Nonlinear Analysis: Real World Applications 11 (2010) 3031–3036

Contents lists available at ScienceDirect

Nonlinear Analysis: Real World Applications

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

Symmetry analysis for the nonlinear model of diffusion and reaction in porous catalysts

R.J. Moitsheki [a,*], T. Hayat [b], M.Y. Malik [b], F.M. Mahomed [a]

[a] Centre for Differential Equations, Continuum Mechanics and Applications, School of Computational and Applied Mathematics, University of the Witwatersrand, Private Bag 3, Wits 2050, South Africa

[b] Department of Mathematics, Quaid-I-Azam University 45320, Islamabad 44000, Pakistan

ARTICLE INFO

Article history:
Received 21 August 2009
Accepted 30 October 2009

Keywords:
Lie point symmetries
Nonlinear problems
Analytic solutions

ABSTRACT

In this paper the nonlinear problem arising due to diffusion and reaction in catalyst is investigated. This problem was studied before using the Adomian decomposition, finite differences and homotopy analysis methods. Mathematical analysis for the case of the nth order reactions is performed and exact analytical solutions are investigated by the Lie symmetry method. Moreover, we look for exact solutions for negative reaction constants and show that the solutions exist for various values of n and the Thiele modulus ϕ. Graphs are plotted for these parameters and discussed.

1. Introduction

Ordinary differential equations (ODEs) have received considerable attention since the days of Lie (see e.g. [1,2]), and as such ODEs are a fertile area of study (many techniques for solving and solutions to these equations exist). A nonlinear second order ODE is linearizable by a point transformation if it satisfies Lie's linearization condition (see e.g. [3]). The theory on Lie symmetry techniques may be found in text such as those of [4,5]. There are many results on ODEs (see [3]). For example, an equation which admits a two-dimensional non-Abelian symmetry algebra may be transformed to one which is at most cubic in the first derivative and may further be linearized or integrated (see e.g. [3]).

The prediction of diffusion and reaction rates in porous catalysts has received increasing attention by investigators, especially in chemical engineering. Such situations become more interesting when the reaction rate depends upon the nonlinear concentration. In such problems the analytic solutions are rare. Recently, Sun et al. [6] used the Adomian decomposition method (ADM) for the solution of the nonlinear problem of diffusion and reaction in porous catalysts. In continuation, Abbasdandy [7] obtained the analytic and numerical solutions of the problem considered in Ref. [6] by the homotopy analysis method (HAM) and finite difference method (FDM) respectively.

In the present communication, we revisit the nonlinear problem of Refs. [7,6] for exact solutions by using classical Lie point symmetries as well as an allied problem when the reaction rate is negative. The authors [7,6] considered the case when the reaction rate was positive. They obtained approximate solutions which we re-look at here. Moreover, we obtain exact solutions for the case when the reaction rate is negative. Our aim is to provide exact solutions which are independent of the choice of the underlying parameters which are the order n and the Thiele modulus ϕ.

In the next section we briefly describe the mathematical model and then in Section 3 we investigate exact solutions for positive reaction constant. In Section 4 we consider exact solutions for negative reaction constant. Concluding remarks are made in Section 5.

* Corresponding author.
E-mail addresses: raseelo.moitsheki@wits.ac.za (R.J. Moitsheki), pensy_t@yahoo.com (T. Hayat), drmymalik@hotmail.com (M.Y. Malik), Fazal.Mahomed@wits.ac.za (F.M. Mahomed).

1468-1218/$ – see front matter © 2010 Published by Elsevier Ltd
doi:10.1016/j.nonrwa.2009.10.023

2. Mathematical model of diffusion and reaction

We assume that for diffusion, all the microscopic details for the porous medium are lumped together into the effective diffusion coefficient D_e for the reactant. The convection boundary effects and coupling between chemical reaction and diffusion are neglected here. In view of such considerations, a mass balance on a volume of the porous medium yields [6]

$$\frac{\partial \acute{c}}{\partial t} = \nabla D_e \nabla \acute{c} - r(\acute{c}). \tag{1}$$

In the above equation t designates the time, $\acute{c}$ the chemical reactant concentration and $r(\acute{c})$ is the rate of reaction per unit volume. We further assume that diffusion in a porous slab reaches the steady state situation. The slab is infinite in two directions, giving a large plane sheet with diffusion through the thickness of the sheet. Eq. (1) for the one-dimensional case becomes

$$\frac{\mathrm{d}^2\acute{c}}{\mathrm{d}\acute{x}^2} - \frac{r(\acute{c})}{D_e} = 0, \tag{2}$$

in which $\acute{x}$ indicates the diffusion distance and D_e is a constant.

Due to one impermeable side of the slab and fixed concentration at the other side of the slab, we have [6]

$$\acute{x}(0) = 0, \qquad -D_e\frac{\mathrm{d}\acute{c}}{\mathrm{d}\acute{x}} = 0; \tag{3}$$

$$\acute{x}(1) = \ell, \qquad \acute{c} = \acute{c}_s \tag{4}$$

where ℓ is the catalyst pore length.

Defining the non-dimensional variables

$$x = \frac{\acute{x}}{\ell}, \qquad u = \frac{\acute{c}}{\acute{c}_s} \tag{5}$$

and taking into account the reaction $A \rightarrow B$ with the rate dependence upon the nth power of concentration A, dependent on $k\acute{c}^n$ (the reaction constant k depends upon temperature), Eqs. (2) to (4) reduce to

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} \pm \frac{l^2ku^{n-1}(0)}{D_e}u^n = 0, \tag{6}$$

$$u(1) = 1, \qquad u'(0) = 0. \tag{7}$$

The reaction constant k is positive or negative. In [6], the authors study the equation

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} - \phi^2u^n = 0 \tag{8}$$

where the Thiele modulus is expressed by

$$\phi^2 = \frac{k\ell^2u^{n-1}(0)}{D_e}, \quad k > 0. \tag{9}$$

Here we show that for such an Eq. (8) and boundary condition (7) there exists no solution for $n \neq 0, 1$. The cases $n = 0, 1$ render the equation linear which is easily tractable. Moreover, we study the equation

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \phi^2u^n = 0 \tag{10}$$

where the Thiele modulus is expressed by

$$\phi^2 = -\frac{k\ell^2u^{n-1}(0)}{D_e}, \quad k < 0. \tag{11}$$

For Eq. (10) together with (7), we show that exact physical solutions exist for different values of n and Thiele modulus ϕ.

3. Symmetry reductions for (8)

We firstly analyze Eq. (8). We seek the symmetries admitted by (8). It turns out that for $n = 0$ and 1, Eq. (8) becomes linear and admits eight-dimensional Lie symmetry algebras for both the cases. These cases are not of our interest and are herein omitted. For $n \neq 0, 1$, Eq. (8) admits a two-dimensional non-Abelian algebra viz.,

$$X_1 = \frac{\partial}{\partial x}, \qquad X_2 = x\frac{\partial}{\partial x} - \frac{2u}{n-1}\frac{\partial}{\partial u}, \qquad n \in \Re,\ n \neq 0, 1. \tag{12}$$

We consider two cases for suitable canonical variables.