

Modeling the Transport of Hydrocarbons in the Subsurface Environment with Chemical Reaction

S. V. Hemalatha, Nirmala P. Ratchagar

Abstract: The objective of the present study is to investigate the transport of hydrocarbons with chemical reaction due to oil flow through the subsurface. The coupled nonlinear differential equations governing the flow and mass transfer are simplified using perturbation technique and solved numerically. The dimensionless velocity and concentration profiles are depicted graphically and discussed for the effects of the parameters involved.

Keywords: Beavers-Joseph slip condition, Buoyancy effects, Concentration of hydrocarbons, Retardation.

I. INTRODUCTION

Solute transport problems involving first order decay reactions and retardation coefficient frequently occurs in soil and groundwater systems. Thus the migration of petroleum hydrocarbon products through the soil causes physical, chemical and biochemical changes depending not only on their own properties, but also on soil properties[1].

Some of the petrochemical products get adsorbed on soil when entering the subsurface and reach the underground water table[2, 3]. Experimental result of Adam et al.[4] showed that addition of oxygenates such as ethanol, reduces the atmospheric pollution, but increase the downward migration of hydrocarbons to groundwater by lessening the adsorptive capacity of the surface soil components. Transport of polycyclic aromatic hydrocarbons in porous medium is studied by Sabbah et al. [5] using break through curves. Mukherjee and Shome [6] presented an analytical solution for a double phase flow of water and oil in saturated porous medium using calculus of variation and similarity theory.

Gawdzik and Zygodlo [7] experimentally verified the results of contamination by hydrocarbons migration in the soil using soil filter test. Abdulkadir and Yahaya[8] studied the dispersion of crude oil on land with the help of MINTAB software. Okop and Ekpo [9] classified the hydrocarbon penetration due to crude oil spillage in the soil depths according to their chemical similarities.

Our objective is to study the movement and characteristics of oil flow during the transport of hydrocarbons in the soil. Soil

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in the subsurface under study is bounded by porous layers on both the upper and lower surfaces. The soil is assumed to be a homogeneous porous medium. The fluids are considered to be incompressible. The transient, two dimensional flow of oil, diffuses and simultaneously undergoes first-order irreversible chemical reaction in the liquid under isothermal conditions. The obtained governing equations are solved using perturbation method.

II. MATHEMATICAL FORMULATION

The mathematical model is a nonlinear system of equations, based on the principle of mass, linear momentum in the presence of concentration buoyancy effects including Darcian term and the solute transport equation with chemical reaction. These results in following equations as:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (1)$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + g\beta_c(C - C_1) - \frac{\nu}{k_p} u \quad (2)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - \frac{\nu}{k_p} v \quad (3)$$

$$\rho_b \frac{\partial S}{\partial t} + \beta_w \frac{\partial C}{\partial t} + \beta_w u \frac{\partial C}{\partial x} + \beta_w v \frac{\partial C}{\partial y} = \beta_w D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) - \beta_w k_1(C - C_1) \quad (4)$$

where, u and v are the components of velocities along x and y directions, respectively, C is the concentration of hydrocarbons in water, S is the concentration of adsorbed oil in soil, ν is the kinematic viscosity of oil, g is the gravitational acceleration, β_c is the concentration expansion coefficient, C_1 is the concentration at the upper surface, ρ is the density of oil, C_p is the specific heat at constant pressure, k_p is the permeability of the medium, ρ_b is the soil bulk density, β_w is the volumetric water content of soil, D is the mass diffusivity and k_1 is the chemical reaction rate parameter.

Accounting for equilibrium in linear sorption process,

the retardation factor $R = 1 + \frac{\rho_b k_d}{\beta_w}$, where,

$S = k_d C$, k_d is the adsorption coefficient, reduces equation (4) to

$$R \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) - k_1(C - C_1) \quad (5)$$

Using the appropriate boundary conditions such as the Beavers-Joseph slip condition [10] for horizontal velocity, we have:

$$\left. \begin{aligned} \frac{\partial u}{\partial y} &= -\frac{\alpha}{\sqrt{k_p}}(u - Q), v = 0, C = C_0 + \varepsilon e^{n+\lambda x}(C_0 - C_1) \text{ at } y = 0 \\ \frac{\partial u}{\partial y} &= \frac{\alpha}{\sqrt{k_p}}(u - Q), v = -\varepsilon e^{n+\lambda x} u_0, C = C_1 \text{ at } y = h \end{aligned} \right\} (6)$$

where, α is the slip parameter and C_0 are the temperature and concentration at the lower surface, respectively, u_0 , n and λ are constants and ε is the perturbation parameter (<1).

