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Two Dimensional Mathematical Models for Convective-Dispersive Flow of Pesticides in Porous Media

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Abstract:
The transport of solutes through porous media where chemicals undergo adsorption or change process on the surface of the porous materials has been a subject of research over the years. Use of pesticides has resulted in production of diverse quantity and quality for the market. Disposal of excess material has also become an acute problem. The concept of adsorption is essential in determining the movement pattern of pesticides in soil in order to assess the effect of migrating chemicals from their disposal sites on the quality of ground water. In this paper, we derive a two dimensional equation accounting for both lateral and axial pesticide flow in a porous media by convective- dispersive transport with steady state water flow. The model is derived from the first principle and solved using Alternation-Direct-Implicit (ADI) method.

Key Words: convective-dispersive, adsorption, pesticides, porous media, solutes

I. INTRODUCTION

Convective-Dispersive equations have been solved using implicit methods. This is due to their unconditional stability but the challenges associated with the matrices have become a concern and a limitation in obtaining solutions [1, 9]. Implicit finite difference methods obtain the solution for the next step from the state of both the current and the next steps, while explicit methods obtain the solution from the current step only. Implicit methods require computation per time step and can implement long time step intervals without suffering numerical instabilities. On the contrary explicit numerical methods suffer from instabilities. Implicit numerical methods are stable in one-dimension problems but they do not guarantee stability in multidimensional problems. Inversion of matrices produced by explicit numerical are easier to solve compared to those of implicit numerical methods, but require smaller time interval thus increasing computation time. In this paper we adopt ADI method. In numerical analysis, the Alternating Direction Implicit (ADI) method is a finite

Difference method for solving parabolic and elliptic partial differential equations.

The advantage of the ADI method is that the equations that have to be solved in each step have a simpler structure and can be solved efficiently with the tridiagonal matrix algorithm., also called Thomas Alogarithm, whis is user friendly [6] Peaceman and Rachford [1] method is the most ideal for 2D. These methods blend implicit numerical methods with explicit numerical methods. ADI method solves the first dimension implicitly and the second dimension explicitly and the next step the first dimension explicitly and the second dimension implicitly and so on. This method is unconditionally stable and since it applies implicit scheme to one dimension at a time, the non-zero terms are present only in three diagonal line matrix, which is simple and friendlier to solve compared to the matrix created by the fully implicit method [7] in 2D. Advantages of ADI method is that it prevents numerical problems encountered by the fully implicit schemes and it shortens computing time by a factor of 2 compared to the implicit method and does not encounter numerical problems such as negative distribution functions or crashes during matrix inversion [6] that are seen in implicit methods.

II. DERIVATION OF CONVECTIVE-DISPERSIVE SOLUTE TRANSPORT EQUATION WITH STEADY STAT WATER FLOW CONDITION

Let the average pore water velocity be $V(LT^{-1}) = \dfrac{q}{\theta}$,[5]

i.e. $q = -K\dfrac{\partial H}{\partial z}$, is the flux density, $\theta = \dfrac{V_W}{V_S}$, in which V_W is volume of water in the porous media and V_S is volume of solids in used instead flow medium before the flow takes place.

In this paper we apply the concept of dispersion through a cylindrically packed soil vessel to derive the convective dispersive equation for pesticide adsorption in a porous media. (See Figure 1 below)

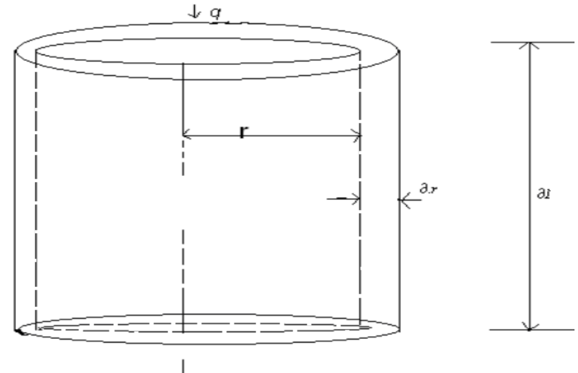

Figure. 1. Cylindrically packed soil vessel

At very low flow rate, the dispersion is different in longitudinal and radial directions. The Dispersion coefficients are denoted by D_L for longitudinal and D_R for radial

$$D(\theta,V) = D_{diff} + D_{dis}, \qquad (1.0)$$

where D_{diff} (L^2T^{-1}) is molecular diffusion coefficient, D_{dis} (L^2T^{-1}) is the hydrodynamic dispersion and is the mixing or spreading of the solute during transport due to differences in velocities within a pore and between pores. The volumetric water content denoted by θ which we can assume to be the void age for saturated soils.

