

The Mathematical modelling of environmental pollution using the Freundlich non-linear contaminant transport formulation

Y. M Aiyesimi
Department of Mathematics and Computer Science
Federal University Of Technology, Minna, Nigeria

Abstract

In this paper environmental pollution has been modeled mathematically using the Freundlich non-linear contaminant transport formulation. An analytical solution of lower order perturbation of the concentration $C(x,t)$ is obtained. Flow profiles for various values of molecular diffusion D and the velocity U are studied and the effects of these parameters on the flow regimes highlighted.

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1.0 Introduction

Computational fluid dynamics has grown to become a versatile tool for the investigation of transport phenomena. Application of this abounds in the various fields of engineering, science and medicine. Great advancement in the numerical techniques and their implementations in very efficient flow simulation codes together with astronomical growth in computer power have provided this field of research with the maturity to compete the more familiar classical methods (experimental and analytical methods) with a similar level of accuracy and hence reliability of results. In addition computational fluid dynamics (CFD) offers a greater flexibility in the specification of problem conditions. Not only the boundary and the fluid properties can be well controlled but certain physical effects may be isolated or supported thus creating new perspectives to the research and application of fluid dynamics. The present work will profit immensely from the above-mentioned advantages of numerical investigation approach and employ them effectively in the detailed analysis of the contaminant transport as it pertains to environmental pollution.

2.0 Mathematical Modelling and Formulation of Physical Problems

The concentration $C(x,t)$ of the contaminant is governed by the differential equation

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + \frac{P_b}{n} \frac{\partial S}{\partial t} - D \frac{\partial^2 C}{\partial x^2} = 0 \quad (2.1)$$

where U is the effective velocity of flow, P_b is the bulk density of porous medium, n the porosity of medium, S the mass of contaminant adsorbed and D is the molecular diffusion/ mechanical dispersion. For simplicity we assume these parameters to be constant. Now since the mass of contaminant adsorbed depends much more on time than on the concentration the equation above is of the form

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + \frac{\partial \Phi(C)}{\partial C} \frac{\partial C}{\partial t} - D \frac{\partial^2 C}{\partial x^2} = 0$$

that is,
$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + \epsilon \frac{\partial C}{\partial t} - D \frac{\partial^2 C}{\partial x^2} = 0 \quad (2.2)$$

Equation (2.2) is therefore the mathematical model representing our physical problem.

2.1 Solution technique

The concentration $C(x,t)$ is expanded with ϵ as the perturbation parameter. That is

$$C(x,t) = C^{(0)}(x,t) + \epsilon C^{(1)}(x,t) + \epsilon^2 C^{(2)}(x,t) + \epsilon^3 C^{(3)}(x,t) + \dots \quad (2.3)$$

The substitution of equation (2.3) into equation (2.2) results in the following:

$$\begin{aligned} & \frac{\partial C^{(0)}}{\partial t} + U \frac{\partial C^{(0)}}{\partial x} + D \frac{\partial^2 C^{(0)}}{\partial x^2} + \varepsilon \left[\frac{\partial C^{(0)}}{\partial t} + \frac{\partial C^{(1)}}{\partial t} + U \frac{\partial C^{(1)}}{\partial x} - D \frac{\partial^2 C^{(1)}}{\partial x^2} \right] \\ & + \varepsilon^2 \left[\frac{\partial C^{(1)}}{\partial t} + \frac{\partial C^{(2)}}{\partial t} + U \frac{\partial C^{(2)}}{\partial x} - D \frac{\partial^2 C^{(2)}}{\partial x^2} \right] + \varepsilon^3 \left[\frac{\partial C^{(2)}}{\partial t} + \frac{\partial C^{(3)}}{\partial t} + U \frac{\partial C^{(3)}}{\partial x} - D \frac{\partial^2 C^{(3)}}{\partial x^2} \right] \\ & + \varepsilon^4 \left[\frac{\partial C^{(3)}}{\partial t} + \frac{\partial C^{(4)}}{\partial t} + U \frac{\partial C^{(4)}}{\partial x} \right] + \Lambda = 0 \end{aligned}$$

Hence neglecting orders two and all higher orders for obvious reason we therefore have to solve the following system of homogenous differential equations:

$$\frac{\partial C^{(0)}}{\partial t} + U \frac{\partial C^{(0)}}{\partial x} - D \frac{\partial^2 C^{(0)}}{\partial x^2} = 0 \quad (2.4)$$

$$\frac{\partial C^{(0)}}{\partial t} + \frac{\partial C^{(1)}}{\partial t} + U \frac{\partial C^{(1)}}{\partial x} - D \frac{\partial^2 C^{(1)}}{\partial x^2} = 0 \quad (2.5)$$

