolution and Thiele's modulus, respectively. Furthermore, Nu_M and Nu_H denote Sherwood and Nusselt numbers and, $f(y)$ is the reaction rate expression in where y is the heat within porous catalyst particle.

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) have been reported by Hlaváček et al. The exact analytical solution of Eqs. (1) and (2) has been given in the case that the reaction rate is a linear term (first order reaction) as $f(y)=y$ and the geometry of the particle is a flat plate as in Ref. [7]. In that article, authors have given a full discussion of existence and multiplicity of solutions and, they have 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.

It is pertinent at this point to ascertain how reaction order influences the extent to which conversion is retarded by back-mixing. Since the mixing process essentially alters the concentration field within the reactor, intuition suggests that higher the reaction order the greater the influence of backmixing upon the reaction rate (and therefore conversion for a given contact time). Intuition is readily supported by quantitative treatment in this instance. Consider cases of zero, one-half, and second-order kinetics. The extent to which backmixing influences the reaction rate in each case is reflected in terms of the required ratio of contact time in a continuous flow stirred-tank reactor (CSTR) relative to that in a plug flow reactor (PFR) model for a given level of conversion and temperature. Non-segregated flow will be assumed in the CSTR analysis for simplicity. While differences were demonstrated for non-linear kinetics between segregated and non-segregated CSTR models, these are secondary in comparison with differences in PFR and CSTR performance [8].

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In the present work, the nth order power kinetics reaction rate, i.e. $f(y)=y^n$, is considered which is more general than that considered in Ref. [7] (first order reaction rate). We show that the problem (1) and (2) is nevertheless exactly tractable in both cases: (1) $Nu_M=Nu_H$, and (2) $Nu_M\neq Nu_H$. As a matter of fact, the motivation of present work has two features: The first one is to show that the mentioned problem is exactly solvable and then, to give exact analytical solution in an implicit form for further physical interpretation (tt is worth mentioning here that to analyze exactly the non-linear phenomena is of consequential matter in science and engineering [9–11]). The second one, which concludes from the first one, is to show that the problem has multiple stationary solutions (unique, dual and triple solutions) depending on the values of the parameters of the model (γ, β, $\lambda=\phi^2$ and n). This paper is organized as follows: the mathematical reformulation and the solution procedure for obtaining exact solution are given in Sections 2 and 4 for $Nu_M=Nu_H$ and $Nu_M\neq Nu_H$, respectively. Sections 3 and 5 contain the graphical results and their discussion. The concluding remarks are included in Section 6.

2. The exact analytical solution when $Nu_M=Nu_H$

In this case, the problem (1)–(4) reduces to

$$\frac{d^2y}{dx^2}+\frac{a}{x}\frac{dy}{dx}=\phi^2 f(y)\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right], \tag{5}$$

with boundary conditions

$$x=0:\quad \frac{dy}{dx}=0, \tag{6}$$

$$x=1:\quad y+\frac{1}{Nu}\frac{dy}{dx}=1. \tag{7}$$

Also, the relation between $y(x)$ and $\tau(x)$ is given by

$$\tau=1+\beta(1-y). \tag{8}$$

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

$$r\approx y^n\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right]. \tag{9}$$

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

$$\frac{dr}{dy}<0. \tag{10}$$

By differentiating (9), condition (10) yields

$$n-\frac{\gamma\beta y}{[1+\beta(1-y)]^2}<0. \tag{11}$$

Let us assume that (10) 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 $\gamma\beta>n$. Finally, by denoting $\lambda=\phi^2$, the problem is converted to

$$\frac{d^2y}{dx^2}-\lambda y^n\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right]=0, \tag{12}$$

$$\frac{dy}{dx}(0)=0,\quad y(1)=1. \tag{13}$$

The above problem has been studied and solved numerically by some researchers, in the case $n=1$, through some methods such as interval analysis and Modified Adomian Decomposition Method (MADM) [6,12]. Ford and Pennline [5] have proved the existence and uniqueness of the solution for this problem in the same case ($n=1$) on some domains for system parameters.

