

Journal of Advanced Research in Fluid Mechanics and Thermal Sciences



Journal homepage: https://semarakilmu.com.my/journals/index.php/fluid_mechanics_thermal_sciences/index ISSN: 2289-7879

Taylor's Dispersion Approach for Modelling Contaminated Solute Transport in Soil Through Two Immiscible Fluids

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ARTICLE INFO

ABSTRACT

Article history:

Received 20 August 2024 Received in revised form 26 December 2024 Accepted 5 January 2025 Available online 10 February 2025

Keywords:

Taylor dispersion method; viscous fluids; two immiscible fluids; diffusion; concentration

Our environment is surrounded by land and water. Everyday activities of humans have an adverse effect on the environment. The leachate water from landfills, industries and companies are passed through water and soil every day. So, it is crucial to understand how the contaminants are transported through the soil from polluted water. This paper depicts the transportation of contaminants through two immiscible fluids in two sub surfaces of the soil region (Top Soil and Parent Rock). Taylor's dispersion method is employed to study the concentration of the contaminants in both sub surfaces. The model contains key parameters such as fluid velocity, density, coefficient of thermal expansion and temperature which helps in understanding the contamination of soil through two layers. This model also elaborates the effects of different heights, diffusion coefficient and various values of dynamics viscosity affecting the concentration profiles through graphs.

1. Introduction

Soil is a complex mixture of minerals, organic material, water and other various lifeforms. Humans have intentionally or unintentionally polluted the soil. For the past two decades, the soil contamination has a huge impact on environment all around the world. The soil by nature is non-toxic, organic and full of minerals in right concentration. Any changes in their organic structure will lead to the contamination of soil.

The contaminated soil will pass the pollutants to groundwater which are absorbed by plants and trees. If the plants that have been affected by the contaminated soil is taken as food by humans will

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https://doi.org/10.37934/arfmts.127.1.2028

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have a huge impact on their physical health. This leads to major health risks and even leads to epidemic or pandemic diseases.

Similarly, the storage of toxic waste from landfills may result in the seepage of pollutants into the soil. The overuse of pesticides, releasing industrial waste with hazardous chemicals, petroleum products also have a major role in soil contamination. The contaminants can be classified into two major groups as liquid waste and solid waste. The liquid wastes include chemicals and effluents. The solid wastes include heavy metals, plastics, garbage from construction and commercial waste and so on.

There is much importance in learning about contaminants in soil. The contaminated soil will lead to ecosystem eutrophication and reduced biodiversity. There is risk of soil losing its fertility which will lead to use of inorganic fertilizers that will lead to even more contamination of soil.

Aris [1] extended the work of Taylor, in which Taylor considered solute dispersion in laminar flow within a circular tube. Aris generalised by considering arbitrary values of the Peclet number providing a proper understanding of process of dispersion. Barton [2] studied the early stages of dispersion of passive solute in three-dimensional fluid flow. Chang and Santiago [3] addressed Taylor dispersion in axisymmetric channels with arbitrary shapes. The study developed analytical and numerical methods to characterize dispersion in channels with complex geometries, extending beyond traditional cylindrical shapes. Kumar *et al.*, [4] investigated the phenomenon of Taylor dispersion in the context of elongated rods within a fluid flow. Taylor dispersion refers to the enhanced spreading of solute particles in a flow due to the combined effects of molecular diffusion and velocity variations.

Kumar et al., [5] investigated fully developed mixed convection flow in a vertical channel that contains alternating porous and fluid layers. The analysis considered both isothermal and isoflux boundary conditions and examines their effects on the flow characteristics. Kumar et al., [6] examined the combined free and forced convection in vertical channel composed of both porous and fluid layers. Kumar et al., [7] analysed the chemical reactions influence solute dispersion in a system comprising two immiscible viscous fluids confined between parallel plates. Moser and Baker [8] discussed the fundamental principles of TDA, focusing its rapid analysis times and minimal sample consumption when using fused silica capillaries.

