Advection Dispersion by Eulerian Lagrangian Finite Element Method

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(Received September 30, 1992)

SYNOPSIS

In this paper the author will be describe phenomena of advection dispersion in subsurface flow by using Eulerian Lagrangian Finite Element Method. Where Finite Element Method with Galerkin formulation and weighted residual method is used to solve seepage and advection dispersion equation. The problem of one dimensional and two dimensional rectangular wave are analyzed in this paper. And the result of numerical analyses will be compared with analytical solutions. The numerical results showed the very good agreement with the analytical solutions.

1. INTRODUCTION

Recently, allot of ground water contaminant problems are discussed to estimate the behaviors of these problems, numerical methods have been used as powerful technics. Generally, there are three numerical methods to solve problems of ground water contaminant, that is Lagrangian method, Eulerian method and Eulerian-Lagrangian method. The typical Lagrangian method is Particle Tracking Method, when we apply this method to practical problem, we need lot of memory of computer Eulerian method is very popular method to solve advection dispersion problem. But in this case of high seepage advection velocity and we have to divide very small mesh size. So there is a limitation to solving practical this kind problem by using Eulerian method. The Eulerian Lagrangian method is the most useful method to estimate the advection dispersion problem. The previous researcher such as S P Neuman (1980) presented this method, where numerical scheme for advection dispersion equation conjugate space time grid is used. It is used two grid that is advection grid and dispersion dispersion grid. Both grids are fixed in space and have distinct spatial and temporal increment [1]. Afterwards, S.P Neuman and S. Shorek (1982) presented Eulerian Lagrangian method for advection and dispersion problem. Where the advection-dispersion problem can be solved

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independently at each time step, this new approach is called Method of Reverse Streaklines, or Conventional Method of Continuous Particle Tracking [2]. The residual dispersion problem can be treated by Eulerian Finite Element Method. Then S P Neuman (1984) discussed Adaptive Eulerian Lagrangian Finite Element Method for advection dispersion problem as this method is based on the composition of concentration field in two part, one advective and one dispersive, in rigorous manner that does not leave room for ambiguity [3]. And then R.Cady and S.P Neuman (1988) presented three dimensional adaptive Eulerian Lagrangian Finite Element Method[4], in this method there is a little difference with S.P Neuman previous method published in 1984. They were developed into three dimensional domain, but unsaturated condition and density dependent phenomena is not considered. In this paper the Eulerian Lagrangian Finite Element analysis will be extend to the saturated-unsaturated seepage problem and density dependent problem. Furthermore, the result of numerical analysis will be discussed.

2. GOVERNING EQUATION

The governing equation the water movement in saturated-unsaturated with density dependent is derived in the form :

$$\frac{\rho f. \gamma. \theta}{\rho} \cdot \frac{\partial C}{\partial t} + (\alpha. Ss + Cs(\theta)) \frac{\partial \psi}{\partial t} - \frac{\partial}{\partial xi} (kij^{(s)}(\theta) \frac{\partial \psi}{\partial xi} + ki3.kr(\theta) \rho r) = 0 \quad(1)$$

Where:

 $\rho f = density of fresh water ; t = time ; \alpha = 0 for unsaturated condition$

 γ = bulk density; ψ = pressure head; α =1 for saturated condition

 $Cs(\theta)$ = specific capacity; $kij^{(s)}$ = saturated hydraulic conductivity tensor

 $\rho r = \rho/\rho f$ = relative fluid density; kr = relative hydraulic conductivity

Ss = specific storage coefficient; Cs = moisture capacity; $\rho = \rho f (1 + \gamma C)$ = fluid density

The initial and boundary condition of the problem take the form

$$\psi(xi,t) = \psi_0(xi)$$
 (2)

$$\psi$$
 (xi,t) = ψ o (xi,t) (3)

- kr.(
$$\theta$$
) (kij^(s) $\frac{\partial \psi}{\partial x_i}$ + ki3. ρ r) = Vn (xi, t) (4)

