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Full Length Research Paper

Symmetry reductions and computational dynamics of a nonlinear reaction-diffusion problem with variable thermal conductivity

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In this paper, the nonlinear model for the reaction-diffusion problem with variable thermal conductivity is investigated. It is assumed that the model source term is an arbitrary function of temperature. Classical symmetry is employed to analyze all forms of the source term for which the governing equation admits extra point symmetries. A number of symmetries are obtained and some reductions are performed. Using the fourth-order Runge-Kutta method with a shooting technique, numerical solution of a reduced boundary value problem is obtained. Pertinent results are displayed graphically and discussed quantitatively.

Key words: Symmetry reduction, reaction-diffusion equation, variable thermal conductivity, shooting technique.

INTRODUCTION

Reaction-diffusion equations model creates many problems in mathematical physics, astrophysics, engineering and science (Cebeci and Bradshaw, 1984). In applications to population biology, the reaction term models growth, and the diffusion term accounts for migration. They arise, quite naturally, in chemistry and chemical engineering especially in systems involving constituents locally transformed into each other by chemical reactions and transported in space by diffusion (Kamenetskii, 1969; Balakrishnan, 1996).

The theory of reaction-diffusion equations has long been a fundamental topic in the field of combustion. For many problems of interest, it is characterized by a gradual increase in temperature due to external heating, followed by a rapid temperature increase over a very short time, often referred to as a thermal explosion, as exothermic reactions begin to occur (Barenblatt et al., 1998; Boddington et al., 1977; Makinde, 2005). The concept lends credence to the logic that a conducting medium with temperature-sensitive internal heat generation will burn under a specific circumstance, if it fails to transfer heat adequately to establish a steady-state temperature distribution in the medium. This logic, though academic, is actually a useful link between a mathematical analysis and common sense, and may be the link between an academic exercise and the life span of industrial products, and even public safety (Moitsheki and Makinde, 2008). Moreover, constant thermo-physical properties and uniform heat transfer coefficient are often assumed in the determination of the temperature distribution in a reactive material (Makinde, 2007; Moitsheki and Makinde, 2010). The mathematical complexity of the reaction-diffusion equation is reduced by this assumption and therefore a well-established closed form analytical solution can be obtained for a number of cases. However, this assumption may lead to poor prediction of the thermal performance of the many reactive materials (Zaturska and Banks, 1985; Moitsheki and Makinde, 2007; Lacey and Wake, 1982, Liu, 1987).

The objective of this study is therefore twofold: firstly, a Lie group symmetry reduction is performed on the non-linear reaction-diffusion problem in order to obtain some close form solution for the reduced transient problem with respect to similarity variable; secondly, the governing

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initial boundary value problem is solved numerically using the fourth-order Runge-Kutta method with a shooting technique. Pertinent results are presented graphically and discussed quantitatively.

Mathematical formulation

The mathematical formulation of the reaction-diffusion problem with variable thermal conductivity problem is based on the conservation of energy equation with arbitrary heat source term. We assume that the temperature dependent thermal conductivity follows a power law given by,

$$k = k_0 \left(\frac{T - T_0}{T_w - T_0} \right)^m , \quad (1)$$

where m is the power law index, T_0 is the initial temperature of the material, T_w is the material surface temperature, k_0 is the thermal conductivity coefficient at material surface. The dimensionless reaction diffusion equation together with the corresponding boundary condition is given as

$$\frac{\partial \theta}{\partial t} = \frac{1}{y^n} \frac{\partial}{\partial y} \left[y^n \theta^m \frac{\partial \theta}{\partial y} \right] + \lambda G(\theta) \quad (2)$$

with

$$\theta(y,0) = 0, \; \frac{\partial \theta}{\partial y}(0,t) = 0, \; \theta(1,t) = 1. \quad (3)$$

where λ is the internal heat generation parameter, n represents the material geometry such that n = 0, 1, 2 denotes rectangular, cylindrical and spherical geometries respectively. Dimensional quantities are denoted with a bar, and dimensionless quantities are defined as,

$$\theta = \frac{T - T_0}{T_w - T_0}, y = \frac{\bar{y}}{a}, t = \frac{k_0 \bar{t}}{\rho c_p a^2}, \lambda = \frac{Qa^2}{k_0 (T_w - T_0)}, \quad (4)$$

where T is the absolute temperature, T_0 is the initial temperature of the material, $\bar{t}$ is the time, T_w is the material surface temperature, k_0 is the material thermal conductivity coefficient, ρ is the density, a is the material half width, Q is the heat source parameter, c_p is the specific heat at constant pressure, $\bar{y}$ is the distance measured transverse direction and a is the material radius.

