

Numerical Modeling of One-Dimensional Longitudinal Dispersion Equation using Eulerian-Lagrangian Method

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ABSTRACT : Various Eulerian-Lagrangian numerical models for the one-dimensional longitudinal dispersion equation are studied comparatively. In the models studied, the transport equation is decoupled into two component parts by the operator-splitting approach; one part governing advection and the other dispersion. The advection equation has been solved using the method of characteristics following fluid particles along the characteristic line and the results are interpolated onto an Eulerian grid on which the dispersion equation is solved by Crank-Nicholson type finite difference method. In solving the advection equation, various interpolation schemes are tested. Among those, Hermite interpolation polynomials are superior to Lagrange interpolation polynomials in reducing both dissipation and dispersion errors.

1. Introduction

Governing equation of contaminant transport in natural channels is one-dimensional (1-D) longitudinal dispersion equation. To solve solution of longitudinal dispersion equation numerically, various Eulerian methods (Leonard, 1979; Lee and Kang, 1987; Abott and Basco, 1989) are developed. However most of these numerical methods are hampered by excess numerical oscillation and dissipation especially when advection mechanism dominates because Eulerian methods cannot describe hyperbolicity describing advection process in advection-dispersion equation. So, it is difficult to predict physical dispersion processes precisely by using Eulerian methods. To avoid spurious numerical error, Lagrangian methods which numerically compute only dispersion term in moving coordinates through flow are sporadically used, but it is difficult to construct numerical grid of complicated geometry or flow field (Noye, 1987).

Eulerian and Lagrangian method (ELM) using merits of both Eulerian method and Lagrangian method has been used to acquire an exact solution of 1-D longitudinal dispersion equation by various researchers (Holly and Preissmann, 1977; Baptista et al., 1979; Yang and Hsu, 1991; Seo and

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Kim, 1993). In ELM, Eulerian computational grid is used to ensure computational convenience and advection equation is solved using the method of characteristics following fluid particles along the characteristic line to control numerical error.

In differentiating total derivative of advection equation, it is necessary to determine concentration value of arbitrary point which the characteristic line is crossing. The concentration value of this point is interpolated using two values at the grid points which are closest to the point of interest. ELM's accuracy is much dependent on this interpolating method. When Lagrange interpolating polynomials are used, the simplest way is to interpolate with first order interpolation using two known concentrations. This method is suffered by numerical dissipation, so in most cases Lagrange second, third and fourth interpolating polynomial is used (Baptista et al., 1979; Cheng et al., 1984). In case of using higher Lagrange interpolating polynomial, we can acquire higher precision and reduce numerical dissipation. However, in this case it is difficult to treat boundary condition because many informations of grid are to be known. Another weakness of higher Lagrange interpolating polynomial is that it is hampered by spurious numerical oscillation.

To overcome these defect of Lagrange interpolating method, Holly and Preissmann (1977) used Hermite interpolating polynomial in which both concentration and concentration derivative are used. Hermite interpolating polynomial gives better solution. Holly and Polatera (1984) applied Hermite interpolating polynomial to compute two-dimensional advection equation. Toda and Holly (1986) considered the direction of characteristic line without splitting advection and dispersion equation into two parts. Yang and Hsu (1991) intended to promote precision of Holly and Preissmann method by reducing the number of interpolation using characteristic line crossing several time step. Jun and Lee (1993, 1994) computed one dimensional longitudinal equation with Hermite fifth degree interpolating polynomial and Crank-Nicholson method and showed that the ELM's computational results are superior to Eulerian method's.

In this study, to increase the ELM's applicability, advection equation has been differentiated using Lagrange third, fourth and fifth interpolating polynomials and Hermite third and fifth interpolating polynomials. The dispersion equation has been differentiated using Crank-Nicholson finite difference method. Error analysis of advection equations of Lagrange fifth degree interpolating polynomial and Hermite third interpolating polynomial was executed.

2. Splitting of Governing Equation

The 1-D longitudinal dispersion equation with constant flow section induced by Taylor (1953) is given below.

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = K \frac{\partial^2 C}{\partial x^2} \quad (1)$$

In this equation, x and t are longitudinal distance and time respectively and C is concentration and u, K are cross-section average velocity and longitudinal dispersion coefficient respectively. In this study, velocity and longitudinal dispersion coefficient are constant. Because Eq. (1) is linear, advection and dispersion process can be splitted as follows.

$$\frac{1}{2} \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = 0, \quad n\Delta t \leq t \leq f\Delta t \tag{2}$$

$$\frac{1}{2} \frac{\partial C}{\partial t} + K \frac{\partial^2 C}{\partial x^2} = 0, \quad f\Delta t \leq t \leq (n+1)\Delta t \tag{3}$$

Eqs. (2) and (3) are differentiated as below.

$$\frac{C^f - C^n}{\Delta t} = u \frac{\partial C}{\partial x} \tag{4}$$

$$\frac{C^{n+1} - C^f}{\Delta t} = K \frac{\partial^2 C}{\partial x^2} \tag{5}$$

in which C^f is concentration when pure advection is occurred; C^n, C^{n+1} are concentrations at present and next time level, respectively; and Δt is time increment.

