Transport of petroleum hydrocarbons in the subsurface with internal heat generation

Nirmala P. Ratchagar and Hemalatha S.V.*

Department of Mathematics, Annamalai University, Annamalainagar, Tamilnadu-608 002, India.

Abstract

The objective of the present study is to investigate the transport of hydrocarbons on the unsteady two dimensional laminar oil flow through the subsurface including internal heat generation and homogeneous first-order chemical reaction. The highly nonlinear coupled differential equations governing the fluid flow, heat and mass transfer are simplified and solved using perturbation technique. The dimensionless velocity of oil flow in the subsurface, temperature of the medium, concentration of the hydrocarbons in water and the coefficient of skin friction for all time are obtained and displayed graphically showing the effects of the different parameters involved.

Keywords: Concentration of hydrocarbons, Buoyancy effects, Retardation, Chemical reaction.

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1 Introduction

Problems of solute transport in two-dimension involving sequential first order decay reactions and retardation coefficient frequently occurs in soil and groundwater systems, for example the migration of simultaneous movement of petroleum hydrocarbons, organic phosphate transport and the transport of pesticides and their metabolites. Water in the soil environment forms a mixture with petroleum products which makes the hydrocarbon components difficult to separate. The flow of hydrocarbon products through the soil causes physical, chemical and biochemical changes. The direction and rate at which these contaminants spread are dependent not only on their own properties, but also on soil properties. When entering the subsurface, some of the petrochemical products get adsorbed on soil while others infiltrate deep into soil and reach the underground water table [1].

Subsurface is the area located immediately below the land surface which has the highest concentration of organic matter and microorganisms and is where most of the earth’s biological soil activity occurs. Several mathematical methods have been reported by many authors for the transport of hydrocarbons in the subsurface. Some of them include, numerical model of multiphase immiscible flow for evaluating nonaqueous phase liquids(NAPL) such as petroleum hydrocarbons and water phase flow in a two phase(water, NAPL) and three phase(air, water and NAPL) system [2,3,4,5,6,7]. Li and Zienkiewicz [8] and Rahman and Lewis [9] extended the above study for deforming soil. Addition of oxygenates such as ethanol, even though reduced the atmospheric pollution due to vehicular emission, increased the downward
migration of hydrocarbons to groundwater by lessening the adsorptive capacity of the surface soil component have been experimentally showed by Adam et al. [10].

Sabbah et al. [11] studied the transport of polycyclic aromatic hydrocarbons in porous medium in the presence of dissolved organic matter and predicted the sorption constants of polycyclic aromatic hydrocarbons to soil and their binding constants to dissolved organic matter using breakthrough curves. An analytical solution of fingering phenomenon arising in double phase flow of water injected with constant velocity into a dipping oil saturated porous medium using calculus of variation and similarity theory have been presented by Mukherjee and Shome [12].

A mathematical model of groundwater contamination by hydrocarbons migrating in the soil have been developed by Gawdzik and Zygodlo [13]. They verified the results experimentally by soil filter test. Abdulkadir and Yahaya[14] proposed a model equation with the aid of MINITAB software for dispersion of crude oil on land. An experimental investigation was carried out by Okop and Ekpo [15] for crude oil spillage contamination of soil to classify the hydrocarbon penetration in the soil depths according to their chemical similarities.

The study of heat generation in moving fluids is important in view of several physical problems such as those dealing with chemical reactions. Possible heat generation effects may change the temperature distribution. El-Hakiem [16] and many authors [17,18,19] studied the effects of heat generation or absorption those dealing with chemical reactions. Possible heat generation effects may change the temperature distribution. El-Hakiem [16] and many authors [17,18,19] studied the effects of heat generation or absorption.

Motivated by these studies, we have investigated the combined effects of chemical reaction and internal heat generation in the subsurface. The study area containing water as native fluid is considered to be homogeneous porous medium bounded by porous layers on both the upper surface and lower surface. The soil and the fluids are supposed to be incompressible and the flow is transient, two dimensional. We assume that the solute diffuses and simultaneously undergoes first order irreversible chemical reaction. The effects of heat generation due to friction has been taken into consideration. The governing equations are simplified using perturbation technique and solved numerically.

