Unsteady Flow Of Chemically Reacting Temperature Dependent Fluid Flows Through A Porous Vertical Surface

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Abstract - The motivation of present research paper is to analyze the Steady Flow of Chemically Reacting Temperature Dependent Fluid Flows through a Porous Vertical Surface analytical technique for temperature equation and numerical technique for velocity field, under which consistency and convergence criterion exist. The results show increase velocity with increases as thermal Grashof number increases, while velocity decreases with increase in viscosity and suction parameters. It is also established that there exist a linear relationship between the thermal buoyancy and the fluid velocity. The temperature on the other hand, is a decreasing function of suction parameter or the spatial variable.

Keywords—Newtonian fluids; non-Newtonian fluid; chemically reacting fluid; combustion; Arrhenius kinetics; incompressible Navier-Stokes equations;

Subject Classification: 76D05, 76V05, 80A32

1. Introduction

A chemically reacting flow is a fluid flow in which a chemical reaction is also occurring. Such flows occur in a wide range of fields including combustion, chemical engineering, biology, and pollution abatement. For most liquids, the viscosity decreases with temperature and increases with pressure. For gases, it increases with both temperature and pressure [1]. In general, the higher the viscosity of a substance, the more resistance it presents to flow (and hence more difficult to pump). Ever since the formulation of the equations of continuity (mass) and momentum (Cauchy, Navier-Stokes), the fluid dynamics of Newtonian fluids has come a long way during the past 300 or so years, albeit significant challenges especially in the field of turbulence and multi-phase flows still remain [2]. It is appropriate to mention here that it has long been a matter of debate and discussion in the literature whether a true yield stress exists or not, for example, [3] and the review of [4] for different viewpoints on this matter. Evidently, the answer to the question whether a substance has a yield stress or not seems to be closely related to the choice of a time scale of observation. In spite of this fundamental difficulty, the notion of an apparent yield stress is of considerable value in the context of engineering applications, especially for product development and design in food, pharmaceutical and healthcare sectors, [5] and [6].

Of the time-independent fluids, this sub-class has generated very little interest and hence very few reliable data are available. Indeed, until up to about early 1980s, this type of flow behavior was considered to be rare, but, however, with the recent growing interest in the handling and processing of systems with high solids loadings, it is no longer so, this is explained in [7], [8], [9], for instance. Exothermic and endothermic chemical reactions and its application to processes of ignition and combustions has been a subject of intense study by scientists. In a study carried out by [10], a three-component model of a system is considered which includes exothermic oxidation and endothermic evaporation process. They report that, the full system can be approximated and the safe and dangerous regions of parameter space can be identified by assuming a slow rate of consumption of fuel and oxygen.

Significant research effort has been expended in seeking a similar expression for \( \sigma \) for non-Newtonian fluids which should be able not only to predict shear-dependent viscosity, yield stress, visco-elastic effects in shear and extensional flows, rheopexy and thixotropy but should also satisfy the requirements of frame indifference, material objectivity, etc. [11], [12], [13], [14], [15] amongst others gives critical appraisals of the current state of the art and useful guidelines for
the selection of an appropriate expression for $\sigma$ (constitutive equation) which are available in the literature. Therefore, if one were able to develop an appropriate constitutive equation and/or to choose one from the existing selection, it is possible to set up the governing differential equations together with suitable boundary conditions, albeit there are situations in which the prescription of boundary conditions is also far from obvious, particularly in flows with a free surface, slip etc.

Rout [16] investigate the influence of chemical reaction and the combined effects of internal heat generation and a convective boundary condition on the laminar boundary layer MHD heat and mass transfer flow over a moving vertical flat plate. The effects of physical parameters on the velocity, temperature, and concentration profiles are illustrated graphically. Other relevant discussion could be found in the work of [17].

For most elementary reactions, the rearrangement of atoms in going from reactants to products via a transition state proceeds through the movements of atomic nuclei that experience a potential energy field that is generated by the rapid motions of the electrons in the system. On this potential energy surface there will be a path of minimum energy expenditure for the reaction to proceed from reactants to products (reaction coordinate). The low energy positions of reactants and products on the potential energy surface will be separated by a higher energy region. The highest energy along the minimum energy pathway in going from reactants to products defines the transition state, [18]. Hence the motivation for this work is to unsteady flow of chemically reacting temperature dependent fluid flows through a porous vertical surface.