3. Advection Model

Advection equation, Eq. (4) is describing that concentration is constant along the characteristic line. Namely, the total derivative of concentration with respect to time is zero.

$$\frac{dC}{dt} = 0 \tag{6}$$

$$\frac{dx}{dt} = u \tag{7}$$

Eqs. (6) and (7) can be written as follows referring Fig. 1.

$$C_R^f = C_P^n \tag{8}$$

$$\frac{x_R - x_P}{\Delta t} = u \tag{9}$$

Eqs. (8) and (9) are describing that concentration of time step n is only advected by $u \Delta t$ without concentration change in Δt . Therefore, accuracy of the characteristic method is heavily dependent on the interpolating method used in calculating concentration at P.

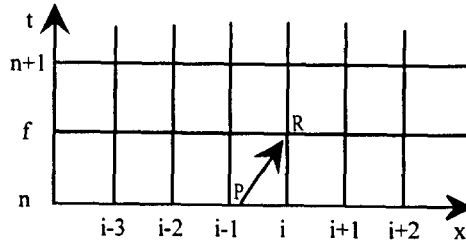


Fig. 1. One-Dimensional Eulerian Computational Grid

3.1 Lagrange Interpolating Polynomial

The general Lagrange interpolating polynomial is given as

$$C(x) = \sum_{i=1}^n C_i \phi_i(x) \quad (10)$$

in which C_i is a concentration of each node. $\phi_i(x)$ is interpolating function which is expressed as follows.

$$\phi_i(x) = \prod_{k=1, k \neq i}^n \left(\frac{x-x_k}{x_i-x_k} \right) \quad (11)$$

In Eq. (11), $n = 2, 3, 4$, and so on make Lagrange first, second and third, and so on degree interpolating polynomials respectively. In this study, advection equation is solved using Lagrange third, fourth and fifth degree interpolating polynomial. Advection model with Lagrange third degree interpolating polynomial is described as

$$C_i^f = C_i^n = L_0 C_{i-2}^n + L_1 C_{i-1}^n + L_2 C_i^n + L_3 C_{i+1}^n \quad (12)$$

in which

$$L_0 = \frac{(\alpha-1)\alpha(\alpha+1)}{6} \quad (13a)$$

$$L_1 = \frac{(2-\alpha)\alpha(\alpha+1)}{2} \quad (13b)$$

$$L_2 = \frac{(2-\alpha)(1-\alpha)(1+\alpha)}{2} \quad (13c)$$

$$L_3 = \frac{(\alpha-2)(1-\alpha)\alpha}{2} \quad (13d)$$

in which α is a Courant number ($\alpha = u \Delta t / \Delta x$).

If Lagrange fourth degree interpolating polynomial is used, then C_1^f is given as

$$C_1^f = C_p^n = M_1 C_{1-2}^n + M_2 C_{1-1}^n + M_3 C_1^n + M_4 C_{1+1}^n + M_5 C_{1+2}^n \quad (14)$$

in which

$$M_1 = \frac{(\alpha-1)\alpha(\alpha+1)(\alpha+2)}{24} \quad (15a)$$

$$M_2 = \frac{(2-\alpha)\alpha(\alpha+1)(\alpha+2)}{6} \quad (15b)$$

$$M_3 = \frac{(2-\alpha)(1-\alpha)(\alpha+1)(\alpha+2)}{4} \quad (15c)$$

$$M_4 = \frac{(\alpha-2)(1-\alpha)\alpha(\alpha+2)}{6} \quad (15d)$$

$$M_5 = \frac{\alpha(\alpha+1)(\alpha-1)(\alpha-2)}{24} \quad (15e)$$

If Lagrange fifth degree interpolating polynomial is used, then C_1^f is written as

$$C_1^f = C_p^n = H_1 C_{1-3}^n + H_2 C_{1-2}^n + H_3 C_{1-1}^n + H_4 C_1^n + H_5 C_{1+1}^n + H_6 C_{1+2}^n \quad (16)$$

in which

$$H_1 = \frac{(\alpha-2)(\alpha+1)\alpha(\alpha+1)(\alpha+2)}{120} \quad (17a)$$

$$H_2 = \frac{(3-\alpha)(\alpha-1)\alpha(\alpha+1)(\alpha+2)}{24} \quad (17b)$$

$$H_3 = \frac{(3-\alpha)(2-\alpha)\alpha(\alpha+1)(\alpha+2)}{12} \quad (17c)$$

$$H_4 = \frac{(3-\alpha)(2-\alpha)(\alpha-1)(\alpha+1)(\alpha+2)}{12} \quad (17d)$$

$$H_5 = \frac{(3-\alpha)(2-\alpha)(\alpha-1)\alpha(\alpha+2)}{24} \quad (17e)$$

$$H_6 = \frac{(\alpha-3)(\alpha-2)(1-\alpha)\alpha(\alpha+1)}{120} \quad (17f)$$

3.2 Hermite Interpolating Polynomial

In Hermite interpolating methods, approximate solution of advection equation is obtained using both concentrations and concentration derivatives. In Hermite third degree interpolating method,

two concentrations and two concentration first derivative are used as

$$C_1^f(\alpha) = A_1\alpha^3 + A_2\alpha^2 + A_3\alpha + A_4 \quad (18)$$

in which coefficients are calculated as follows.