We now introduce the following non-dimensional quantities:

$$\begin{aligned} u^* &= \frac{u}{u_0}, v^* = \frac{v}{u_0}, t^* = \frac{tu_0^2}{\nu}, x^* = \frac{xu_0}{\nu}, y^* = \frac{yu_0}{\nu}, \\ \phi &= \frac{C - C_1}{C_0 - C_1}, Q^* = \frac{Q}{u_0} \end{aligned}$$

where, ϕ is the dimensionless concentration.

Making use of the non-dimensional variables in equations (1) to (3) and (5) neglecting the '*' symbol gives

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (7)$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + Gc\phi - \sigma^2 u \quad (8)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} - \sigma^2 v \quad (9)$$

$$R \frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} = \frac{1}{Sc} \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) - K\phi \quad (10)$$

where,

$$Gc = \frac{\nu g \beta_C (C_0 - C_1)}{u_0^3} \text{ is the mass Grashof number,}$$

$$\sigma = \frac{\nu}{u_0 \sqrt{k_p}} \text{ is the porous parameter,}$$

$$Sc = \frac{\nu}{D} \text{ is the Schmidt number and}$$

$K = \frac{k_1 \nu}{u_0^2}$ is the dimensionless chemical reaction rate parameter.

The boundary conditions (6) in non-dimensional form are:

$$\left. \begin{aligned} \frac{\partial u}{\partial y} &= -\alpha \sigma (u - Q), v = 0, \phi = 1 + \varepsilon e^{n+\lambda x} \text{ at } y = 0 \\ \frac{\partial u}{\partial y} &= \alpha \sigma (u - Q), v = -\varepsilon e^{n+\lambda x}, \phi = 0 \text{ at } y = 1 \end{aligned} \right\} (11)$$

III. METHOD OF SOLUTION

Applying the perturbation method in the form,

$$\left. \begin{aligned} u(x, y, t) &= u_0(y) + \varepsilon e^{n+\lambda x} u_1(y) + O(\varepsilon^2) \\ v(x, y, t) &= \varepsilon e^{n+\lambda x} v_1(y) + O(\varepsilon^2) \\ \phi(x, y, t) &= \phi_0(y) + \varepsilon e^{n+\lambda x} \phi_1(y) + O(\varepsilon^2) \end{aligned} \right\} (12)$$

the system of partial differential equations (8) to (10), reduces to a system of ordinary differential equations. Neglecting the higher order of (ε^2) gives the following set of equations for u_0, ϕ_0 and u_1, v_1, ϕ_1 in simplified form.

Zeroth order equations:

$$u_{0,yy} - \sigma^2 u_0 + Gc\phi_0 = 0 \quad (13)$$

$$\phi_{0,yy} - Sc K \phi_0 = 0 \quad (14)$$

First order equations:

$$u_{1,yy} + (\lambda^2 - \sigma^2 - \lambda u_0 - n)u_1 - v_1 u_{0,y} + Gc\phi_1 = 0 \quad (15)$$

$$v_{1,yy} + (\lambda^2 - \sigma^2 - \lambda u_0 - n)v_1 = 0 \quad (16)$$

$$\phi_{1,yy} + (\lambda^2 - Sc(\lambda u_0 + nR + K))\phi_1 - Sc v_1 \phi_{0,y} = 0 \quad (17)$$

subject to the boundary conditions,

$$\left. \begin{aligned} u_{0,y} &= -\alpha \sigma (u_0 - Q), \phi_0 = 1 \text{ at } y = 0 \\ u_{0,y} &= \alpha \sigma (u_0 - Q), \phi_0 = 0 \text{ at } y = 1 \end{aligned} \right\} (18)$$

$$\left. \begin{aligned} u_{1,y} &= -\alpha \sigma u_1, v_1 = 0, \phi_1 = 0 \text{ at } y = 0 \\ u_{1,y} &= \alpha \sigma u_1, v_1 = -1, \phi_1 = 0 \text{ at } y = 1 \end{aligned} \right\} (19)$$

The numerical solutions for the coupled equations (13)-(17) using the boundary conditions (18) and (19) give the velocity profiles and concentration distributions.

IV. RESULTS AND DISCUSSION

Numerical evaluation for the velocity profiles and concentration distributions have been computed using MATHEMATICA 8.0. To understand the nature of movement of oil spill and the distribution of concentration of hydrocarbons in the real field, physical numbers for Schmidt number, chemical reaction rate parameter, retardation factor and porous parameter are chosen and the results obtained



are discussed through Figures 1 to 6.

The values of other physical parameters are set as real constants.

Figures 1 and 2 indicate the velocity(u) and the velocity(v) for different porous parameter, respectively. From Figure 1, it is seen that the velocity decreases with increase in porous parameter. This is due to the frictional drag resistance against the flow. But for vertical flow, the velocity(v) increases for increasing porous parameter as in Figure 2.