2. Physical Processes and Mathematical Formulation of Problem

Three physical processes are involved in a reacting flow: (1) the fluid dynamics, (2) the thermodynamics, and (3) the chemical reactions. The fluid dynamics process is the balance between the temporal evolution and the spatial convection of the flow properties due to conservation of mass, momentum, and energy. The thermodynamics of the reactive fluid include microscopic heat transfer between gas molecules, work done by pressure, and the associated volume change. And, chemical reactions determine the generation/destruction of chemical species under the constraint of mass conservation.

Each of the above processes could be either evolving or in equilibrium. For the evolving condition, each above process has its own space and time scales, and they are very different from that of other processes. Such differences in space and time scales, on one hand, could allow simplification in the theoretical model. On the other hand, they could be the source of numerical difficulties. In this work, we assume that the space and time scales of fluid dynamics and chemical reactions are much larger than that of thermodynamics. Thus, the thermodynamic process is always considered to be in equilibrium. From the viewpoint of thermodynamics, the chemical composition of the reactive gas mixture is locally frozen, and the gas mixture is locally motionless a condition which is referred to as thermal equilibrium.

Thus, we restrict our discussion to the flow part only. In principle, one can always set up the equation of continuity and Cauchy’s momentum equations (written in their compact form for an incompressible fluid) as follows:

$$\nabla \cdot \mathbf{V} = 0$$

$$\frac{\rho \partial \mathbf{V}}{\partial t} = -\nabla p + \rho g + \nabla \cdot \mathbf{\sigma}$$

For Newtonian fluids, the deviatoric stress tensor $\mathbf{\sigma}$ is related to the rate of deformation tensor.

In particular, all three of these quantities are coupled. The fluid flow moves around the chemicals and the chemicals react, which produces or absorbs heat and affects the temperature; and, finally, the temperature affects the fluid flow through buoyancy effects.

Considering mass fractions instead of concentrations, we then have the properties

$$\sum_{i=1}^{N} Y_i(x, t) = 1 \quad \text{for all } x \in \Omega \quad \text{and } t \geq 0,$$

and

$$0 \leq Y_i(x, t) \leq 1, \quad \text{for all } x \in \Omega \quad \text{and } t \geq 0.$$

We assume that the equations hold in a $C^2$ bounded domain $\Omega \subset \mathbb{R}^3$. Using the above notation our model for incompressible reacting flows takes the form

$$\nabla \cdot \mathbf{u} = 0,$$

$$\partial_t \mathbf{u} - Pr \Delta \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = f_0(T),$$

$$\partial_t \nabla T + (\mathbf{u} \cdot \nabla) T = \sum_{i=1}^{N} h_i W_i(Y_{i}, \cdots, Y_{v}, T)$$
\[
\partial_t Y_i - \frac{1}{Le} \Delta Y_i + (u \cdot \nabla) Y_i = W_i(Y_i, \cdots, Y_j, T) \tag{6}
\]

\( W_i(Y_i, \cdots, Y_j, T) \) describes the change in mass fractions due to the reaction. The first two equations are the usual Navier-Stokes equations, and the second two are reaction-diffusion equations with a transport term added. The central assumption made in deriving these equations is that the fluid has constant density. Further physical background on these equations, are contained in [19] and [20].

The most common model of chemical kinetics is the so-called Arrhenius model in which the \( W_i \) take the form

\[
W_i(Y_i, \cdots, Y_j, T) = \sum_{j=1}^{m_i} A_i e^{-E_j/RT} \prod_{k=1}^{N} c_i^{v_{j,k}},
\]

where \( v_{j,k} \) are nonnegative integers, where at least one of \( v_{j,k} \), for \( k = 1, \ldots, N \), is nonzero for each \( j \).

We consider schematically pictured in Fig. 1. In this case one set of reactants enters on one portion of the boundary, another set enters on another portion, they mix and react in the middle, and then the products leave.