Lohrasbi and Sahai [9] focused on the effects of an applied magnetic field on the flow and heat transfer behaviour of the two-phase system. They developed a mathematical model to describe the velocity and temperature distributions with the flow with factors such as the magnetic field strength and the properties of the two phases. Parasa and Meduri [10] aimed at finding the analytic solution for an oscillatory flow of couple stress fluid flow over a contaminated fluid sphere, filled with a couple stress fluid which is considered with interfacial slip on the boundary. The stream functions and drags related to the findings were analytically obtained. Rudraiah and Ng [11] covered theoretical models, experimental observations, and practical applications of dispersion in various types of porous media. The review highlights the impact of reactions on dispersion characteristics and discussed the implications for environmental and engineering applications. Shail [12] examined the behaviour of steady, fully developed laminar flow of two immiscible incompressible, electrically conducting fluids between two parallel plates under the influence of a transverse magnetic field. Smith [13] analysed the time period before the contaminant distribution reaches a Gaussian profile and also the initial dispersion behaviour of a contaminant introduced into a shear flow.

Taylor [14] derived an analytical solution to describe the concentration distribution of the solute along the length of the tube and explores the effects of various flow conditions on dispersion rates. Taylor [15] developed a model to describe how turbulence affects the dispersion of solutes and presented analytical results for concentration profiles in turbulent flows. Zeng *et al.*, [16] evaluated the performance of various analytical solutions for modelling Taylor dispersion in open channel flows.

The model compared these solutions by applying them to different flow scenarios and assessing their accuracy in predicting dispersion behaviour.

Little to no work is found in the literature on dispersion of solute for two fluid flow between two layers of soil. The objective of this work is to analyze the unsteady dispersion of a solute for two immiscible viscous fluids in a channel using the Taylor's Model.

2. Problem Formulation

A laminar flow of two immiscible viscous fluids flowing between two parallel layers of soil is considered with the distance of h_1+h_2 apart, taking x-axis along the mid – section of the channel (soil layers) and the y-axis perpendicular to the walls (Figure 1). Subsurface $1(-h_1 \le y \le 0)$ is filled with contaminated fluid with viscosity μ_1 under uniform pressure gradient ∇p_1 and subsurface $2(0 \le y \le h_2)$ is filled with contaminated fluid with viscosity μ_2 under uniform pressure gradient ∇p_2 .

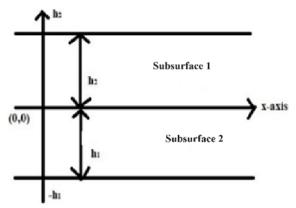


Fig. 1. Physical configuration

It is assumed that the flow is steady, laminar, fully developed and some fluid properties are constants. g is gravitational acceleration, β_1 and β_2 are the thermal expansion coefficients, T_0 , T_1 , T_2 are the temperature coefficients of initial subsurface, subsurface 1 and subsurface 2 respectively.

The governing equations are given by

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0$$

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u = -\frac{1}{\rho}\nabla p + \nu \nabla^2 u + \rho g \beta (T_1 - T_0)$$

Subsurface 1:

$$\nabla^2 u_1 = P_1 + \rho g \beta (T_1 - T_0) \tag{1}$$

where
$$P_1 = \frac{1}{\mu_1} \nabla p_1$$
.

Subsurface 2:

$$\nabla^2 u_2 = P_2 + \rho g \beta (T_2 - T_0) \tag{2}$$

where
$$P_2 = \frac{1}{\mu_2} \nabla p_2$$
.

where u_i is the x – component of fluid velocity and p_i is the pressure gradient. The boundary conditions on velocity are no – slip conditions requiring that the velocity must vanish at the boundary. In addition, continuity of velocity and shear stress at the interface is assumed. With these assumptions, the boundary and interface conditions on velocity becomes,

$$u_1 = 0 \text{ at } y_1 = -h_1$$

$$u_2 = 0 \text{ at } y_2 = h_2$$

$$u_1 = u_2 \text{ at } y_1 = y_2 = 0$$

$$\text{where } h_1 \text{ and } h_2 \text{ are the heights of the subsurface 1 and subsurface 2.}$$

$$(3)$$

where h_1 and h_2 are the heights of the subsurface 1 and subsurface 2.