Figures 3 and 4 show the effect of Schmidt number and chemical reaction rate parameter on the concentration profile, respectively. It reveals that the concentration decreases with increasing Schmidt number and chemical reaction rate parameter. This causes the concentration buoyancy to decrease yielding a reduction in the fluid velocity.

Figures 5 and 6 signify the porous parameter and retardation factor of concentration profile with respect to time. They indicate that concentration of hydrocarbon in water increases with increase in time. Figure 5 shows that the concentration increases with increasing porous parameter. From Figure 6, we see that when the retardation factor increases the concentration decreases. This shows less retardation factor at higher concentrations, and higher retardation factor at lower concentrations.

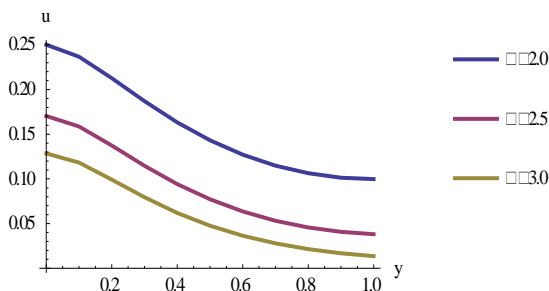


Fig. 1. Effect of porous parameter on u velocity

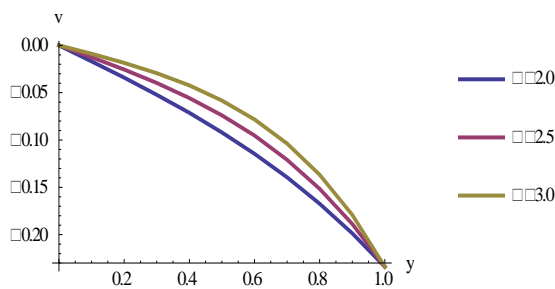


Fig. 2. Effect of porous parameter on v velocity

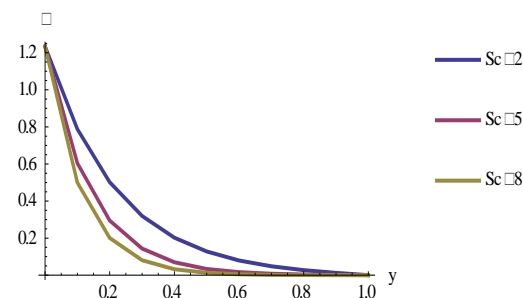


Fig. 3. Effect of Schmidt number on concentration distribution

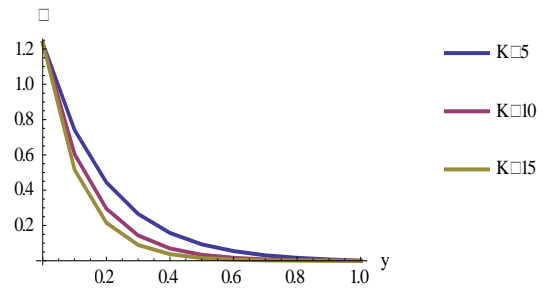


Fig. 4. Effect of chemical reaction rate parameter on concentration distribution

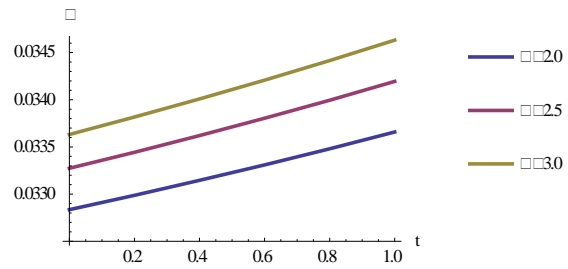


Fig. 5. Time evolution of concentration distribution for different porous parameter

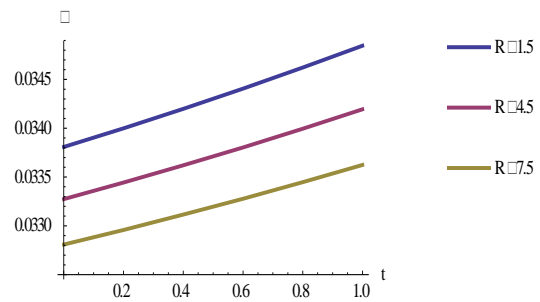


Fig. 6. Time evolution of concentration distribution for different retardation parameter

V. CONCLUSION

Transport problems are in much need of multi-dimensional solutions as they widely applied to solute dispersal in any direction. This paper is focused on the study of transport of hydrocarbons through the subsurface including chemical reaction. The numerical solution predicts the evolution of oil penetration into soil and its characteristics that describe the transport of hydrocarbons dissolved in the water, both in the period immediately after the spill, and over the subsequent time. Obtained results may serve as a predictive tool in environmental / groundwater management and applies to real-world applications.

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