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FINITE ELEMENT SOLUTION OF DISPERSION IN GROUNDWATER

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ABSTRACT

This report presents a finite element solution and the corresponding computer model that simulates two-dimensional transient solute transport in flowing groundwater. The model is both general and flexible and can be applied to a wide range of problem types. It computes changes in concentration over time caused by the processes of convective transport, hydrodynamic dispersion and mixing (or dilution) from fluid sources. The model includes adsorption and radioactive decay phenomena. It is assumed that gradients of fluid density, temperature, and viscosity do not affect the groundwater velocity distribution. This assumption allows us to solve separately groundwater flow and mass transport problems.

Finite element formulation of the mass transport equation leads to a set of integral equations. This set of equations is solved assuming third-order approximation of the dependent variable, concentration, over the elements.

The validity of the computer model is established by comparing its numerical results with existing analytical solutions. The analysis of the influence of time step, numerical Peclet number, and time integration weighting factor upon the accuracy of numerical calculations is presented.

As a hypothetical example, we will present an analysis of groundwater contamination caused by leakage from a waste disposal site situated above a fresh water aquifer.

The report includes a listing of the computer program, which is written in FORTRAN IV, and the users manual.

INTRODUCTION

This report describes and documents a finite element solution and computer model for calculating transient changes in concentration of solute in flowing groundwater. The computer program solves the partial differential equation of mass transport. The purpose of this simulation model is to compute the concentration of a dissolved chemical species in an aquifer at any specified place and time. Changes in chemical concentration occur within a dynamic groundwater system primarily due to four processes (Bear, 1972, Konikov and Bredehoeft, 1978): 1) convective transport, in which dissolved chemicals are moving with the flowing groundwater; 2) hydrodynamic dispersion, in which small-scale variations in the groundwater velocity and diffusion cause the paths of dissolved species to spread from the average direction of groundwater flow; 3) fluid sources and sinks, where water of one concentration is introduced into water of different concentration, or is withdrawn; and 4) chemical reactions, in which some amount of a dissolved chemical species may be added to or removed from the groundwater due to chemical and physical reactions in the water or between the water and the solid aquifer materials. The possible reactions assumed in this model are equilibrium adsorption, first-order irreversible kinetic adsorption and radioactive decay. The model also includes the presence of a sink-source term.

It is assumed that changes in concentration do not affect fluid density and viscosity. This assumption allows us to solve separately the groundwater flow and mass transport equations.

The model may be applied to a wide variety of practical problems. The computer program is offered as a basic working tool that may have to be modified by the user for efficient application to specific field problems.

The program is written in FORTRAN IV and is compatible with most high-speed computers. The data requirements, input format specifications, program options and output formats are all structured in a general manner that should be readily adaptable to many field problems.

This report includes a detailed description of the finite element solution of the mass transport equation. The reader is assumed to have moderate familiarity with groundwater pollution and finite element method.

MATHEMATICAL MODEL FOR DISPERSION IN GROUNDWATER

In this study the movement of a solute through saturated porous media is considered. This solute will be referred to as "tracer." The symbol c will be used to denote the concentration of the tracer

$$c = \frac{\text{mass of solute}}{\text{volume of solution}} \qquad [ML^{-3}] \qquad (1)$$

BASIC ASSUMPTIONS

Fickian Law:

It is assumed that macroscopic dispersion is a Fickian process; that is, there is a linear relationship between macroscopic dispersive flux and the product of the mean concentration gradient and mean velocity of the fluid (Fried, 1975). The dispersive flux is defined to be the total mass flux ($\overline{q_i c}$) less the mean convective flux ($\overline{q_i}\,\overline{c}$) . In terms of expectations (indicated by overbar),

$$\overline{q_i' c'} = \overline{q_i c} - \overline{q_i}\,\overline{c} \qquad i = 1,2,3 \qquad (2)$$

where q_i is the specific discharge and c is concentration.

what is i ?

$\overline{q_i' c'}$ is ?

If this dispersion flux is Fickian in nature, we may then write (ref. ?)

$$\overline{q_i'c'} = - |q| \; \alpha_{ij} \frac{\partial \overline{c}}{\partial x_j} \qquad (3)$$

where α_{ij} is the effective or macroscopic dispersivity tensor, and $|q|$ is the magnitude of the specific discharge vector. The dispersion coefficient tensor is related to α_{ij} by $D_{ij} = |u| \; \alpha_{ij}$, where $|u| = |q|/n$, $|u|$ is the magnitude of the pore water velocity and n is the effective porosity. In the direction of groundwater flow the longitudinal (D_L) and transverse (D_T) dispersion coefficients are given by (Bear, 1972; Fried, 1975):

$$D_L = \alpha_L |u| \qquad (4a)$$

$$D_T = \alpha_T |u| \qquad (4b)$$

where α_L and α_T = longitudinal and transverse dispersivity, respectively.

In global coordinates xy the components of the dispersion coefficient tensor may be written as: x-y

$$D_{xx} = \alpha_L u_x^2/|u| + \alpha_T u_y^2/|u| \qquad (5a)$$

$$D_{yy} = \alpha_L u_y^2/|u| + \alpha_T u_x^2/|u| \qquad (5b)$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T) \; u_x u_y/|u| \qquad (5c)$$

where u_x, u_y are the components of the pore water velocity vector.

Separation of Groundwater Flow and Mass Transport Equations:

It is assumed that variation of concentration does not ~~e~~affect the viscosity and density of a fluid. This assumption allows the separation of the groundwater flow and mass transport equations.

Presence of Adsorption:

There are two models of adsorption used in this study. A common equilibrium model is given by (Cameron and Klute, 1977)

$$S = kc \tag{6}$$

where k is an empirical equilibrium constant $[M^{-1}L^{3}]$, S is the adsorbed phase concentration in units of mass of adsorbed chemical per mass of solid media $[M^{0}]$.

If the local equilibrium assumption is not considered valid, a kinetic mode of the reaction is required. In general, the kinetic relationship may be of any order, reversible or irreversible of single or multiple reaction. In this study the first-order irreversible kinetic model has been used. This model may be written as (Cameron and Klute, 1977):

$$\frac{\partial S}{\partial t} = K_1 c \tag{7}$$

where K_1 is the adsorption rate constant $[M^{-1}L^{3}T^{-1}]$

Presence of Radioactive Decay:

If a tracer undergoes radioactive decay, the resulting change in tracer concentration may be expressed by (Ven Genuchten, 1981):

$$\frac{\partial c}{\partial t} = -\lambda c \qquad (8)$$

where λ is the decay constant $[T^{-1}]$.

This equation may be integrated with the limits chosen as the time necessary for the initial concentration to decrease by one-half.

$$\int_{C_o}^{C_o/2} \frac{dc}{c} = -\lambda \int_{0}^{t_{1/2}} dt \qquad (9)$$

where C_o = initial concentration $[ML^{-3}]$

$t_{1/2}$ = half life of species [T]

The equation is integrated and solved for λ to obtain

$$\lambda = \frac{0.693}{t_{1/2}} \qquad (10)$$

where .693 is?

Sinks and Sources:

In the mass transport equation, there are a variety of sink and source terms that may be considered. The most common ones are inputs and outputs in the system caused by wells or leakage through the aquifer. Concentration changes caused by the convective flow of solute in or out of an aquifer can occur through wells or areas normal to the flow field. The term representing the effect of ~~recharge~~ is (Grove, 1977) given by:

sink or source ?

$$\gamma = \frac{c'W}{bn} \qquad [ML^{-3}T^{-1}] \qquad (11)$$

where: c' = concentration of the fluid recharging the system $[ML^{-3}]$

W = recharge rate, the volume flux per unit area $[LT^{-1}]$

b = saturated thickness of the aquifer $[L]$

n = effective porosity $[L^0]$

ad γ = ?

The term representing pumping wells is given by (Bredehoeft and Pinder, 1972):

$$\Sigma\eta_i c = \frac{c}{nb} \sum_{i=1}^{m} Q_i(x_i,y_i)\ \delta(x - y_i) \cdot \delta(y - y_i) \qquad (12)$$

where Q_i = pumping rate $[L^3T^{-1}]$

δ = dirac delta function, which assures values for the term only at nodal points where wells are present

m = number of wells

η_i = discharge constant, defined by eq. 12 ? $[T^{-1}]$

how does (12) relate to (11) ?

THE GOVERNING MASS TRANSPORT EQUATION

The advective-dispersion may be obtained by combining the conservation of mass equation for a tracer and Fickian law. The partial differential equation describing two dimensional transient mass transport is given by (Van Genuchten, 1981)

$$\frac{\partial}{\partial x_i}\left(nD_{ij}\frac{\partial c}{\partial x_j} - q_i c\right) - \frac{\partial}{\partial t}(nc+\rho S) = \alpha nc + \beta\rho S - \gamma n + n\Sigma\eta_{\textcircled{i}} c \qquad (13)$$

$$i,j = 1,2$$

use differ. + let this one goes from 1 to m where c = tracer concentration $[ML^{-3}]$

S = adsorbed concentration $[M^0]$

n = effective porosity $[L^0]$

D_{ij} = dispersion coefficient tensor $[L^2T^{-1}]$

q_i = specific discharge vector $[LT^{-1}]$

ρ = porous medium bulk density $[ML^{-3}]$

α, β = first order rate constants for decay, associated with liquid and soil, respectively $[T^{-1}]$ explain why zero-order

γ = zero-order liquid-phase source term $[ML^{-3}T^{-1}]$ see eq. (11)

Substitution of the equilibrium adsorption model (eq. 6) into eq. 13 gives:

$$\frac{\partial}{x_i}\left(D_{ij}\frac{\partial c}{\partial x_j} - u_i c\right) - \frac{\partial (Rc)}{\partial t} = \mu c - \gamma + \Sigma \eta_{\textcircled{i}} c \qquad (14)$$

where the retardation factor R is defined by:

$$R = 1 + \rho k/n \qquad \xleftarrow{\text{no units?}} [-] \qquad (15)$$

and where the general decay constant μ is given by:

$$\mu = \alpha + \beta\rho k/n \qquad [T^{-1}] \qquad (16)$$

Substitution of the first-order irreversible kinematic model of adsorption (eq. 7) into eq. 13, without presence of radioactive decay, gives

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j} - u_i c\right) - \frac{\partial c}{\partial t} = \mu_1 c + \sum_{\textcircled{i}=1}^{\overset{m?}{\textcircled{k}}} \eta_{\textcircled{i}} c - \gamma \qquad (17)$$

use other index

where: $\mu_1 = k_1 \rho/n$ what is i? species?

(14)

In the global system of coordinates xy, the mass transport equation may be written as:

$$\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x} + D_{xy}\frac{\partial c}{\partial y} - u_x c\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c}{\partial y} + D_{yx}\frac{\partial c}{\partial x} - u_y c\right) - \frac{\partial (Rc)}{\partial t} = \mu c - \gamma + \Sigma \eta_i c \qquad (18)$$

Assuming that the velocity vector ~~is coincident~~ coincides with the x-axis, the simplified form of ~~the~~ eq. 18 may be written:

$$\frac{\partial}{\partial x}\left(D_L\frac{\partial c}{\partial x} - u_x c\right) + \frac{\partial}{\partial y}\left(D_T\frac{\partial c}{\partial y}\right) - \frac{\partial (Rc)}{\partial t} = \mu c - \gamma + \Sigma \eta_i c \qquad (19)$$ ✓

Initial and Boundary Conditions:

In order to solve eq. 18 initial and boundary conditions have to be specified for the domain of the problem. The initial conditions are to be given by the distribution of the tracer concentration $c_0(x,y)$ for initial time t_0. There are two types of boundary conditions used in this study: 1) constant concentration, when the concentration on the boundary is given; and 2) no-flow boundary, when no tracer flows through the boundary. Flow specified boundary can be handled through the recharge — term, can't it?

DEVELOPMENT OF FINITE ELEMENT SOLUTION

In this development the Galerkin procedure and isoparametric elements have been used to formulate the finite element solution of the mass transport equation. The Galerkin method is an old numerical technique, classically used to solve differential equations not amenable to analytical techniques. Recent advances in computing techniques have popularized this method by coupling it with the finite element technique. The principle of the finite element method is to approximate the unknown function by a set of functions discretized in space but continuous in time. This set of approximating functions is given by time dependent coefficients and basis functions that are only space dependent. The basis functions are to be continuous and piecewise continuously differentiable in the domain of the region. Thus the approximation of the unknown function is given by (Zienkiewicz, 1971):

? why use this? Does it mean $C \cong \bar{C}$?

$$\bar{c}(t,x,y) = \sum_{i=1}^{m} c_i(t)\, N_i(x,y) \tag{20}$$

where: $c_i(t)$ = values of approximating function at nodal points

$N_i(x,y)$ = the basis functions of nodal points

m = number of nodal points

The differential equation of the dependent variable $c(x,y,t)$ may be represented by ~~the~~ a differential operator (L), such that

$$L[c(x,y,t)] = 0 \tag{21}$$

~~where L is a differential operator~~

The Galerkin method uses the concept of a residual, Res, in its development (Zienkiewicz, 1971). This residual is formed by substituting into the differential operator the previously described approximation for the dependent variable. Thus:

$$L[c(x,y,t)] \approx L[\bar{c}(x,y,t)] = L[\sum_{i=1}^{m} c_i(t)\, N_i(x,y)] = \text{Res} \tag{22}$$

The residual vanishes in the entire domain of interest or is identically equal to zero for a true solution to the equation. In general, the true solution will not result and the residual will not be equal to zero. The Galerkin method's approach is to make the residual orthogonal to each of m weighting functions w_i

$$\int_A \text{Res}\ w_i\ dA = \int_A L[\bar{c}(x,y,t)]\ w_i\ dA = 0 \qquad (23)$$

$$\text{for } i = 1,2,\ \ldots,\ m$$

Galerkin chose these weighting functions identical to the basis functions used in the original approximation and set this weighted average equal to zero. The weighted average of the residuals can be defined and set equal to zero as follows (Grove, 1977):

$$\frac{\int_A \text{Res}\ N_i\ dA}{\int_A N_i\, dA} = 0 \quad ; \quad i = 1,2,\ \ldots,\ m \qquad (24)$$

or

$$\int_A L[\bar{c}(x,y,t)]\ N_i(x,y)\ dA = 0 \quad , \quad i = 1,2,\ \ldots,\ m \qquad (25)$$

Thus, we have m unknown ~~values of~~ coefficients, c_i, and ~~the~~ a system of m equations. By solving this system of equations, one can calculate the values of the coefficients c_i.