Vn = darcy velocity of normal direction

The Governing Equation Advection Dispersion for the Analysis of Contaminant Transport

$$R.\frac{\partial C}{\partial t} = \nabla .(D.\nabla.C) - Vs.\nabla.C - \frac{\lambda.R}{\rho}.C + \frac{QpC^*}{\rho.\theta} \dots (5)$$

$$R = (1 + \frac{\rho'}{n} . Kd)$$
 (6)

Where:

C = concentration; D = dispersion coefficient; n = porosity

Vs = real velocity; ρ = fluid density; QpC^* = source; θ = moisture content

 λ = radio active coefficient; ρ = fluid density; QpC^* = source

p = bulk density of the solid; Kd = infiltration coefficient

In cartesian coordinate the dispersion tensor can be written in the form (Bear 1972) [6]:

$$D_{11} = a_L \frac{V1 \ V1}{|V|} + a_T \frac{V3 \ V3}{|V|} + a_m \tau$$
 (7)

$$D_{12} = D_{21} = (a_L - a_T) \frac{V1 V3}{|V|}$$
 (8)

$$D_{33} = a_L \frac{V1 \ V1}{|V|} + a_T \frac{V3 \ V3}{|V|} + a_m \tau$$
 (9)

Where:

a_L = longitudinal dispersivity

a_T = tranversal dispersivit

am = diffusion coefficient

V1 = real velocity in y direction; V3 = real velocity in x direction; |V| = real velocity absolute

 τ = tortuosity

Advection Dispersion Equation with Eulerian Lagrangian Finite Element Method

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{V.\nabla}{R} \qquad (10)$$

We can rewrite in Eq.(5) in Lagrangian form as

$$R.(\frac{dC}{dt} - \frac{V.\nabla.C}{R}) = \nabla.(D.\nabla.C) - V.\nabla.C - \frac{\lambda.R}{\rho} \cdot C - q \quad (11)$$

Where q = source term $(-q = \frac{QpC^*}{\rho \cdot \theta})$

Afterwards in Eq (11), left side of second part and right side of second part yield and we obtain in the form

$$R \cdot \frac{dC}{dt} = \nabla \cdot (D \cdot \nabla C) - \frac{\lambda \cdot R}{\rho} \cdot C - q$$
 (12)

Then Neuman introduces an expression of C as the sum of two functions [2],[3]

$$C(x,t) = \widetilde{C}(x,t) + \widehat{C}(x,t) \quad (13)$$

Where \tilde{C} = Concentration of Advection

 \hat{C} = Concentration of Dispersion

 $\widetilde{\mathbf{C}}$ satisfies the homogeneous differential equation

$$R.\frac{d\tilde{C}}{dt} = -\frac{R\lambda}{\rho}.\tilde{C}$$
 (14)

In the Condition the advection problem, Eq. (14) can be solved for \widetilde{C} independent of \widehat{C} . Subtracting Eq.(14) from Eq.(12) leads to residual dispersion problem for C, defined by

$$R.\left[\frac{dC}{dt} - \frac{d\tilde{C}}{dt}\right] = \nabla.(D.\nabla.C) - \frac{R \lambda}{\rho}.(C - \tilde{C}) + q \quad(15)$$

3. NUMERICAL APPROACH

In the present work, an iterative Galerkin Finite Element Method is used to solve equation of transient seepage in saturated-unsaturated porous medium (Eq. (1)) and Eulerian Lagrangian Finite Element is used to solve equation advection dispersion (Eq. (5)). The method was implemented using quadrilateral Galerkin Finite Element of relative ease of transforming from the global coordinate system into the local coordinate system. This transformation is needed to evaluate interpolation that relies upon the finite element basis function for particle locations.