The element height is denoted by $\partial\ell$. Inner radius is r and outer radius is $r+\partial r$, C is the concentration of the material to be dispersed and is a function of axial position l , radial position r, time t and dispersion coefficients D_R and D_L radial and axial respectively.

The rate of entry of reference material due to flow in axial direction is $q(2\pi r\partial rC)$. The corresponding efflux rate is

$$q(2\pi r\partial r)\left(C+\frac{\partial C}{\partial l}\partial l\right). \qquad (1.1)$$

The net accumulation rate in element due to flow in axial direction is :

$$-q(2\pi r\partial r)\left(\frac{\partial C}{\partial l}\partial l\right). \qquad (1.2)$$

Rate of diffusion in axial direction across inlet boundary is:

$$-(2\pi r\partial r\,\theta)\left(D_L\frac{\partial C}{\partial l}\right) \qquad (1.3)$$

The corresponding rate at outlet boundary is:

$$(2\pi r\partial r\,\theta)\ D_L\left(\frac{\partial C}{\partial l}+\frac{\partial^2 C}{\partial l^2}\partial l\right) \qquad (1.4)$$

The net accumulation rate due to diffusion from boundaries in axial direction is:

$$(2\pi r\partial r\,\theta)\,D_L\frac{\partial^2 C}{\partial l^2}\partial l \qquad (1.5)$$

Diffusion in radial direction at r is:

$$-(2\pi r\partial r\,\theta)\,\partial l D_R\frac{\partial C}{\partial r}\ . \qquad (1.6)$$

The corresponding rate at radius $r+\partial r$ is

$$-[2\pi(r+\partial r)\theta]\partial l$$

$$D_R\left[\frac{\partial C}{\partial r}+\frac{\partial^2 C}{\partial r^2}\partial r\right]. \qquad (1.7)$$

The net accumulation rate due to diffusion from boundaries is:

$$-[2\pi.r\partial r\theta]\partial l$$

$$D_R\frac{\partial C}{\partial r}+[2\pi(r+\partial r)\partial l(\theta)]D_R\left(\frac{\partial C}{\partial r}+\frac{\partial^2 C}{\partial r^2}\partial r\right). \qquad (1.8)$$

If we ignore the last term, because we are considering infinite small changes and that makes the second derivative negligible, it becomes:

$$-2\pi\theta D_R\partial l\left[\partial r\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right)\right]. \qquad (1.9)$$

For a representative elementary volume of soil, the total amount of a given chemical species X (ML^{-3}) is represented by the sum of the amount retained by the soil matrix and the amount present in the soil as

$$X=\rho_b S+\theta C \qquad (1.10)$$

where, ρ_b is the bulky density, and S is the amount of solute adsorbed,

Differentiating (1.10) with respect to t, yields,

$$\frac{\partial X}{\partial t}=\rho_b\frac{\partial S}{\partial t}+\theta\frac{\partial C}{\partial t}\ . \qquad (1.11)$$

Now the total accumulation rate is:

$$(2\pi r\partial r\partial l)\frac{\partial X}{\partial t}$$

$$=(2\pi r\partial r\partial l)\left(\rho_b\frac{\partial S}{\partial t}+\theta\frac{\partial C}{\partial t}\right). \qquad (1.12)$$

From equations (1.0) to (1.12), we have:

$$\left(\rho_b\frac{\partial S}{\partial t}+\theta\frac{\partial C}{\partial t}\right)2\pi r\partial r\partial l=-q(2\pi r\partial r)\frac{\partial C}{\partial l}\partial l$$

$$+(2\pi r\partial r\theta)D_L\left(\frac{\partial^2 C}{\partial l^2}\partial l\right)+2\pi\theta l D_R\left[\partial r\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right)\right]$$

(1.13)

Dividing through by $(2\pi r\partial r)\partial l\theta$, we get

$$\left(\frac{\rho}{\theta}\frac{\partial S}{\partial t}+\frac{\partial C}{\partial t}\right)=D_L\frac{\partial^2 C}{\partial l^2}+\frac{1}{r}D_R\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right)-\frac{q}{\theta}\frac{\partial C}{\partial l}\ .$$

(1.14)