GALERKIN-FINITE ELEMENT SOLUTION OF MASS TRANSPORT EQUATION

The differential operator for the mass transport equation is given by (eq. 18):

$$L[c(x,y,t)] = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x} + D_{xy}\frac{\partial c}{\partial y} - u_x c\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c}{\partial y} + D_{yx}\frac{\partial c}{\partial x} - u_y c\right)$$

$$- \frac{\partial (Rc)}{\partial t} - \mu c - \Sigma \eta_i c + \gamma = 0 \qquad (26)$$

here c is the analytical sol. previously used $\bar{c}$

Perhaps we should define $C' = \Sigma \bar{\bar{C}} N_i$ where C' is an approximation of c

Substituting this equation into eq. 25 we obtain

$$\iint_A N_i\left[\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c}{\partial y}\right)\right] dxdy + \iint_A N_i\left[\frac{\partial}{\partial x}\left(D_{xy}\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial y}\left(D_{yx}\frac{\partial c}{\partial x}\right)\right] dxdy$$

$$- \iint_A N_i\left[\frac{\partial}{\partial x}(u_x c) + \frac{\partial}{\partial y}(u_y c) + \frac{\partial}{\partial t}(Rc) + \Sigma \eta_i c + \mu c - \gamma\right] dxdy = 0 \qquad (27)$$

$$\text{for } i = 1,2.., m$$

This integral equation contains second order derivatives, and requires continuity of the first differentials at all interface regions (boundaries of the elements) to avoid infinities in the second differentials. If we want to avoid this restriction, Green's theorem may be used. It is given by:

I think ok Carl

I believe

$$\iint_A \left(\overset{\checkmark}{\phi}\,\overset{2}{\frac{\partial \psi}{\partial x}} + \overset{\checkmark}{\theta}\,\overset{2}{\frac{\partial Q}{\partial y}}\right) dxdy = - \iint_A \left(\overset{\checkmark}{\psi}\,\overset{\checkmark}{\frac{\partial \phi}{\partial x}} + \overset{\checkmark}{Q}\,\overset{\checkmark}{\frac{\partial \theta}{\partial y}}\right) dxdy$$

$$+ \int_S (\overset{\checkmark}{\phi\psi} l_x + \overset{\checkmark}{Q\theta} l_y)\, dS \qquad (28)$$

in which l_x, l_y are the direction cosines of the outward normal to the boundary S and the x or y direction, respectively. Integral S is taken over the whole boundary of the region.

Substituting $\phi = D_{xx}N_i$, $\theta = D_{yy}N_i$, $\psi = \frac{\partial c}{\partial x}$, $Q = \frac{\partial c}{\partial y}$ into the first integral of the eq. 28 gives

This assumes all D's are constants

$$\iint_A \overbrace{N_i\left[D_{xx}\frac{\partial^2 c}{\partial x^2} + D_{yy}\frac{\partial^2 c}{\partial y^2} + \frac{\partial D_{xx}}{\partial x}\frac{\partial c}{\partial x} + \frac{\partial D_{yy}}{\partial y}\frac{\partial c}{\partial y}\right]}^{\text{1st. o.r.h.s. of 27}} dxdy =$$

$$- \iint_A \left(D_{xx}\frac{\partial N_i}{\partial x}\frac{\partial c}{\partial x} + D_{yy}\frac{\partial N_i}{\partial y}\frac{\partial c}{\partial y}\right) dxdy + \int_S N_i\left(D_{xx}\frac{\partial c}{\partial x}l_x + D_{yy}\frac{\partial c}{\partial y}l_y\right) dS$$

(29)

Substituting $\phi = \theta = D_{xy} N_i$ ($D_{xy} = D_{yx}$ - see eq. 5), D's are constant
$\psi = \frac{\partial c}{\partial y}$, $Q = \frac{\partial c}{\partial x}$ into eq. 28 gives

$$\iint_A N_i\left(D_{xy}\frac{\partial^2 c}{\partial x\partial y} + D_{xy}\frac{\partial^2 c}{\partial x\partial y} + \frac{\partial D_{xy}}{\partial x}\frac{\partial c}{\partial y} + \frac{\partial D_{xy}}{\partial y}\frac{\partial c}{\partial x}\right) dxdy =$$

$$- \iint_A \left[D_{xy}\frac{\partial N_i}{\partial x}\frac{\partial c}{\partial y} + D_{xy}\frac{\partial N_i}{\partial y}\frac{\partial c}{\partial x}\right] dxdy + \int_S N_i\left(D_{xy}\frac{\partial c}{\partial y}l_x + D_{xy}\frac{\partial c}{\partial x}l_y\right) dS$$

(30)

The left sides of eqs. 29 and 30 are equivalent to the first two integrals in eq. 27, f. constant D's so we can substitute the right hand sides of eqs. 29 and 30 for these two integrals. Notice that the right hand sides of eqs. 29 and 30 do not have the second differentials.

It is of interest to remark that the sum of the boundary integrals of equations 29 and 30 has a certain physical meaning. It represents in fact a weighted boundary integral of the dispersive flux. The boundary conditions sometimes specify this rather than the actual distribution of concentration. In the latter case the boundary integration is not performed, since the concentration on the boundary is given, and the value of each of the N_i basis functions of the interior nodes is equal to zero on the boundary. In the former case the values of the boundary integrals are prescribed by the given dispersive flux and included in the system of equations as a known value.

For convenience in presenting the numerical solution, we drop the boundary integral terms of eqs. 29 and 30. Substituting the results of integration by parts into the eq. 27, we obtain:

$$- \iint_A \left(D_{xx} \frac{\partial N_i}{\partial x} \frac{\partial c}{\partial x} + D_{yy} \frac{\partial N_i}{\partial y} \frac{\partial c}{\partial y} \right) dxdy - \iint_A \left(D_{xy} \frac{\partial N_i}{\partial x} \frac{\partial c}{\partial y} + D_{xy} \frac{\partial N_i}{\partial y} \frac{\partial c}{\partial x} \right) dxdy$$

$$- \iint_A N_i \left(\frac{\partial}{\partial x} (u_x c) + \frac{\partial}{\partial y} (u_y c) + \frac{\partial}{\partial t} (Rc) + \Sigma \eta_i c + \mu c - \gamma \right) dxdy = 0 \qquad (31)$$

Substituting for the dependent variable c(x,y,t) [redacted] its approximation $\bar{c}(x,y,t) = \sum_{i=1}^{m} c_i(t) \, N_i(x,y)$, we obtain

why is this needed? Have not talked about finite differences yet.

$$[H] \, \{c\}_{\boxed{t, t+\Delta t}} + [M] \left\{ \frac{\partial c}{\partial t} \right\} = \{B\} \qquad (32)$$

where:

$$H_{ij} = \sum_e h_{ij}^e \qquad \text{for } i \neq j \qquad (33a)$$

$$H_{ij} = \sum_e h_{ij}^e + \bar{h}_{ii} \qquad \text{for } i = j \qquad (33b)$$

$$M_{ij} = \sum_e m_{ij}^e \qquad (33c)$$

$$B_i = \sum_e b_i^e \qquad (33d)$$

$$h_{ij}^{e} = \iint_{A_e} \Big[D_{xx} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + D_{yy} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + D_{xy} \Big(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} \Big)$$

$$+ N_i \Big(u_x \frac{\partial N_j}{\partial x} + u_y \frac{\partial N_j}{\partial y} \Big) + N_i N_j \Big(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \Big) + \mu N_i N_j \Big] \, dxdy \qquad (33e)$$

$$\overline{h}_{ii} = \iint_{A} N_i \, \eta_i \, dxdy = Q_i/nb \qquad (33f)$$

$$m_{ij}^{e} = \iint_{A_e} R \, N_i N_j \, dxdy \qquad (33g)$$

$$b_i^{e} = \iint_{A_e} \gamma \, N_i \, dxdy \qquad (33h)$$

in which the summation Σ_e is performed over all the elements, and the integrals are calculated for each element. In these equations it has been assumed that R, μ and γ do not vary over an element. In the numerical calculations it has been also assumed that the pore water velocity components are represented in the same manner as the function c

$$\bar{u}_x = \sum_{k=1}^{m} u_{xk} \, N_k(x,y) \qquad (34a)$$

$$\bar{u}_y = \sum_{k=1}^{m} u_{yk} \, N_k(x,y) \qquad (34b)$$

Thus, the components of the dispersion coefficient are given at any point by:

$$D_{xx} = \alpha_L \overline{u}_x^2/|\overline{u}| + \alpha_T \overline{u}_y^2/|\overline{u}| \qquad (35a)$$

$$D_{yy} = \alpha_L \overline{u}_y^2/|\overline{u}| + \alpha_T \overline{u}_x^2/|\overline{u}| \qquad (35b)$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T)\, \overline{u}_x \, \overline{u}_y/|\overline{u}| \qquad (35c)$$

this shows that D is space dependent. why didn't you consider terms involving $\frac{\partial D}{\partial x}$ or $\frac{\partial D}{\partial y}$ in equation 31.

where: $|\overline{u}| = (\overline{u}_x^2 + \overline{u}_y^2)^{1/2}$

In order to integrate eq. 32 in time ~~the~~ a weighted finite difference scheme is used.

use Φ ~~perhaps in letters~~

$$\frac{\partial\{c\}}{\partial t} = \frac{\overset{\cancel{\psi}}{\{c\}^{t+\Delta t}} - \overset{\cancel{(1-\psi)}}{\{c\}^{t}}}{\Delta t} \qquad (36a)$$

~~Or~~

$$\{c\}^{t,t+\Delta t} = \psi\{c\}^{t+\Delta t} + (1-\psi)\,\{c\}^{t} \qquad (36b)$$

~~use some other symbol if you can~~

in which $\{c\}^{t+\Delta t}$ is the vector of the values of concentration at the nodes at the time t+Δt, and ψ is the weighting coefficient, which is equal to 1.0 for strictly implicit scheme and to 0.0 for explicit scheme. $\frac{1}{2}$ for Crank-Nicolson

The final set of equations which includes Dirichlet type boundary conditions is given by

$$[H^*]\,\{c_{un}\}^{t+\Delta t} = \{B^*\} \qquad (37)$$

where: $\{c_{un}\}^{t+\Delta t}$ = concentration at the active nodes (where the value of concentration is unknown) at ~~the~~ time $t+\Delta t$; the subscript un refers to unknown values.

$$H^*_{ij} = \psi\, H_{ij} + M_{ij}/\Delta t \quad \text{for active nodes } i,j \tag{38a}$$

$$B^*_i = \bar{B}_i + B_i \tag{38b}$$

$$\bar{B}_i = \sum_j \left[(\psi-1)\, H_{ij} + M_{ij}/\Delta t\right] \cdot C^t_j \tag{38c}$$

for active nodes i,j

$$\bar{B}_i = \frac{1}{2} \sum_k H_{ik}\left(c^{t+\Delta t}_k + c^t_k\right) \tag{38d}$$

I don't follow this

for active node i and passive (known value of c) node k

Eq. 37 forms a system of linear equations whose solution is the vector of the values of concentration at the active nodes at time $t+\Delta t$. This solution is the initial condition for the next time step.

Order of Elements

In this study ~~the~~ third-order (cubic) isoparametric elements are used. The shape of these elements in local and global coordinate systems is depicted by Figures 1 and 2, respectively. The basi~~c~~s functions ~~of~~ at corner nodes are given ~~for~~ in local coordinates $\zeta\eta$ by (Zienkiewicz, 1971):

$$N_i(\zeta,\eta) = \frac{1}{32}(1+\zeta_0)(1+\eta_0)[-10+9(\zeta^2+\eta^2)] \qquad (39a)$$

$$\zeta_i = \pm 1 \text{ and } \eta_i = \pm 1$$

and for mid-side nodes

$$N_i(\zeta,\eta) = \frac{9}{32}(1+\zeta_0)(1-\eta^2)(1+9\,\eta_0) \qquad (39b)$$

$$\text{for } \zeta_i = \pm 1 \text{ and } \eta_i = \pm \frac{1}{3}$$

$$N_i\ (\zeta\ \eta) = \frac{9}{32}(1+\eta_0)(1-\zeta^2)(1+9\,\zeta_0) \qquad (39c)$$

Comma?

$$\text{for } \zeta_i = \pm \frac{1}{3} \text{ and } \eta_i = \pm 1$$

in which $\zeta_0 = \zeta\,\zeta_i$; $\eta_0 = \eta\,\eta_i$; and ζ_i, η_i are coordinates of the i^{th} node.

may be worthwhile to give an indication as how you plan to integrate N_i at this point. In a way wrap up your math. development as much as possible.

Figure 1. Cubic element in local system of coordinates.

Figure 2. Cubic element in global of coordinates.

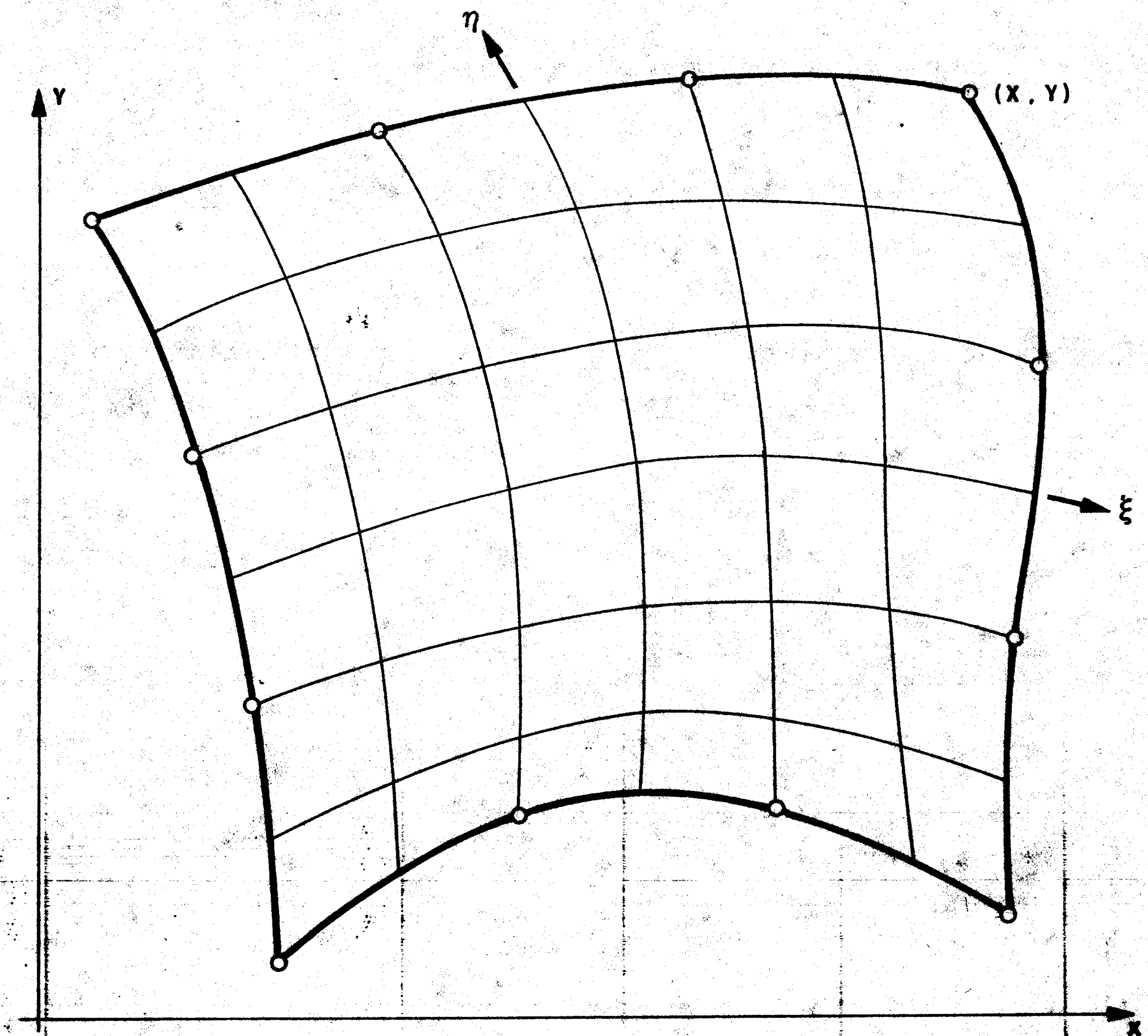


Figure 2

NUMERICAL RESULTS FOR SIMULATION OF MASS TRANSPORT

In this section the results of numerical simulation of some dispersion problems are presented and compared with analytical solutions. The effects upon accuracy of the weighting factor ψ, time step Δt and numerical Peclet number P_e are discussed.

