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Finite element analysis of one–dimensional hydrodynamic dispersion of a reactive solute in electroosmotic flow

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Abstract

In this research work, we consider the one dimensional hydrodynamic dispersion of a reactive solute in electroosmotic flow. We present results demonstrating the utility of finite element methods to simulate and visualize hydrodynamic dispersion in the electroosmotic flow. From examination of concentration profile, effective diffusion coefficients were numerically determined for different peclet numbers. Our result shows close approximation to analytic solution.

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1.0 Introduction

Chromatographic separation using electric fields to drive electro-osmotic flow are usually performed in packed columns. The role of the packing is to provide a large surface area for solute adsorption and thereby to improve column performance. However, recent advances in manufacturing methods now enable the fabrication of electrochromatographic columns having characteristics transverse dimensions in the micron to submicron range.

Axial dispersion is important in chromatographic process because it tends to spread the solute peaks. As a result, closely packed peaks cannot be resolved when dispersion is excessive. Estimating the magnitude of the dispersion and identifying the conditions leading to minimum dispersion are thus important to optimizing the process.

As a solute is converted in open column transverse variations in the velocity field produce transverse variations in the solute concentration. At the same time, transverse diffusion tends to reduce induce concentration gradients. At sufficiently late times transport in the axial direction is just balance by diffusive transport in the transverse direction. This is the phenomenon of hydrodynamic dispersion. Such dispersion yields a mean axial profile of the solute concentration that is consistent with diffusive transport alone, although the apparent diffusivity is larger than the actual value.

Various forms of (I.I.I) has been solved by various researchers for various boundary conditions. Bear (1979) [2] provides some analytical solutions for the one dimensional case using the laplace transform.

Varoglu (1982) [10] applied a finite element model for the diffusion convection equation with application to air pollution. (HromadkaII and Guymon (1982) [6] use the nodal integration model to solve the one dimensional advection diffusion problem. Barker (1982) also solved the case of solute transport in fissured aquifer using the method of laplace transform. Tim and Mostaghimi (1989) [9] used the finite element to analyse the one dimensional form of the transport of of pesticides and their metabolites in the unsaturated zone. But the problem of flow of solute in an electroosmotic flow has only been treated sparingly for example Griffiths and Roberts (2002) [4] considered the case of a non-reactive neutral solute using the method of asymptotic series solution. The difference between the above literatures and ours is that we are considering the problem of the flow of a reactive solute.in electroosmotic flow which involves solving three partial differential equations simultaneously. In this paper we applied the finite element solution to the time dependent problem to determine the effect of the dispersion coefficient for various times.

2.0 Governing Equation

In this research work we consider the flow of a two dimensional planar transport of a reactive solute in an electro-osmotic flow. The flow is assumed to be incompressible and transport properties are assumed constant. Under this restriction the time dependent concentration field is governed by

$$\frac{\partial c}{\partial t} = Dx\frac{\partial \xi}{\partial x^2} + Dy\frac{\partial^2 c}{\partial y^2} - U\frac{\partial c}{\partial x} + \lambda c \tag{2.1}$$

Where c is the local solute concentration t is the time, u is the local fluid velocity Dx, Dy are the coefficients of hydrodynamic dispersion in the x and y direction respectively. λ is the rate of chemical reaction.

Further assuming that flow is steady and that inertial effects are small, the momentum equation may be written as

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{\ell}{\mu}\frac{\partial \phi}{\partial x} \tag{2.2}$$

Where μ is the viscosity, ℓ is the net local charge density, and ϕ is the local electric potential.

Finally, for a dielectric constant $\in$ that does not vary with position the poison equation governing the electric field is:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = \frac{-\ell}{\in} \tag{2.3}$$

and the local charge density may be related to the electric field potential through the Boltzmann distribution given by:

$$\ell = -2FZCeSinh(ZF\phi/RT)$$

where F is the Faraday constant, Z is the ion charge number, Ce is the bulk fluid ion concentration R is the universal gas constant and T is the temperature.