$$C_1^f(0) = C_1^n \quad (19a)$$

$$C_1^f(1) = C_{i-1}^n \quad (19b)$$

$$CX_1^f(0) = CX_1^n \quad (19c)$$

$$CX_1^f(1) = CX_{i-1}^n \quad (19d)$$

in which CX means a first derivative of variable C .

If we calculate coefficients of Eq. (18) using Eqs. (19a)–(19d), we will obtain finite difference equation as follows.

$$C_1^f = a_1C_{i-1}^n + a_2C_i^n + a_3CX_{i-1}^n + a_4CX_i^n \quad (20)$$

in which

$$a_1 = \alpha^2(3-2\alpha) \quad (21a)$$

$$a_2 = 1-a_1 \quad (21b)$$

$$a_3 = \alpha^2(1-\alpha)\Delta x \quad (21c)$$

$$a_4 = -\alpha(1-\alpha)\Delta x \quad (21d)$$

Solution of first order derivative advection equation is obtained using equation given below.

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial \alpha} \frac{\partial \alpha}{\partial x} = -\frac{1}{\Delta x} \frac{\partial}{\partial \alpha} \quad (22)$$

So,

$$CX_1^f = -\frac{1}{\Delta x}(3A_1\alpha^2 + 2A_2\alpha + A_3) \quad (23)$$

If we substitute coefficients obtained using Eqs. (19a)–(19d) to Eq. (23), Eq. (23) becomes

$$CX_1^f = b_1C_{1-1}^n + b_2C_1^n + b_3CX_{1-1}^n + b_4CX_1^n \tag{24}$$

in which

$$b_1 = 6\alpha(\alpha-1)/\Delta x \tag{25a}$$

$$b_2 = -b_1 \tag{25b}$$

$$b_3 = \alpha(3\alpha-2) \tag{25c}$$

$$b_4 = (\alpha-1)(3\alpha-1) \tag{25d}$$

Similarly in Hermite fifth degree interpolating method, concentrations, first order concentration derivatives and second order concentration derivatives are used. Hermite fifth degree finite difference equation are derived as

$$C_1^f = c_1C_{1-1}^n + c_2C_1^n + c_3CX_{1-1}^n + c_4CX_1^n + c_5CXX_{1-1}^n + c_6CXX_1^n \tag{26}$$

$$CX_1^f = d_1C_{1-1}^n + d_2C_1^n + d_3CX_{1-1}^n + d_4CX_1^n + d_5CXX_{1-1}^n + d_6CXX_1^n \tag{27}$$

$$CXX_1^f = e_1C_{1-1}^n + e_2C_1^n + e_3CX_{1-1}^n + e_4CX_1^n + e_5CXX_{1-1}^n + e_6CXX_1^n \tag{28}$$

in which

$$c_1 = \alpha^3(10-15\alpha+6\alpha^2) \tag{29a}$$

$$c_2 = 1-c_1 \tag{29b}$$

$$c_3 = \alpha^3(1-\alpha)(4-3\alpha)\Delta x \tag{29c}$$

$$c_4 = -\alpha(1-\alpha)^3(1+3\alpha)\Delta x \tag{29d}$$

$$c_5 = \alpha^3(1-\alpha)^2\Delta x^2/2 \tag{29e}$$

$$c_6 = -\alpha^2(1-\alpha)^3\Delta x^2 \tag{29f}$$

$$d_1 = -30\alpha^3(1-\alpha^2)/\Delta x \tag{30a}$$

$$d_2 = -d_1 \tag{30b}$$

$$d_3 = -\alpha^2(2-3\alpha)(6-5\alpha) \tag{30c}$$

$$d_4 = (1-\alpha)^3(1-3\alpha)(1+5\alpha) \tag{30d}$$

$$d_5 = -\alpha^3(1-\alpha)(3-5\alpha)\Delta x/2 \tag{30e}$$

$$d_6 = -\alpha(1-\alpha)^2(2-5\alpha)\Delta x/2 \tag{30f}$$

$$e_1 = 60\alpha(1-3\alpha+2\alpha^2)/\Delta x^2 \tag{31a}$$

$$e_2 = -e_1 \tag{31b}$$

$$e_3 = 12\alpha(1-\alpha)(2-5\alpha)/\Delta x \tag{31c}$$

$$e_4 = 12\alpha(1-\alpha)(3-5\alpha)/\Delta x \tag{31d}$$

$$e_5 = \alpha(3-12\alpha+10\alpha^2) \tag{31e}$$

$$e_6 = (1-\alpha)(1-8\alpha+10\alpha^2) \tag{31f}$$

4. Error Analysis of Advection Equation

In this study, Lagrange fifth degree interpolating polynomial which is the most accurate method among Lagrange interpolating polynomials and Hermite third interpolating polynomial is analyzed by Fourier analysis. The basic assumptions in the Fourier analysis are that advection equation is linear, and thus superposition of arbitrary solutions is possible.