Is there any other type of Peclet number?

LONGITUDINAL TRANSIENT DISPERSON WITH THE STEP-INPUT FUNCTION

In homogeneous and isotropic porous media ~~the~~ one-dimensional dispersion without adsorption, radioactive decay or source is described by the equation

$$\frac{\partial}{\partial x}(D_L \frac{\partial c}{\partial x}) - u \frac{\partial c}{\partial x} = \frac{\partial c}{\partial t} \qquad (40)$$

For initial and boundary conditions given by

$$c(0,t) = C_0; \qquad t > 0 \qquad (41a)$$

$$c(x,0) = 0; \qquad x > 0 \qquad (41b)$$

$$c(\infty,t) = 0; \qquad t > 0 \qquad (41c)$$

Equations 40 and 41 describe hydrodynamic dispersion in a semi-infinite column ($x > 0$) with a source of tracer with concentration C_0 maintained at $x = 0$ at time $t > 0$. The flow of a water solutant is maintained at a constant velocity u, and initially ($t = 0$) the concentration in the column is equal to zero. The analytical solution of this problem is given by (Fried, 1975)

Figure 3. Finite element network for one-dimensional mass transport.

$$D_L \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x} - R \frac{\partial c}{\partial t} = \mu c - \gamma \tag{47}$$

and initial and boundary conditions

$$c(x,0) = C_i \tag{48a}$$

$$c(0,t) = C_0 \qquad t > 0 \tag{48b}$$

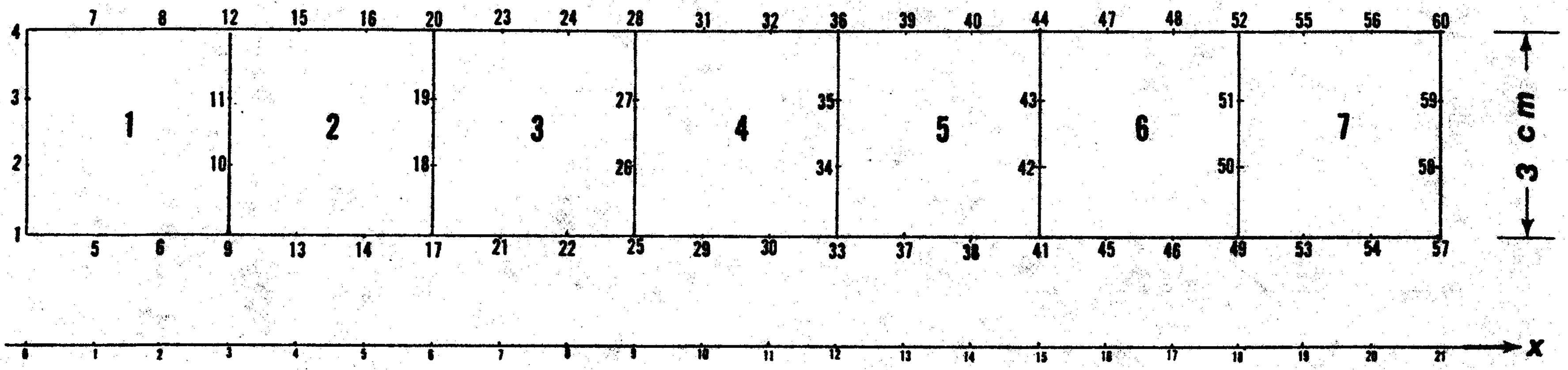
$$\frac{\partial c}{\partial t}(\infty,t) = 0 \tag{48c}$$

The analytical solution for this case is as follows:

$$c(x,t) = (c_0 - \gamma/\mu)\, H(x,t) + M(x,t) \tag{49}$$

where

$$\begin{aligned} H(x,t) = {} & \frac{1}{2} \exp\left[\frac{(u - v)x}{2D_L}\right] \operatorname{erfc}\left[\frac{Rx - vt}{2(D_L Rt)^{1/2}}\right] \\ & + \frac{1}{2} \exp\left[\frac{(u + v)x}{2D_L}\right] \operatorname{erfc}\left[\frac{Rx + vt}{2(D_L Rt)^{1/2}}\right] \\ M(x,t) = {} & \left(\frac{\gamma}{\mu} - C_i\right) \exp\left(-\frac{\mu t}{R}\right) \left\{\frac{1}{2} \operatorname{erfc}\left[\frac{Rx - ut}{2(D_L Rt)^{1/2}}\right]\right. \\ & \left. + \frac{1}{2} \exp\left(\frac{ux}{D_L}\right) \operatorname{erfc}\left[\frac{Rx + ut}{2(D_L Rt)^{1/2}}\right]\right\} + \frac{\gamma}{\mu} \\ & + \left(C_i - \frac{\gamma}{\mu}\right) \exp\left(-\frac{\mu t}{R}\right) \end{aligned} \tag{50}$$



is x in cm?

Figure 3

Is there a range of
u, & D_L for which s.t.o.r.h.s.
may be neglected?

$$\frac{c}{c_0} = \frac{1}{2} \left[\mathrm{erfc} \left(\frac{x - ut}{2(D_L t)^{1/2}}\right) + \exp \left(\frac{ux}{D_L}\right) \mathrm{erfc} \left(\frac{x + ut}{2(D_L t)^{1/2}}\right)\right] \tag{42}$$

where erfc(z) is a complementary error function, erfc(z) = 1 - erf(z). The second term in eq. 41 may be neglected in most cases.

you mean 42
and why it can be
droped?

The numerical simulation of this problem has been done in order to investigate the accuracy of the numerical solution depending on some numerical parameters. These parameters are: 1) Peclet number P_e, 2) Courant number C_u, 3) weighting factor ψ. The numerical Peclet number is given by

$$P_e = \frac{u\Delta x}{D_L} \tag{43}$$

not neccessarily.

where Δx is assumed the distance between nodes. This number describes the proportion between advective and dispersive terms in numerical simulation (i.e., the larger P_e, the larger the influence of the advective term).

The Courant number is given by

$$C_u = \frac{u\Delta t}{\Delta x} \tag{44}$$

✓

The value of Courant number is equal to the part of the distance Δx which is covered by a solutant in one time step Δt.

The weighting factor ψ is described in an earlier section. For a certain time t + Δt it represents the proportion between the concentrations at the time t and t + Δt, whose weighted average is assumed to be representative for the time between t and t + Δt. This weighted average is given by:

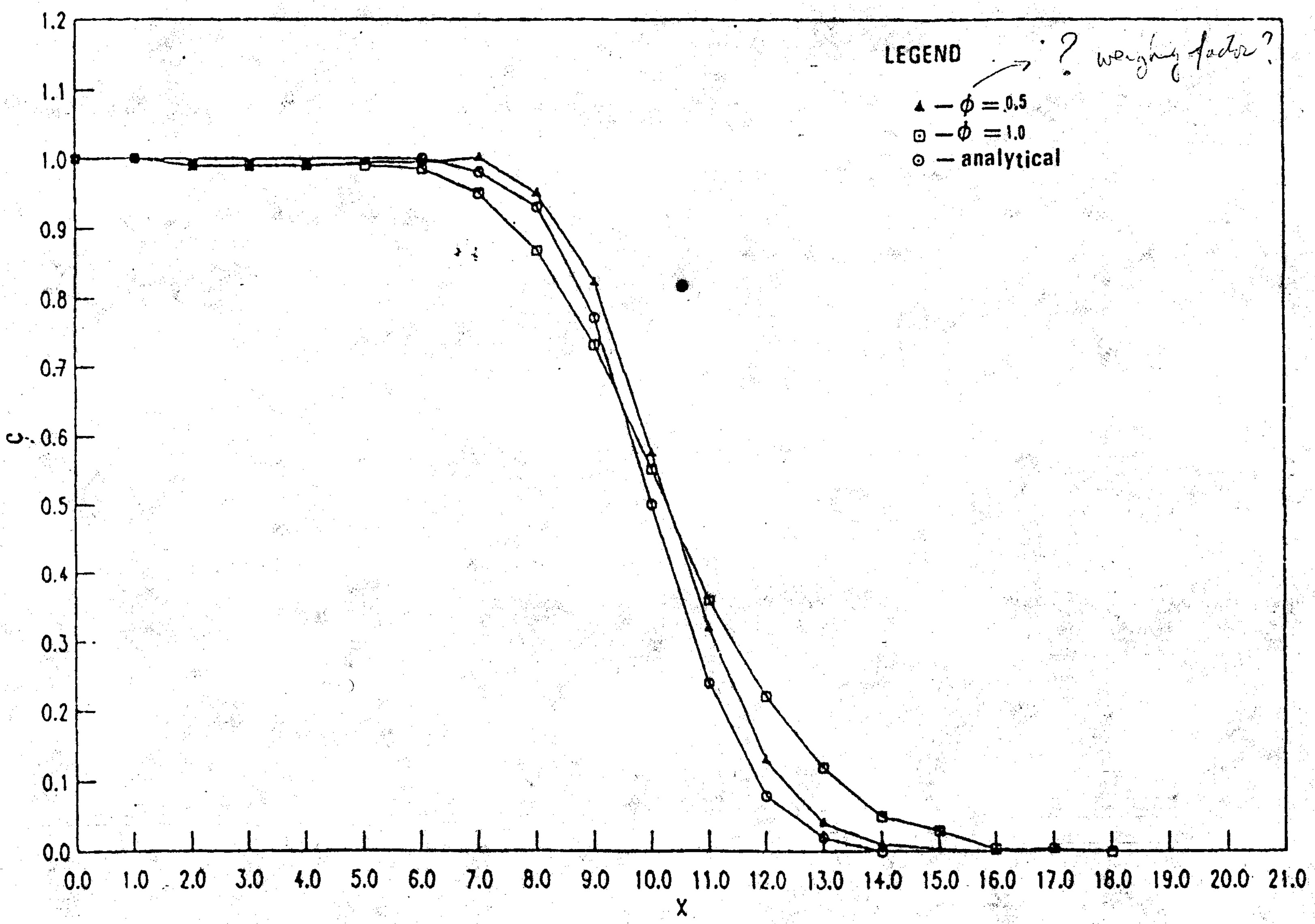
$$\{c\}^{t,t+\Delta t} = \psi\{c\}^{t+\Delta t} + (1-\psi)\ \{c\}^{t} \qquad (45)$$

The finite element grid for numerical simulation is shown in Figure 3. The distance between nodes, Δx, is assumed to be 1.0, and the pore water velocity is assumed as 1.0. The values of numerical parameters which have been used are: P_e: 10; 100; ∞; C_u = 0.25; 0.5; 1.0; 2.0; ψ = 0.25; 0.5; 0.75; 1.0. The results of numerical simulation are shown in Figures 4-12.

Analysis of the result shows that the best accuracy is obtained when C_u = 0.5 and ψ = 0.5. As it has been expected, the better accuracy is obtained for lower Peclet numbers, which simply implies that the finer grid or smaller velocity gives the higher accuracy. However, it is more important for practical applications to have satisfactory accuracy for large ~~numerical~~ Peclet numbers, since in order to lessen the Peclet number one has to decrease the grid size Δx, which results in a large number of nodes. This requires a large computer storage and long computer time, which is at some point neither possible nor economical. The results of numerical simulation for P_e = 100 and P_e = ∞ are shown in Figures 10 and 12. The finite element method for this value gives satisfactory agreement with the analytical solution.

It may be worthwhile to justify some of the numerical dispersions we see in Figs. For example $P_e = \infty$ means what? ~~Do~~ Are we ever going to have such a case? What is the average velocity of G.W. and average value of D to create a P_e = say 100. M. H.

Figure 4. Longitudinal dispersion in uniform one-dimensional flow, $P_e = 10.0$, $Cu = 0.25$.



? weighing factor?

Figure 4

Figure 5. Longitudinal dispersion in uniform one-dimensional flow, $P_e = 10.0$, $Cu = 0.5$.

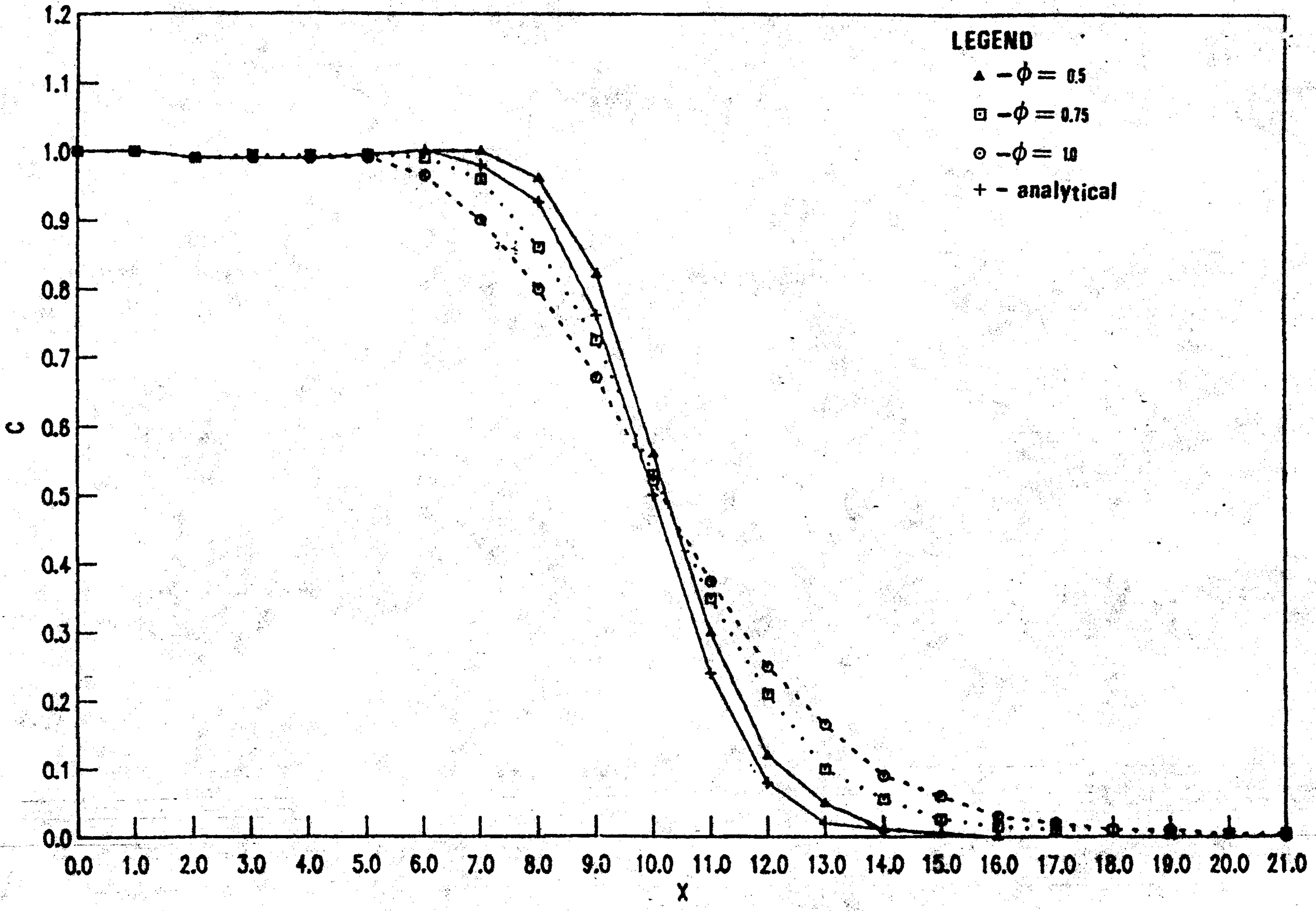

LEGEND
▲ –ϕ= 0.5
⊡ –ϕ= 0.75
⊙ –ϕ= 1.0
+ – analytical
C
X
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0

Figure 5

Figure 6. Longitudinal dispersion in uniform one-dimensional flow, $P_e = 10.0$, $Cu = 1.0$.