The solution of our contaminant problem is therefore given as;

$$C(x, t) = C^{(0)}(x, t) + \varepsilon C^{(1)}(x, t) \quad (2.6)$$

2.1.1 Solution of the order (1) problem

We recall that the order (1) problem is represented by the following initial boundary value problem:

$$\frac{\partial C^{(0)}}{\partial t} + U \frac{\partial C^{(0)}}{\partial x} - D \frac{\partial^2 C^{(0)}}{\partial x^2} = 0 \quad (2.7)$$

$$C^{(0)}(0, t) = 1, C^{(0)}(l, t) = 0 \text{ and } C^{(0)}(x, 0) = 1$$

Adopting the separation of variable technique we have the following two uncoupled ordinary differential equations in the independent variables x and t :

$$D \frac{\partial^2 \chi}{\partial x^2} + -U \frac{d\chi}{dx} - \lambda^2 \chi(x) = 0,$$

$$\text{and } \frac{dT}{dt} + \lambda^2 T(t) = 0 \quad (2.8)$$

where we have assumed here that $C^{(0)}(x, t) = \chi(x)T(t) \neq 0$ and λ^2 is an arbitrary constant. On applying the boundary and initial conditions after solving we have that $T(t) = e^{-\lambda^2 t}$

$\chi(x) = e^{\frac{Ux}{2D}} (CoshKx - coth kl \sinh kx)$ where $k = \frac{\sqrt{U^2 + 4D\lambda^2}}{2D}$. Thus the solution to the order (1) problem is given as;

$$C^{(0)}(x, t) = e^{\frac{Ux}{2D} - \lambda^2 t} (\cosh kx - Cothkl \sinh kx) \quad (2.9)$$

Consequently the order (ε) problem is governed by the initial boundary value problem;

$$\frac{\partial C^{(1)}}{\partial t} + U \frac{\partial C^{(1)}}{\partial x} - D \frac{\partial^2 C^{(1)}}{\partial x^2} = \lambda^2 e^{\frac{Ux}{2D} - \lambda^2 t} (\cosh kx - coth kl \sinh kx) \quad (2.10)$$

$$C^{(1)}(0, t) = 0 = C^{(1)}(l, t) = C^{(1)}(x, 0)$$

Taking the Laplace transform of equation (2.1.4) in the time domain results in the following ordinary differential equation:

$$D \frac{\partial^2 y}{\partial x^2} - U \frac{dy}{dx} - sy = -\frac{\lambda^2}{\lambda^2 + s} e^{\frac{Ux}{2D}} (\cosh kx - coth kl \sinh kx), \quad y(0) = y(l) = 0 \quad (2.11)$$

where y is the Laplace transform of $C^{(1)}(x, t)$ and s is the Laplace parameter the complimentary function

of equation (2.11) is given as $y_c(x) = e^{\frac{Ux}{2D}} (\alpha \sinh \mu x + \beta \cos \mu x)$ where $\mu = \frac{\sqrt{U^2 + 4sD}}{2D}$ and α and β

are arbitrary constants of integration. Adopting the variation of parameter technique the particular integral

of equation (2.11) is given as $y_p(x) = \frac{\lambda^2 e^{\frac{Ux}{2D}}}{2\mu(\lambda^2 + s)} \left[\frac{\cosh kx - \coth kl \sinh kx}{k + \mu} - \frac{\cosh kx - \coth kl \sinh kx}{k - \mu} \right]$.

Hence by virtue of our earlier definitions we finally have that,

$$y(x) = e^{\frac{Ux}{2D}} (\alpha \sinh \mu x + \beta \cosh \mu x) - \frac{\lambda^2 e^{\frac{Ux}{2D}} (\coth kl \sinh kx - \cosh kx)}{(s + \lambda^2)(s - \lambda^2)}$$

that is
$$y(x) = e^{\frac{Ux}{2D}} \left[(\alpha \sinh \mu x + \beta \cosh \mu x) - \frac{\lambda^2 (\coth kl \sinh kx - \cosh kx)}{(s + \lambda^2)(s - \lambda^2)} \right].$$

On applying the corresponding boundary conditions we thus obtain;

$$y(x) = \frac{\lambda^2 e^{\frac{Ux}{2D}}}{(s + \lambda^2)(s - \lambda^2)} [\cosh \mu x - \coth kl \sinh kx] + (\cosh \mu x - \coth kl \sinh kx)$$

that is

$$y(x) = \frac{D\lambda^2 e^{\frac{Ux}{2D}}}{(\lambda^2 + s)(s - \lambda^2)} [(\cosh kx - \coth kl \sinh kx) + (\cosh \mu x - \coth kl \sinh kx)]$$