Symmetry techniques for differential equations

The theory and applications of continuous symmetry groups were founded by Lie in the 19th century (Lie, 1881). Modern accounts of this theory may be found in seminal texts such as those of Bluman and Anco (2002), Bluman and Kumei (1989) and Olver (1986). We restrict our discussion to classical Lie point symmetries, since we will only use such symmetries. The reader is referred to Bluman and Anco (2002), Bluman and Kumei (1989) and Olver (1986) for more details on this theory. Given a continuous one parameter symmetry group, it is possible to reduce the number of independent variables by one. Lie's fundamental result is that the whole of one parameter group can be determined from the transformation laws up to the first degree of the parameter ε, that is determination of symmetry groups involves transformations of the form

$$\begin{aligned} y_* &= y + \varepsilon \xi(t, y, \theta) + O(\varepsilon^2); \\ t_* &= t + \varepsilon \tau(t, y, \theta) + O(\varepsilon^2); \\ \theta_* &= \theta + \varepsilon \eta(t, y, \theta) + O(\varepsilon^2); \end{aligned} \quad (5)$$

generated by the vector field

$$X = \tau(t,y,\theta)\frac{\partial}{\partial t} + \xi(t,y,\theta)\frac{\partial}{\partial y} + \eta(t,y,\theta)\frac{\partial}{\partial \theta}, \quad (6)$$

and leave the *2nd* order governing partial differential equation (2) invariant. The infinitesimal criterion for invariance of a PDE such as Equation 2 is given by

$$X^{(2)} Eq.(2)|_{Eq.(2)} = 0, \quad (7)$$

where $X^{(2)}$ is the second extension or prolongation of the infinitesimal generator X. The invariance condition (7) results in an over-determined linear system of determining equations for the coefficients τ, ξ and η. Manipulation of these determining equations to find their solutions is very long and tedious. We omit the calculation but list the results in "Lie point symmetry analysis of Equation 3". It is possible to find all possible functions or cases for the source term $G(\theta)$ such that extra symmetries are admitted by Equation 2. Determination of such cases and symmetries admitted is called *group or symmetry classification*. The problem of group classification was introduced by Lie (Lie, 1881) and recent accounts on this topic may be found for example in Bluman and Kumei (1989), Ivanova and Sophocleous (2006), Ovsiannikov (1959) and Vaneeva et al. (2007). We adopt methods in Bluman and Kumei (1989) (which exclude explicit equivalence transformation analysis) to perform group classification of Equation 2. In this work

Table 1. Extra symmetries admitted by Equation 2.

Forms of *G(θ)*	**Parameters**	**Symmetries**
Θ^p, p, $p \neq 0, 1$	*m* and *n* arbitrary	$X_2 = \frac{1}{2(p-1)}\left[-2\theta\frac{\partial}{\partial\theta} + (p-m-1)y\frac{\partial}{\partial y} + 2(p-1)t\frac{\partial}{\partial t}\right]$
pθ , p	*m* and *n* arbitrary	$X_2 = -\frac{e^{-\lambda pt}}{\lambda mp}\left[\lambda p\theta\frac{\partial}{\partial\theta} + \frac{\partial}{\partial t}\right]$, $X_3 = -\frac{n}{m(n-1)}\left[2\theta\frac{\partial}{\partial\theta} + my\frac{\partial}{\partial y}\right]$.
	n =0, m arbitrary	$X_4 = \frac{\partial}{\partial y}$
p ≠ 0	*m,n* arbitrary	$X_2 = 2\theta\frac{\partial}{\partial\theta} + (m+1)y\frac{\partial}{\partial y} + 2t\frac{\partial}{\partial t}$.
0	*m,n* arbitrary	$X_2 = -\frac{1}{2m}\left[-2\theta\frac{\partial}{\partial\theta} + my\frac{\partial}{\partial y}\right]$, $X_3 = y\frac{\partial}{\partial y} + 2t\frac{\partial}{\partial t}$.