Taking $l=x$ and $r=y$, equation(1.14) becomes,

$$\frac{\rho}{\theta}\frac{\partial S}{\partial t}+\frac{\partial C}{\partial t}=D_x\frac{\partial^2 C}{\partial x^2}+\frac{1}{y}D_y\frac{\partial}{\partial y}\left(y\frac{\partial C}{\partial y}\right)-\frac{q}{\theta}\frac{\partial C}{\partial x} \qquad (1.15)$$

But $\frac{q}{\theta} = V_X$ (pore water velocity), therefore equation (1.15) comes to

$$\left(\frac{\rho}{\theta}\frac{\partial S}{\partial C} * \frac{\partial C}{\partial t} + \frac{\partial C}{\partial t}\right) = D_x \frac{\partial^2 C}{\partial x^2} + \frac{1}{y} D_y \frac{\partial}{\partial y}\left(y \frac{\partial C}{\partial y}\right) - V_x \frac{\partial C}{\partial x} \quad (1.16)$$

From the Freundlich equation, [10]

$$S = KC^N, \quad \frac{\partial S}{\partial C} = KNC^{N-1}, \quad \frac{\partial S}{\partial t} = \frac{\partial S}{\partial C}\frac{\partial C}{\partial t}, = KNC^{N-1}\frac{\partial C}{\partial t}. \quad (1.17)$$

Putting equation (1.17) in (1.16)

$$R(C)\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - V_x \frac{\partial C}{\partial x} + \frac{1}{y} D_y \frac{\partial}{\partial y}\left(y \frac{\partial C}{\partial y}\right), \quad (1.18)$$

where, $R(C) = \left(1 + \frac{\rho}{\theta} KNC^{N-1}\right)$.

Equation (1.18) is our model equation describing two-dimensional movement of solute in the soil or porous media.

2. Solution of the Equation using Numerical Method

The expanded equation (1.18) is

$$R(C)\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - V_x \frac{\partial C}{\partial x} + \frac{1}{y} D_y \frac{\partial C}{\partial y} + D_y \frac{\partial^2 C}{\partial y^2}$$

The finite difference method is ideal for solving nonlinear equations. We replace the differential with its finite difference equivalent. We shall establish grids based on dimensions we are to consider. We use the (i, j) notation that is used to designate the pivot point for two-dimensional space (x, y) direction and (i, j) being the counters in the (x, y) directions. The partial derivative of C with respect to x implies that t is kept constant and vice versa.

The initial condition is that the concentration of pesticide at all positions in the soil at time zero is constant and equal to C_i. That is $C(x,0) = C_i$ for $x > 0$, $C(0,y)=C_j$

Boundary conditions: two conditions are necessary:

i. In the first case the concentration of the pesticides at the position x = 0, y=0 is specified for a period of time, the concentration at the surface is zero. That is

$$C(0,0,t) = C_0 \text{ for } 0<t \le t_o$$
$$C(0,0,t) = 0 \text{ for } t > t_o$$

ii. In the second case, the concentration of the pesticides in the solution entering the soil system at position x or y = 0 is specified for a period time. Following that time, the concentration at the surface is zero.

Thus

$$\{VC_0, \text{for}, 0 < t \le t_0$$
$$-D_x \frac{dC}{dx} + D_y \frac{\partial C}{\partial y} + VC\big|_{x=0} = 0, \text{ for, } t>0.$$

Assumptions

i. The pore water velocity is constant in time and space. This condition can be met for a uniform soil if the flux density of water velocity and volumetric water content are constant for all positions all the times.

ii. The spread of solute is dominated by hydraulic dispersion rather than diffusion.

iii. The hydrodynamic dispersion can be approximated as the product of the dispersivity and pour water velocity.

iv. The adsorption process is instantaneous and reversible and the adsorption isotherm can be described by the model i.e the concentration of pesticide absorbed on the soil solids is proportional to the concentration in the solution, [8]

The second order accuracy in time can be obtained by using the Crank-Nicolson Method.