We recall here that $C^{(1)}(x, t) = L^{-1}[y(x)]$, that is

$$\begin{aligned} C^{(1)}(x, t) &= L^{-1} \left[\frac{\lambda^2 e^{\frac{Ux}{2d}}}{(s + \lambda^2)(s - \lambda)} [Cosh\mu x - Coth\mu l \sinh \mu x] - (Coshkx - Cothkl \sinh kx) \right] \\ &= \lambda^2 e^{\frac{Ux}{2D}} L^{-1} \left[\frac{1}{(s + \lambda^2)(s - \lambda^2)} [(Cosh\mu x - Coth\mu l \sinh \mu x) + (Coshkx - Cothkl \sinh kx)] \right] \\ &= \lambda^2 e^{\frac{Ux}{2D}} \left\{ L^{-1} \left[\frac{1}{(s + \lambda^2)(s - \lambda^2)} [(Cosh\mu x - Coth\mu l \sinh \mu x)] \right] + L^{-1} \left[\frac{1}{(s + \lambda^2)(s - \lambda^2)} [Coshkx - Cothkl \sinh kx] \right] \right\} \\ &= \lambda^2 e^{\frac{Ux}{2D}} [Coshkx - Cothkl \sinh kx] L^{-1} \left[\frac{1}{(s + \lambda^2)(s - \lambda^2)} \right] + \lambda^2 e^{\frac{Ux}{2D}} \left[\frac{1}{(s + \lambda^2)(s - \lambda^2)} [(Cosh\mu x - Cothkl \sinh kx] \right] \\ &= e^{\frac{Ux}{2D}} Sinh\lambda^2 t [Coshkx - Cothkl \sinh kx] + e^{\frac{Ux}{2D}} \left[\frac{e^{\lambda^2 t} \sinh(1-x)\xi}{2Sinh\xi l} - \frac{e^{-\lambda^2 t} Sinh(1-x)\eta}{2Sinh\eta l} \right] \\ &+ \frac{2\pi D\lambda^2 e^{\frac{Ux}{2D}}}{1^2} \sum_{p=0}^{\infty} \frac{pe^{s_p^1}}{(s_p + \lambda^2)(s_p - \lambda^2)} Sin \left[\frac{p\pi}{1} x \right] \end{aligned}$$