3.1 NUMERICAL APPROACH OF SEEPAGE IN SATURATED UNSATURATED POROUS MEDIA

By adapting Galerkin Finite Element Method to Eq (1), we obtained matrix differential equation such as follow

$$A_{nm}\psi_m + F_{nm}\frac{\partial \psi_m}{\partial t} + X_{nm}\frac{\partial C_m}{\partial t} - Q_n - B_n = 0 \dots (16)$$

Where:

$$A_{nm} = \int_{V} \frac{\partial N_{n}}{\partial x_{i}} \cdot \frac{\partial N_{m}}{\partial x_{j}} \cdot kij^{S} \cdot kr (\theta) dV \qquad (17)$$

$$F_{nm} = \int_{V} Nn \cdot Nm \cdot (\alpha \cdot Ss + Cs \cdot (\theta)) dV$$
 (18)

$$X_{nm} = \int_{V} N_n \cdot N_m \cdot \frac{\rho f \cdot \gamma \cdot \theta}{\rho} \cdot dV \qquad \dots \dots (19)$$

$$Q_n = \int_S n_i \cdot N_n \cdot Vd \cdot dS$$
 (20)

$$B_{n} = \int_{V} \frac{\partial N_{n}}{\partial x_{i}} \cdot (kij^{S} \cdot Kr(\theta) \cdot \rho r) \cdot dV \qquad(21)$$

3.2 NUMERICAL APPROACH OF ADVECTION-DISPERSION IN POROUS MEDIA

The advection problem is generally solved by Single Step Reverse Particle Tracking (SRPT) combined with the solution of Eq.(14) over time step. And Forward Particle Tracking (FWPT) is used in the vicinity of steep concentration front to define the concentration field and residual dispersion problem is solved to obtaine the nodal concentration at the end of the time step by using finite element of fixed grid.

 $C^{N}(x,t)$ is used to approximated C(x,y) and is defined as

$$C(x,t) = C^{N}(x,t) = \sum_{n} Cn(t).\xi_{n}(x)$$
 (22)

Where N = the total number of nodes in the finite element grid

Cn = the concentration at node n.

 ξ = finite element basis function for node n.

3.2.1 SINGLE REVERSE PARTICLE TRACKING METHOD

Consider a fictitious particle that moves from a location Kx_n at t_k to a new location X_n^{k+1} at t^{k+1} which coincides with node n. Its initial location is then given by

$$Kx_n = X_n^{k+1} - \int_{k}^{t_{k+1}} \frac{V}{R} \cdot D.t$$
 (23)

The final C value of the same particle upon reaching node n, \tilde{C}_n^{k+1} , is obtained by solving Eq.(14) analytically over Δt .

$$\widetilde{C}_n^{k+1} = C_n^k \exp \left[- \int_{t_n}^{t_{k+1}} \frac{\lambda}{\rho} dt \right]$$
 (24)

3.2.2 CONTINUOUS FORWARD PARTICLE TRACKING METHOD

Steep concentration fronts are tracked with the aid of particle cloud that covers the fronts until their gradient dissipate. A particle p moves from its initial location at t^k , X_p^k , to a new location

$$X_p^{k+1} = X_p^k + \int_{t_k}^{t_{k+1}} \frac{V}{R} dt$$
 (25)

at t^{k+1} where the integration is performed by the same method as in Eq.(23). If the particle concentration at t^k is C_p^k , its concentration at t^{k+1} is in analogy to Eq.(24)

$$\widetilde{C}_p^{k+1} = C_p^k \exp \left[- \int_{k}^{k+1} \frac{\lambda}{\rho} dt \right] \quad (26)$$

3.2.3 RESIDUAL DISPERSION BY FINITE ELEMENT

By applying the Galerkin method to Eq.(15), we obtained matrix differential equation such as follow

$$\frac{\partial C_n}{\partial t} W_{nm} - \frac{\partial \widetilde{C}_n}{\partial t} W_{nm} + G_{nm} \cdot C_m + H_{nm} C_m + (C_n - \widetilde{C}_n) L_n + U_n = 0 \quad \dots (27)$$