4.1 Lagrange Fifth Degree Interpolating Polynomials

To carry out error analysis using Fourier analysis, C_1^n in Eq. (16) is substituted to $\bar{C}^n \exp(j\sigma i)$ as follows.

$$\bar{C}^j = G\bar{C}^n \tag{32}$$

in which \bar{C}^n is an amplitude at arbitrary time step, n and $j \equiv \sqrt{-1}$. Amplification factor, G is given below.

$$G = H_1 \cos 3\sigma + (H_2 + H_6) \cos 2\sigma + (H_3 + H_5) \cos \sigma + H_4 - j(H_7 \sin 3\sigma + (H_2 - H_6) \sin 2\sigma + (H_3 - H_5) \sin \sigma) \tag{33}$$

in which σ is $2\pi\Delta x/L$ and L is a specific wave length of Fourier sine curve. Amplitude portraits and celerity portraits by Eq. (33) are depicted in Fig. 2. Amplitude error and celerity error are defined as follows.

$$\text{Amplitude Error} = \text{mod}(G) \tag{34}$$

$$\text{Celerity Error} = -\frac{\arctan\left(\frac{\text{Im}(G)}{\text{Re}(G)}\right)}{\alpha \sigma} \tag{35}$$

Fig. 2 shows that numerical dissipation is greatest but celerity error is zero when Courant number is 0.5.

4.2 Hermite Third Degree Interpolating Polynomials

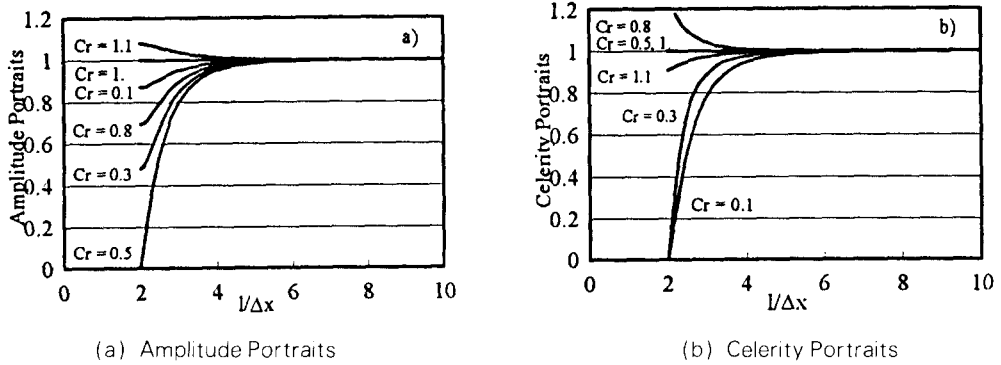


Fig. 2. Lagrange Fifth Degree Interpolating Polynomials

Holly and Preissmann (1977) obtained following equation by substituting C_1^n to $\bar{C}^n \exp(j\sigma t)$ in Eqs. (20) and (24).

$$\left(\frac{\bar{C}^{n+1}}{CX^{n+1}}\right) = F\left(\frac{\bar{C}^n}{CX^n}\right) \tag{36}$$

in which F is amplification matrix given as

$$F = \begin{bmatrix} k_1 & k_2 \\ k_3 & k_4 \end{bmatrix} \tag{37}$$

in which each component are given as follows

$$k_1 = a_1 \exp(-j\sigma) + a_2 \tag{38a}$$

$$k_2 = a_3 \exp(-j\sigma) + a_4 \tag{38b}$$

$$k_3 = b_1 \exp(-j\sigma) + b_2 \tag{38c}$$

$$k_4 = b_3 \exp(-j\sigma) + b_4 \tag{38d}$$

This amplification matrix is independent of time, so Eq. (28) becomes

$$\left(\frac{\bar{C}^n}{CX^n}\right) = F^n \left(\frac{\bar{C}^0}{CX^0}\right) \tag{39}$$

in which \bar{C}^0 and CX^0 are defined arbitrarily by means of initial conditions.