We perform symmetry classification of the source term. Note that we seek point symmetries that leave a single Equation 2 invariant rather than the entire BVP, and apply boundary conditions onto the obtained invariant solutions. It is a well known fact that the symmetry algebra may be reduced if invariance is sought for the entire BVP.

If a differential equation is invariant under some point symmetry, one can often construct similarity solutions which are invariant under some subgroup of the full group admitted by the equation in question. These solutions result from solving a reduced equation in fewer variables.

Lie point symmetry analysis of Equation 3

In the initial Lie point symmetry analysis of Equation 2, where the source term *G(θ)* together with the constants appearing in the Equation 2 are all arbitrary, the admitted principal Lie algebra is one-dimensional and spanned by a translation in time variable. Note that we omit the case m = 0, n = 2 as this renders the governing equation linear. Also, the case *G(θ) = pθ* was dealt with in details in Moitsheki (2008), and here we list some of the results. Furthermore, we have successfully employed symmetry techniques and Adomain methods to determine solutions for nonlinear diffusion with power law heat capacity and source term (Makinde and Moitsheki, 2010). The cases for which the principal Lie algebra extends are listed in Table 1.

Symmetry reduction: Some illustrative examples

Constant G(θ)

Given a non zero constant source term and using the symmetry generator X_2 listed in Table 1 we obtain the functional form of the invariant solution for Equation 2

$\theta = tF(\gamma)$ where $\gamma = yt^{-(m+1)/2}$ and *F* satisfies the nonlinear ordinary differential equation

$$\left\{F + \frac{m+1}{2}\gamma\frac{dF}{d\gamma}\right\} = \frac{1}{\gamma^n}\frac{d}{d\gamma}\left[\gamma^n F^m \frac{dF}{d\gamma}\right] + \lambda p\,. \qquad (8)$$

Linear G(θ)

Given *G(θ) = p θ*, *p* ≠ 0 and using the vector field X_2 listed in Table 1, we obtain the functional form of the

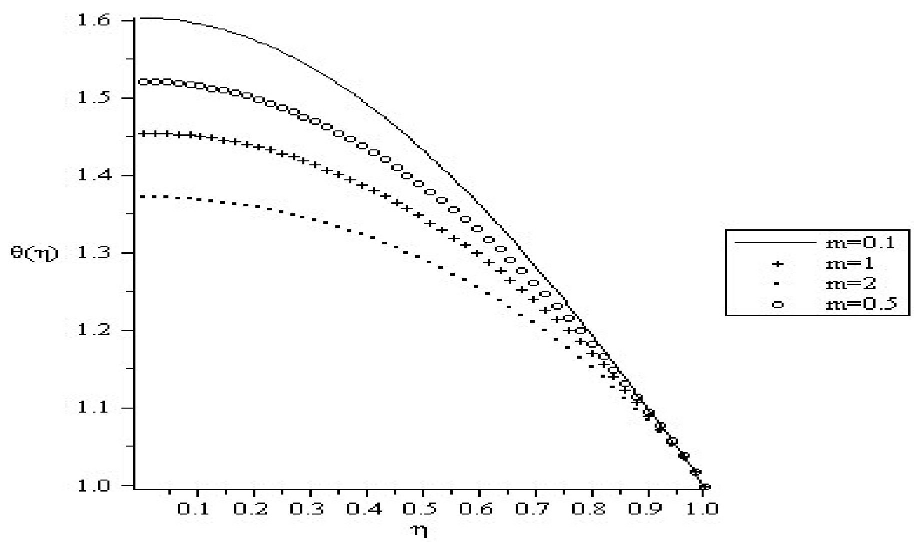

Figure 1. Temperature profiles with increasing thermal conductivity for b=1, λ=0.3, n=0.