3.0 Solution of the one-dimensional contaminant dispersion problem.

Consider the one dimensional contaminant dispersion equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - U\frac{\partial c}{\partial x} + \lambda c \tag{3.1}$$

together with the following boundary and initial conditions

$$\left.\begin{aligned} C(x,o) &= 0 \\ C(o,t) &= C_m \\ C(L,t) &= 0 \end{aligned}\right\} \tag{3.2}$$

Let

$$C^{(e)} = \sum N_i^{(e)}(x)C(t) \tag{3.3}$$

where $N_i = \dfrac{x_{i+1} - x}{x_{i+1} - x_i}$ and $N_i = \dfrac{x - x_i}{x_{i+1} - x_i}$ are the linear Lagrange interpolating functions. Suppose that U_n, C_n and ϕ_n are some approximate solutions Huebner[5] the Galerkin procedure applied at node i of an isolated element becomes

$$\int N_i\left(\frac{\partial C^{(e)}}{\partial t}-D\frac{\partial^2 C^{(e)}}{\partial x^2}+U_n\frac{\partial C^{(e)}}{\partial x}-\lambda C^{(e)}(t)\right)dx=0 \qquad (3.4)$$

$$\Rightarrow\int N_i\left(\frac{\partial N^{(e)}C(t)}{\partial t}-D\frac{\partial^2 N^{(e)}C(t)}{\partial x^2}+U_n\frac{\partial N^{(e)}C(t)}{\partial x}-\lambda n^{(e)}C(t)\right)dx=0 \qquad (3.5)$$

$$\Rightarrow\int\left[N_iN^{(e)}\frac{\partial C(t)}{\partial t}-DN_i\frac{\partial^2 N}{\partial x^2}C(t)+U_nN_i\frac{\partial N^{(e)}}{\partial x}C(t)-\lambda N_iN^{(e)}C(t)\right]dx=0 \qquad (3.6)$$

$$\Rightarrow\int N_iN^{(e)}\frac{\partial C(t)}{\partial t}dx-D\int N_i\frac{\partial N^{(e)}}{\partial x}C(t)-\int\frac{\partial N_i}{\partial x}.\frac{\partial N^{(e)}}{\partial x}C(t)dx$$
$$+U_n\int N_i\frac{\partial N^{(e)}}{\partial x}C(t)dx-\lambda\int N_iN^{(e)}C(t)dx=0 \qquad (3.7)$$

$$\Rightarrow\int N_iN^{(e)}\frac{\partial C(t)}{\partial t}dx+D\int\frac{\partial N_i}{\partial x}.\frac{\partial N^{(e)}}{\partial x}C(t)$$
$$+U_n\int N_i\frac{\partial N^{(e)}}{\partial x}C(t)dx-\lambda\int N_iN^{(e)}C(t)dx=0 \qquad (3.8)$$

Integrating (3.8) between x_j and x_k we have

$$\int_{x_j}^{x_k}\begin{bmatrix}N_jN_j & N_JN_I\\ N_kN_j & N_kN_k\end{bmatrix}\begin{bmatrix}C_j^{/}(t)\\ C_k^{/}(t)\end{bmatrix}dx+D\int_{x_j}^{x_k}\begin{bmatrix}N_j^{/}N_j^{/} & N_j^{/}N_k^{/}\\ N_k^{/}N_j^{/} & N_k^{/}N_k^{/}\end{bmatrix}\begin{bmatrix}C_j^{/}(t)\\ C_k^{/}(t)\end{bmatrix}dx+U_n\int_{x_j}^{x_k}\begin{bmatrix}N_j^{/}N_j^{/} & N_j^{/}N_k^{/}\\ N_k^{/}N_j^{/} & N_k^{/}N_k^{/}\end{bmatrix}$$
$$\begin{bmatrix}C_j^{/}(t)\\ C_k^{/}(t)\end{bmatrix}dx-\lambda\int_{x_j}^{x_k}\begin{bmatrix}N_jN_j & N_jN_k\\ N_kN_j & N_kN_k\end{bmatrix}\begin{bmatrix}C_j(t)\\ C_k(t)\end{bmatrix}dx=0 \qquad (3.9)$$