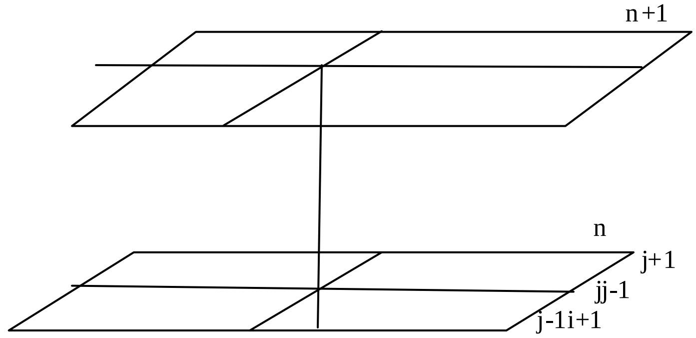

Figure.2.Grid showing second order accuracy in time is Obtain using Crank Nicolson Method.

$$R(C)\frac{\left(C^{n+1} - C^n\right)}{\Delta t} = D_x \frac{\partial_x^2 C^{n+1} + \partial_x^2 C^n}{2\Delta x^2} - V_x \frac{\partial_x C^{n+1} + \partial_x C^n}{4\Delta x}$$
$$+ D_y \frac{\partial_y C^{n+1} + \partial_y C^n}{4y\Delta y} + D_y \frac{\partial_y^2 C^{n+1} + \partial_y^2 C^n}{2\Delta y^2} \quad (1.20)$$

If $\Delta x = \Delta y = h$

$$C_{i,j}^{n+1} = C_{i,j}^n + \frac{\Delta t D_x}{2h^2 R(C_{i,j}^n)}\left[\left(C_{i+1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i-1,j}^{n+1}\right) + \left(C_{i+1,j}^n - 2C_{i,j}^n + C_{i-1,j}^n\right)\right]$$
$$- \frac{V_x \Delta t}{4hR(C_{i,j}^n)}\left[\left(C_{i+1,j}^{n+1} - C_{i-1,j}^{n+1}\right) + \left(C_{i+1,j}^n - C_{i-1,j}^n\right)\right]$$
$$+ \frac{D_x \Delta t}{4hy_j R(C_{i,j}^n)}\left[\left(C_{i,j+1}^{n+1} - C_{i,j-1}^{n+1}\right) + \left(C_{i,j+1}^n - C_{i,j-1}^n\right)\right]$$
$$+ \frac{D_y \Delta t}{2h^2 R(C_{i,j}^n)}\left[\left(C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}\right) + \left(C_{i,j+1}^n - 2C_{i,j}^n + C_{i,j-1}^n\right)\right] \quad (1.21)$$

Using Matrix, this equation is expensive to solve.

The most practical solution to this came with the development of Alternation-Direct-Implicit (ADI) Method by Peace man and Richford[1]. This consists of first treating one row implicit with backward Euler and reversing the roles and treating the other one by backward Euler.

III. COMPUTATION MOLECULE FOR THE ADI METHOD

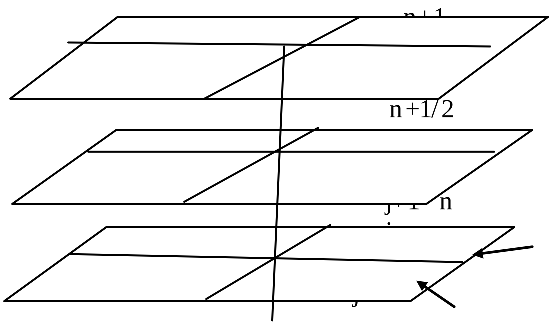

Figure.3.Computation Molecule for ADI Method

These methods involve solving one set of linear equations for two dimensional systems, solve 1D equation for grid line. It also provides for solving by alternating direction to prevent bias.

$$C_{i,j}^{n+\frac{1}{2}} - C_{i,j}^{n} = \frac{D_x \Delta t}{2h^2 R(C_{i,j}^n)}\left[\left(C_{i-1,j}^{n+\frac{1}{2}} - 2C_{i,j}^{n+\frac{1}{2}} + C_{i+1,j}^{n+\frac{1}{2}}\right) + \left(C_{i-1,j}^{n} - 2C_{i,j}^{n} + C_{i+1,j}^{n}\right)\right]$$

$$+\frac{V_x \Delta t}{4hR(C_{i,j}^n)}\left[\left(C_{i-1,j}^{n+\frac{1}{2}} - C_{i+1,j}^{n+\frac{1}{2}}\right) + \left(C_{i-1,j}^{n} - C_{i+1,j}^{n}\right)\right]$$

$$-\frac{D_y \Delta t}{4hy_j R(C_{i,j}^n)}\left[\left(C_{i,j-1}^{n+\frac{1}{2}} - C_{i,j+1}^{n+\frac{1}{2}}\right) + \left(C_{i,j-1}^{n} - C_{i,j+1}^{n}\right)\right]$$

$$+\frac{D_y \Delta t}{2h^2 R(C_{i,j}^n)}\left[\left(C_{i,j-1}^{n+\frac{1}{2}} - 2C_{i,j}^{n+\frac{1}{2}} + C_{i,j+1}^{n+\frac{1}{2}}\right) + \left(C_{i,j-1}^{n} - 2C_{i,j}^{n} + C_{i,j+1}^{n}\right)\right] \qquad (1.22)$$

