Ch.8 Numerical Modeling

Contents

Objectives

8.1 River and Estuary Models

8.1.1 Considerations in Choosing a Model

Table 8.1 Types of Transport Models

Code	Name	Description
1A	One-dimensional tidally averaged	A numerical solution of 1-D tidally averaged dispersion equation [Eq. (7.38)] ①steady state model: coefficients are constant in time. ② unsteady model: flow parameters and dispersion coefficient vary between tidal cycles.
1T	One-dimensional tidally varying	A numerical solution of Eq. (7. 46) Tidal evaluation, velocity and dispersion coefficient vary during tidal cycle.
1TB	Branching 1-D tidally averaged	A network of 1T models connected at junctions.
2VA 2HA	Two-dimensional tidally averaged	A numerical solution of 2-D tidally averaged dispersion equation. 2V : horizontally averaged model 2H : vertically averaged model
2VT 2HT	Two-dimensional tidally varying	A numerical solution of 2-D tidally varying dispersion equation
3A	Three-dimensional tidally averaged	A numerical solution of 3-D tidally averaged dispersion equation
3T	Three-dimensional tidally varying	A numerical solution of 3-D tidally varying dispersion equation
P	Physical model	A small-scale physical replica of the prototype geometry with provisions of generating tidal and river flows

NP	Hybrid numerical physical	A combination of a physical and a numerical model, using one model to generate input information for the other

◎ Dispersion mechanisms to be replicated by models

Mixing mechanism	Appropriate Model	Description
Trapping	2HT physical model	Well verified for simulation of trapping mechanism
	1TB	Branches represent traps.
Density-driven circulation	2VA 2VT	In case transverse gravitational circulation is not important.
	3A 3T	If density-driven currents are important, the equations determining the flow and the salinity distribution are coupled.
Tidal pumping	2HT physical model	Accuracy of 2HT may be difficult to establish.
Shear flow dispersion	2HT 2VT	
Wind effects	2HT 3T	Fig. 8.1
Rotational effects	2HT	Easily modeled in 2HT models.
Catastrophic/ seasonal changes	1A physical model	Long term simulation for a period of a year of more

8.1.2 Numerical Models

8.1.2.1 One-Dimensional Models

• 1-D model is accurate in any case where the time scale of the process being studied is substantially greater than the time scale for cross sectional mixing

→ In practical use of 1-D models, instantaneous complete cross sectional mixing is assumed.

(1) Finite Difference Models

• 1A (tidally averaged model)

$$A\frac{\partial C}{\partial t} + Q_f\frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(KA\frac{\partial C}{\partial x}\right) + \text{source/sink} \qquad (7.\ 38)$$

• 1T (tidally varying model)

$$\frac{\partial}{\partial t}(AC) + \frac{\partial}{\partial x}(\bar{u}AC) = \frac{\partial}{\partial x}\left(K_t A\frac{\partial C}{\partial x}\right) + \text{source/sink} \qquad (7.\ 46)$$

• Numerical solution of 1-D Eq. of motion

→ method of characteristics solution by Streeter and Wylie (1967)

• Finite-difference representation of derivatives

(i) Explicit technique

- all the derivatives are expressed in terms of known values

  (values of C at time level n)

- easier to program

① backward difference operator

$$\frac{\partial C}{\partial x} \approx \frac{C_{j,n} - C_{j-1,n}}{\Delta x} \tag{8.1}$$

② forward difference operator

$$\frac{\partial C}{\partial x} \approx \frac{C_{j+1,n} - C_{j,n}}{\Delta x} \tag{8.2}$$

③ central difference operator

$$\frac{\partial C}{\partial x} \approx \frac{C_{j+1,n} - C_{j-1,n}}{2\Delta x} \tag{8.3}$$

(ii) Implicit technique

- use some of unknown values of *C* at time level $n+1$

- a set of simultaneous equations must be solved to obtain all the values at the new time level at the same time

- implicit schemes are more stable and a longer time step can be used.

• central difference operator

$$\frac{\partial C}{\partial x} \approx \frac{1}{2}\left[\frac{C_{j+1,n+1} - C_{j-1,n+1}}{2\Delta x} + \frac{C_{j+1,n} - C_{j-1,n}}{2\Delta x}\right] \tag{8.4}$$

○ Numerical diffusion

· Most numerical schemes induce unwanted numerical spreading

· Numerical diffusion is an apparent diffusivity caused by the numerical process.

· Numerical diffusion in Pure Advection Problem

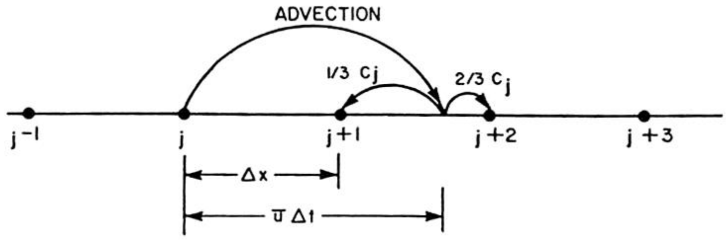


Figure 8.2 An illustration of the origin of numerical diffusion in a simple model, showing the case where $\bar{u}\Delta t/\Delta x = 1\frac{2}{3}$. The mass originating at point j is proportioned $\frac{2}{3}$ to point $j + 2$ and $\frac{1}{3}$ to point $j + 1$.

① The mass represented by the concentration at a grid point is advected forward during a time step a distance $\bar{u}\Delta t / \Delta x$ grid points.

② Then, mass is divided between the two nearest grid points proportionally according to the distance from each.

③ Division between the grid points is necessary because the numerical scheme has no way of representing a concentration except at grid point.