Carrying out the necessary integration and differentiation we have

$$\frac{Le}{6}\begin{bmatrix}2 & 1\\ 1 & 2\end{bmatrix}\begin{bmatrix}\dot{C}_j\\ \dot{C}_k\end{bmatrix}+\frac{D}{Le}\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix}\begin{bmatrix}C_j\\ C_k\end{bmatrix}+\frac{U_n}{2}\begin{bmatrix}-1 & 1\\ -1 & 1\end{bmatrix}\begin{bmatrix}C_j\\ C_k\end{bmatrix}-\frac{\lambda Le}{6}\begin{bmatrix}2 & 1\\ 1 & 2\end{bmatrix}\begin{bmatrix}C_j\\ C_k\end{bmatrix}=0 \qquad (3.10)$$

We shall now proceed to sum up the element equations for $x_i < x_j < x_k$ to give

$$\frac{Le}{6}\begin{bmatrix}2 & 1 & 0\\ 1 & 4 & 1\\ 0 & 1 & 2\end{bmatrix}\begin{bmatrix}\dot{C}_i\\ \dot{C}_j\\ \dot{C}_k\end{bmatrix}+\frac{D}{Le}\begin{bmatrix}1 & -1 & 0\\ -1 & 2 & -1\\ 0 & -1 & 1\end{bmatrix}\begin{bmatrix}C_i\\ C_j\\ C_k\end{bmatrix}+\frac{U_n}{2}\begin{bmatrix}-1 & 1 & 0\\ -1 & 0 & 1\\ 0 & -1 & 1\end{bmatrix}\begin{bmatrix}C_i\\ C_j\\ C_k\end{bmatrix}-\frac{\lambda Le}{6}\begin{bmatrix}1 & -1 & 0\\ -1 & 2 & -1\\ 0 & -1 & 1\end{bmatrix}\begin{bmatrix}C_i\\ C_j\\ C_k\end{bmatrix}=0 \qquad (3.11)$$

$$\Rightarrow \frac{1}{6}\begin{bmatrix} 2 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 2 \end{bmatrix}\begin{bmatrix} \dot{C}_i \\ \dot{C}_j \\ \dot{C}_k \end{bmatrix} + \frac{D}{L_e^2}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}\begin{bmatrix} C_i \\ C_j \\ C_k \end{bmatrix} + \frac{U_n}{2Le}\begin{bmatrix} -1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{bmatrix}\begin{bmatrix} C_i \\ C_j \\ C_k \end{bmatrix}$$

$$-\frac{\lambda}{6}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}\begin{bmatrix} C_i \\ C_j \\ C_k \end{bmatrix} = 0 \qquad (3.12)$$

which can be written in the form:

$$\frac{1}{6}\left[\dot{C}_{i-1} + 4\dot{C}_i + \dot{C}_{i+1}\right] + \frac{D}{h^2}\left[-C_{i-1} + 2C_i - C_{i+1}\right]$$

$$+\frac{U_n}{2h}\left[-C_{i-1} + C_{i+1}\right] - \frac{\lambda}{6}\left[C_{i-1} + 4C_i + C_{i+1}\right] = 0 \qquad (3.13)$$

Taking $Le = h$ i.e.

$$\frac{1}{6}\left[\dot{C}_{i-1} + 4\dot{C}_i + \dot{C}_{i+1}\right] + \frac{D}{h^2}\left[C_{i-1} - 2C_{i_i} + C_{i+1}\right]$$

$$+\frac{U_n}{2h}\left[-C_{i-1} + C_{i+1}\right] - \frac{\lambda}{6}\left[C_{i-1} + 4C_i + C_{i+1}\right] = 0 \qquad (3.14)$$

