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

Okedoye A. M.

Department of Mathematics and Computer Science, Federal University of Petroleum Resources, Effurun, Nigeria, E – mail: okedoye.akindele@fupre.edu.ng,

Okewale A. O.

Department of Chemical Engineering, Federal University of Petroleum Resources, Effurun, Nigeria, E – mail: okewale.akindele@fupre.edu.ng,

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 viscousity 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 flow; combustion; Arrhenius kinetics; incompressible Navier-Stokes equations;

Subject Classification: 76D05, 76V05, 80A32

¹Corresponding Authour

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 the fluid momentum (Cauchy, Navier-Stokes), 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 Onifade Y. S.

Department of Physics, Federal University of Petroleum Resources, Effurun, Nigeria, E – mail: onifade.yemi@fupre.edu.ng

Akinrinmade V. A.

Department of Mathematics and Statistics, osun State College of Technology, Esa-Oke, Osun State, Nigeria

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 σ for non-Newtonian fluids which should be able not only to predict sheardependent 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



Figure 1. Domain Ω configuration

the selection of an appropriate expression for σ (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 eauilibrium.

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:

$$\nabla \cdot V = 0 \tag{1}$$

$$\frac{\rho DV}{Dt} = -\nabla p + \rho g + \nabla \cdot \sigma \tag{2}$$

For Newtonian fluids, the deviatoric stress tensor σ 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

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

and

$$0 \le Y_i(x,t) \le 1$$
, for all $x \in \Omega$ and $t \ge 0$

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

$$\nabla \cdot u = 0, \tag{3}$$

$$\partial_t u - Pr\Delta u + (u \cdot \nabla)u + \nabla p = f_0(T),$$
 (4)

$$\partial_t u - \Delta T + (u \cdot \nabla)T = \sum_{i=1}^N h_i W_i(Y_1, \cdots, Y_1, T) \quad (5)$$

$$\partial_t Y_i - \frac{1}{Le} \Delta Y_i + (u \cdot \nabla) Y_i = W_i(Y_1, \cdots, Y_1, T)$$
 (6)

 $W_i(Y_1, \dots, Y_1, T)$ 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

$$W_i(Y_1, \cdots, Y_1, T), = \sum_{j=1}^{m_i} A_j e^{-E_j/R_0 T} \prod_{k=1}^N C_k^{\nu_{j,k}},$$

where $v_{j,k}$ are nonnegative integers, where at least one of $v_{j,k}$, for k = 1, ..., 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.

$$\partial_t \int_{\Omega} Y_i \, dx = \int_{\Omega} \partial_t Y_i \, dx = \int_{\Omega} \frac{1}{Le} \Delta Y_i + (u \cdot \nabla) Y_i + W_i dx$$
$$\partial_t \int_{\Omega} Y_i \, dx = \int_{\Omega} \frac{1}{Le} \Delta Y_i + (u \cdot \nabla) Y_i + W_i dx \tag{7}$$

Now using the identity

$$\nabla \cdot (uY_i) = Y_i \nabla \cdot u + (u \cdot \nabla)Y_i$$

the divergence free property of u, and the divergence theorem, we get

$$\partial_t \int_{\Omega} Y_i dx = \int_{\Omega} \frac{1}{Le} \nabla \cdot \nabla Y_i - \nabla \cdot (uY_i) + W_i dx$$
$$= \int_{\partial \Omega} \frac{1}{Le} \frac{\partial Y_i}{\partial n} - Y_i (u \cdot n) dS + \int_{\Omega} W_i dx \quad (8)$$

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 $\partial \Omega = \Gamma_1 \cup \Gamma_0 \cup \Gamma_w$ 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 Neuman 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

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

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

The appropriate initial and boundary conditions are

$$t \le 0: \ u = 0 \quad T = T_0 \quad \forall y \\ t > 0: \begin{cases} u = U_0 \ T = T_1 \ y = 0 \\ u = 0 \ T = T_0 \ y \to \infty \end{cases}$$
 (11)

Where all the variables and parameters have their usual meaning.

3. Method of Solution

The viscousity is define as $\mu = e^{-E/_{RT}}$

Using the following dimensionless quantities

$$\frac{E(T-T_0)}{RT_0^2} = \theta, \frac{u}{U_0} = \phi, t = \frac{\rho U_0^2}{\mu_0} t', y = \frac{1}{h} y'$$

Equations (9) and (10) becomes

$$\frac{\partial}{\partial t} \phi(y,t) - s \frac{\partial}{\partial y} \phi(y,t) = \frac{\partial}{\partial y} \left(e^{\frac{\lambda \theta(y,t)}{1 + \epsilon \theta(y,t)}} \frac{\partial}{\partial y} \phi(y,t) \right) + Grt \theta(x,t) \quad (12)$$
$$\frac{\partial \theta(y,t)}{\partial t} - s \frac{\partial}{\partial y} \phi(y,t) = \frac{1}{Pr} \frac{\partial^2}{\partial y^2} \theta(x,t) \quad (13)$$

where

$$s = \frac{v_0}{U_0}, U_0 = \frac{\mu_0}{\rho h} Grt = \frac{g\beta\mu_0 RT_0^2}{\epsilon T_0}, Pr = \frac{\mu c_p}{k},$$