Where:

$$W_{nm} = R \int_{\Omega} \zeta_n \zeta_m dv = R \int_{\Omega} \zeta_n \zeta_m dv \qquad \dots (28)$$

$$G_{nm} = \int_{\Omega} D_{ij} \frac{\partial \zeta_n}{\partial x_i} \frac{\partial \zeta_m}{\partial x_j} dv \qquad \dots (29)$$

$$H_{nm} = \int_{\Omega} n_i v_i \zeta_n \zeta_m ds \qquad (30)$$

$$L_n = \int_{\Omega} \frac{\lambda R}{\rho} \zeta_n dv \qquad (31)$$

$$U_n = \int_{\Omega} \zeta_n q \, dv \qquad \dots (32)$$

In the equation (31), we can approximated in the form:

$$L_n = \lambda R \int_{v} \frac{1}{\rho_e} N_n dv \qquad (33)$$

where ρ_e = density of element

3.2.4 INTEGRATION OVER TIME

To integrate matrix differential Eq.(16), the time domain is discretized into sequence of finite intervals, Δ t, and the time derivatives of φ_n and C_n are replaced by Finite Differences. And by the approximated difference partial, Eq. (16) can be written as follow

$$(\frac{F_{nm}^{k+1/2}}{\Delta \, t^k} \, + \, \omega. \, A_{nm}^{k+1/2} \,) \, \psi_m^{k+1} \, = \, Q_n^{k+1} \, - \, B_n^{k+1/2} \, - \, \frac{C_m^{k+1} - C_m^k}{\Delta \, t^k} \, X_{nn}^{k+1/2} \, + \, (\frac{F_{nm}^{k+1/2}}{\Delta \, t^k} - (1 - \omega) \, A_{nm}^{k+1/2}) \, \psi_m^k \, \, (34)$$

In this case ω is depend on the scheme integration

Where $\omega = 1/2$ = central difference $\omega = 1$ = backward difference

And also matrix differential Eq.(27), can be written in the matrix differential partial, this equation can be written i the matrix differential equation in the form:

$$\left\{ \left(G_{nm} + H_{nm} + L_{nn} \right) + \frac{W_{nn}}{\Delta t} \right\} C_n^{k+1} = \left(L_{nn} + \frac{1}{\Delta t} W_{nn} \right) \widetilde{C}_n^{k+1} - U_{nn} \qquad (35)$$

In analyzing for advection-dispersion matrix differential equation, we used backward difference, so matrix differential equation (27) can be shown such as the above equation.

At the beginning of each time step, these are predicted by linear extrapolation according to

$$\psi_n^{k+1/2} = \psi_n^k + \frac{\Delta t^k}{2 \Delta t^{k-1}} (\psi_n^k - \psi_n^{k-1}) \qquad \dots (36)$$

The resulting set of simultaneous equation is solved by Gaus Elimination method. At each iteration, the most recent values of ψ_n^{k+1} are used to obtain an improved value of $\psi_n^{k+1/2}$ from

$$\psi_n^{k+1/2} = 1/2 (\psi_n^k + \psi_n^{k+1})$$
 (37)

And the next step, the matrix differential equation for residual dispersion is written such as in Eq.(35), we will obtained the value for concentration each node and time step.

4. PROGRAMING

The program consists of over 16000 lines of fortran 77 code, this code includes 161 subroutines or function sub programs. The main program component of the code found in the Elus 90 files, consists of dimensioning parameters to allocate space for the many variables that occur throughout the program and to define number of permanent files and temporary files used in the program. The major of the code is depicted in the general flow diagram shown as Fig.1.

Input data model is divided 22 types and the using of each types depends on the model that will be analyzed. The program consists of three kinds of model analyses, that is perpendicular analyses, plane surface analyses and axissimetry analyses. In particular, the program is used Eulerian-Lagrangian Finite Element Method to analyses Advection-Dispersion Problem. In general processes of calculation Eulerian-Lagrangian method is follow: the seepage equation by using Galerkin Finite Element method and weighted residual method will be shaped matrix equation of integral, and we call the lump mass integration. And the coordinate system will be transferred from global coordinate to local coordinate with using the Isoparametric elements. The problem of transferring coordinate will be solved with integral gaus legendre, so we will obtain the equation matrix consisted of number that is possible to calculate all the coefficient matrix. From this calculation we will obtained the pressure head for each node. The calculation

of matrix is used Gaus Elimination Method.