Amplification matrix of analytical solution is given as following.

$$F_0 = \begin{bmatrix} \exp(-j\sigma\alpha) & 0 \\ 0 & \exp(-j\sigma\alpha) \end{bmatrix} \tag{40}$$

Amplitude error and celerity error are induced by comparing Eqs. (37) and Eq. (39). The comparison of amplification matrix is equal to comparison of eigenvalue of the amplification matrix. The amplitude of eigenvalue of amplification matrix of Eq. (39) is always unity and there is no celerity error. The eigenvalue of amplification matrix of Eq. (37) is obtained as following.

$$(F-\lambda I)X=0 \quad (41)$$

Since Eq. (40) doen not have a trivial solution, we have

$$(k_1-\lambda)(k_4-\lambda)-k_2k_3=0 \quad (42)$$

so,

$$\lambda_{1,2}=\frac{(k_1+k_4)\pm\sqrt{(k_1+k_4)^2-4(k_2k_3-k_1k_4)}}{2} \quad (43)$$

In Eq. (42), we can obtain two complex eigenvalue. As σ goes to zero, λ_1 goes to $\exp(-j\sigma i)$ and λ_2 is very different to $\exp(-j\sigma i)$. Namely,

$$|\lambda_2| < |\lambda_1| \leq 1, \text{ for } \alpha \leq 1 \quad (44)$$

An amplitude error and celerity error of primary mode, λ_1 are depicted in Fig. 3. To compare to the results shown in Fig. 2, Hermite third degree interpolating polynomial gives much better results. The influence of secondary mode, λ_2 is rapidly reduced as time goes on because absolute value of secondary mode (about 0.5) is less than one. Namely, if concentration and concentration derivative are arbitrarily given as a initial condition, we can think that initial condition is equal to linear sum of eigenvectors. Namely,

$$\begin{pmatrix} \overline{C^0} \\ \overline{CX^0} \end{pmatrix} = A_1 \begin{pmatrix} \overline{C_1} \\ \overline{CX_1} \end{pmatrix} + A_2 \begin{pmatrix} \overline{C_2} \\ \overline{CX_2} \end{pmatrix} \quad (45)$$

Using Eqs. (38) and (40) at time step n, we have

$$\begin{aligned} \overline{C^n} &= A_1 \lambda_1^n \overline{C_1} + A_2 \lambda_2^n \overline{C_2} \\ \overline{CX^n} &= A_1 \lambda_1^n \overline{CX_1} + A_2 \lambda_2^n \overline{CX_2} \end{aligned} \quad (46)$$

In Eq. (44), it is postulated that influence of secondary mode about solution is rapidly reduced as time goes on. In Eqs. (44) and (45), A_1 and A_2 are arbitrary constants, and $(\overline{C_1}, \overline{CX_1})^T$ and $(\overline{C_2}, \overline{CX_2})^T$

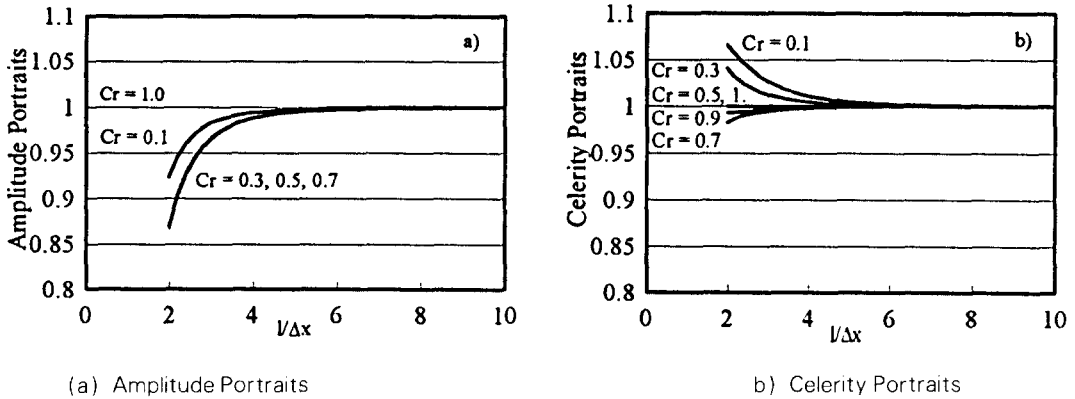


Fig. 3. Hermite Third Degree Interpolating Polynomial

are eigenvectors of λ_i and λ_i , respectively.

5. Dispersion Model

By differentiating Eq. (5) and using Crank–Nicholson finite difference method, we obtain following equation.

$$\frac{C_i^{n+1} - C_i^f}{\Delta t} = \frac{K}{2\Delta x^2} (C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1} + C_{i+1}^f - 2C_i^f + C_{i-1}^f) \tag{47}$$

Eq. (47) is rearranged as

$$-0.5\beta C_{i+1}^{n+1} + (1 + \beta)C_i^{n+1} - 0.5\beta C_{i-1}^{n+1} = 0.5\beta C_{i+1}^f + (1 - \beta)C_i^f - 0.5\beta C_{i-1}^f \tag{48}$$

in which is defined as diffusion number ($\beta = K\Delta t / \Delta x^2$).

Because Eq. (47) is a tridiagonal matrix, it can be solved easily by using Thomas algorithm. If Hermite interpolating polynomial is used, linear equation of CX and CXX as well as C are also solved by differentiating Eq. (3) with respect to x because concentration derivatives are also diffused (Jun and Lee, 1994). Zero concentration derivatives are imposed as a boundary condition.