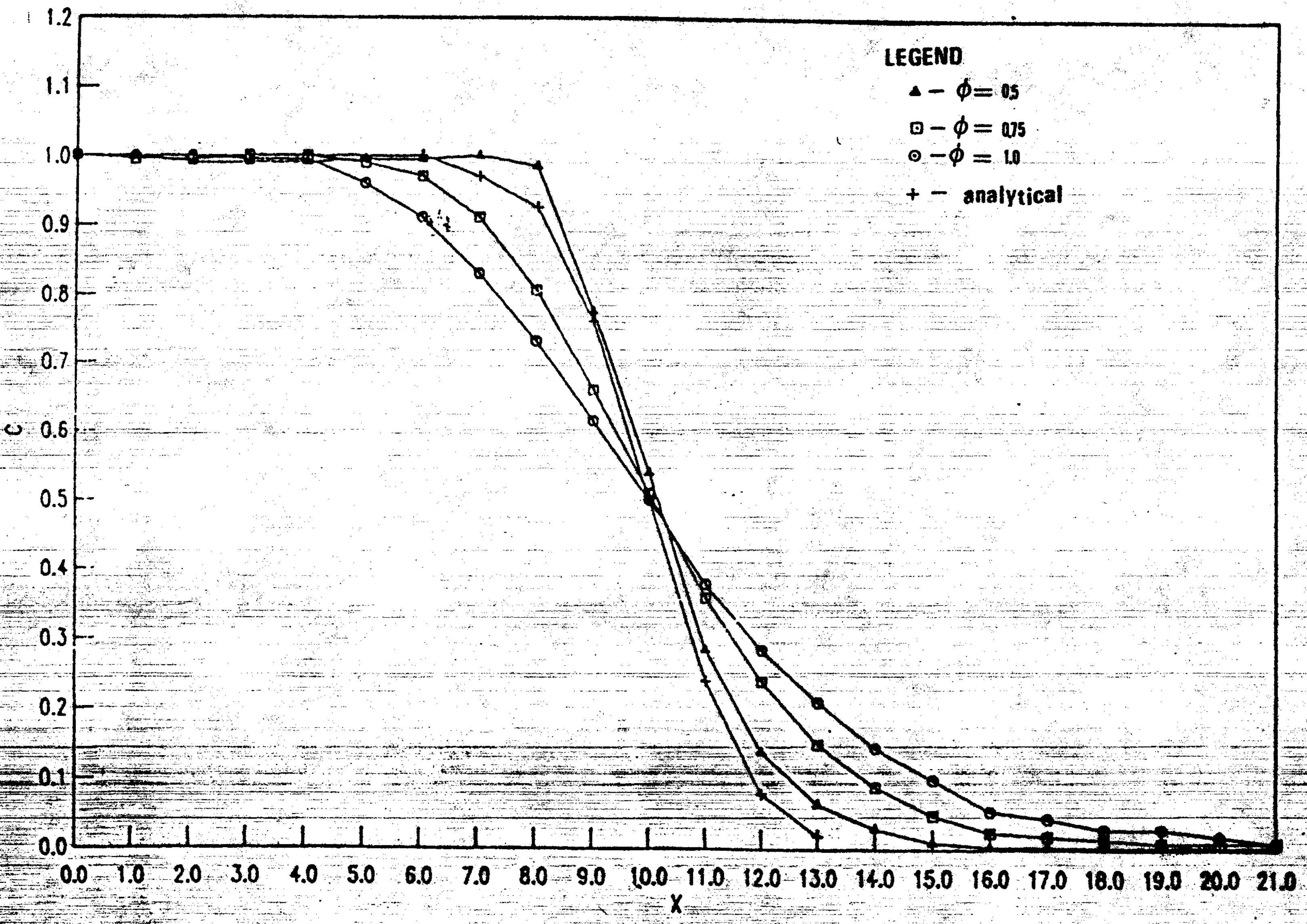

LEGEND
▲ – φ = 0.5
□ – φ = 0.75
⊙ – φ = 1.0
+ – analytical
C
X
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0

Figure 6

Figure 7. Longitudinal dispersion in uniform one-dimensional flow, $P_e = 10.0$, $Cu = 2.0$.

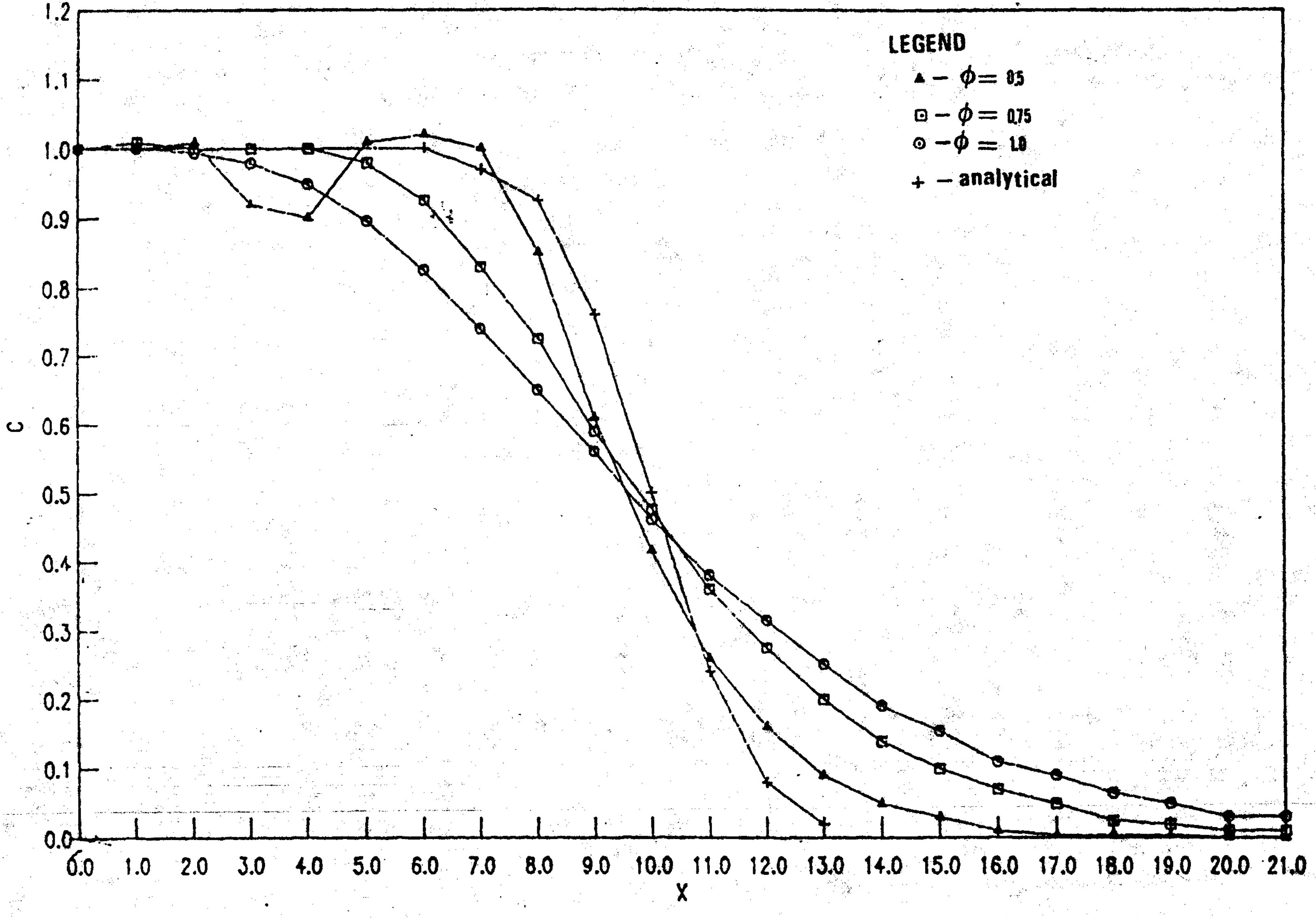
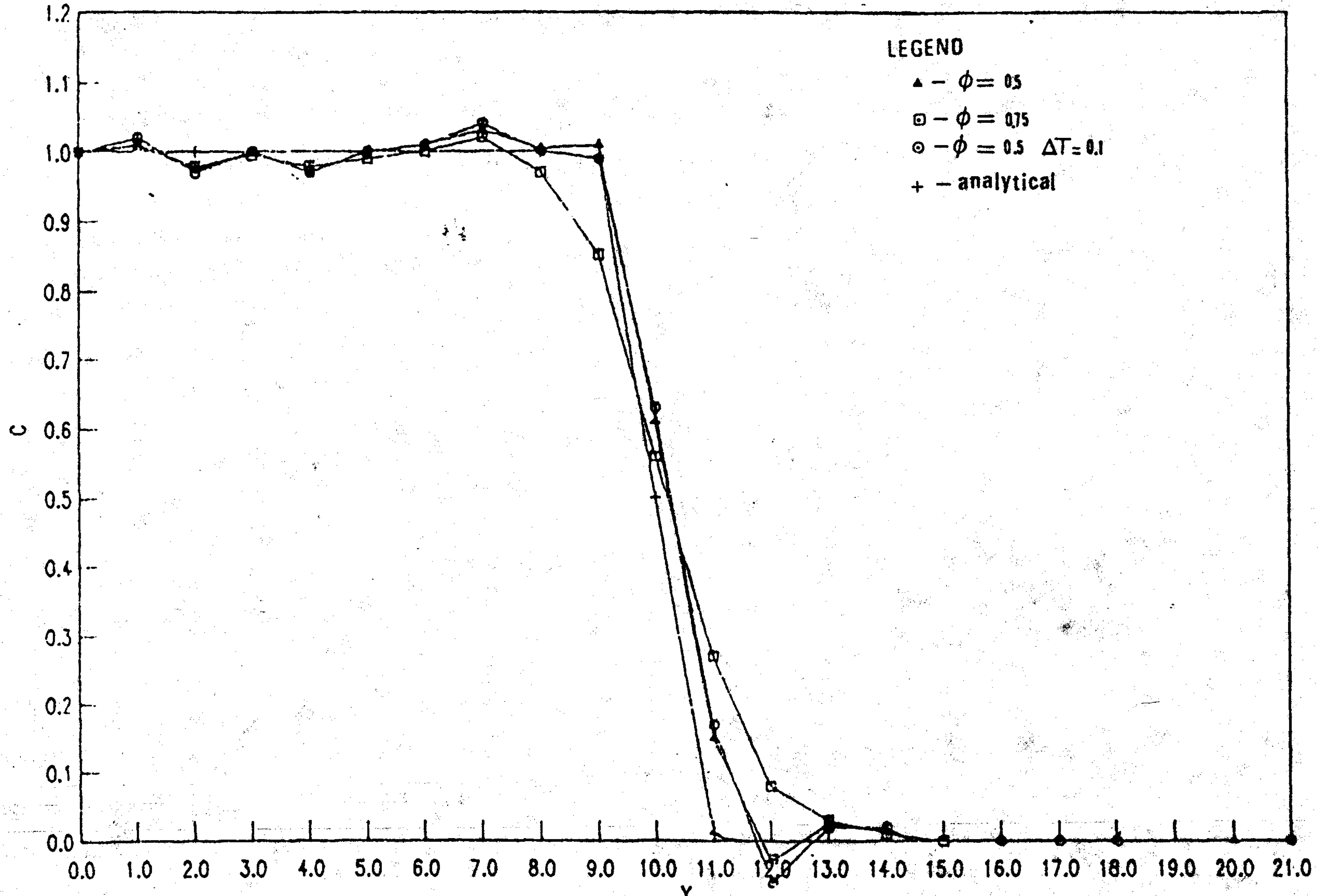

LEGEND
▲ – φ = 0.5
⊡ – φ = 0.75
⊙ – φ = 1.0
+ – analytical
C
X
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0

Figure 7

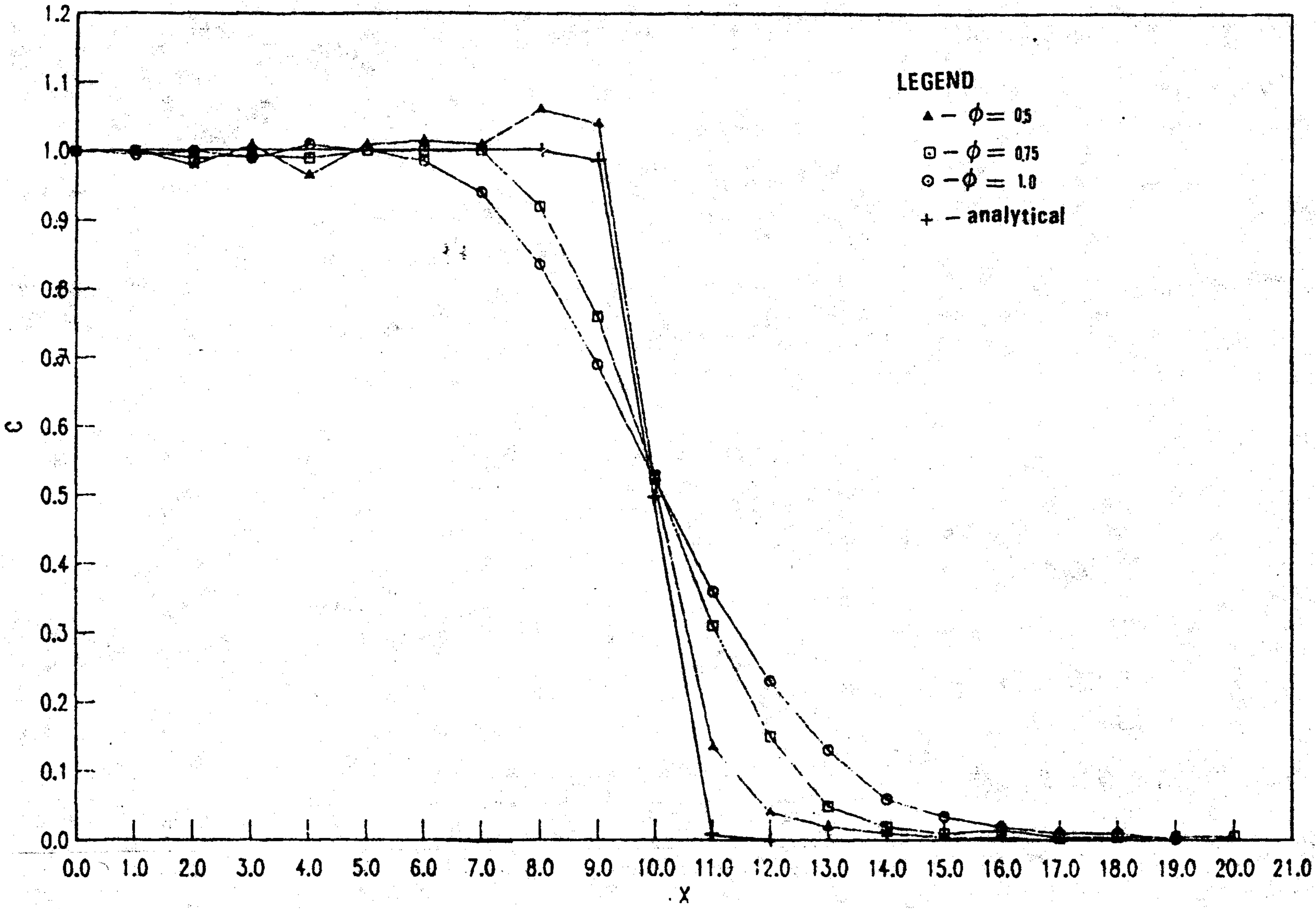
Figure 8. Longitudinal dispersion in uniform one-dimensional flow, $P_e = 100.0$, $Cu = 0.25$.