## 2 Mathematical Formulation

The mathematical model is a nonlinear system that includes the continuity equation, equation of momentum in the presence of thermal and concentration buoyancy effects including Darcian term, the energy equation with heat generation and the species equation with homogeneous first order chemical reaction defined by equations (2.1)-(2.5). These are written as:

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0
\]  

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \nu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + g \beta_T (T - T_1) + g \beta_C (C - C_1) - \frac{v}{k_p} u
\]  

\[
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = \nu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - \frac{v}{k_p} v
\]  

\[
\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{k_T}{\rho C_p} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \frac{Q_0}{\rho C_p} (T - T_1)
\]  

\[
\beta_w \frac{\partial C}{\partial t} + \beta_T \frac{\partial C}{\partial x} + \beta_T \frac{\partial C}{\partial x} + \beta_T \frac{\partial C}{\partial y} = \beta_w D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) - \beta_w k_1 (C - C_1)
\]  

where, \(u\) and \(v\) are the components of velocities along \(x\) and \(y\) directions, respectively, \(T\) is the temperature distribution in the region, \(Q_0\) is the heat generation constant, \(C\) is the concentration of hydrocarbons in water, \(S\) is the concentration of adsorbed oil in soil, \(\nu\) is the kinematic viscosity of oil, \(g\) is the gravitational acceleration, \(\beta_T\) and \(\beta_C\) are the thermal and concentration expansion coefficients, respectively, \(k_p\) is the permeability of the medium, \(T_1\) and \(C_1\) are the temperature and concentration at the upper surface, respectively, \(\rho\) is the density of oil, \(C_p\) is the specific heat at constant pressure, \(k_T\) is the thermal conductivity, \(\rho_b\) is the soil bulk density, \(\beta_w\) is the volumetric water content of soil, \(D\) is the mass diffusivity and \(k_1\) is the chemical reaction rate parameter.
We now introduce the following non-dimensional quantities: 

\[ u \]

which form a system of nonlinear partial differential equations are simplified using perturbation technique. 

Making use of the non-dimensional variables in equations (2.1) to (2.4) and (2.6), neglecting the '*' symbol \( \theta \) where, 

\[ \alpha \]

where, \( u \) and \( v \) are dimensionless temperature and concentration respectively. Under these assumptions, the appropriate boundary conditions for the velocity, temperature and concentration fields are:

\[
\begin{align*}
\frac{\partial u}{\partial y} &= -\frac{\alpha}{\sqrt{k_p}} u, \quad v = 0, \quad u = T_0 + e^{\epsilon t + \lambda x} (T_0 - T_1), \quad C = C_0 + e^{\epsilon t + \lambda x} (C_0 - C_1) \quad \text{at} \quad y = 0, \quad t > 0 \\
\frac{\partial u}{\partial y} &= \frac{\alpha}{\sqrt{k_p}} u, \quad v = -e^{\epsilon t + \lambda x} u_0, \quad T = T_1, \quad C = C_1 \quad \text{at} \quad y = h, \quad t > 0 
\end{align*}
\]

(2.7)

where, \( \alpha \) is the slip parameter, \( T_0 \) and \( C_0 \) are the temperature and concentration at the lower surface, respectively, \( u_0 \), \( n \) and \( \lambda \) are constants and \( \epsilon \) is the perturbation parameter \(< 1 \).

We now introduce the following non-dimensional quantities:

\[
\begin{align*}
&u^* = \frac{u}{u_0}, \quad v^* = \frac{v}{v_0}, \quad t^* = \frac{t}{u_0^2}, \quad x^* = \frac{x}{u_0}, \quad y^* = \frac{y}{u_0}, \quad \theta = \frac{T - T_1}{T_0 - T_1}, \quad \phi = \frac{C - C_1}{C_0 - C_1}
\end{align*}
\]

where, \( \theta \) and \( \phi \) are dimensionless temperature and concentration respectively.

Making use of the non-dimensional variables in equations (2.1) to (2.4) and (2.6), neglecting the '*' symbol gives

\[
\begin{align*}
\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} &= \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + Gr \theta + Gc \phi - \sigma^2 u \\
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} &= \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} - \sigma^2 v \\
\frac{\partial \theta}{\partial t} + u \frac{\partial \theta}{\partial x} + v \frac{\partial \theta}{\partial y} &= \frac{1}{Pr} \left( \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} \right) + Q_1 \theta \\
R \frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} &= \frac{1}{Sc} \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) - K \phi
\end{align*}
\]

(2.8)

(2.9)

(2.10)

(2.11)

(2.12)

where, \( Gr = \frac{v \beta \theta (T_0 - T_1)}{u_0^3} \) is the Grashof number, \( Gc = \frac{v g \beta C (C_0 - C_1)}{u_0^3} \) is the modified Grashof number, \( \sigma = \frac{\nu}{u_0 \sqrt{k_p}} \) is the porous parameter, \( Q_1 = \frac{Q_0 u}{\rho C_p u_0^2} \) is the heat generation parameter, \( Pr = \frac{\rho C_p v}{k} \) is the Prandtl number, \( Sc = \frac{D}{D} \) is the Schmidt number and \( K = \frac{k_1 v}{u_0^2} \) is the dimensionless chemical reaction rate parameter.