6. Numerical Experiment

6.1 Input Data

In this study, five numerical models of different interpolating schemes are tested. Δx , u and simulation time are 500m, 0.5m/sec and 30,000 sec, respectively. The longitudinal dispersion coefficient, K and Δt are changed to simulate various Courant number and Peclet number (Peclet number is a dimensionless constant that represents relative importance of advection and dispersion). Gaussian distribution is used as a initial condition given as

$$C(x, 0) = \exp\left(-\frac{(x-x_0)^2}{2\sigma_0^2}\right) \quad (49)$$

in which σ_0 and x_0 are 400 and 3000 m, respectively. At time t , analytical solution of the governing equation is as

$$C(x,t) = \frac{\sigma_0}{\sigma_t} \exp\left(-\frac{(x-x_0-ut)^2}{2\sigma_t^2}\right) \quad (50)$$

$$\text{in which } \sigma_t = \sqrt{\sigma_0^2 + 2Kt} \quad (51)$$

In this study, following error index (Baptista et al., 1984) is used to compare the behavior of the numerical models more quantitatively.

$$\text{RMS Error} = \frac{1}{N} \sum_{i=1}^N \sqrt{(C_i^a - C_i^n)^2} \quad (52)$$

$$\text{Dissipation Error} = \frac{C_{\max}^a - C_{\max}^n}{C_{\max}^a} \quad (53)$$

$$\text{Dispersion Error} = \left| \frac{C_{\min}^n}{C_{\max}^a} \right| \quad (54)$$

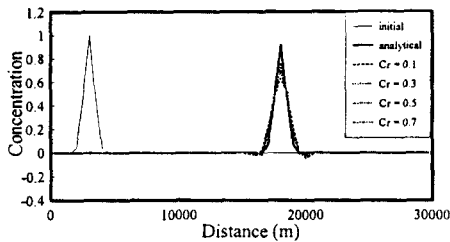
in which N is the total number of node and C_i^a, C_i^n and are analytical solution and numerical solution of arbitrary node respectively. $C_{\max}^a, C_{\max}^n, C_{\min}^n$ are maximum value of analytical solution and numerical solution, and minimum value of numerical solution respectively. RMS Error is a overall error index. Dissipation Error is a index of numerical dissipation. Dispersion Error is a index of spurious numerical oscillation.

6.2 Influence of Initial Condition

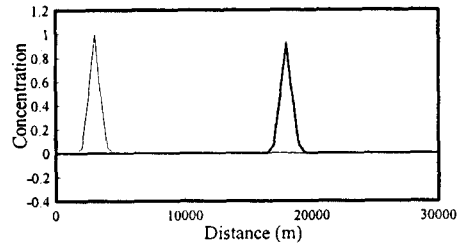
When Hermite interpolating polynomial is used, it is important to investigate influence of concentration derivative because concentration derivative is given as a initial condition. Figs. 4 and 5 are concentration distributions computed by each method in time 30,000sec. Abbreviations used in Figs. 4 and 5 are listed in Table 1. Fig. 4 is a concentration distribution when as a initial condition of concentration derivative, derivative of initial Gaussian concentration distribution is used. Figs. 5(d) and (e) are concentration distributions when initial concentration derivative is set to be zero. There is just a little difference between two cases.

Table 1. Abbreviation of Numerical Models Used in This Study

Abbreviation	Description
3-L	Lagrange third degree interpolating polynomial is used(i-2, i-1, i, i+1 node are used)
4-L	Lagrange fourth degree interpolating polynomial is used(i-2, i-1, i, i+1, i+2 node are used)
5-L	Lagrange fifth degree interpolating polynomial is used(i-3, i-2, i-1, i, i+1, i+2 node are used)
3-HP	Hermite third degree interpolating polynomial is used
5-HP	Hermite fifth degree interpolating polynomial is used

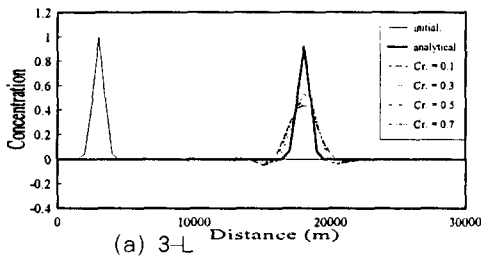


(a) 3-HP

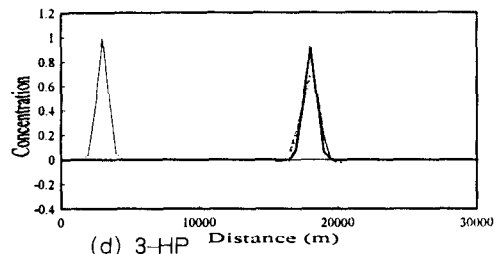


(b) 5-HP

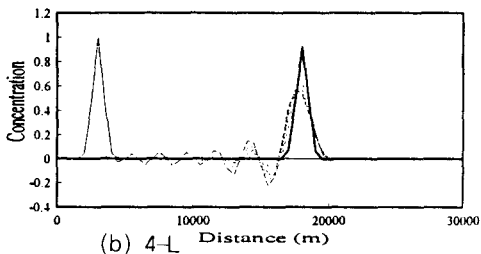
Fig. 4. Computational Results of Hermite Model Using Real Concentration Derivative, Peclet Number = 500