Since we have chemicals and heat flowing into and out of the system, an important quantity to consider is how much of each flows in and out of the system. We can formally derive this quantity from the equations in (6) in the following way. We consider first the rate of change of the total amount of \( Y_i \) in the domain.

\[
\partial_t \int_\Omega Y_i \, dx = \int_\Omega \partial_t Y_i \, dx = \int_\Omega \frac{1}{Le} \Delta Y_i + (u \cdot \nabla) Y_i + W_i \, dx
\]

Now using the identity

\[
\nabla \cdot (u Y_i) = Y_i \nabla \cdot u + (u \cdot \nabla) Y_i
\]

the divergence free property of \( u \), and the divergence theorem, we get

\[
\partial_t \int_\Omega Y_i \, dx = \int_\Omega \frac{1}{Le} \nabla \cdot (\nabla Y_i - \nabla \cdot (u Y_i)) + W_i \, dx
\]

where \( n \) is the outward unit normal to \( \partial \Omega \). This implies that the rate of change of the total amount of \( Y_i \) in the domain is due to three terms which we can physically interpret as diffusion across the boundary, fluid transport across the boundary, and changes due to reactions in the domain.

Now, for the physical boundary conditions to be used, we will assume the existence of a partition \( \partial \Omega = \Gamma_u \cup \Gamma_g \cup \Gamma_w \) corresponding to the portions of the boundary where fluid flows into the domain, portions where fluid flows out, and the walls of the container, respectively. On all of \( \partial \Omega \), the fluid flow \( u \) will be specified by Neumann boundary data; however, the boundary conditions for \( T \) and \( Y_i \) will vary across the partition.

Combining equations (3) to (8), velocity and Temperature fields could be expressed as

\[
\rho \left( \frac{\partial u}{\partial t} + v_0 \frac{\partial u}{\partial y} \right) = \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right) + \rho g \beta (T - T_0) \tag{9}
\]

\[
\rho c_p \left( \frac{\partial T}{\partial t} + v_0 \frac{\partial T}{\partial y} \right) = \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) \tag{10}
\]

The appropriate initial and boundary conditions are

\[
t \leq 0: u = 0 \quad T = T_0 \quad \forall y
\]

\[
t > 0: \begin{cases} u = U_0 & T = T_1 & y = 0 \\ u = 0 & T = T_0 & y \to \infty \end{cases}
\]

(11)

Where all the variables and parameters have their usual meaning.

3. Method of Solution

The viscosity is define as \( \mu = e^{-E/RT} \)

Using the following dimensionless quantities

\[
e \left( \frac{T - T_0}{RT_0^2} \right) = \theta, \quad \frac{u}{U_0}, \quad \frac{t}{t_0}, \quad \frac{y}{h}
\]

Equations (9) and (10) becomes

\[
\frac{\partial}{\partial t} \phi(y,t) = -s \frac{\partial}{\partial y} \phi(y,t) = \frac{\partial}{\partial y} \left( e^{\theta(y,y)} \frac{\partial}{\partial y} \phi(y,t) \right) + Gr \theta(x,t) \tag{12}
\]

\[
\frac{\partial \theta(y,t)}{\partial t} - s \frac{\partial}{\partial y} \phi(y,t) = \frac{\partial^2}{\partial y^2} \theta(x,t) \tag{13}
\]

where

\[
s = \frac{v_0}{U_0}, U_0 = \frac{\mu_0}{\rho h} Gr t, \quad s = e^\frac{\theta(y,y)}{E/RT_0^2}, P = \frac{\mu c_p}{k}
\]

The above system is solved using Maple module for solving partial differential equations. The method used support pdsolve(PDEsys,conditions, numeric, vars, options) command which returns a module that can be used to compute numerical solutions for time-based PDE systems over a fixed finite 1-space interval. The pdsolve/numeric routine uses finite difference methods to obtain these numerical solutions [21]. Time-based Solver mode of operation uses the default method, which is a centered implicit scheme, the PDE system is sufficiently close to a standard form for the method to find the numerical solution. The optional equations for the default method used is ‘time’ = name,’range’ = l..r. The values of both options are determined automatically since the boundary conditions are specified for both end points of the domain. This option related to error estimation, and error control. Plot and plot3d are
methods used to compute/or view the solution of our input PDE returned by pdsolve/numeric module. In addition, the settings method is configured to query/set certain parameters of the solution process [22].