1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
C
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
X
LEGEND
▲ – φ = 0.5
⊡ – φ = 0.75
⊙ – φ = 0.5 ΔT = 0.1
+ – analytical

Figure 8

Figure 9. Longitudinal dispersion in uniform one-dimensional flow, $P_e = 100.0$, $Cu = 0.5$.



LEGEND
▲ – ϕ = 0.5
□ – ϕ = 0.75
○ – ϕ = 1.0
+ – analytical
C
X
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0

Figure 9

Figure 10. Longitudinal dispersion in uniform one-dimensional flow, $P_e = 100.0$, $Cu = 1.0$.

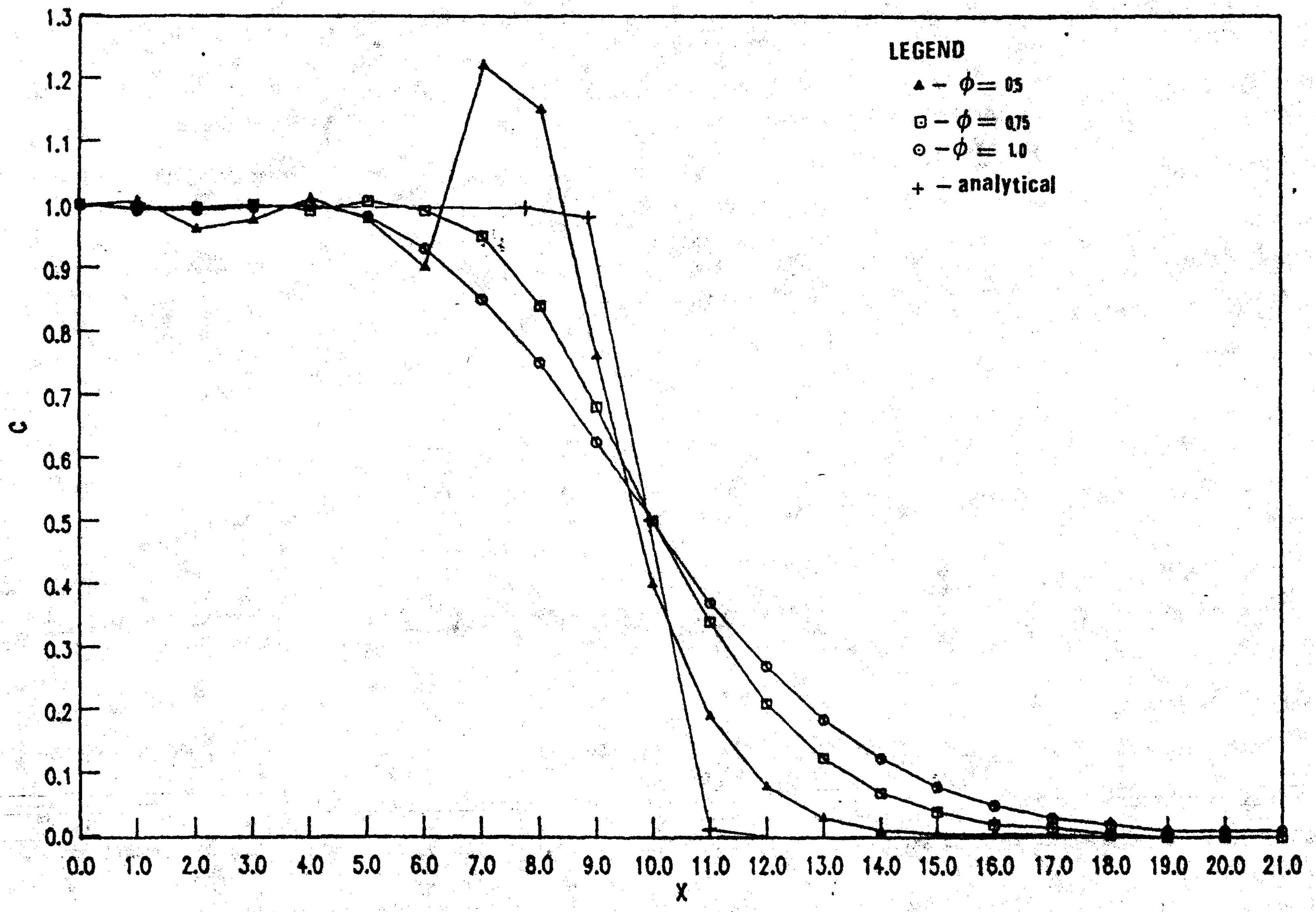

1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
C
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
X
LEGEND
▲ – $\phi = 0.5$
□ – $\phi = 0.75$
⊙ – $\phi = 1.0$
\+ – analytical

Figure 10

Figure 11. Longitudinal dispersion in uniform one-dimensional flow, $P_e = 100.0$, $Cu = 2.0$.

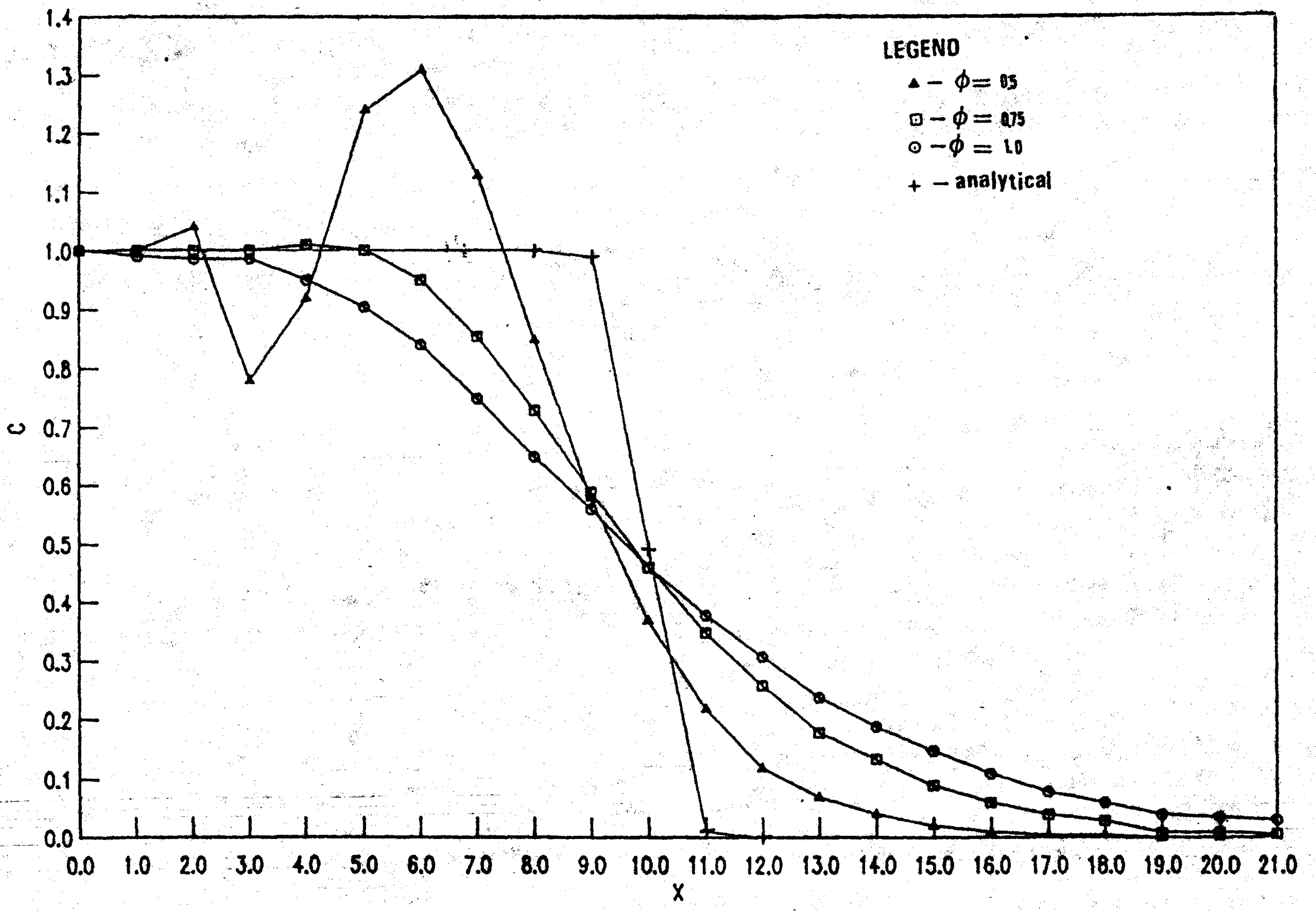

LEGEND
▲ – φ = 0.5
⊡ – φ = 0.75
⊙ – φ = 1.0
+ – analytical
C
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
X
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0

Figure 11

Figure 12. Longitudinal dispersion in uniform one-dimensional flow, $P_e = \infty$, Cu = 0.25 and 0.5

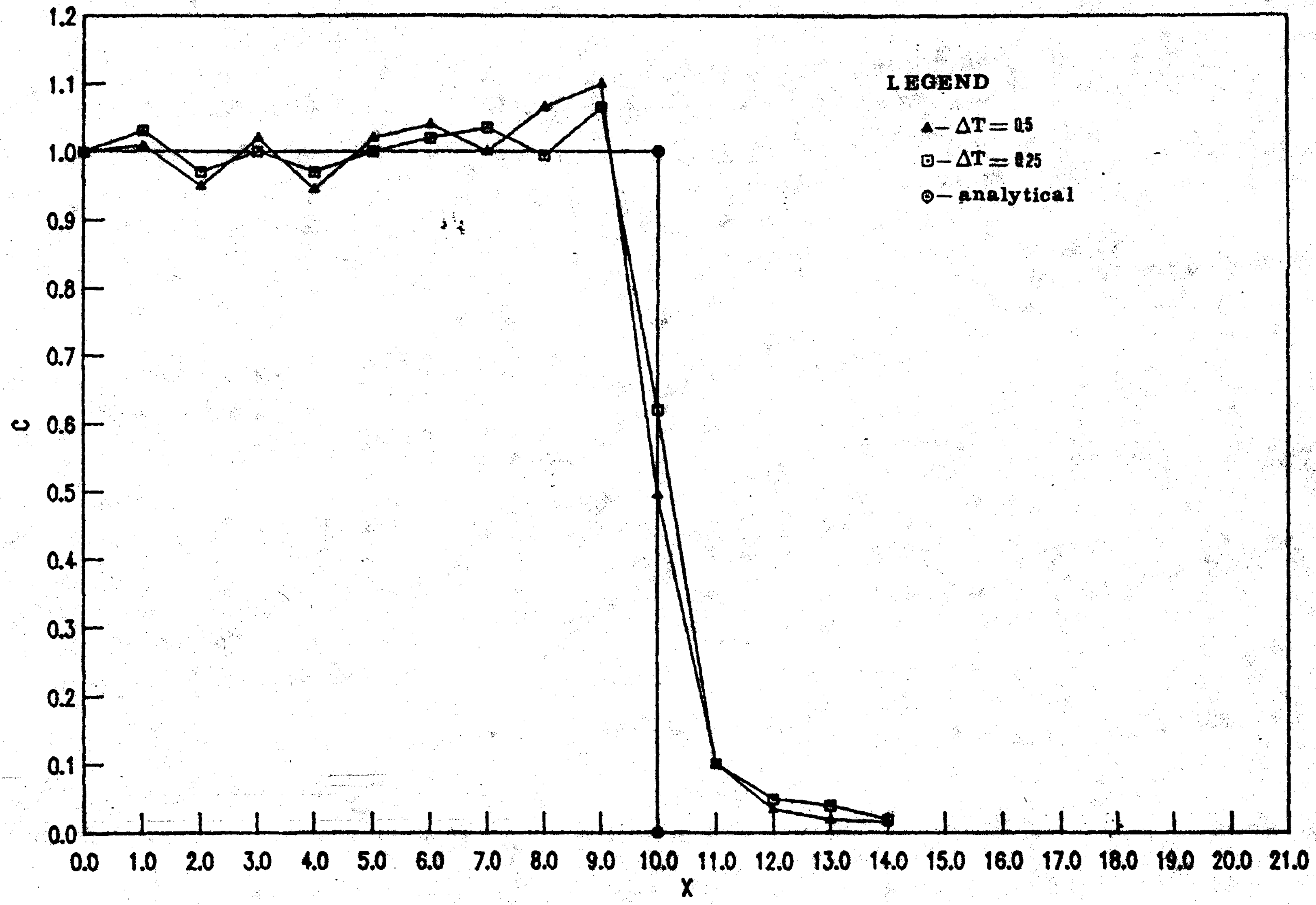

1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
C
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
X
LEGEND
▲– ΔT = 0.5
☐– ΔT = 0.25
⊙– analytical

Figure 12

LONGITUDINAL TRANSIENT DISPERSION WITH THE PRESENCE OF ADSORPTION, RADIOACTIVE DECAY AND SOURCE

The equation of mass transport in semi-infinite column ($x > 0$), with a concentration C_0 maintained at $x = 0$ for time $t > 0$, the flow of solutant maintained at a constant velocity u, and with presence of adsorption, radioactive decay, and source, is given by

$$D_L \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x} - R \frac{\partial c}{\partial t} = \mu c - \gamma \qquad (47)$$

[illegible] μ and γ are ______ as explained in ______.

and initial and boundary conditions

$$c(x,0) = C_i \qquad (48a)$$

$$c(0,t) = C_0 \qquad t > 0 \qquad (48b)$$

$$\frac{\partial c}{\partial t} (\infty,t) = 0 \qquad (48c)$$

The analytical solution for this case is as follows (Van Genuchten, 1981):

$$c(x,t) = (c_0 - \gamma/\mu)\, H(x,t) + M(x,t) \qquad (49)$$

where

$$H(x,t) = \frac{1}{2} \exp\left[\frac{(u - v)x}{2D_L}\right] \operatorname{erfc}\left[\frac{Rx - vt}{2(D_L Rt)^{1/2}}\right]$$

$$+ \frac{1}{2} \exp\left[\frac{(u + v)x}{2D_L}\right] \operatorname{erfc}\left[\frac{Rx + vt}{2(D_L Rt)^{1/2}}\right]$$

$$M(x,t) = \left(\frac{\gamma}{\mu} - C_i\right) \exp\left(-\frac{\mu t}{R}\right) \left\{\frac{1}{2} \operatorname{erfc}\left[\frac{Rx - ut}{2(D_L Rt)^{1/2}}\right]\right.$$

$$\left. + \frac{1}{2} \exp\left(\frac{ux}{D_L}\right) \operatorname{erfc}\left[\frac{Rx + ut}{2(D_L Rt)^{1/2}}\right]\right\} + \frac{\gamma}{\mu}$$

$$+ \left(C_i - \frac{\gamma}{\mu}\right) \exp\left(-\frac{\mu t}{R}\right) \tag{50}$$

and where

$$v = u(1 + 4\mu D_L/u^2)^{1/2} \tag{51}$$

The finite element grid is shown in Figure 3. The numerical results for the ~~data~~ dimensionless data: $\Delta x = 1.0$, $R = 10.0$, $\mu = 1$, $\gamma = 0.12$, $u = 1.0$, $D_L = 0.1$, $t = 100.0$ are shown in Figure 13. The results show very good agreement with the analytical solution. show how the equation was made dimensionless. is $\Delta X = \frac{\Delta x}{L}$ what's L? etc.