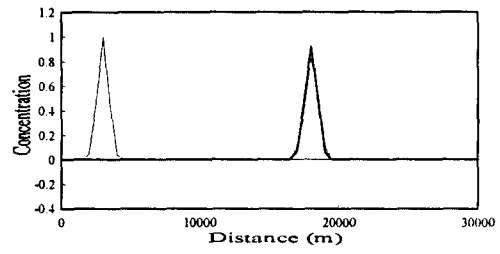
(a) 3-L



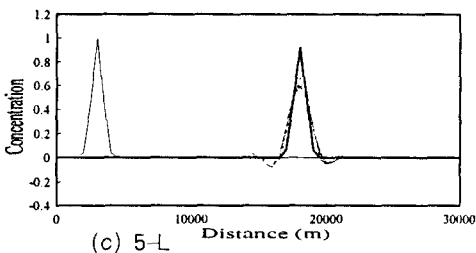
(d) 3-HP



(b) 4-L



(e) 5-HP



(c) 5-L

Fig.5 Computational Results of Each Method, Peclet Number = 500

6.3 Analysis of Result

Behavior of numerical models when Peclet number is 500 are shown in Fig. 5. Both dissipation error and dispersion error are very large for Lagrange third degree interpolating polynomial. For the case of Lagrange fourth degree interpolating polynomial, dissipation error is reduced little bit compared to third degree polynomial, however phase shift or dispersion error grows very largely because of nonsymmetrical use of node information of both of characteristic line. Dissipation error for Lagrange fifth degree interpolating polynomial is relatively small but numerical dispersion error is still large. Both dissipation error and dispersion error for Hermite third degree interpolating polynomial are reduced quite much compared to Lagrange polynomials. Hermite fifth degree interpolating polynomial gives almost the same as analytical solution and both dissipation and dispersion errors are almost suppressed.

RMS errors are depicted in Fig. 6. This figure shows that as Peclet number increases, error also increases. When Peclet number is 500, all methods except Hermite fifth degree interpolating polynomial give some error.

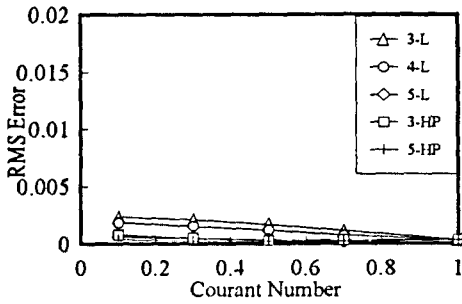
Fig. 7 is a picture of dissipation error. When Peclet number is 20, Lagrange third degree interpolating polynomial has comparatively large error, but other method give error smaller than 5%. When Peclet number is 500, all methods except Hermite fifth degree interpolating polynomial give noticeable dissipation error.

Fig. 8 is a picture of dispersion error. When Peclet number is more than 20, especially, Lagrange fourth degree interpolating polynomial gives excess numerical dispersion error. We can see that Hermite fifth degree interpolating polynomial gives the best result.

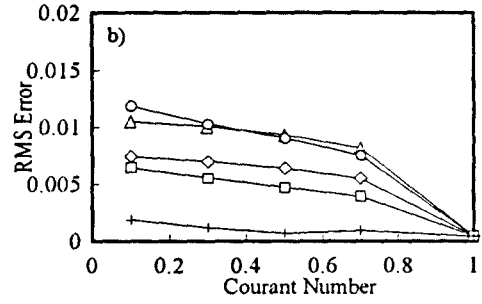
7. Summary and Conclusions

ELM is used to solve 1-D longitudinal dispersion equation. In this study, advection equation is solved using the method of characteristics and dispersion equation is solved by Crank-Nicholson finite difference method. Lagrange third, fourth and fifth degree and Hermite third and fifth degree interpolating polynomial are used to solve advection equation. Following results is obtained from analysis of behavior of numerical models.

- 1) When dispersion dominates all the proposed models give good results.
- 2) In case of advection dominated problems, Hermite fifth degree interpolating polynomial gives almost the same result as the analytical solution. However all other methods give noticeable dissipation errors.
- 3) Generally speaking, Hermite interpolating polynomials give better results but execution time becomes larger because for Hermite interpolating polynomials another Thomas algorithm need to be solved to solve concentration derivative equation.