Introducing the following non-dimensional quantities

$$u_1^* = \frac{u_1}{u_0}; \ u_2^* = \frac{u_2}{u_0}; \eta_1 = \frac{y_1}{h_1}; \eta_2 = \frac{y_2}{h_2}$$

Solutions of Eq. (1) and Eq. (2) using boundary and interface conditions (4) become, for subsurface 1,

$$u_1 = [P_1 + \rho g \beta_1 (T_1 - T_0)] \frac{y_1^2}{2} + l_1 y_1 + l_2$$
 (5)

Similarly for subsurface 2,

$$u_2 = [P_2 + \rho g \beta_2 (T_2 - T_0)] \frac{y_2^2}{2} + l_3 y_2 + l_4$$
 (6)

From Eq. (5) and Eq. (6),

$$l_{2} = l_{1}h_{1} - [P_{1} + \rho g\beta_{1}(T_{1} - T_{0})] \frac{h_{1}^{2}}{2}$$

$$l_{1} = \frac{\mu_{2}}{h_{1}\mu_{1} + h_{2}\mu_{2}} + \left[\frac{[P_{1} + \rho g\beta_{1}(T_{1} - T_{0})]}{2} - \frac{[P_{2} + \rho g\beta_{2}(T_{2} - T_{0})]}{2}\right]$$

$$l_{3} = \frac{l_{1}\mu_{1}}{\mu_{2}}; l_{2} = l_{4}$$
(7)

The average velocity for the first subsurface is defined by

$$\overline{u_1} = [P_1 + \rho g \beta_1 (T_1 - T_0)] \frac{h_1^2}{6} - \frac{l_1 h_1}{2} - l_2$$
(8)

Similarly,
$$\overline{u_2} = [P_2 + \rho g \beta_2 (T_2 - T_0)] \frac{h_2^2}{6} - \frac{l_3 h_2}{2} + l_4$$
 (9)

A solute is assumed to diffuse in the absence of a first-order irreversible chemical reaction in the liquid under isothermal conditions. Equation for concentration \mathcal{C}_1 of the solute for subsurface 1 satisfies

$$\frac{\partial C_1}{\partial t_1} + u_1 \nabla C_1 = D_1 \nabla^2 C_1 \tag{10}$$

Similarly, equation for concentration \mathcal{C}_2 of the solute for subsurface 2 satisfies

$$\frac{\partial C_2}{\partial t_2} + u_2 \nabla C_2 = D_2 \nabla^2 C_2 \tag{11}$$

in which D_1 and D_2 are the molecular diffusion coefficients (assumed constants) for the 1st and 2nd subsurface, respectively.

$$|\nabla^2 C_1| \ll \left| \frac{\partial^2 C_1}{\partial v_1^2} \right| \text{ and } |\nabla^2 C_2| \ll \left| \frac{\partial^2 C_2}{\partial v_2^2} \right|$$

Convection across a plane moving with the mean speed of the flow is assumed, then relative to this plane the fluid velocity for the 1st and 2nd sub surfaces are given by,

$$u_{1x} = u_1 - \overline{u_1} = \left[P_1 + \rho g \beta_1 (T_1 - T_0) \right] \frac{h_1^2}{2} \left[\eta_1^2 - \frac{1}{3} \right] + l_1 h_1 \left[\eta_1 + \frac{1}{2} \right]$$
(12)

$$u_{2x} = u_2 - \overline{u_2} = \left[P_2 + \rho g \beta_2 (T_2 - T_0) \right] \frac{h_2^2}{2} \left[\eta_2^2 - \frac{1}{3} \right] + l_3 h_2 \left[\eta_2 - \frac{1}{2} \right]$$
(13)

Using the non-dimensional variables

$$\theta_{1} = \frac{t_{1}}{\overline{t_{1}}}, \overline{t_{1}} = \frac{L_{1}}{u_{1}}, \xi_{1} = \frac{(x_{1} - \overline{u_{1}}t_{1})}{L_{1}}, \eta_{1} = \frac{y_{1}}{h_{1}}$$

$$\theta_{2} = \frac{t_{2}}{\overline{t_{2}}}, \overline{t_{2}} = \frac{L_{2}}{u_{2}}, \xi_{2} = \frac{(x_{2} - \overline{u_{2}}t_{2})}{L_{2}}, \eta_{2} = \frac{y_{2}}{h_{2}}$$
(14)