where

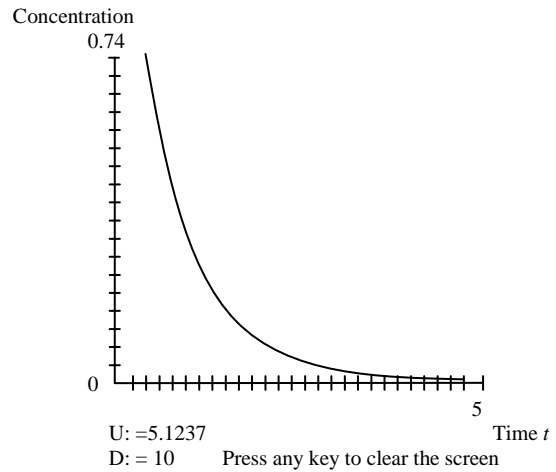
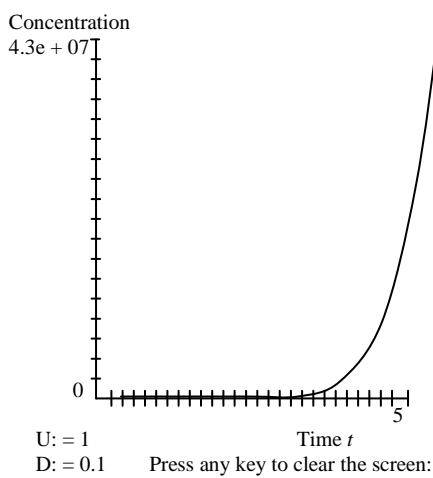
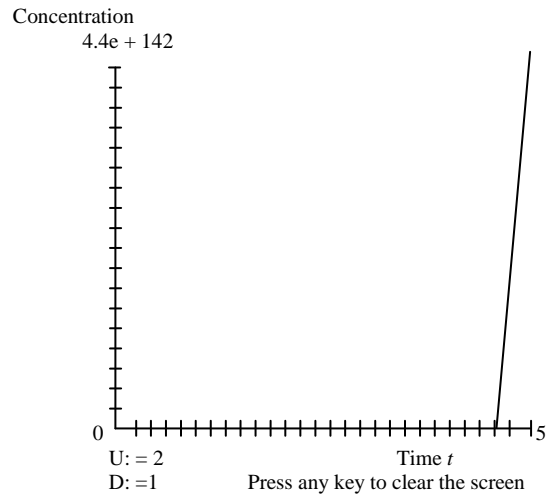
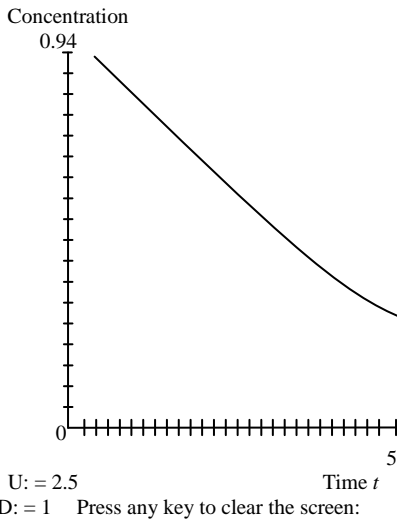
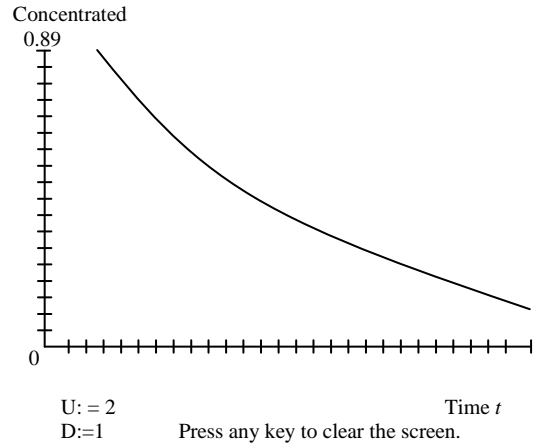
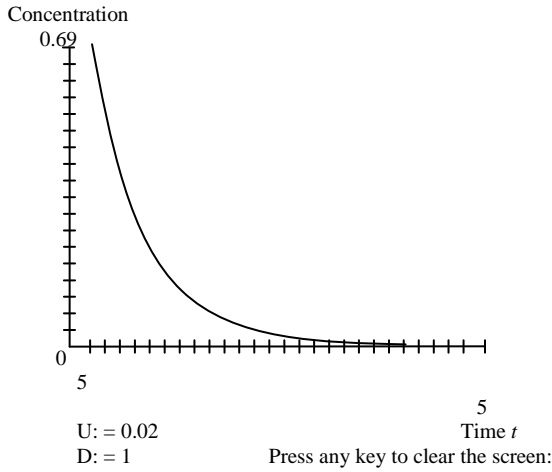
$$\xi = \frac{\sqrt{U^2 + 4D\lambda^2}}{2D} \quad \eta = \frac{\sqrt{U^2 - 4D\lambda^2}}{2D}, \quad s_p = \frac{4D^2 p^2 \pi^2 + U^2 l^2}{4Dl^2}; \quad \mu_p = \frac{ip\pi}{1}, \quad i = \sqrt{-1}$$

We thus have as the final result of our initial boundary value problem given as;

$$\begin{aligned} C(x, t) &= e^{\frac{Ux}{2D} \lambda^2 t} (Coshkx - Cothkl \sinh kx) \\ &+ \mathcal{E} \left[e^{\frac{Ux}{2D} \sinh \lambda^2 t} [Coshkx - Cothkl \sinh kx] + e^{\frac{Ux}{2D}} \left[\frac{e^{\lambda^2 t} Sinh(1-x)\xi}{2Sinh\xi l} - \frac{e^{-\lambda^2 t} Sinh(1-x)\eta}{2Sinh\eta l} \right] \right] \\ &+ \frac{2\pi D\lambda^2 e^{\frac{Ux}{2D}}}{1^2} \sum_{p=0}^{\infty} \frac{pe^{s_p^1}}{(s_p + \lambda^2)(s_p - \lambda^2)} Sin \left[\frac{p\pi}{1} x \right] \end{aligned}$$

3.0 Numerical Computation

In what follows we investigate the influence of the parameters such as the molecular diffusion (D), the velocity (U) and distance (x) on the concentration profiles $C(x, t)$.



4.0 **Result**

The numerical simulations above indicate decrease in the concentration with increasing molecular diffusion (D) and decreasing velocity (U). It also shows decrease in the concentration of the pollutant as we move from the source point which agrees completely with physical observation.

Refereces

- [1] Dawson, C. (1998) Analysis of an upwind finite element method for non-linear contaminant transport equation. Journal of the society for industrial and applied mathematics.
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- [3] Spiegel, M. R Theory and problems of advanced mathematics for engineers and scientist. Schaum outline series. McGraw-hill Book Company. SI (metric edition).