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 timebased 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, λ and Grt and for fixed values of Pr and ϵ . 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 fromas 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 in corroborated in Fig. 3, where it is seen that velocity increases with time. In addition, at the initial stageof 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 effecte of suction parameter is shown in Fig. 4. We observe the occurrence of peak in the profile but fissuled out when s > 1. The when s < 1implication 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 obersve 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 thermak buoyancy effect on the velocity. It is observed that increase in the thermal buoyancy brings about increase in velocity boundary layer. We also oberve a reverse flow within the bodu 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 decreasesassymptotically 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



Figure 3: Velocity distributions at different time



Figure 4: Velocity distributions at different suction values



Figure 5: Velocity distributions at different viscousity parameter



Figure 6: Velocity distributions at different values of thermal buoyancy



Figure 7: 3d Temperature distributions

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



Figure 8: Temperature distributions at different time t



Figure 9: Temperature distributions at different values of suction parameter

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

и	dimensional velocity field	t	Time
T_1	surface temperature	R	universal gas
Т	dimensional temperature field	θ	dimensionless temperature
у	Spatial coordinate	Ø	dimensionless velocity
k	thermal conductivity	Pr	Prandtl number
T_0	free stream temperature	ρ	density
m_i	molecular weight of chemical species <i>i</i>	ε	$0 < \epsilon \ll 1$
c_p	specific heat at constant pressure	μ	Dynamic viscousity
Ε	the activation energies		

Nomenclature

References

[1.] Reid R. C., Prausnitz JM, Sherwood TK. The properties of gases and liquids. 3rd edn. McGraw-Hill, New York. (1977)

[2.] Uhlherr P. H. T, Guo J, Zhang XM, Zhou JZQ, Tiu C (2005). The shear-induced solid-liquid transition in yield stress materials with chemically different structures. J Non-Newt Fluid

[3.] Barnes H. A., Walters K (1985) The yield stress myth? Rheol Acta 24: 323-326.

[4.] Barnes H. A. (1989). Review of shearthickening (dilatancy) in suspensions of nonaggregating solid particles dispersed in Newtonian liquids. J Rheol 33:329-366.

[5.] Barnes H. A. (1999). The yield stress- a review or everything flows? J Non-Newt Fluid Mech 81: 133-178.

[6.] Steffe J. F. (1996). Rheological methods in food process engineering. Freeman, East Lansing, MI.

[7.] Barnes H. A., Hutton JF, Walters K (1989). An introduction to rheology. Elsevier, Amsterdam.

[8.] Boersma W. H., Laven J, Stein HN (1990). Shear thickening (dilatancy) in concentrated suspensions. AIChEJ 36: 321-332.

[9.] Goddard J. D, Bashir Y. M. (1990). On Reynolds dilatancy. In: recent developments in structured continua. Longman, London.

[10.] Truscott, J. E.; Brindley, J.; Mcintosh, A; and Griffiths J (1996). The effect of diffusion on the antiignition of combustible fluids in insulation materials. IMAG of Appl. Maths 57,pp 257-271.

[11.] Bird R. B., Armstrong RC, Hassager O (1987). Dynamics of polymeric liquids. Vol I and II, 2nd edn. Wiley, New York.

[12.] Graessley W. W. (2004). Polymer liquids and networks: structure and properties. Garland science, New York.

[13.] Kroger M. (2004). Simple models for complex non-equilibrium fluids. Phy. Rep. 390: 453-551.

[14.] Morrison F. A. (2001). Understanding rheology. Oxford university press, New York.

[15.] Tanner R. I. (2000). Engineering rheology. 2nd edn. Oxford university press, London.

[16.] Rout B. R., Parida, S. K., and Panda, S. (2013). MHD Heat and Mass Transfer of Chemical Reaction Fluid Flow over a Moving Vertical Plate in Presence of Heat Source with Convective Surface Boundary Condition

[17.] Chhabra R. P., Richardson JF (2008) Non-Newtonian flow and applied rheology. 2nd edn. Butterworth-Heinemann, Oxford.

[18.] Mark E. Davis and Robert J. Davis Fundamentals of Chemical Reaction Engineering, *McGraw-Hill Higher Education*, (2003)

[19.] Buckmaster, J. D. and Ludford, G. S. S. (1983). ``Lectures on Mathematical Combustion," CBMS-NSF Regional Conference Series in Applied Mathematics, No. 43, SIAM, Philadelphia.

[20.] Williams, F. A. ``Combustion Theory: The Fundamental Theory of Chemically Reacting Flow Systems," 2nd ed., Benjamin_Cummings, Menlo Park, CA, 1985.

[21.] Boyce, W.E., and DiPrima, R.C. Elementary Differential Equations and Boundary Value Problems. New York: John Wiley & Sons, 1997.

[22.] Strikwerda, J. C. Finite Difference Schemes and Partial Differential Equations. Wadsworth and Brooks/Cole, 1989.