Consider a kind of generalization case of Eqs. (12)–(13) by taking into account the original boundary condition (7) i.e.

$$\frac{d^2y}{dx^2}-\lambda y^n\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right]=0, \tag{14}$$

$$\frac{dy}{dx}(0)=0,\quad y(1)+\frac{1}{Nu}\frac{dy}{dx}(1)=1, \tag{15}$$

the problem (14)–(15) is equivalent to (12) and (13) when $Nu\to\infty$. By changing the function $u=\frac{dy}{dx}$, we have

$$\frac{d^2y}{dx^2}=\frac{du}{dx}=\frac{du}{dy}\frac{dy}{dx}=u\frac{du}{dy}. \tag{16}$$

Therefore, Eq. (14) is converted to the following:

$$u\frac{du}{dy}=\lambda y^n\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right], \tag{17}$$

which is the first order ordinary differential equation of a separable type, then by integration and replacing u by $\frac{dy}{dx}$, it takes the form

$$\frac{1}{2}\left(\frac{dy}{dx}\right)^2=\lambda\mathbf{IF}(y;\beta,\gamma,n)+C, \tag{18}$$

where C is the integral constant and **IF** is defined so that

$$\frac{d\mathbf{IF}(y;\beta,\gamma,n)}{dy}=y^n\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right], \tag{19}$$

for example,

$$\mathbf{IF}(y;\beta,\gamma,0)=\frac{e^{\gamma}\left((\beta(y-1)-1)e^{\gamma/\beta(y-1)-1}-\gamma\mathrm{Ei}\left(\frac{\gamma}{(y-1)\beta-1}\right)\right)}{\beta}, \tag{20}$$

$$\begin{aligned}\mathbf{IF}(y;\beta,\gamma,1)&=\frac{e^{\gamma}\left(\beta y e^{\gamma/\beta(y-1)-1}(\gamma+\beta y)-\gamma(2\beta+\gamma+2)\mathrm{Ei}\left(\frac{\gamma}{(y-1)\beta-1}\right)\right)}{2\beta^2}\\&\quad-\frac{(\beta+1)(\beta+\gamma+1)e^{\gamma(1/\beta(y-1)-1+1)}}{2\beta^2}\end{aligned} \tag{21}$$

$$\begin{aligned}\mathbf{IF}(y;\beta,\gamma,2)&=\frac{e^{\gamma}\begin{pmatrix}\beta y e^{\gamma/\beta(y-1)-1}\left(\gamma(4\beta+\gamma+4)+2\beta^2y^2+\beta\gamma y\right)\\-\gamma\left(6\beta^2+6\beta(\gamma+2)+\gamma^2+6\gamma+6\right)\mathrm{Ei}\left(\frac{\gamma}{(y-1)\beta-1}\right)\end{pmatrix}}{6\beta^3}\\&\quad-\frac{(\beta+1)\left(2\beta^2+\beta(5\gamma+4)+\gamma^2+5\gamma+2\right)e^{\gamma(1/\beta(y-1)-1+1)}}{6\beta^3}\end{aligned} \tag{22}$$

$$\mathbf{IF}(y;\beta,\gamma,3)=\frac{e^{\gamma}\begin{pmatrix}\beta y e^{\frac{\gamma}{\beta(y-1)-1}}\begin{pmatrix}\gamma\left(18\beta^2+2\beta(5\gamma+18)+\gamma^2+10\gamma+18\right)\\+6\beta^3y^3+2\beta^2\gamma y^2+\beta\gamma y(6\beta+\gamma+6)\end{pmatrix}\\-\gamma\begin{pmatrix}24\beta^3+36\beta^2(\gamma+2)+12\beta(\gamma^2+6\gamma+6)\\+\gamma^3+12\gamma^2+36\gamma+24\end{pmatrix}\mathrm{Ei}\left(\frac{\gamma}{(y-1)\beta-1}\right)\end{pmatrix}}{24\beta^4}$$