

A Computational Study of Transmission of Various Pollutants

Dr. Mahesh Chandra¹ and Mr. Prashant Kumar²

¹Professor, Department of Mathematics, F.S. University, Shikohabad, Uttar Pradesh, INDIA.

²Research Scholar, Department of Mathematics, F.S. University, Shikohabad, Uttar Pradesh, INDIA.

¹Corresponding Author: maheshchandra2047@gmail.com



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ABSTRACT

The present paper deals with Numerical Simulation of Pollutant Transport in Surface Media. The contamination of surface media, such as rivers, lake and open soil layers, due to industrial run off and agriculture waste represents a critical environmental challenge. Understanding how these contaminants disperse over time and space is vital for effective environmental management and remediation. This paper presents a robust mathematical framework and numerical simulation designed to predict the transport dynamics of pollution in surface media. The physical phenomena primarily advection, dispersion and chemical reactions are mathematically formulated using partial differential equations specially the advection-diffusion reaction equation given the geometrical irregularity and varying flow dynamics inherent in surface system. In the present study numerical techniques such as the Finite Difference method, Finite Element method, to simulate the transport process under diverse conditions.

Keywords- Numerical Simulation, Pollutant Transport, Advection-Diffusion, Surface Media.

I. INTRODUCTION

Most of researchers have already done on some similar topics. They have motivated me to do on this topic. Here we will like to show their valuable contributions. Tian, L., Gu, S, Wu, Y and Zhang, C. (2022) focused on deployed coupled Smooth Particle Hydrodynamics and shallow water equation. They used numerical strategy to solve the advection diffusion reaction dynamics across real world surface topographies. They have demonstrated how particle-based Lagrangian models outperforms classical mesh solvers when dealing with complex highly irregular boundary gradients.

Nasrudin, F.S.M., Phang, C. & Kanwal, A. (2023) has focused on a Ritz approximation framework to solve fractal-fractional advection-diffusion reaction equation analyzing how non local derivative structure impact localized concentration peaks over complex geometry. Xuan, W., Yang, C., Wu, X., Shao, Y., & Bai, Y. (2024) investigated solute and pollutant transport through open river domain using multilayer rigid

vegetation matrix. Their numerical models illustrate how biological obstruction introduce non-uniform mechanical dispersion tensors.

Hao, D. N., Thanh, N. T., Duc, N.V. & Thang, N.V. (2025) conducted a comprehensive numerical modelling review targeting leaching kinematics and transport boundaries across complex multi-process surface-subsurface matrices. Hafiyyan, Q., and Nirmala, A. (2026) formulated a stabilized modifier with numerical filter for 1D pollutant transport tracking. The scheme resolves sharp Gaussian concentration pulse with highly localized absolute errors.

II. MATHEMATICAL MODELING OF GOVERNING EQUATION

The governing equation Which was given (Pinder-1976) Bear (1979) Freeze and Cherry in (1979).

$$L(h) = \frac{d}{dx} \left[T_{xx} \frac{dh}{dx} \right] + \frac{d}{dy} \left[T_{yy} \frac{dh}{dy} \right] + \frac{d}{dz} \left[T_{zz} \frac{dh}{dz} \right] + R - Q = S \frac{dh}{dt} \dots\dots\dots(1)$$

$$L(c) = \frac{dc}{dt} + \frac{d}{dx}(V_x c) + \frac{d}{dy}(V_y c) + \frac{d}{dz}(V_z c) - \frac{d}{dx}(d_{xx} \frac{dc}{dx}) - \frac{d}{dy}(d_{yy} \frac{dc}{dy}) - \frac{d}{dz}(d_{zz} \frac{dc}{dz}) + RC - QC = 0 \dots (2)$$

$$\text{Where } V_x = -\frac{1}{b} \frac{d}{dx}(T_{xx} h)$$

$$v_y = -\frac{1}{b} \frac{d}{dx}(T_{xy} h)$$

$$v_z = -\frac{1}{b} \frac{d}{dz}(T_{zz} h)$$

$$D_{xx} = \alpha L \frac{V_x^2}{V}, D_{yy} = \alpha T \frac{V_y^2}{V} + \alpha L \frac{V_y^2}{V^2}, D_{zz} = \alpha L \frac{V_z^2}{V^2}$$