Applying the trapezoidal rule (Segerlind 1976) we obtain the Crank Nicolson Method

$$\left[1 - 3rD - \frac{3}{2}r_0U_n - \frac{k\lambda}{2}\right]C_{i-1}^{n+1} + \left[4 + 6rD - 2k\lambda\right]C_i^{n+1}$$

$$+\left(1 - 3rD + \frac{3}{2}r_0U_n - \frac{k\lambda}{2}\right)C_{i-1}^{n+1}$$

$$= \left[1 + 3rD + \frac{3r_0U_n}{2} + \frac{k\lambda}{2}\right]C_{i-1}^{n}$$

$$+\left(4 - 6rD + 2k\lambda\right)C_i^n + \left[1 + 3rD - \frac{3r_0U_n}{2} + \frac{k\lambda}{2}\right]C_{i+1}^{n} \qquad (3.15)$$

Multiplying through by 2 we shall have

$$\left(2 - 6rD - 3r_0U_n - k\lambda\right)C_{i-1}^{n+1} + \left(8 + 12rD - 4k\lambda\right)C_i^{n+1}$$

$$+\left(2 - 6rD + 3r_0U_n - k\lambda\right)C_{i+1}^{n+1}$$

$$= \left(2 - 6rD + 3r_0U_n + k\lambda\right)C_{i-1}^{n}$$

$$+\left(8 - 12rD - k\lambda\right)C_i^n + \left(1 + 6rD - 3r_0U_n + k\lambda\right)C_{i+1}^{n} \qquad (3.16)$$

which is the difference equation for equation (3.15), where $r = \dfrac{Dk}{h^2}, r_0 = \dfrac{Uk}{h}, k = \Delta t$ and $h = \Delta x$.

We also have

$r_0 =$ Corrant number

$r =$ Diffusion number

and $\frac{r_0}{r} =$ Pedet number

4.0 Solution of the one–dimension momentum equation.

The one dimensional momentum equation is given by

$$\mu \frac{\partial^2 u}{\partial x^2} = \ell \frac{\partial \phi}{\partial x} \tag{4.1}$$

together with the following boundary conditions

$$\left.\begin{array}{l} U(0) = 0 \\ U(L) = U_1 \end{array}\right\} \tag{4.2}$$

We can choose the velocity and Electric potential components as field variables and apply the method of weighted residuals with Galerkins criterion. For a general element domain we select U and ϕ as nodal variables and interpolate the variables as follows $U^{(e)} = N_i U_i(x); \phi^{(e)} = N_i \phi_i(x)$ Zienkiewicz and Taylor [12], Taylor and Hood [8], Yamada et'al [11]; Tim and Mostaghimi [9], Smith and Ariffiths [7] Chung [3].

Now applying the Galerkin's method as said above we have

$$\int_n N_i \left[\frac{\partial^2 u^{(e)}}{\partial x^2} - e \frac{\partial \phi^{(e)}}{\partial x} \right] dx = 0 \tag{4.3}$$

on integration by parts of the first term of (4.3) we have

$$N_i \frac{\partial N^{(e)} U_i}{\partial x} \Big/_B - \int \frac{\partial N_i}{\partial x} . \frac{\partial N^{(e)}}{\partial x} U_i dx - \ell \int N_i \frac{\partial N^{(e)}}{\partial x} \phi_i \partial x = 0 \tag{4.4}$$

Integration between the limits $x_i < x < x_j$ we have

$$N_i \frac{\partial N^{(e)} U_i}{\partial x} \Bigg|_{x_i}^{x_j} - \int_{x_i}^{x_j} \frac{\partial N_i}{\partial x} . \frac{\partial N^{(e)}}{\partial x} .U_i dx - \frac{\ell}{\mu} \int N_i \frac{\partial N^{(e)}}{\partial x} \phi_i \partial x = 0 \tag{4.5}$$