The matrix form, for each row is,

$$\begin{bmatrix} C_{1,j}^{n+\frac{1}{2}} \\ C_{2,j}^{n+\frac{1}{2}} \\ ,, \\ ,, \\ C_{I,j}^{n+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} C_{1,j}^{n} \\ C_{2,j}^{n} \\ ,, \\ ,, \\ C_{I,j}^{n} \end{bmatrix} + \frac{D_x \Delta t}{2h^2 R(C_{i,j}^n)}\left\{\begin{bmatrix} -2 & 1 & ,, & ,, & 0 \\ 1 & -2 & 1 & ,, & ,, \\ ,, & - & - & - & ,, \\ ,, & ,, & - & - & 1 \\ 0 & ,, & ,, & 1 & -2 \end{bmatrix}\left(\begin{bmatrix} C_{1,j}^{n+\frac{1}{2}} \\ C_{2,j}^{n+\frac{1}{2}} \\ ,, \\ ,, \\ C_{I,j}^{n+\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} C_{1,j}^{n} \\ C_{2,j}^{n} \\ ,, \\ ,, \\ C_{I,j}^{n} \end{bmatrix}\right)\right\}$$

$$+\frac{V_x \Delta t}{4hR(C_{i,j}^n)}\left\{\begin{bmatrix} 0 & -1 & ,, & ,, & 0 \\ 1 & 0 & -1 & ,, & ,, \\ ,, & - & - & - & ,, \\ ,, & ,, & - & - & -1 \\ 0 & ,, & ,, & 1 & 0 \end{bmatrix}\left[\begin{bmatrix} C_{1,j}^{n+\frac{1}{2}} \\ C_{2,j}^{n+\frac{1}{2}} \\ ,, \\ ,, \\ C_{I,j}^{n+\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} C_{1,j}^{n} \\ C_{2,j}^{n} \\ ,, \\ ,, \\ C_{I,j}^{n} \end{bmatrix}\right]\right\}$$

$$-\frac{D_y \Delta t}{4hy_j R(C_{i,j}^n)}\left\{\begin{bmatrix} 0 & -1 & ,, & ,, & 0 \\ 1 & 0 & -1 & ,, & ,, \\ ,, & - & - & - & ,, \\ ,, & ,, & - & - & -1 \\ 0 & ,, & ,, & 1 & 0 \end{bmatrix}\left[\begin{bmatrix} C_{i,1}^{n+\frac{1}{2}} \\ C_{i,2}^{n+\frac{1}{2}} \\ ,, \\ ,, \\ C_{i,J}^{n+\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} C_{i,1}^{n} \\ C_{i,2}^{n} \\ ,, \\ ,, \\ C_{i,J}^{n} \end{bmatrix}\right]\right\}$$

$$+\frac{D_y \Delta t}{2h^2 R(C_{i,j}^n)}\left\{\begin{bmatrix} -2 & 1 & ,, & ,, & 0 \\ 1 & -2 & 1 & ,, & ,, \\ ,, & - & - & - & ,, \\ ,, & ,, & - & - & 1 \\ 0 & ,, & ,, & 1 & -2 \end{bmatrix}\left(\begin{bmatrix} C_{i,1}^{n+\frac{1}{2}} \\ C_{i,2}^{n+\frac{1}{2}} \\ ,, \\ ,, \\ C_{i,J}^{n+\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} C_{i,1}^{n} \\ C_{i,2}^{n} \\ ,, \\ ,, \\ C_{I,j}^{n} \end{bmatrix}\right)\right\}$$