Intertidal and boundary conditions will take the form

$$h(x, y, 0) = h_0 \quad c(x, y, 0) = C_0$$

$$\text{for } 0 \leq x \leq L, 0 \leq y < w$$

$$D_{xx} \frac{dc}{dx} n_x = 0 \dots (3)$$

$$T_{xx} \frac{dh}{dx} n_x = 0 \dots (4)$$

$$D_{xx} \frac{dc}{dx} n_x = 0 \dots (5)$$

$$D_{yy} \frac{dc}{dy} n_y = 0 \dots (6)$$

$$D_{zz} \frac{dc}{dz} n_z = 0 \dots (7)$$

III. NUMERICAL TECHNIQUES

Finite Element Method: in this investigation we have replied weak formulation

$$\hat{h} = \sum_{i=1}^N h_i \phi_i$$

$$C^A = \sum_{i=1}^N c_i \phi_i$$

The weighted Residual at all nodes by taking in account $\int \int_r \phi_i L(h^A) dx dy = 0, \int \int_r$

Applying Green's Theorem to eliminate Partial Differential equation of 2nd order

$$[A^k] [h^T] [B^h] \left\{ \frac{dh}{dt} \right\} = [F^h]$$

The elements of coefficient matrix vector for both system of equation are

$$A_{ij}^c = \int \int -D_{xx} \frac{d\phi_i}{dx} \frac{d\phi_j}{dx} - d_{xy} \frac{d\phi_i}{dx} \cdot \frac{d\phi_j}{dy} - d_{yx} \frac{d\phi_i}{dy} \frac{d\phi_j}{dx} - D_{yy} \frac{d\phi_i}{dy} \cdot \frac{d\phi_j}{dy} - D_{zz} \frac{d\phi_i}{dz} + v_x \frac{d\phi_i}{dx} + v_y \frac{d\phi_i}{dy} + v_z \frac{d\phi_i}{dz}$$

The integration of coefficient matrix of triangular elemental is

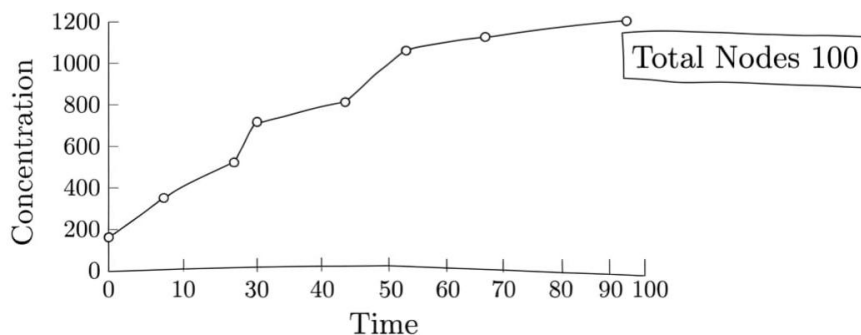
$$\int \int \int_e \frac{d\phi_i^k}{dx} \cdot \frac{d\phi_j^k}{dz} dx dy dz \dots (8)$$

After the disperse movement equal to random adjective location

$$x_{pk+1} = x_P, k + 1 \sqrt{2 \alpha_L V_x \Delta t} \dots (9)$$

$$y_{pk+1} = y_P, k + 1 \sqrt{2 \alpha_L V_y \Delta t} \dots (10)$$

IV. RESULT & DISCUSSION



The graph displays the clear, progressive increase in concentration over time showing a non-linear or stepped upward trajectory before starting to level off near the observed concentration. A notable sharp increase in concentration occurs between $t = 25$ and $t = 28$ as well as between $t = 40$ and $t = 50$. The developed model reproduce observed pollutant behavior.

FUTURE SCOPE

In future we will work to 3D models reactive pollutant or coupling with GIS / remote sensing.

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