Since the first term of (4.5) satisfies the boundary conditions we have

$$\int_{x_i}^{x_j} \frac{\partial N_i}{\partial x} . \frac{\partial N^{(e)}}{\partial x} .U_i dx + \frac{\ell}{\mu} \int N_i \frac{\partial N^{(e)}}{\partial x} \phi_i \partial x = 0 \tag{4.6}$$

$$\Rightarrow \int_{x_i}^{x_j} \begin{bmatrix} N_i^/ N_i^/ & N_i^/ N_j^/ \\ N_j^/ N_j^/ & N_j^/ N_j^/ \end{bmatrix} \begin{bmatrix} U_i \\ U_j \end{bmatrix} dx + \frac{\ell}{\mu} \int \begin{bmatrix} N_i^/ N_i^/ & N_i^/ N_j^/ \\ N_j^/ N_i^/ & N_j^/ N_j^/ \end{bmatrix} \begin{bmatrix} \phi_i \\ \phi_j \end{bmatrix} dx = 0 \tag{4.7}$$

on evaluation of (4.7) we have

$$\frac{1}{Le} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} U_i \\ U_j \end{bmatrix} + \frac{\ell}{2\mu} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} \phi_i \\ \phi_j \end{bmatrix} = 0$$

Summary up the element equations between $x_i < x_i < x_k$ we have

$$\frac{1}{Le}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}\begin{bmatrix} U_i \\ U_j \\ U_k \end{bmatrix} + \frac{\ell}{2\mu}\begin{bmatrix} -1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{bmatrix}\begin{bmatrix} \phi_i \\ \phi_j \\ \phi_k \end{bmatrix} = 0 \qquad (4.8)$$

which can be written in difference form as

$$\frac{1}{Le}\left[-U_{i-1} - 2U_i - U_{i+1}\right] + \frac{\ell}{2\mu}\left[-\phi_{i-1} + \phi_{i+1}\right] = 0 \qquad (4.9)$$

where the ϕ_i can be determined from the solution of the potential equation

5.0 Solution of the one–dimensional electric potential equation.

The one dimensional electric potential equation is given by

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\ell}{\in} = 0 \qquad (5.1)$$

Together with the conditions

$$\left.\begin{aligned} U(0) &= \phi_0 \\ U(L) &= 0 \end{aligned}\right\} \qquad (5.2)$$

Given that $\phi^{(e)} = N_i\phi_i$, we have using the Galerkin's method

$$\int_{x_i}^{x_j} N_i\left[\frac{\partial^2\phi}{\partial x} + \frac{\ell}{\in}\right]dx = 0 \qquad (5.3)$$

Integrating the first by parts we have

$$N_i \frac{\partial\phi_i}{\partial x}\bigg|_{x_i}^{x_j} - \int_{x_i}^{x_j} \frac{\partial N_i}{\partial x}.\frac{\partial N^{(e)}}{\partial x}\phi_i dx + \int_{x_i}^{x_j} N_i \frac{\ell}{\in}dx = 0 \qquad (5.4)$$

Since, the first term satisfies the boundary conditions we have

$$-\int_{x_i}^{x_j} \frac{\partial N_i}{\partial x}.\frac{\partial N^{(e)}}{\partial x}\phi_i dx + \int_{x_i}^{x_j} N_i \frac{\ell}{\in}dx = 0 \qquad (5.5)$$

$$\int_{x_j}^{x_k}\begin{bmatrix} N_iN_i & N_iN_j \\ N_jN_i & N_jN_j \end{bmatrix}\begin{bmatrix} \phi_i \\ \phi_j \end{bmatrix}dx - \frac{\ell}{\in}\begin{bmatrix} N_i \\ N_j \end{bmatrix}dx = 0 \qquad (5.6)$$

Evaluating (5.6) we have

$$\frac{1}{Le}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} \phi_i \\ \phi_j \end{bmatrix} - \frac{\ell}{2\in}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = 0 \qquad (5.7)$$

Summing up the element matrix $x_i < x_j < x_k$ we have

$$\frac{1}{Le}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}\begin{bmatrix} \phi_{i-1} \\ \phi_i \\ \phi_{i+1} \end{bmatrix} + \frac{\ell Le}{2\in}\begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} = 0 \qquad (5.8)$$

which in recurrence form we have

$$\frac{1}{L_e^2}\left[-\phi_{i-1} - 2\phi_i - \phi_{i+1}\right] = \frac{\ell}{\in} \qquad (5.9)$$

which is the difference solution to equation (5.8)