In the next processes with the similar method that explained above, by using Eulerian Lagrangian Finite Element Method we will obtain concentration for each nodal point. The subroutine in the program generally is divided into four classifications:

The first classification, to read variation of input data that used for processes calculation, for example coefficient of permeability, coefficient of dispersion, to generate of node point and element and to read boundary and initial condition, we will approximate the model. The second classification, to calculate seepage matrix which was formed from each element, we will obtain the pressure head of each point. The third classification, to calculate darcy velocity for each element and with the correlation of shape function, we will obtain the real velocity. The final classification, from the real velocity by using Eulerian Lagrangian Method, we will obtaine the concentration each nodal point.

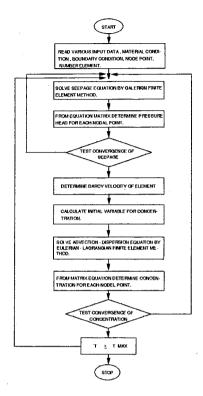


Fig.1 Flow Chart of Advection-Dispersion

5. COMPARISON OF ANALYTICAL AND NUMERICAL RESULT

To illustrate some of the problems with particular treatment of advection dispersion, simple examples of one and two dimensional will be solved by the various Peclet number (Pe = V L/D), and Courant number (Pe = V L/D). Where V = M magnitude of velocity, L = M characteristic length, T = M time step and D = M dispersion coefficient. Afterward the results will be compared with analytical solutions.

5.1 ANALYTICAL AND NUMERICAL SOLUTION OF ONE DIMENSIONAL CASE

5.1.1 ANALYTICAL SOLUTION

In this case, we will approximate the one dimensional dispersion problem in a nonsteady state and uniform velocity field over infinite one dimensional region by

$$\frac{\partial C}{\partial t} = Dx \frac{\partial^2 C}{\partial x^2} - Vx \frac{\partial C}{\partial x} \quad \text{on} \quad 0 \le x \le x_{\infty} \qquad \dots (38) \stackrel{?}{\underset{\begin{subarray}{c}}{\bigcirc}}$$

subject to

$$C(x,0) = 0.0$$

 $C(0,t) = 1.0$ (39)
 $C(x_{\infty},t) = 0.0$

Fig.2 Boundary conditions and initial condition

Analytically solution to this case is [2],[3]

$$C(x,t) = 0.5. \left\{ erfc \left(\frac{x - Vx \cdot t}{\sqrt{4 Dx \cdot t}} \right) + exp \left(\frac{Vx \cdot x}{Dx} \right) erfc \left(\frac{x + Vx \cdot t}{\sqrt{4 Dx \cdot t}} \right) \right\} \dots (40)$$

5.1.2 MODEL AND RESULT OF NUMERICAL ANALYSIS

The finite element consists of 50 rectangular elements and 102 nodes point. Fig.2 shown the boundary and initial condition. All the parameters for the one dimensional problem can be seen in table 1. In this case we used various Pe number and Cr number. The results of numerical analysis for various Pe number can be shown in Fig 3, Fig 4 and Fig 5, in these figure, solid lines are analytical solutions.

Table.1 Parameter values for one dimensional

Case	Pc	Cr	Vx (m/sec)	Δt (sec)	Δ x (m)	D (m2/sec)	F.W.F
I-1	0.25	0.1	0.05	0.1	0.05	0.01	0
1-2	0.25	0.01	0.05	0.01	0.05	0.01	0
1-3	0.25	0.1	0.05	0.1	0.05	0.01	63
1-4	0.25	0.01	0.05	0.01	0.05	0.01	63
2-1	5.0	5.0	1000.0	0.0001	0.02	4.0	0
2-2	5.0	0.5	1000.0	0.00001	0.02	4.0	0
2-3	5.0	5.0	1000.0	0.0001	0.02	4.0	63
2-4	5.0	0.5	1000.0	0.00001	0.02	4.0	63
3-1 2	0.02	5.0	1000.0	0.0001	0.02	1.0	0
3-2 2	0.0	0.5	1000.0	0.00001	0.02	0.1	0
3-3 2	0.0	5.0	1000.0	1000.0	0.02	1.0	63
3-4 2	0.0	0.5	1000.0	0.00001	0.02	1.0	63