By the above equations and the non - dimensional quantities,

$$\frac{1}{t_1}\nabla \cdot C_1 + \boldsymbol{u}_1 \cdot \nabla C_1 = \boldsymbol{D}_1 \nabla^2 C_1 \tag{15}$$

where $oldsymbol{u_1} = rac{u_{1x}}{L_1}$, $oldsymbol{D}_1 = rac{D_1}{h_1^2}$

$$\frac{1}{t_2}\nabla \cdot \mathcal{C}_2 + \boldsymbol{u}_2 \cdot \nabla \mathcal{C}_2 = \boldsymbol{D}_2 \nabla^2 \mathcal{C}_2 \tag{16}$$

where $u_2 = \frac{u_{2x}}{L_2}$, $D_2 = \frac{D_2}{h_2^2}$, where L_1 and L_2 are the typical lengths along the flow direction for the 1st and 2nd subsurface respectively.

From the above Eq. (15) and Eq. (16),

$$\nabla^2 C_1 = \frac{u_1}{D_1} \nabla C_1 \tag{17}$$

$$\nabla^2 C_2 = \frac{u_1}{D_1} \nabla C_2 \tag{18}$$

$$\frac{\partial C_1}{\partial \eta_1} = 0 \text{ at } \eta_1 = -1 \text{ and } \frac{\partial C_2}{\partial \eta_2} = 0 \text{ at } \eta_2 = 1$$

Using the conditions above,

$$C_1 = \frac{h_1^2}{D_1 L_1} \frac{\partial C_1}{\partial \xi_1} \left[P_1 + \rho g \beta_1 (T_1 - T_0) \right] \frac{h_1^2}{2} \left[\frac{\eta_1^4}{12} - \frac{\eta_1^2}{6} \right] + l_1 h_1 \left[\frac{\eta_1^3}{6} + \frac{\eta_1^2}{4} \right] + a_1$$
 (19)

$$C_2 = \frac{h_2^2}{D_2 L_2} \frac{\partial C_2}{\partial \xi_2} \left[P_2 + \rho g \beta_2 (T_2 - T_0) \right] \frac{h_2^2}{2} \left[\frac{\eta_2^4}{12} - \frac{\eta_2^2}{6} \right] + l_3 h_2 \left[\frac{\eta_2^3}{6} + \frac{\eta_2^2}{4} \right] + a_2$$
 (20)

where a_1 and a_2 are constants.

The volumetric rates at which the solute is transported across a section of the channel of unit breadth Q_1 subsurface 1 and Q_2 subsurface 2, Eq. (12), Eq. (13), Eq. (19) and Eq. (20)

$$Q_{1} = \int_{-1}^{0} C_{1} u_{1x} d\eta_{1} = -\frac{h_{1}^{7} \{P_{1} + \rho g \beta_{1} (T_{1} - T_{0})\}^{2}}{D_{1} L_{1}} \frac{\partial C_{1}}{\partial \xi_{1}} \left(\frac{2}{945}\right) + \frac{\{P_{1} + \rho g \beta_{1} (T_{1} - T_{0})\}}{D_{1} L_{1}} h_{1}^{6} l_{1} \frac{\partial C_{1}}{\partial \xi_{1}} \left(\frac{1}{120}\right) - \frac{h_{1}^{5} l_{2}^{2}}{D_{1} L_{1}} \frac{\partial C_{1}}{\partial \xi_{1}} \left(\frac{1}{120}\right)$$

$$Q_2 = \int_0^1 C_2 u_{2x} \, d\eta_2 = -\frac{h_2^7 \{P_2 + \rho g \beta_2 (T_2 - T_0)\}^2}{D_2 L_2} \, \frac{\partial C_2}{\partial \xi_2} \left(\frac{2}{945}\right) + \frac{\{P_2 + \rho g \beta_2 (T_2 - T_0)\}}{D_2 L_2} \, h_2^6 l_3 \, \frac{\partial C_2}{\partial \xi_2} \left(\frac{1}{120}\right) - \frac{h_2^5 l_3^2}{D_2 L_2} \, \frac{\partial C_2}{\partial \xi_2} \left(\frac{1}{120}\right)$$

3. Results and Discussion

Effects of pressure gradient p_1 and p_2 are shown in the Figure 2, that depicts how the concentration varies according to the variations in pressure gradient. It is observed that when there is an increase in the pressure, the concentration in the subsurface 1 and subsurface 2 decreases. Since the pressure gradient suppresses the flow, the concentration gets reduced. As there is no flow when the pressure is zero, the concentration also becomes zero.