[illegible] what Pe & Cu are [illegible].

TWO-DIMENSIONAL MASS TRANSPORT

For a solutant which flows with constant pore water velocity u in semi-infinite column ($x > 0$, $0 < y < 2b$) of homogeneous porous media, the dispersion equation for the steady-state case is given by:

$$D_L \frac{\partial^2 c}{\partial x^2} + D_T \frac{\partial^2 c}{\partial y^2} - u \frac{\partial c}{\partial x} = 0 \tag{52}$$

Boundary conditions are given by (Fig. 14).

$$c(0,y) = c_0 \qquad 0 < y < 2b$$

$$c(0,y) = 0 \qquad \overset{0}{\boxed{b}} < y < 2b$$

$$\frac{\partial c}{\partial y}(x,0) = 0 \qquad x > 0 \tag{53}$$

$$\frac{\partial c}{\partial y}(x,2b) = 0 \qquad x > 0$$

$$c(\infty,y) = \text{bounded} \qquad 0 < y < 2b$$

For the assumption $D_L = 0$, the approximate analytical solution is given by:

[illegible] $D_L = 0$ makes (52) a 1-D eq. . Then why call it 2-D

$$\frac{c}{c_0} = \frac{1}{2}\,\mathrm{erfc}\left(\frac{y-b}{2(D_T x/u)^{1/2}}\right) \tag{54}$$

The finite element grid used for this problem is shown in Figure 15. The comparison of the numerical and analytical results for $u = 0.1$ and $D_T = 0.001$ is presented in Figure ~~15~~ 16. The numerical results show satisfactory agreement with the approximate analytical solution, thus proving the capability of the presented numerical method to simulate two-dimensional problems.

Figure 13. Longitudinal dispersion with the presence of adsorption, source and decay.

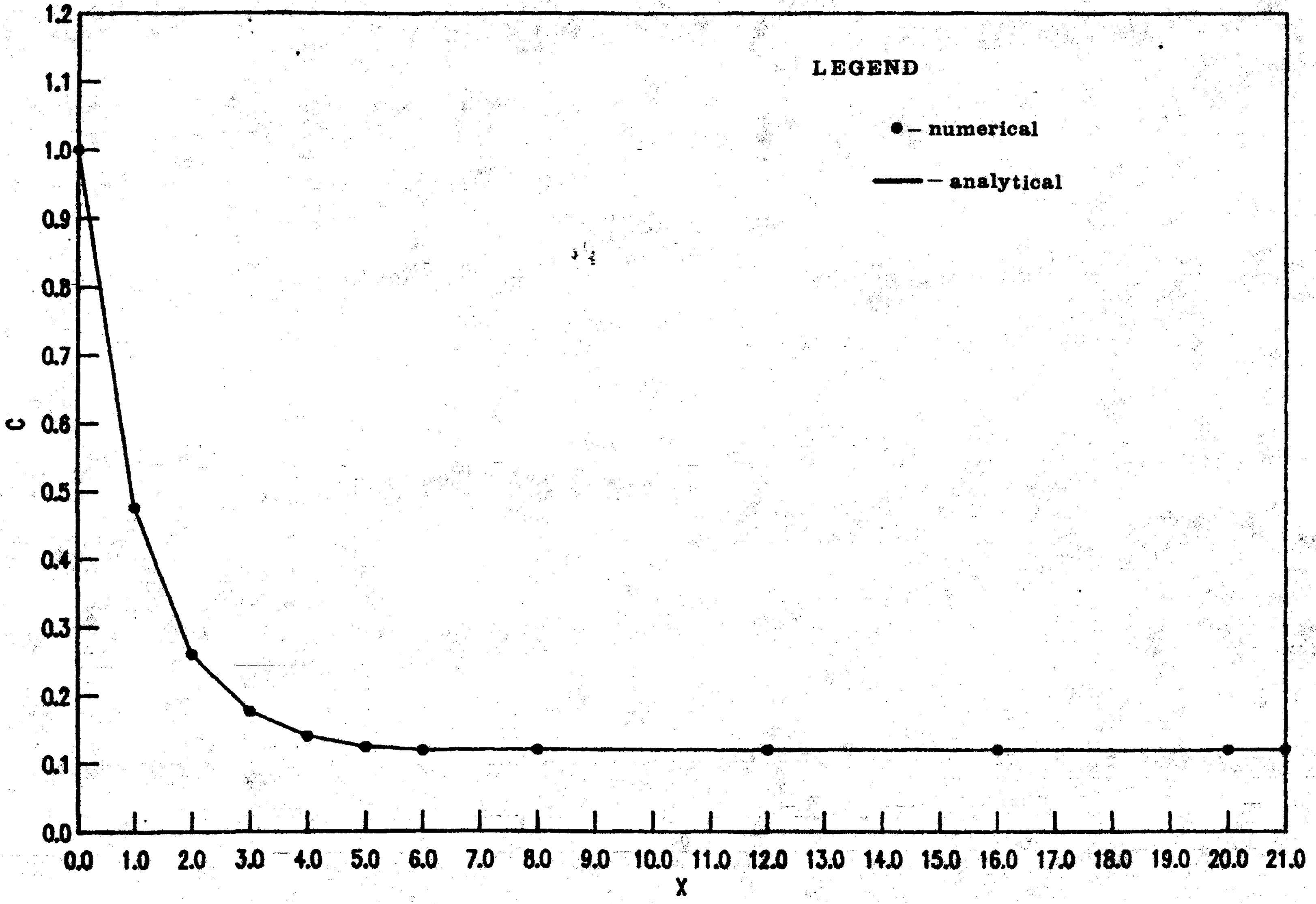

1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
C
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
X
LEGEND
● – numerical
— – analytical

Figure 13

Figure 14. Boundary conditions for two-dimensional mass transport.

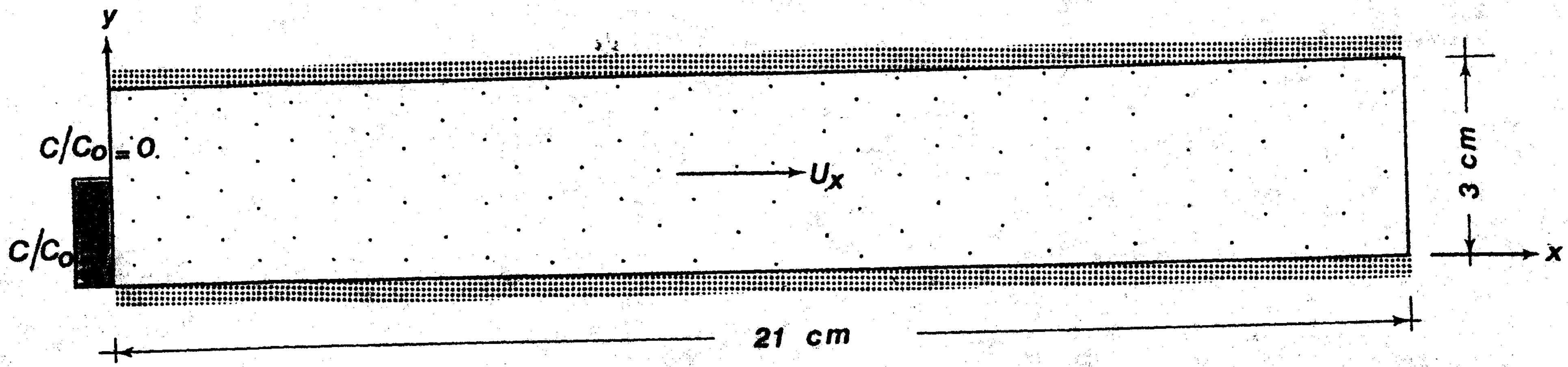
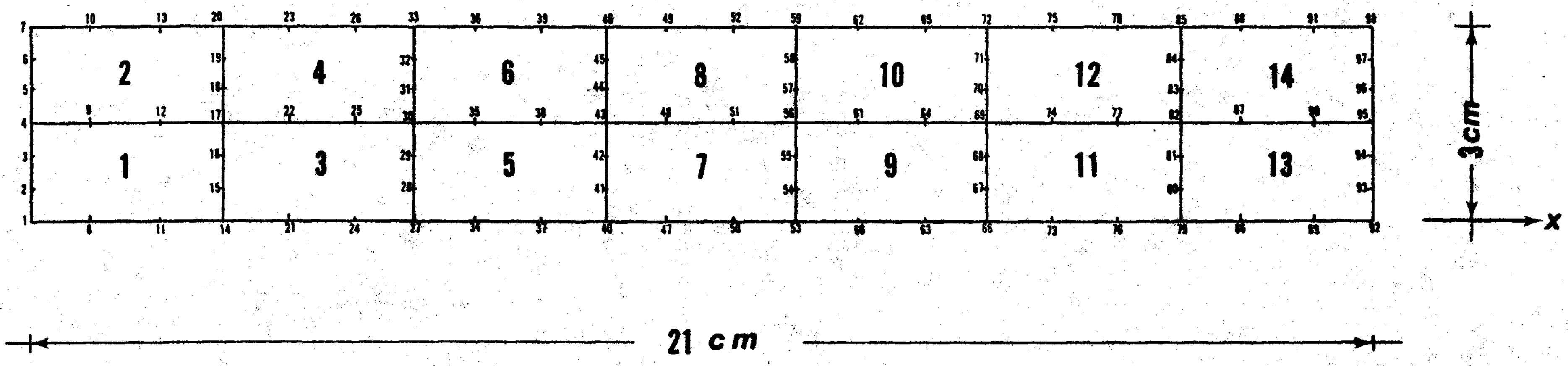


Figure 14

Figure 15. Finite element network for two-dimensional mass transport.



7
6
5
4
3
2
1
10 13 20 23 26 33 36 39 46 49 52 59 62 65 72 75 78 85 88 91 98
19 32 45 58 71 84 97
2 4 6 8 10 12 14
18 31 44 57 70 83 96
9 12 17 22 25 30 35 38 43 48 51 56 61 64 69 74 77 82 87 90 95
16 29 42 55 68 81 94
1 3 5 7 9 11 13
15 28 41 54 67 80 93
8 11 14 21 24 27 34 37 40 47 50 53 60 63 66 73 76 79 86 89 92
3cm
x
21 cm

Figure 15

is this correct?

Figure 16. Steady-state solution of two-dimensional mass transport.

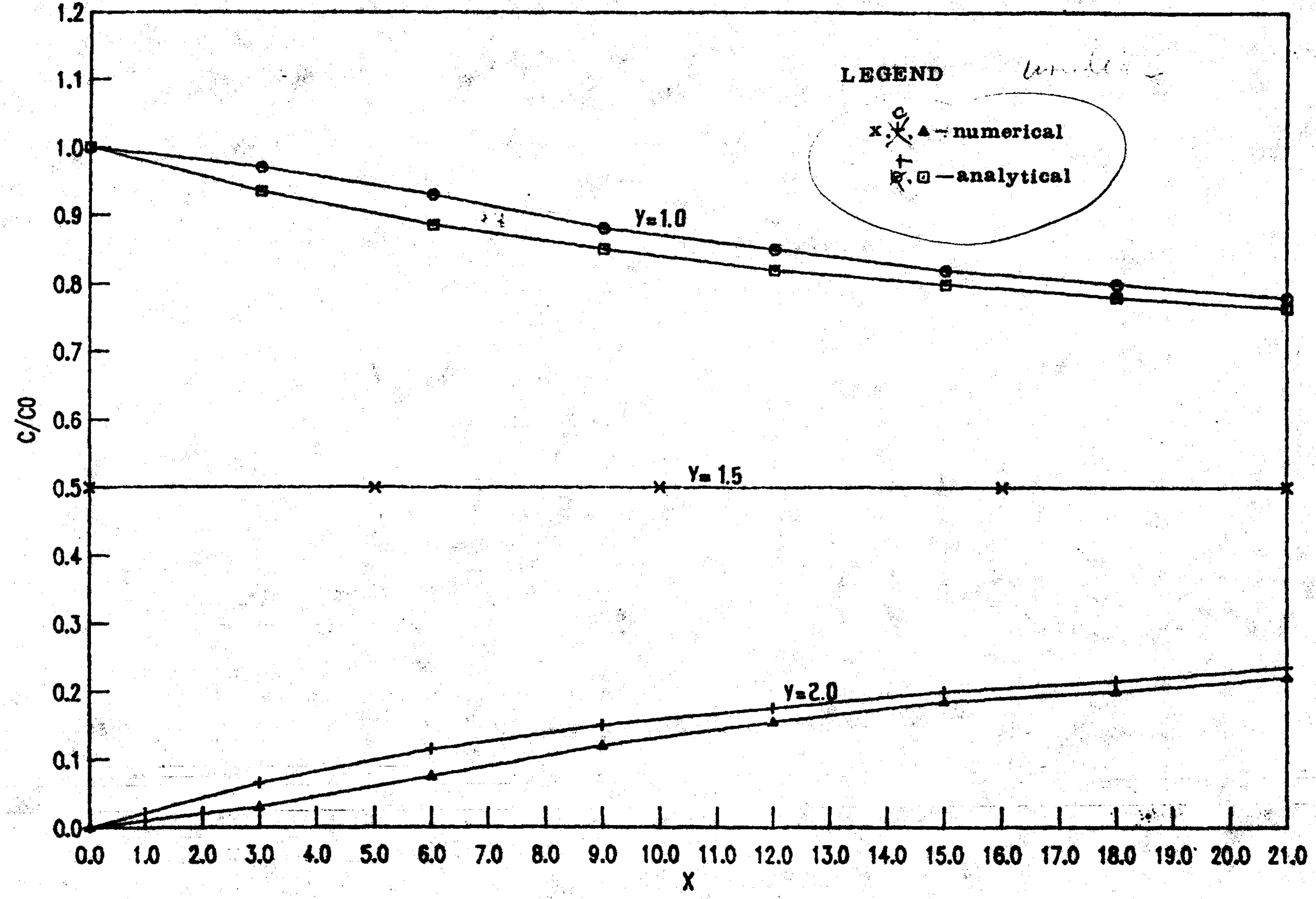

1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
C/C0
LEGEND
x, ✕, ▲ – numerical
⊙, ⊡ – analytical
Y=1.0
Y= 1.5
Y=2.0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
X