4. Results and Discussion

For the purpose of discussing the effect of various parameters on the reaction behavior, calculations have been carried out for different values of $s, \lambda$ and $Grt$ and for fixed values of $Pr$ and $\epsilon$. In order to point out the effects of these parameters on flow characteristic, to be realistic, the value of Prandtl number is chosen to be $Pr = 0.71$ which represents air at temperature $25^\circ C$ and one atmospheric pressure. All parameters are primarily chosen as follows: $s = 0.1, Grt = 0.5$ and $\lambda = 0.1$ for a fixed value of $Pr = 0.71$ and $\epsilon = 0.05$ unless otherwise stated.

Fig. 2 shows the velocity distribution with respect to space and time. It could be seen that maximum velocity occur close to the surface but not on the surface as previously reported in the literature, and decreases away from the fluid moves along the channel. Also, initially the fluid flow velocity increases with time until a time when the steady state is reached after which the velocity decreases. This is corroborated in Fig. 3, where it is seen that velocity increases with time. In addition, at the initial stage of the flow, the maximum velocity was on the surface but drifted afterward to the body of the fluid close to the surface. This is confirmed by profile of $\phi(y,t)$ at $t = 2$.

The effect of suction parameter is shown in Fig. 4. We observe the occurrence of peak in the profile when $s < 1$ but fissured out when $s > 1$. The implication of this is that when there is suction, the maximum velocity is on the surface, otherwise in the body of the fluid if suction is zero. We also observe that increase in suction reduces the velocity as well as the velocity boundary layers. We displayed the effect of viscousity parameter on the flow velocity in Fig. 5. It is observed that the velocity is maximum when viscousity is zero but reduces with an increase in viscousity. This confirm the scenario that the higher the viscousity the more difficult it is for fluid to flow. While in Fig. 6, we show the variation of thermal buoyancy effect on the velocity. It is observed that increase in the thermal buoyancy brings about increase in velocity boundary layer. We also observe a reverse flow within the body of flow as $y \rightarrow 3$ unit.

Fig. 7 to 9 displays the variation of temperature distributions. In Fig. 7, we shows the 3d temperature distribution with respect to time and spatial variables. From the figure, we observe that the temperature decreases asymptotically along the channel but increases with respect to spatial variable until a steady state is attained when further increase in time is less significant as shown in figure 8. While in Fig. 9, we show the effect of suction parameter on temperature distributions. It could be seen from the figure that increase in suction reduces temperature as well as temperature boundary layer.

![Figure 2: 3d velocity profile in $(t,y)$ Coordinates](image)

![Figure 3: Velocity distributions at different time](image)

![Figure 4: Velocity distributions at different suction values](image)

![Figure 5: Temperature distributions](image)
7. Conclusion

The motivation of present research paper is to analyze the Steady Flow of Chemically Reacting Temperature Dependent Fluid Flows through a Porous Vertical Surface analytical technique for temperature equation and numerical technique for velocity field, under which consistency and convergence criterion exist. The theoretical non-linear model for velocity has been derived by employing the Cauchy momentum equation. From our analysis, the following deductions were made:

- that velocity increases as thermal Grashof number increases
- that there is a linear relationship between the thermal buoyancy and the fluid velocity
- that the momentum boundary thickens as Grashof number increases
- that increase in viscousity parameter brings about reduction in the fluid flow
- that increase in suction parameter brings about reduction in the fluid flow
- that temperature is a decreasing function of suction parameter or the spatial variable
**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$u$</td>
<td>dimensional velocity field</td>
</tr>
<tr>
<td>$T_1$</td>
<td>surface temperature</td>
</tr>
<tr>
<td>$T$</td>
<td>dimensional temperature field</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Spatial coordinate</td>
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<tr>
<td>$k$</td>
<td>thermal conductivity</td>
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<tr>
<td>$R$</td>
<td>universal gas</td>
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<td>$T_0$</td>
<td>free stream temperature</td>
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<tr>
<td>$\rho$</td>
<td>density</td>
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<tr>
<td>$m_i$</td>
<td>molecular weight of chemical species $i$</td>
</tr>
<tr>
<td>$c_p$</td>
<td>specific heat at constant pressure</td>
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<td>$E$</td>
<td>the activation energies</td>
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<td>Prandtl number</td>
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<td>dimensionless temperature</td>
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<tr>
<td>$\phi$</td>
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<td>$\epsilon$</td>
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**References**