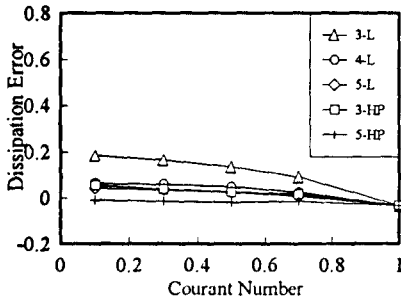


(a) Peclet Number = 20

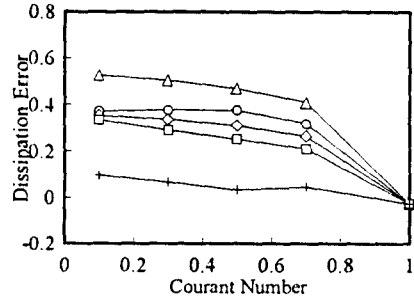


(b) Peclet Number = 500

Fig. 6. RMS Error

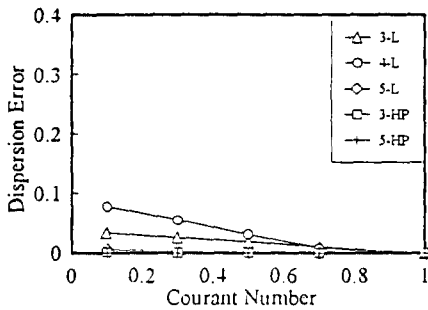


(a) Peclet Number = 20

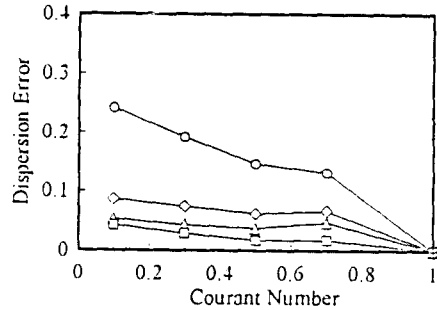


(b) Peclet Number = 500

Fig. 7. Dissipation Error



(a) Peclet Number = 20



(b) Peclet Number = 500

Fig. 8. Dispersion Error

References

Abott, M.B., and Basco, D.R. (1989). *Computational fluid dynamics: An introduction for engineers*. Longman Scientific & Technical, London.

Baptista, A.E.M., Adams, E.E., and Stolzenbach, K.D. (1984). "Eulerian-Lagrangian analysis of pollutant transport in shallow water." *Report No. 296*, Ralph M. Parsons Laboratory Aquatic Sciences and Environmental Engineering, Department of Civil Engineering, Massachusetts Institute of Technology.

- Cheng, R.T., Vinenzo, C., and Nevil, M. (1984). "Eulerian-Lagrangian solution of the convection-dispersion equation in natural coordinates." *Water Resources Research*, Vol. 20, No. 7, pp. 944-952.
- Holly, F.M., and Preissmann, A. (1977). "Accurate calculation of transport in two dimensions." *J. Hyd. Div.*, ASCE, Vol. 103, No. HY11, pp. 1259-1277.
- Holly, F.M., and Usseglio-Polatera, J.M. (1984). "Pollutant dispersion in tidal flow." *J. Hyd. Eng.*, ASCE, Vol. 110, No. 7, pp. 905-926.
- Jun, K.S., and Lee, K.S. (1993). "An Eulerian-Lagrangian hybrid numerical method for the longitudinal dispersion equation." *J. of Korean Association of Hydrological Sciences*, Vol. 26, No. 3, pp. 137-148.
- Jun, K.S., and Lee, K.S. (1994). "Eulerian-Lagrangian split-operator method for the longitudinal dispersion equation." *Proc. of the Korean Society of Civil Engineers*, Vol. 14, No. 1, pp. 131-141.
- Lee, K.S., and Kang, J.W. (1987). "Characteristics of the finite difference approximations for the convective dispersion model." *Proc. of the Korean Society of Civil Engineers*, Vol. 7, No. 4, pp. 147-157.
- Leonard, B.P. (1979). "A stable accurate convective modeling procedure based on quadratic upstream interpolation." *Computer Methods in Applied Mechanics and Eng.*, Vol. 19, pp. 59-98.
- Noye, J. (1987). "Numerical methods for solving the transport equation." *Numerical Modelling: Applications to Marine Systems*, J. Noye, ed., Elsevier, Amsterdam, pp. 195-229.
- Seo, I.W., and Kim, D.G. (1993). "Numerical modeling of 1-D advection-dispersion equation using Eulerian-Lagrangian method." *Proceeding of the 35th Conference of Hydraulic Engineering*, Korean Association of Hydrological Science, pp. 151-157.
- Suh, S.W. (1993). "Coastal dispersion analysis using two-dimensional Eulerian-Lagrangian model." *J. Korean Society of Coastal and Ocean Engineers*, Vol. 5, No. 3, pp. 173-181.
- Taylor, G.I. (1953). "Dispersion of soluble matter in solvent flowing slowly through a tube." *Proceedings of the Royal Society of London, Series A*, Vol. 219, pp. 186-203.
- Toda, K., and Holly, F.M. (1986). "Hybrid numerical method for linear advection-dispersion." Iowa Institute of Hydraulic Research, The University of Iowa, Iowa City, Iowa.
- Yang, J.E., and Hsu, E.L. (1991). "On the use of the reach-back characteristics method for calculation of dispersion." *International J. for Numerical Methods in Fluids*, Vol. 12, pp. 225-235.