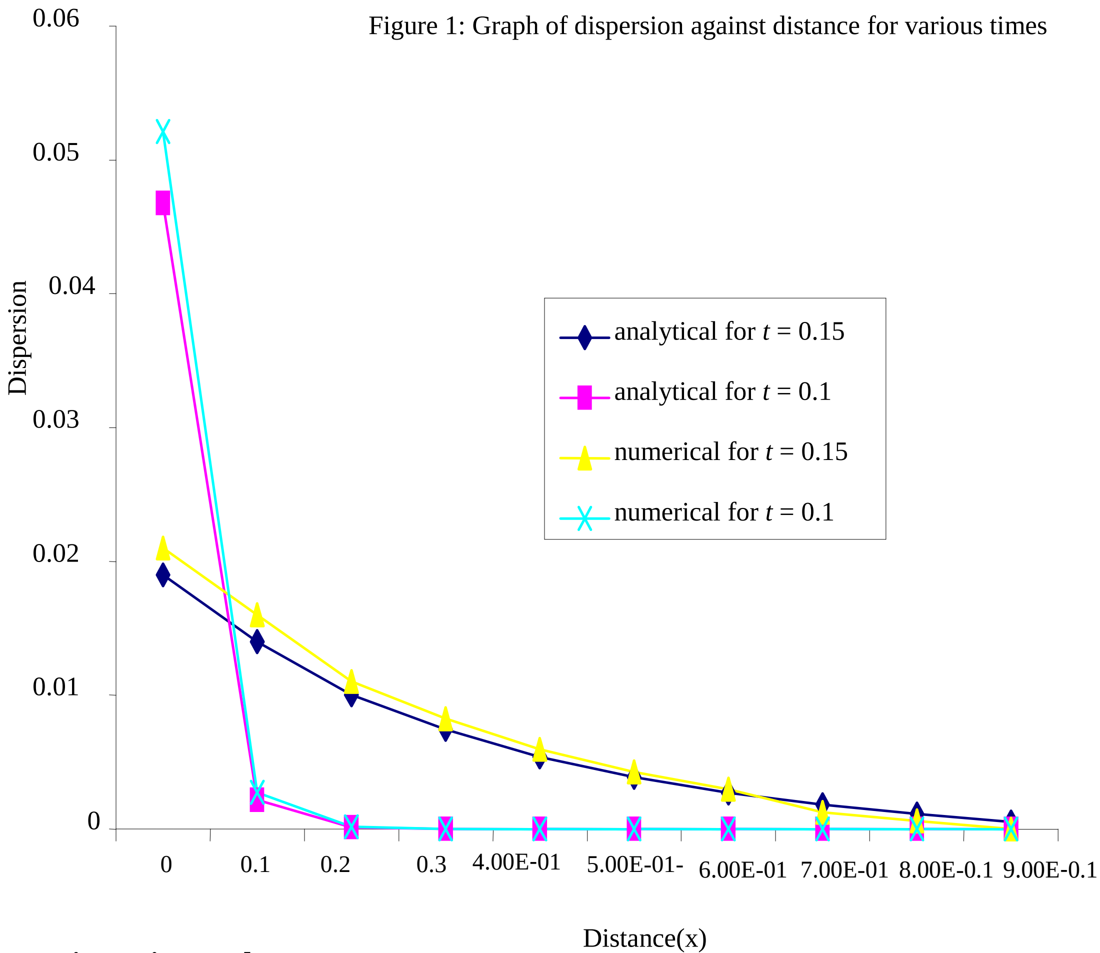

Figure 1: Graph of dispersion against distance for various times

6.0 Discussion and summary

From the graph it can be observed that the concentration of the contaminant decrease sharply with distance for particular times and then steady state is reach, also the concentration increases with time. The effects of oscillations and numerical dispersion which are common to finite difference has been eliminated which is an advantage of the finite element over the finite difference methods.

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