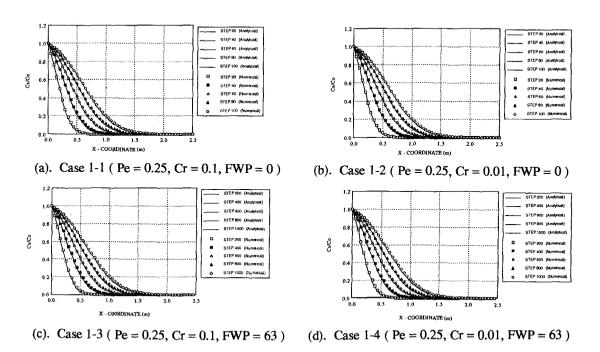


Fig. 3 Comparison of analytical and numerical solutions for low Pe number

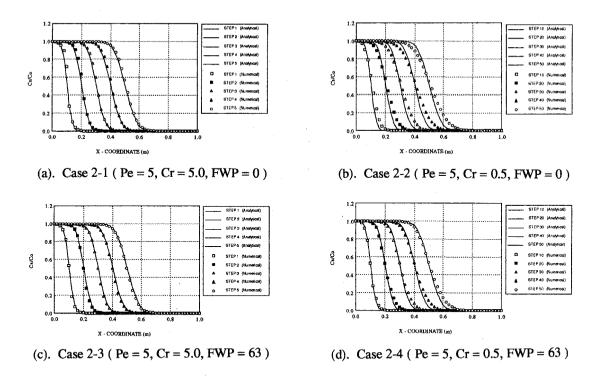


Fig.4 Comparison of analytical and numerical solutions for middle Pe number

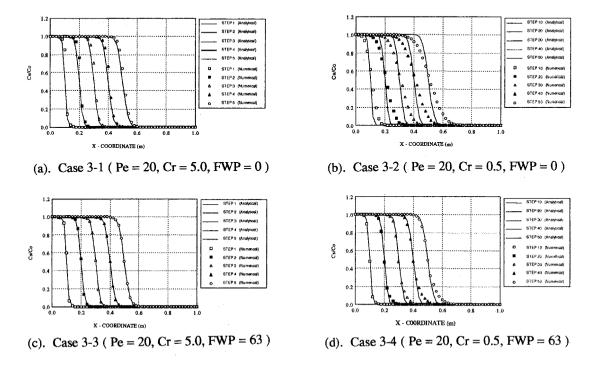


Fig.5 Comparison of analytical and numerical solutions for high Pe number

5.2 ANALYTICAL AND NUMERICAL SOLUTION OF TWO DIMENSIONAL CASE

5.2.1 ANALYTICAL SOLUTION

Partial Differential equation for two dimensional problem can be shown as follow

$$Dx \frac{\partial^2 C}{\partial x^2} + Dy \frac{\partial^2 C}{\partial y^2} - Vx \frac{\partial C}{\partial x} - Vy \frac{\partial C}{\partial y} = \frac{\partial C}{\partial t} \qquad \dots (41)$$

Initial and boundary condition are as follow

$$C(x, y, 0) = 1.0 \text{ when } x_c - a \le x \le x_c + a$$

$$y_c - b \le y \le y_c + b$$

$$C(x, y, 0) = 0.0$$
 otherwise

$$C(\infty, y, t) = C(\infty, y, t) = C(x, \infty, t) = C(x, \infty, t) = 0.0$$

Analytically Solution to this case is [3],[5]

$$C(x,y,t) = 0.25 \left[erf \left\{ \frac{a - (x - x_c) + Vx \cdot t}{\sqrt{4 Dx \cdot t}} \right\} + erf \left\{ \frac{a + (x - x_c) - Vx \cdot t}{\sqrt{4 Dx \cdot t}} \right\} \right]$$

$$\left[erf \left\{ \frac{b - (y - y_c) + Vy \cdot t}{\sqrt{4 Dy \cdot t}} \right\} + erf \left\{ \frac{b + (y - y_c) - Vy \cdot t}{\sqrt{4 Dy \cdot t}} \right\} \right] \qquad \dots (42)$$