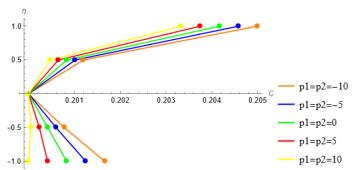


Fig. 2. Effects of pressure gradients p_1 and p_2 on concentration profiles

Concentration profiles with the effects of viscosity of the fluids passing through the two subsurface of soil layers is depicted in Figure 3 and Figure 4. Viscosities of the fluids are varied from μ =0.5 to μ =3. Higher viscosity tends to decrease the mobility of immiscible fluids in soil. This can result in slower flow rates and reduced spreading of the contaminants, leading to more localized contamination.

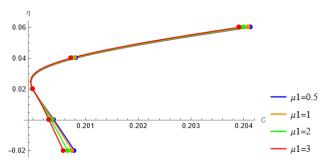


Fig. 3. Effects of various values of μ_1 on concentration profiles

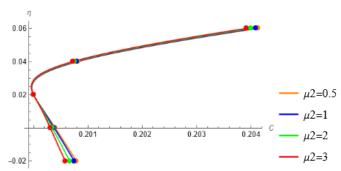


Fig. 4. Effects of various values of μ_2 on concentration profiles

Concentration for different heights of the two subsurface 1 and subsurface 2 in shown in Figure 5 and Figure 6 in which the height and arrangement of soil layers affect the vertical movement of contaminants. The is decrease in the concentration is shown, as the fluid approaches the depths of subsurface 2. (i.e.) the concentration decreases as the h_2 (height of subsurface 2) increases.

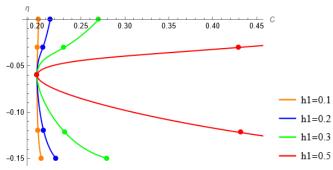


Fig. 5. Effects of various values of h_1 on concentration profiles

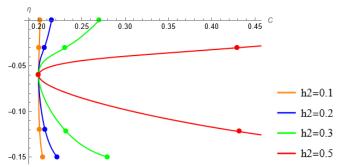


Fig. 6. Effects of various values of h_2 on concentration profiles

Outcomes of diffusion coefficient on concentration profiles are shown in Figure 7 and Figure 8 show that the diffusion coefficient is varied from D=0.1 to D=2. The steepness of the parabola at its vertex reflects how sensitive the concentration profile is to changes in the diffusion coefficient. A steeper parabola indicates higher sensitivity, while a shallower curve suggests that changes in the diffusion coefficient have a less pronounced effect.

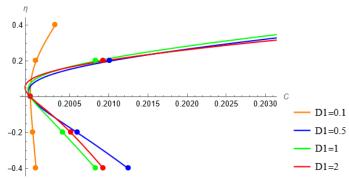


Fig. 7. Effects of Diffusion coefficient ${\cal D}_1$ on concentration profiles

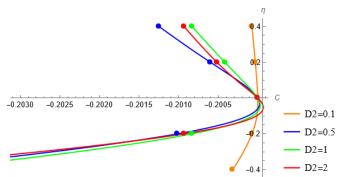


Fig. 8. Effects of Diffusion coefficient D_2 on concentration profiles

where i=1,2. The subscripts 1,2 represents the quantities of subsurface 1 and subsurface 2 respectively.

4. Conclusion

The dispersion of contaminants seeping through two sub surfaces of the soil by two immiscible fluids is studied in this model. Advection diffusion equation is used in the mathematical model to analyse the fluid flow velocities, densities, temperature and concentration of leachate water for each layer separately. The proposed model provides insight to the researchers and helps them understand the complexity of the contamination in soil. The graphs depict the effects of concentration profiles, velocity profiles on the soil sub surfaces. For future research, two types of pressure, density and concentration for each layer can be used. Also, multi-immiscible fluids with multi-soil layer can be discussed or considered.

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