The boundary conditions (2.7) in non-dimensional form are:

\[
\begin{align*}
&u = 0, \quad v = 0, \quad \theta = 1, \quad \phi = 1 \quad \forall \quad y, \quad t \leq 0 \\
&\frac{\partial u}{\partial y} = -\sigma u, \quad v = 0, \quad \theta = 1 + e^{\epsilon t + \lambda x}, \quad \phi = 1 + e^{\epsilon t + \lambda x} \quad \text{at} \quad y = 0, \quad t > 0 \\
&\frac{\partial u}{\partial y} = \sigma u, \quad v = -e^{\epsilon t + \lambda x}, \quad \theta = 0, \quad \phi = 0 \quad \text{at} \quad y = 1, \quad t > 0 
\end{align*}
\]

(2.13)

3 Method of Solution

The flow equations (2.9) and (2.10) coupled with the energy and concentration equations (2.11) and (2.12), which form a system of nonlinear partial differential equations are simplified using perturbation technique.
This can be done by representing the velocities, temperature and concentration as:

\[
\begin{align*}
    u(x, y, t) &= u_0(y) + e^{nt+\lambda x} u_1(y) + O(e^2) \\
    v(x, y, t) &= e^{nt+\lambda x} v_1(y) + O(e^2) \\
    \theta(x, y, t) &= \theta_0(y) + e^{nt+\lambda x} \theta_1(y) + O(e^2) \\
    \phi(x, y, t) &= \phi_0(y) + e^{nt+\lambda x} \phi_1(y) + O(e^2)
\end{align*}
\] (3.14)

Substituting equations (3.14) into equations (2.9) to (2.12), neglecting the higher order of \(e^2\) and simplifying we obtain the following set of nonlinear ordinary differential equations for \(u_0, \theta_0, \phi_0\) and \(u_1, \theta_1, \phi_1\).

Zeroth order equations:

\[
\begin{align*}
    u_{0yy} - \sigma^2 u_0 + Gr \theta_0 + Gc \phi_0 &= 0 \\
    \theta_{0yy} + Pr Q_1 \theta_0 &= 0 \\
    \phi_{0yy} - Sc K \phi_0 &= 0
\end{align*}
\] (3.15) (3.16) (3.17)

First order equations:

\[
\begin{align*}
    u_{1yy} + \left(\lambda^2 - \sigma^2 - \lambda u_0 - n\right) u_1 - v_1 u_{0y} + Gr \theta_1 + Gc \phi_1 &= 0 \\
    v_{1yy} + \left(\lambda^2 - \sigma^2 - \lambda u_0 - n\right) v_1 &= 0 \\
    \theta_{1yy} + \left(\lambda^2 + Pr(Q_1 - \lambda u_0 - n)\right) \theta_1 - Pr v_1 \theta_{0y} &= 0 \\
    \phi_{1yy} + \left(\lambda^2 - Sc(\lambda u_0 + n R + K)\right) \phi_1 - Sc v_1 \phi_{0y} &= 0
\end{align*}
\] (3.18) (3.19) (3.20) (3.21)

subject to the boundary conditions,

\[
\begin{align*}
    u_{0y} &= -a \sigma u_0 , \quad \theta_0 = 1 , \quad \phi_0 = 1 \quad \text{at} \quad y = 0 \\
    u_{0y} &= a \sigma u_0 , \quad \theta_0 = 0 , \quad \phi_0 = 0 \quad \text{at} \quad y = 1
\end{align*}
\] (3.22)

\[
\begin{align*}
    u_{1y} &= -a \sigma u_1 , \quad v_1 = 0 , \quad \theta_1 = 1 , \quad \phi_1 = 1 \quad \text{at} \quad y = 0 \\
    u_{1y} &= a \sigma u_1 , \quad v_1 = -1 , \quad \theta_1 = 0 , \quad \phi_1 = 0 \quad \text{at} \quad y = 1
\end{align*}
\] (3.23)

The numerical solutions to the coupled equations (3.15)-(3.21) using the boundary conditions (3.22) and (3.23) gives the velocity, temperature and concentration distributions.

From the point of view of applications in technology, it is of interest to know the coefficient of skin friction which physically indicate wall shear stress.

In non-dimensional form, the coefficient of skin friction \(C_f\) is defined as

\[C_f = \frac{\tau_w}{\rho u_0^2} = \frac{\partial u}{\partial y}\]

4 Results and Discussion

Numerical evaluation for the velocity, temperature and concentration distributions as well as coefficient of skin friction for all time have been computed. The results obtained are discussed for various values of Grashof number, Prandtl number, heat generation parameter, Schmidt number, chemical reaction rate parameter, retardation factor and porous parameter. The values of other physical parameters are fixed as real constants.