Figure 16

RADIAL DISPERSION FROM AN INJECTION WELL

In this problem we consider an injection well, which is pumping water into an aquifer. After reaching the steady state condition of groundwater flow the solutant with the concentration c_o is injected from the time t_o on. Assuming injection rate Q_o, the pore water velocity may be computed as follows:

$$u = \frac{Q_o}{2\pi nbr} = \frac{A}{r} \qquad \text{A is just a constant?} \tag{55}$$

The data used for this example are: $Q_o = 1.256 \times 10^5$ m^3/day, $b = 10$ m; $n = .2$; $\alpha_L = 50$ m; and $\alpha_T = 0$. The partial differential equation of radial mass transport may be written in cylindrical coordinates as follows (source):

$$\alpha_L \frac{A}{r} \frac{\partial^2 c}{\partial r^2} - \frac{A}{r} \frac{\partial c}{\partial r} = \frac{\partial c}{\partial t} \tag{56}$$

The analytical solution of this problem is given by (Gelhar and Collins, 1971):

$$\frac{c}{C_o}(r,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{r^2 - r^{*2}}{\left(16\alpha_L \dfrac{r^3 - r_w^3}{3}\right)^{1/2}}\right] \tag{57}$$

in which r_w is the injection well radius and r^* is calculated according to the equation

$$t = \frac{r^{*2} - r_w^2}{2A} \tag{58}$$

The results from the numerical simulation and analytical solution after 50 days of tracer injection are shown in Figure 17.

HYPOTHETICAL EXAMPLE OF WASTE DISPOSAL

In this section the simulation of groundwater contamination as a result of leakage from hypothetical waste disposal is presented (Fig. 18). The waste disposal's size is 50 by 50 m and it is leaking at the rate $W = 1.8 \times 10^{-8}$ m/sec. The concentration of Chloride? tracer in the leaking solutant is assumed either 20000 mg/l or 40000 mg/l. The waste disposal is underlaid by a homogeneous and isotropic fresh water aquifer, which has the uniform pore water velocity in x direction $u_x = 10^{-4}$ m/Sec (or 8.64 m/day), saturated thickness $b = 10$ m, effective porosity $n = 0.2$, longitudinal dispersivity $\alpha_L = 100$ m, and transverse dispersivity $\alpha_T = 50$ m. It is assumed that the groundwater flow pattern is not affected by leakage from the disposal site.

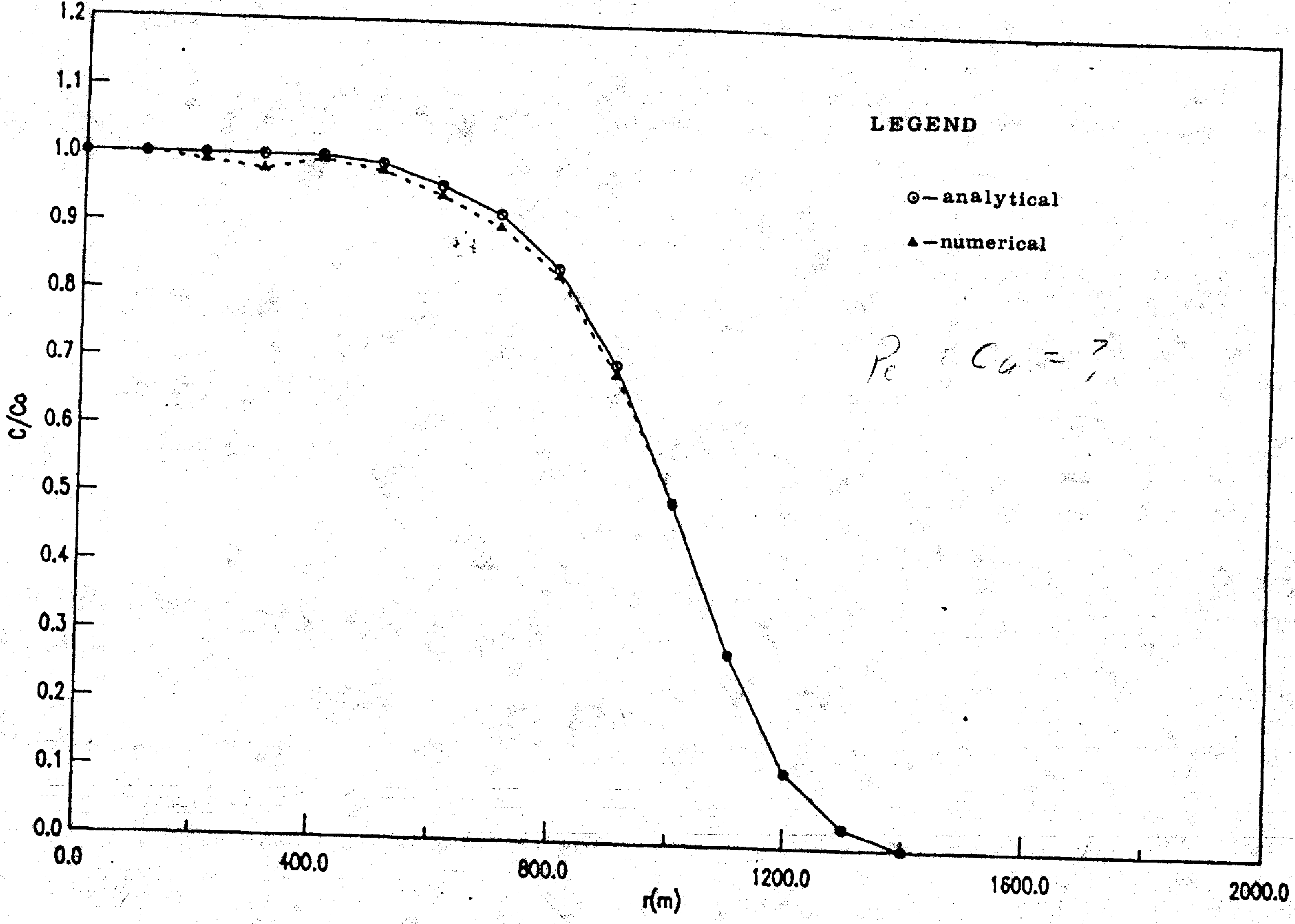
The mass transport equation for this case is given by

$$\frac{\partial c}{\partial t} = \alpha_L u \frac{\partial^2 c}{\partial x^2} + \alpha_T u \frac{\partial^2 c}{\partial y^2} - u \frac{\partial c}{\partial x} - \Upsilon \qquad (59)$$

where $\Upsilon = \frac{Wc'}{nb}$

Where c' is?

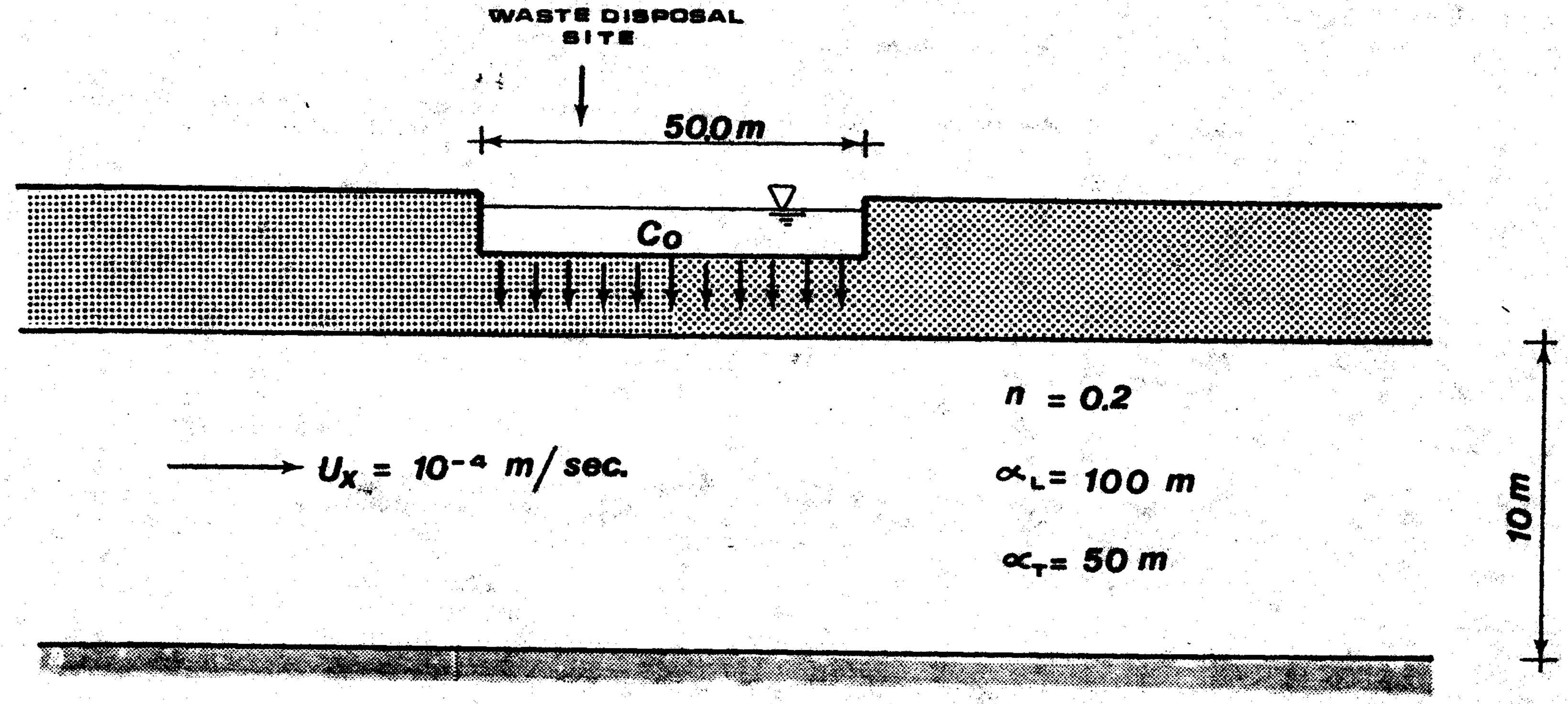
Figure 17. Radial dispersion from an injection well.



Pe ; Co = ?

Figure 17

Figure 18. Hydrologic conditions of groundwater contamination caused by leakage from the waste disposal site.


WASTE DISPOSAL SITE
500 m
C_0
$U_x = 10^{-4}$ m/sec.
$n = 0.2$
$\alpha_L = 100$ m
$\alpha_T = 50$ m
10 m

Fi ju

Figure 19. Finite element network for simulation of aquifer contamination.

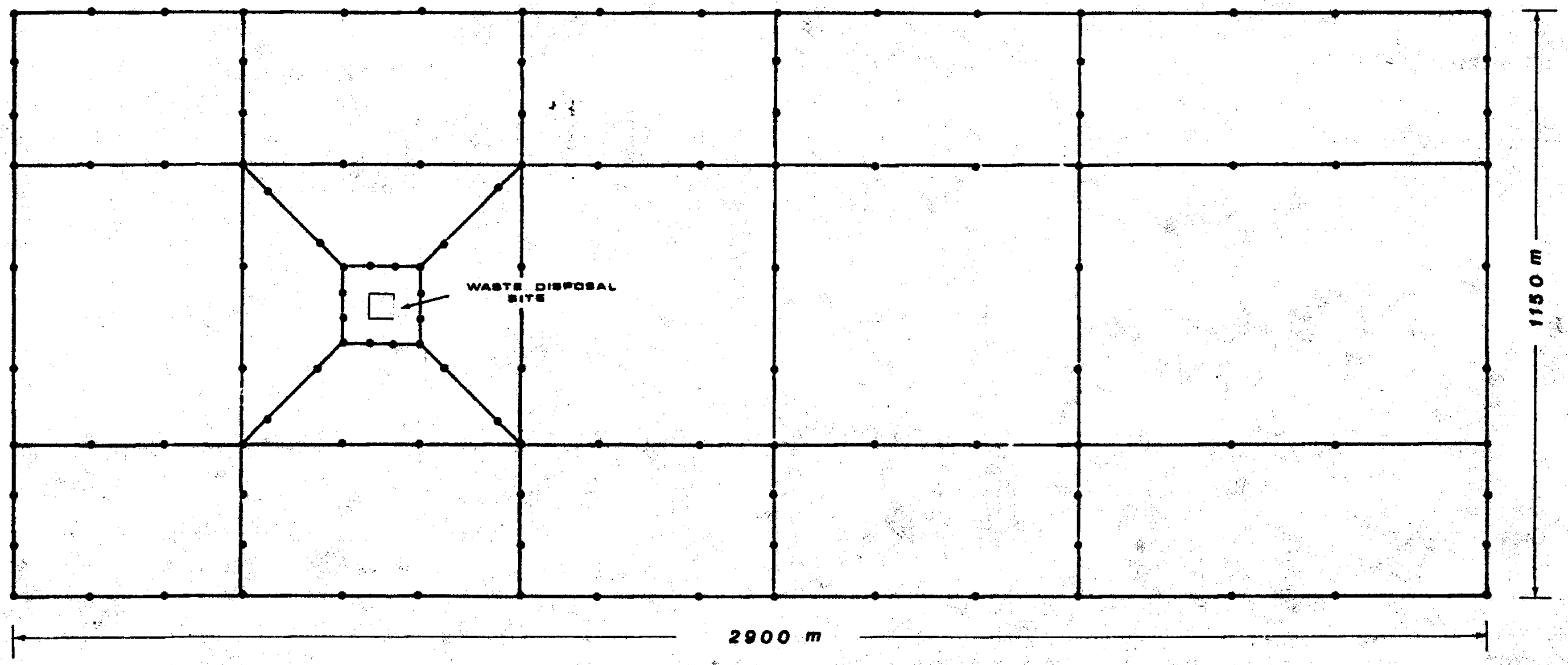


Figure 19

Figure 20. Chloride concentration ~~at~~ in the aquifer at the time t = 578.7 days; brine concentration c_0= 20000 mg/l.

If you use at that means just at the upper surface of the aquifer. Aren't these results averaged in the z direction?