Step 2

$$C_{i,j}^{n+1} - C_{i,j}^{n+\frac{1}{2}} = \frac{D_x \Delta t}{2h^2 R(C_{i,j}^n)}\left[\left(C_{i-1,j}^{n+\frac{1}{2}} - 2C_{i,j}^{n+\frac{1}{2}} + C_{i+1,j}^{n+\frac{1}{2}}\right) + \left(C_{i-1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i+1,j}^{n+1}\right)\right]$$

$$+\frac{V_x \Delta t}{4hR(C_{i,j}^n)}\left[\left(C_{i-1,j}^{n+\frac{1}{2}} - C_{i+1,j}^{n+\frac{1}{2}}\right) + \left(C_{i-1,j}^{n+1} - C_{i+1,j}^{n+1}\right)\right]$$

$$-\frac{D_y \Delta t}{4hy_j R(C_{i,j}^n)}\left[\left(C_{i,j-1}^{n+\frac{1}{2}} - C_{i,j+1}^{n+\frac{1}{2}}\right) + \left(C_{i,j-1}^{n+1} - C_{i,j+1}^{n+1}\right)\right]$$

$$+\frac{D_y \Delta t}{2h^2 R(C_{i,j}^n)}\left[\left(C_{i,j-1}^{n+\frac{1}{2}} - 2C_{i,j}^{n+\frac{1}{2}} + C_{i,j+1}^{n+\frac{1}{2}}\right) + \left(C_{i,j-1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j+1}^{n+1}\right)\right]$$

The matrix form, for each row is,

$$\begin{bmatrix} C_{i,1}^{n+1} \\ C_{i,2}^{n+1} \\ ,, \\ ,, \\ C_{i,J}^{n+1} \end{bmatrix} = \begin{bmatrix} C_{i,1}^{n+\frac{1}{2}} \\ C_{i,2}^{n+\frac{1}{2}} \\ ,, \\ ,, \\ C_{i,J}^{n+\frac{1}{2}} \end{bmatrix} + \frac{D_x \Delta t}{2h^2 R(C_{i,j}^n)} \left\{ \begin{bmatrix} -2 & 1 & ,, & ,, & 0 \\ 1 & -2 & 1 & ,, & ,, \\ ,, & - & - & - & ,, \\ ,, & ,, & - & - & 1 \\ 0 & ,, & ,, & 1 & -2 \end{bmatrix} \left(\begin{bmatrix} C_{1,j}^{n+\frac{1}{2}} \\ C_{2,j}^{n+\frac{1}{2}} \\ ,, \\ ,, \\ C_{I,j}^{n+\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} C_{1,j}^{n+1} \\ C_{2,j}^{n+1} \\ ,, \\ ,, \\ C_{I,j}^{n+1} \end{bmatrix} \right) \right\}$$

$$+ \frac{V_x \Delta t}{4hR(C_{i,j}^n)} \left\{ \begin{bmatrix} 0 & -1 & ,, & ,, & 0 \\ 1 & 0 & -1 & ,, & ,, \\ ,, & - & - & - & ,, \\ ,, & ,, & - & - & -1 \\ 0 & ,, & ,, & 1 & 0 \end{bmatrix} \left[\begin{bmatrix} C_{1,j}^{n+\frac{1}{2}} \\ C_{2,j}^{n+\frac{1}{2}} \\ ,, \\ ,, \\ C_{I,j}^{n+\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} C_{1,j}^{n+1} \\ C_{2,j}^{n+1} \\ ,, \\ ,, \\ C_{I,j}^{n+1} \end{bmatrix} \right] \right\}$$

$$+ \frac{D_y \Delta t}{4hy_j R(C_{i,j}^n)} \left\{ \begin{bmatrix} 0 & -1 & ,, & ,, & 0 \\ 1 & 0 & -1 & ,, & ,, \\ ,, & - & - & - & ,, \\ ,, & ,, & - & - & -1 \\ 0 & ,, & ,, & 1 & 0 \end{bmatrix} \left[\begin{bmatrix} C_{i,1}^{n+\frac{1}{2}} \\ C_{i,2}^{n+\frac{1}{2}} \\ ,, \\ ,, \\ C_{i,J}^{n+\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} C_{i,1}^{n+1} \\ C_{i,j}^{n+1} \\ ,, \\ ,, \\ C_{i,J}^{n+1} \end{bmatrix} \right] \right\}$$

$$+ \frac{D_y \Delta t}{2h^2 R(C_{i,j}^n)} \left\{ \begin{bmatrix} -2 & 1 & ,, & ,, & 0 \\ 1 & -2 & 1 & ,, & ,, \\ ,, & - & - & - & ,, \\ ,, & ,, & - & - & 1 \\ 0 & ,, & ,, & 1 & -2 \end{bmatrix} \left(\begin{bmatrix} C_{i,1}^{n+\frac{1}{2}} \\ C_{i,2}^{n+\frac{1}{2}} \\ ,, \\ ,, \\ C_{i,J}^{n+\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} C_{i,1}^{n+1} \\ C_{i,2}^{n+1} \\ ,, \\ ,, \\ C_{i,J}^{n+1} \end{bmatrix} \right) \right\}$$

The equations can be solved to avoid forward elimination and backward substitution.