invariant solution for Equation 2 (Moitsheki, 2008);

$\theta = e^{\lambda pt} F(y)$ with F satisfying the easily integrated equation

$$\frac{1}{y^n}\frac{d}{dy}\left[y^n F^m \frac{dF}{dy}\right] = 0. \tag{9}$$

In terms of the original variables we obtain the general solution

$$\theta = e^{\lambda pt}\left\{\left(\frac{m+1}{1-n}\right)c_1 y^{1-n} + (m+1)c_2\right\}^{\frac{1}{m+1}}, \quad m \neq -1. \tag{10}$$

Nonlinear G(θ)

Given $G(\theta) = \theta^p$ and using the symmetry generator X_2 listed in Table 1, we obtain the functional form of the invariant solution for Equation 2

$$\theta = t^{\frac{1}{1-p}} F(\gamma)$$

where $\gamma = y t^{(p-m-1)/2(1-p)}$ and F satisfies the nonlinear ordinary differential equation

$$\left\{\frac{1}{1-p}F + \frac{p-m-1}{2(1-p)}\gamma\frac{dF}{d\gamma}\right\} = \frac{1}{\gamma^n}\frac{d}{d\gamma}\left[\gamma^n F^m \frac{dF}{d\gamma}\right] + \lambda F^p. \tag{11}$$

Unfortunately the reduced ordinary differential equations are highly nonlinear and may only be solved numerical.

Computational method

In order to tackle the problem, we first transform Equation 2 into a non-linear ordinary differential equation using the Boltzmann similarity variable $\eta = y/\sqrt{t}$, and we obtain

$$\frac{1}{\eta^n}\frac{d}{d\eta}\left[\eta^n \theta^m \frac{d\theta}{d\eta}\right] + \frac{\eta}{2}\frac{d\theta}{d\eta} + \lambda H(\theta) = 0 \tag{12}$$

with

$$\frac{d\theta}{d\eta}(0) = 0, \quad \theta(1) = 1, \tag{13}$$

where the arbitrary heat source function in Equation 2 is defined as $G(\theta)=H(\theta)/t$. The non-linear differential Equation 12 together with the boundary conditions in Equation 13 is solved numerically using the fourth-order Runge-Kutta method with a shooting technique and implemented in Maple (Heck, 2003). The step size 0.001 is used to obtain the numerical solution with seven-decimal place accuracy as the criterion of convergence.

RESULTS AND DISCUSSION

Figures 1 to 3 illustrate the effects of various thermo-physical parameters on the material temperature profiles. Here, we have assumed an exponentially increasing temperature dependent heat source term given by $H(\theta) = e^{b\theta}$, where $b > 0$ is the internal heat generation parameter. Generally, the material temperature is highest