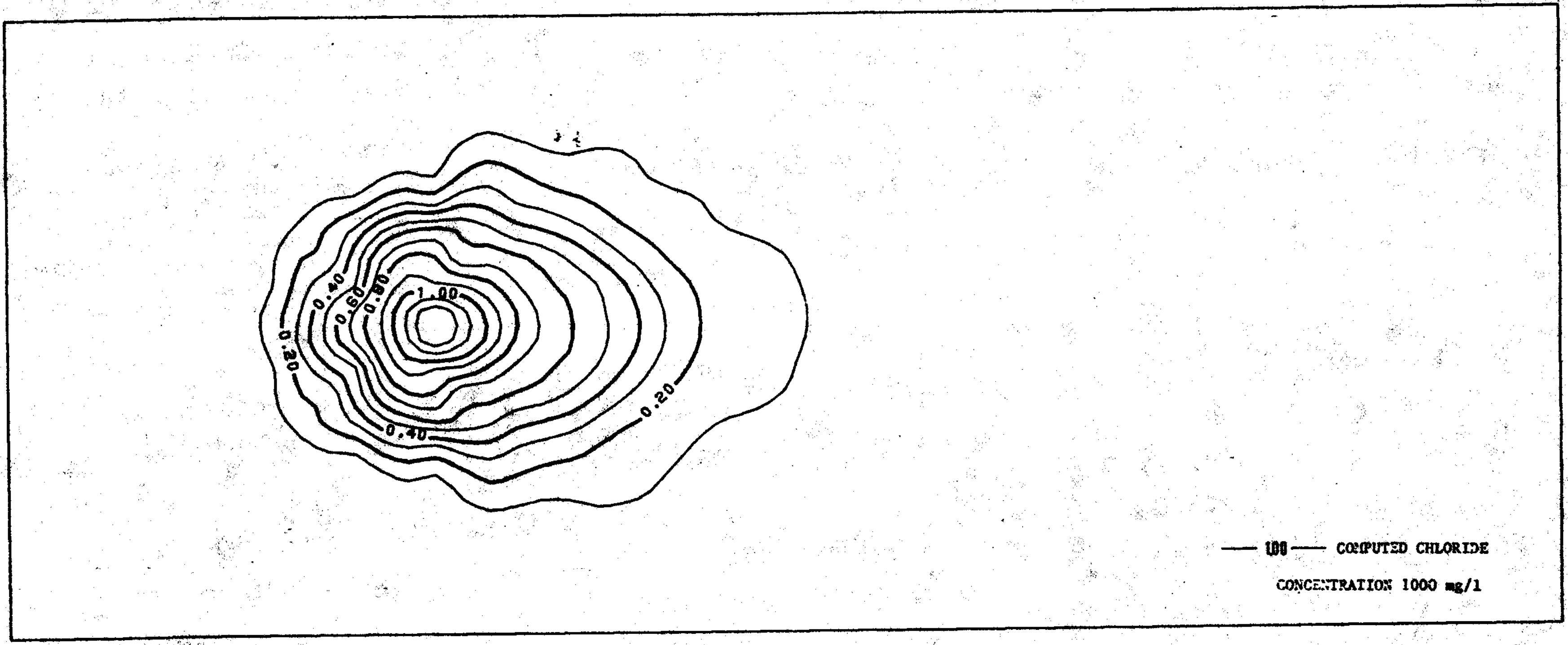

0.40
0.60
0.80
1.00
0.20
0.40
0.20
100 COMPUTED CHLORIDE
CONCENTRATION 1000 mg/l

Figure 20

Figure 21. Chloride concentration ~~at~~ in the aquifer at the time t = 1157.4 days; brine concentration c_0 = 20000 mg/l.

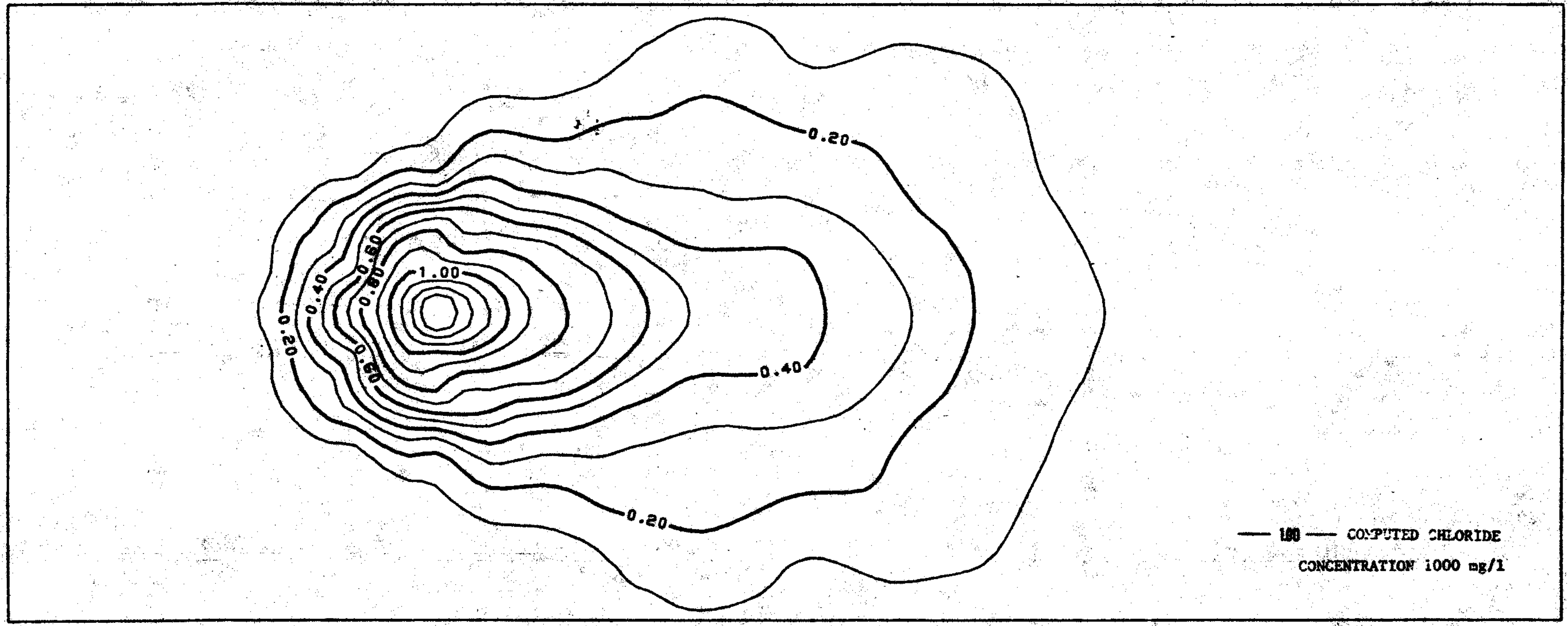

0.20
0.60
0.40
0.80
1.00
0.20
0.60
0.40
0.20
— 100 — COMPUTED CHLORIDE
CONCENTRATION 1000 mg/1

Figure 21

Figure 22. Chloride concentration ~~at~~ in the aquifer at the time $t = 578.7$ days; brine concentration $c_0 = 40000$ mg/l.

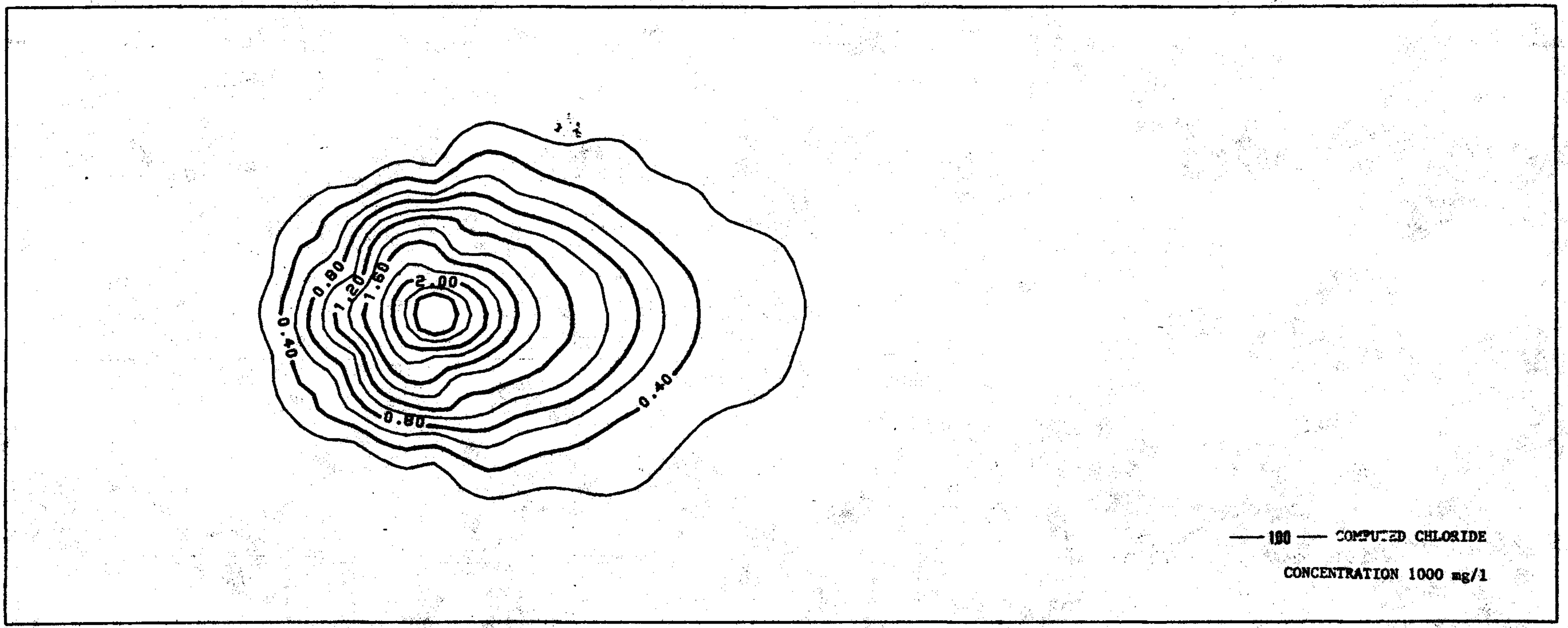

0.40
0.80
1.20
1.60
2.00
0.80
0.40
—100— COMPUTED CHLORIDE
CONCENTRATION 1000 mg/l

Figure 22

Figure 23. Chloride concentration ~~at~~ in the aquifer at the time t = 1157.4 days; brine concentration c = ~~2~~40000 mg/l.

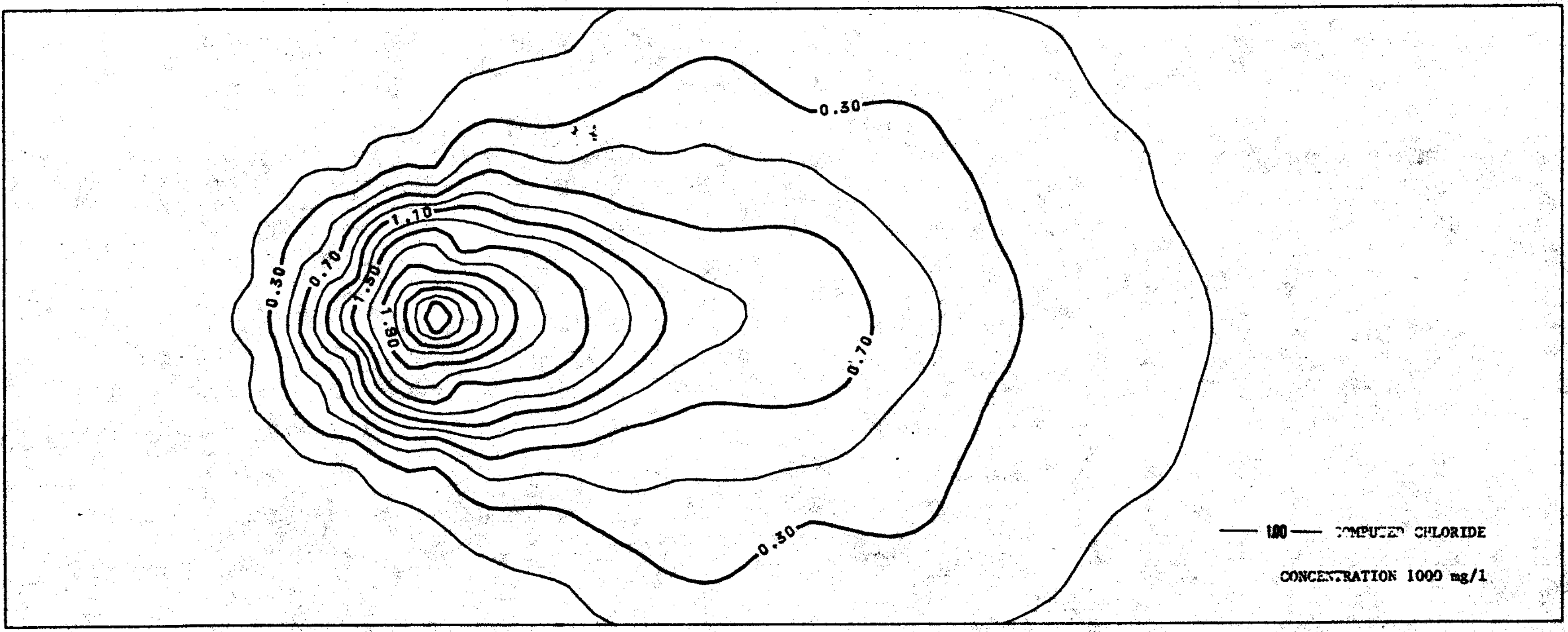

0.30
0.70
1.10
1.50
1.90
0.30
0.70
0.30
— 100 — COMPUTED CHLORIDE
CONCENTRATION 1000 mg/1

Figure 23

The finite element grid is depicted in Figure 19. The results of numerical calculations are shown in Figures 20-23. Figures 20 and 21 show the concentration distribution for assumed leachate concentration c' = 20000 mg/l at the times $t_1 = 5\overset{\times}{(.)}10^7$ sec (578.7 day) and $t_2 = 10^8$ sec (1157.40 day), respectively. The results shown in Figures 22 and 23 were obtained for doubled leachate concentration c' = 40000 mg/l and times $t_1 = \overset{.5\times10^7}{\boxed{5.}10^7}$ sec and $t_2 = 10^8$ sec, respectively.

For all above example a listing of CPU and other relevant information are required

CONCLUSIONS

The model presented in this report can simulate the two-dimensional mass transport of reactive solute in flowing groundwater. The program is general and flexible in that it can be directly applied to a wide range of types of problems, as defined by aquifer properties, chemical and physical reactions, boundary conditions and stresses. However, some program modifications may be required for application to specific field problems and conditions.

The accuracy of the numerical results can be evaluated by comparison with analytical solutions only for relatively simple problems; in these cases there is good agreement between the numerical and analytical results. The accuracy of the numerical simulation is dependent on the numerical Peclet number, Courant number and time integration weighting factor. The analysis of their influence is presented in an earlier section. These parameters should be carefully examined when solving field problems.

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