Stability analysis

Using Von Neumann Analysis

$$C_{i,j}^n = \hat{C}^n \varepsilon^{\lambda\theta_x i} \varepsilon^{\lambda\theta_y j}$$

Step 1

$$\hat{C}^{n+\frac{1}{2}} - \hat{C}^n = \frac{D_x \Delta t}{h^2 R(\hat{C}^n \varepsilon^{\lambda\theta_x i} \varepsilon^{\lambda\theta_y j})} \left[-\hat{C}^{n+\frac{1}{2}}(1 - Cos\theta_x) - \hat{C}^n (1 - Cos\theta_x) \right]$$

$$+ \frac{V_x \Delta t}{2hR(\hat{C}^n \varepsilon^{\lambda\theta_x i} \varepsilon^{\lambda\theta_y j})} \left[\hat{C}^{n+\frac{1}{2}}(\iota Sin\theta_x) + \hat{C}^n (\iota Sin\theta_x) \right]$$

$$+ \frac{D_y \Delta t}{2hR(\hat{C}^n \varepsilon^{\lambda\theta_x i} \varepsilon^{\lambda\theta_y j})} \left[\hat{C}^{n+\frac{1}{2}}(\iota Sin\theta_y) + \hat{C}^n (\iota Sin\theta_y) \right]$$

$$+ \frac{D_y \Delta t}{h^2 R(\hat{C}^n \varepsilon^{\lambda\theta_x i} \varepsilon^{\lambda\theta_y j})} \left[-\hat{C}^{n+\frac{1}{2}}(1 - Cos\theta_y) - \hat{C}^n (1 - Cos\theta_y) \right]$$

Let $R(\hat{C}^n \varepsilon^{\lambda\theta_x i} \varepsilon^{\lambda\theta_y j}) = \mathrm{A}$

$$\frac{\hat{C}^{n+\frac{1}{2}}}{C^n} = \frac{\left[1 - \frac{D_x \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_x) - \frac{D_y \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_y) + \frac{V_x \Delta t}{2h\mathrm{A}} \iota Sin\theta_x + \frac{D_y \Delta t}{2h\mathrm{A}} \iota Sin\theta_y \right]}{\left[1 + \frac{D_x \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_x) + \frac{D_y \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_y) - \frac{V_x \Delta t}{2h\mathrm{A}} \iota Sin\theta_x - \frac{D_y \Delta t}{2h\mathrm{A}} \iota Sin\theta_y \right]}$$

Step 2

$$\hat{C}^{n+\frac{1}{2}} = \frac{D_x \Delta t}{h^2 R(\hat{C}^n \varepsilon^{\lambda\theta_x i} \varepsilon^{\lambda\theta_y j})} \left[-\hat{C}^{n+\frac{1}{2}}(1 - Cos\theta_x) - \hat{C}^{n+1} (1 - Cos\theta_x) \right]$$

$$+ \frac{V_x \Delta t}{2hR(\hat{C}^n \varepsilon^{\lambda\theta_x i} \varepsilon^{\lambda\theta_y j})} \left[\hat{C}^{n+\frac{1}{2}}(\iota Sin\theta_x) + \hat{C}^{n+1} (\iota Sin\theta_x) \right]$$

$$+ \frac{D_y \Delta t}{2hR(\hat{C}^n \varepsilon^{\lambda\theta_x i} \varepsilon^{\lambda\theta_y j})} \left[\hat{C}^{n+\frac{1}{2}}(\iota Sin\theta_y) + \hat{C}^{n+1} (\iota Sin\theta_y) \right]$$

$$+ \frac{D_y \Delta t}{h^2 R(\hat{C}^n \varepsilon^{\lambda\theta_x i} \varepsilon^{\lambda\theta_y j})} \left[-\hat{C}^{n+\frac{1}{2}}(1 - Cos\theta_y) - \hat{C}^{n+1} (1 - Cos\theta_y) \right]$$

$$\frac{\left[1 - \frac{D_x \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_x) - \frac{D_y \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_y) + \frac{V_x \Delta t}{2h\mathrm{A}} \iota Sin\theta_x + \frac{D_y \Delta t}{2h\mathrm{A}} \iota Sin\theta_y \right]}{\left[1 + \frac{D_x \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_x) + \frac{D_y \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_y) - \frac{V_x \Delta t}{2h\mathrm{A}} \iota Sin\theta_x - \frac{D_y \Delta t}{2h\mathrm{A}} \iota Sin\theta_y \right]} \tag{1.25}$$