5,2,2 MODEL AND RESULT OF NUMERICAL ANALYSIS

For this example, the elements consists of 2000 elements and 2121 nodal points and the informations of parameter values for two dimensional model are shown in Table. 2. The boundary condition is shown in Fig.6. In this case, a rectangular wave dispersion phenomena was calculated in an uniform velocity field over an infinite domain at relatively low Peclet numbers, the background concentration is zero and the wave has an initial concentration of one. It is centered at $(x_c, y_c) = (0.15, 0.00)$ and a = 0.05 m, b= 0.008 m. Size of mesh has a length of 0.04 m parallel to the x - coordinate and 0.01 m parallel y coordinate. And the results of numerical analysis are shown in Fig.7 and Fig.8. These figures shown the behavior of concentration in the section through the wave center parallel to the x direction and y direction at six concecutive times.

Table.2 Parameter for two dimensional model

Parameter	Case - 1	Case - 2	
Pe (x)	10.0	10.0	
Pc (y)	1.6	1.6	
Cr (x)	5.45	5.45	
Cr (y)	0.545	0.545	
Vx (m/sec)	1000	1000	
Vy (m/sec)	40	40	
Δt(sec)	0.0000545	0.0000545	
Δx (m)	0.01	0.01	
Δ y (m)	0.004	0.004	
Dx (m2/acc)	1.0	1.0	
Dy (m2/sec)	0.1	0.1	
FWP	0	329	

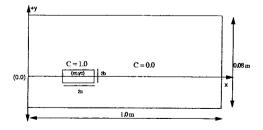
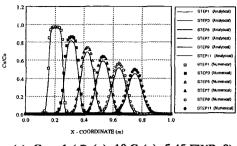
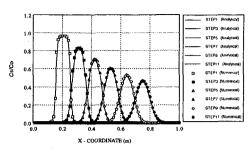


Fig. 6 Boundary conditions for two dimension

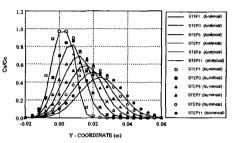


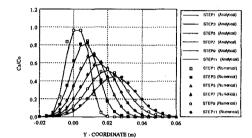


(a). Case 1 (Pe(x)=10,Cr(x)=5.45,FWP=0)

(b). Case 2 (Pe(x)=10,Cr(x)=5.45,FWP=329)

Fig.7 Comparison of analytical and numerical solutions for x-coordinate





(c). Case 1 (Pe(y)=1.6,Cr(y)=0.545,FWP=0)

(d). Case 2 (Pe(y)=1.6,Cr(y)=0.545,FWP=329)

Fig.8 Comparison of analytical and numerical solutions for y-coordinate

6. CONCLUSION

In this paper the numerical analysis by Eulerian Lagrangian Finite Element method have been shown. And also basic theory of saturated and unsaturated seepage flow and the Eulerian Lagrangian Finite Element Method have combined. From the result of calculation, it become appear that the Eulerian Lagrangian Finite Element Method is appropriate to solve the advection dispersion problem. This is caused that in the Eulerian-Lagrangian method the advection dispersion problem with initial and boundary condition can be formally decomposed into pure advection and residual dispersion. And from the result of one dimensional case, we obtained that when Pe is small, dispersion dominates and equation is parabolic in characteristic, and on the contrary when Pe is large, advection dominates and equation changes to hyperbolic. Then the effect of forward particle to the result of calculation become obvious. This method strongly influences to the steep concentration front.

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