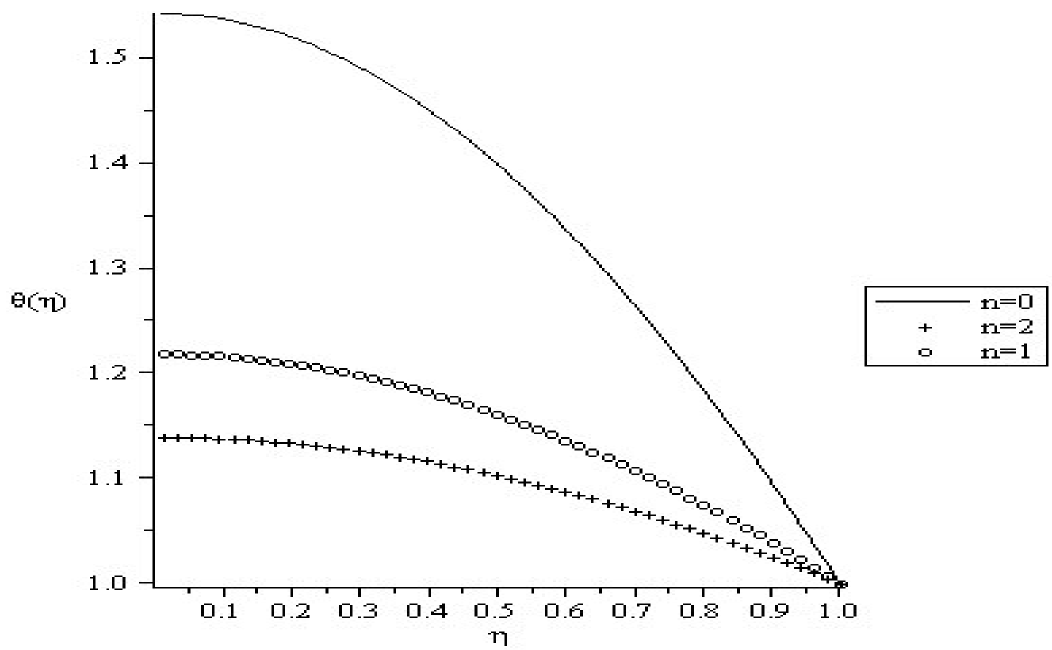

Figure 2. Temperature profiles for varying geometry *b*=1, *λ*=0.3, *m*=0.3.

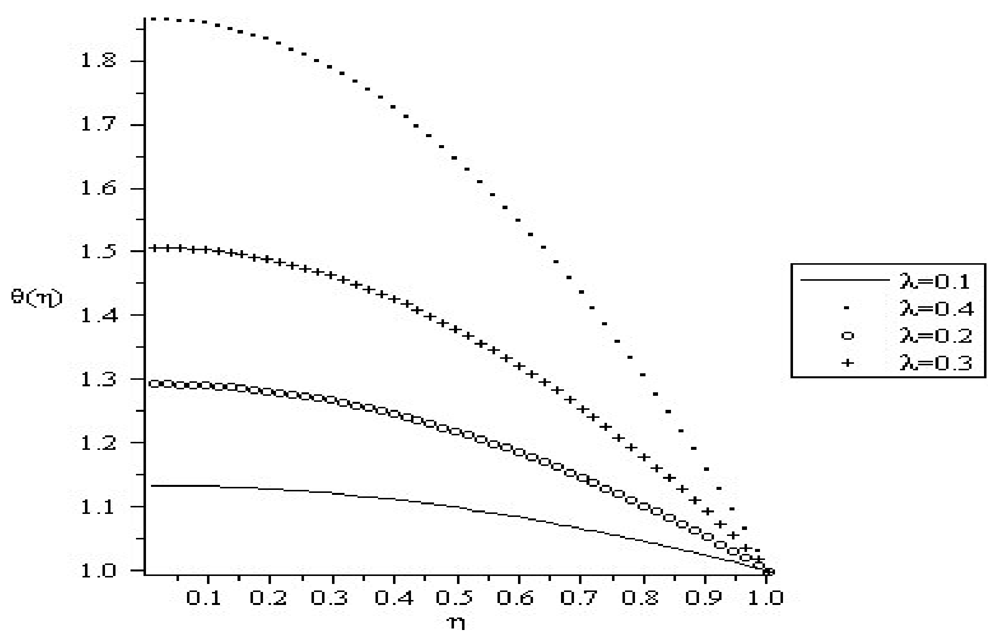

Figure 3. Temperature profiles increasing hest source parameter *b*=1, *n*=0.3, *m*=0.3.

along the centerline and minimum at the surface. Figure 1 shows that the temperature decreases with increasing thermal conductivity of the material. Moreover, it is interesting to note that for a given set of parameter values, highest temperature is observed for materials with rectangular geometry (*n*=0) and lowest temperature for materials with spherical geometry (*n*=2) as illustrated in Figure 2. In Figure 3, we observe that the material temperature increases with an increase in the values of heat source parameter. This clearly implies that an increase in the internal heat generation invariably leads to an elevation in the material temperature.

Conclusion

We have successfully applied the symmetry techniques to a model for reaction-diffusion with variable thermal conductivity. The group classification of Equation 2 is a significant improvement on the results obtained in Moitsheki (2008). The class of equations considered here is in fact a subclass of equations in Moitsheki and Makinde (2010). However, in this manuscript we have provided not only the symmetry analysis but also the numerical results. Pertinent results are presented graphically and discussed quantitatively.

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