When we combine equations (1.24) and (1.25) we get

$$\frac{\hat{C}^{n+1}}{\hat{C}^n} = \frac{\left[1 - \frac{D_x \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_x) - \frac{D_y \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_y) + \frac{V_x \Delta t}{2h\mathrm{A}} \iota Sin\theta_x + \frac{D_y \Delta t}{2h\mathrm{A}} \iota Sin\theta_y \right]}{\left[1 + \frac{D_x \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_x) + \frac{D_y \Delta t}{h^2 \mathrm{A}}(1 - Cos\theta_y) - \frac{V_x \Delta t}{2h\mathrm{A}} \iota Sin\theta_x - \frac{D_y \Delta t}{2h\mathrm{A}} \iota Sin\theta_y \right]}$$

$$\times\frac{\left[1-\frac{D_x\Delta t}{h^2A}(1-Cos\theta_x)-\frac{D_y\Delta t}{h^2A}(1-Cos\theta_y)+\frac{V_x\Delta t}{2hA}\iota Sin\theta_x+\frac{D_y\Delta t}{2hA}\iota Sin\theta_y\right]}{\left[1+\frac{D_x\Delta t}{h^2A}(1-Cos\theta_x)+\frac{D_y\Delta t}{h^2A}(1-Cos\theta_y)-\frac{V_x\Delta t}{2hA}\iota Sin\theta_x-\frac{D_y\Delta t}{2hA}\iota Sin\theta_y\right]}$$

Fromm's scheme keeps track of whether the wave speed is positive or negative, and alters the direction of information transfer accordingly.
This scheme is stable for

$$\left[\frac{\hat{C}^{n+1}}{\hat{C}^n}\right]^2\angle 1,$$

$$\frac{\left[1-\frac{D_x\Delta t}{h^2A}\left(1-\cos\theta_x\right)-\frac{D_y\Delta t}{h^2A}\left(1-Cos\theta_y\right)\right]^2}{\left[1+\frac{D_x\Delta t}{h^2A}\left(1-Cos\theta_x\right)+\frac{D_y\Delta t}{h^2A}\left(1-Cos\theta_y\right)\right]^2}$$

$$\frac{-\left[\frac{V\Delta t}{2hA}Sin\theta_x+\frac{D_y\Delta t}{2hA}Sin\theta_y\right]^2}{+\left[\frac{V\Delta t}{2hA}Sin\theta_x+\frac{D_y\Delta t}{2hA}Sin\theta_y\right]^2}\angle 1$$

Unconditionally For $\theta_x=\theta_y\neq 0$

IV. REFERENCES

[1] Peaceman, D. W.; Rachford Jr., H. H. (1955), "The numerical solution of parabolic and elliptic differential equations", Journal of the Society for Industrial and Applied Mathematics 3 (1): 28–41

[2] Douglas Jr., Jim (1962), "Alternating direction methods for three space variables", Numerische Mathematik 4 (1): 41–63.

[3] J. Douglas Jr and J. E. Gunn, "A general formulation of alternating direction Methods-Part I. Parabolic and hyperbolic problems," Numerische Mathematik, vol. 6, pp. 428–453, 1964.

[4] Van Genuchten M. Th, Davidson J.M & Wierenga, P. J: (1974). An Evaluation of Kinetic and equilibrium equation for predicting pesticide movement through porous media. Soil Sci. Soc. Am.

[5] Weil I, Morris J.C. (1949) Caulson and Richardson 4th Edition Chemical Engineering. (Ame. Chem society 71: 1664).

[6] Thomas, L.H. (1949), Elliptic Problems in Linear Differential Equations over a Network, Watson Sci. Comput. Lab Report, Columbia University, New York.

[7] J. S. CHANG and G. COOPER: A practical difference scheme for Fokker-Planck equations. J. Comput. Phys., Vol. 6, Issue 1, August 1970

[8] Faust S.D and Osman Aly.: (1983). Chemistry of water treatment. (Published by American Book Society

[9] T. Witelski and M. Bowen ''ADI Schemes for higher order nonlinear diffusion equations'' App. Numer. Math., 45:331-351, 2003.

(10) Freundlick H. (1926). Colloid and Capillarity Chemistry (London Methuen and Company)