Figures 1 to 3 depict the horizontal velocity\((u)\) profile for different Grashof numbers, heat generation parameter and porous parameter, respectively. Figure 1 evidently proves that improving Grashof number promotes the velocity profile. This is because advancement in the buoyancy ratio tends to accelerate the fluid flow. From figure 2, we see that when the heat is generated the buoyancy force increases which induces the flow rate to enhance the velocity profile. Hence, rise in heat generation parameter results in potentiating velocity. Figure 3 shows that the velocity reduces with rise in porous parameter. For large porous parameter, the frictional drag resistance against the flow in the porous region is very large and as a result, the velocity decelerate for accelerating porous parameter. But in the case when flow is in the vertical direction, we see that the porous parameter enhances the vertical velocity\((v)\) as given in Figure 4.
With the model prediction of temperature of a particular layer thickness and the particular time, we see that spillage usually affects the thermal properties of the soil and thus causes a departure of the soil thermal properties from normality and abnormality. Figure 5 shows the behavior of temperature distribution for different values of Prandtl number. It is observed that Prandtl number promotes the temperature distribution. The oil viscosity is greater than the thermal diffusivity which results in high Prandtl number \( Pr > 1 \) and hence the momentum diffusion governs the flow, in comparison to thermal diffusion. Figure 6 shows the effect of heat generation parameter on the temperature profile. The increase in heat generation parameter causes increase in temperature, which has the tendency to increase thermal buoyancy effects. \( Q_1 = 0 \) corresponds to the case of no heat generation. With increase in \( Q_1 \), the flow becomes more convective, having wide variation of temperature along the mid-vertical axis, and the higher temperature is observed towards the bottom of the subsurface. The effects of porous parameter on temperature profile is illustrated through Figure 7. It reveals that porous parameter enhances heat transfer in the subsurface.

Figures 8 and 9 display the effect of the Schmidt number and chemical reaction rate parameter on the concentration profile, respectively. Both these figures reveal that the hydrocarbon concentration reduces due to a rise in Schmidt number and chemical reaction rate parameter. This causes the concentration buoyancy to decrease yielding a reduction in the fluid velocity. Figures 10 and 11 represent the temporal variation of concentration profile for different porous parameter and retardation factor, respectively. Both these figures show that concentration of hydrocarbon in water increases with growing time. This evidently shows that more separation of hydrocarbons occur as the hydrocarbons have been in the water longer. From Figure 10 we see that porous parameter enhances the hydrocarbon concentration. Sorption between hydrocarbons and the soil surface play an important role in the transport of hydrocarbons. The result is the development of retardation factor. From the Figure 11, it is clear that the retardation factor retards the hydrocarbon concentration. This means that at higher concentrations, retardation factor is less and at lower concentrations, retardation factor is greater.

The coefficient of skin friction \( (C_f) \), the non-dimensional parameter that characterizes the viscous frictional forces of the flow over a solid surface is analyzed at the lower surface \( y=0 \) and upper surface \( y=1 \), for different values of porous parameter through Figure 12. It reveals that the skin friction coefficient at the bottom surface descends for ascending value of porous parameter. A reverse trend happens at the upper surface. It can be seen that Grashof number enhances \( C_f \) at the lower surface, while it retards \( C_f \) at the upper surface.

5 Conclusion

A mathematical model has been developed to study the movement of oil flow in the subsurface and its characteristics that describe the transport of hydrocarbons dissolved in the water that occupy the void space, or part of it. Numerical results have been reported for large length and time scales over a wide range of parameters. As the transport of hydrocarbons in the subsurface is affected by different processes including advection, diffusion, adsorption and chemical reaction effects, the results obtained provides information on the migration rate, temperature as well as the concentration distribution. The effect of temperature-dependent heat generation in the flow region is also taken into consideration.

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Figure 3. Effect of porous parameter on u velocity

Figure 4. Effect of porous parameter on v velocity

Figure 5. Effect of Prandtl number on temperature distribution

Figure 6. Effect of heat generation parameter on temperature distribution

Figure 7. Effect of porous parameter on temperature distribution

Figure 8. Effect of Schmidt number on concentration distribution

Figure 9. Effect of chemical reaction parameter on concentration distribution

Figure 10. Time evolution of concentration distribution for different porous parameter

Figure 11. Time evolution of concentration distribution for different retardation factor

Figure 12. Effect of porous parameter on coefficient of skin friction
References


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