④ A mass originally concentrated at one point is now spread numerically two points.

• Variance at the end of time step

$$\sigma^2 == \int_{-\infty}^{\infty} (x-\bar{x})^2 c dx = \left(\frac{2}{3}\Delta x\right)^2 \left(\frac{1}{3}\right) + \left(\frac{1}{3}\Delta x\right)^2 \left(\frac{2}{3}\right) = \frac{2}{9}\left(\Delta x\right)^2$$

$$K' = \frac{1}{2} d\sigma^2 / dt = \frac{1}{2}\left[\frac{2}{9}\left(\Delta x\right)^2 - 0\right] / \Delta x = \frac{1}{9}\frac{\Delta x^2}{\Delta t}$$

→ numerical diffusivity

○ How to control numerical diffusion

i) The numerical diffusion represented by K' must be kept much smaller than the actual (real) dispersion represented by K.

ii) Bella and Grenny (1970) suggested that if the K' is forecast accurately and K' is less than K, the value of K can be reduced accordingly.

$$K_{new} = K - K'$$

• K' can be estimated by setting $K = 0$ in the numerical program and observing the results.

iii) Higher order scheme by Stone and Brian (1963)

- spread form forward difference for time derivative

$$\left.\frac{\partial C}{\partial t}\right|_{x=j} = \left[\frac{1}{6}\left(C_{j-1,n+1} - C_{j-1,n}\right) + \frac{2}{3}\left(C_{j,n+1} - C_{j,n}\right) + \frac{1}{6}\left(C_{j+1,n+1} - C_{j+1,n}\right)\right] / \Delta t \tag{8.6}$$

- Crank -Nicholson approximation for diffusive term

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{1}{2}\left[\frac{C_{j+1,n+1} - 2C_{j,n+1} + C_{j-1,n+1}}{\Delta x^2} + \frac{C_{j+1,n} - 2C_{j,n} + C_{j-1,n}}{\Delta x^2}\right] \tag{8.7}$$

• This scheme is the most accurate for the problems for which the diffusion coefficient is relatively small.

• Stone and Brian's method can be used equally well for a tidally averaged or a tidally varying analysis.

8.1.2.2 Multidimensional Models

• In multidimensional models, it is mostly important to understand and express properly physics of flow and exchange.

• The mixing coefficients used in the numerical models express the net results of all processes whose scale is less than the grid size of the model.

• In river and estuary models, turbulent mixing is smaller than the mixing caused by the skewed shear flow of the velocity profile (Fig. 4.8)

• For numerical models which are averaged over at least one spatial dimension, over the tidal cycle, or over both, the mixing coefficient represents what has been averaged.

◎ Two-dimensional models

- in section models : horizontally averaged
- in plan models : vertically averaged

- 2HA : tidally averaged model
- 2HT : tidally varying model

◎ 2HA models

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}+V\frac{\partial C}{\partial y}=\frac{1}{d}\left[\frac{\partial}{\partial x}\left(dK_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(dK_y\frac{\partial C}{\partial y}\right)\right] \tag{8.11}$$

where $\partial/\partial t$ means a change per tidal cycle ; U , V are tidal averages of the vertical averaged x- and y- direction velocities ; d is the local depth; K_x, K_y express the results of all the mechanisms (shear flow mixing, pumping, trapping) that cause mixing within a tidal cycle

• Terms like $\frac{\partial}{\partial x}\left(dK_{xy}\frac{\partial C}{\partial y}\right)$ ought to be included, but usually not because it is difficult to evaluate K_{xy} and K_{yx}.

• 2HA models should be used only in conjunction with extensive field data to define the magnitude of the dispersion coefficients.

◎ 2HT models

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}+V\frac{\partial C}{\partial y}=\frac{1}{d}\left[\frac{\partial}{\partial x}\left(dK_{x}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(dK_{y}\frac{\partial C}{\partial y}\right)\right]$$

• 2HT models are in common use and have the advantage that they represent the important dispersion mechanisms of trapping, pumping, and wind and Coriolis driven circulations.

• 2HT models appear to be practical for smaller bodies of water.

→ Leendertse model (1970) applied to Jamaica Bay

• If coarse spatial grid is used for large water bodies, advantages of replicating the tidal cycle may be lost.

◎ Limitations of 2HT models

① The model should be operated to simulate at least as much real time as is needed to reach an equilibrium distribution of tracer.

<Example> $T_{equil}\approx 100$ days in large estuary

$\Delta t = 1$ min

N (no. of time step) = 144,000

② The water column must not be sufficiently stratified to inhibit vertical mixing.

Ⓐ : $$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}+V\frac{\partial C}{\partial y}=\frac{1}{d}\left[\frac{\partial}{\partial x}\left(dK_{x}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(dK_{y_t}\frac{\partial C}{\partial y}\right)\right]$$

Where $U_t, V_t =$ tidal velocity ; K_{x_t}, K_{y_t} = dispersion coefficient which represent only the effect of the vertical velocity profile. (shear flow dispersion)

$$K_{x_t}, K_{y_t} << K_x, K_y$$

• Bigger mixing by tidal pumping and tidal trapping are now represented by the time-variable advection

i. e., u_t and v_t

③ Since a time-varying flow field must be obtained from a first-stage 2HT flow model, the flow model must produce the complex flows which leads to trapping, pumping, and other dispersion mechanisms.

→ The residual circulations are caused by the nonlinear frictional and inertial terms in the equations of motion.

→ Leendertse's (1967) model included nonlinear friction and inertial terms; however the no-slip boundary condition was not imposed.

→ Tee's (1976) model incorporated the no-slip boundary condition.

→ Tee computed a residual circulation from boundary layer separation

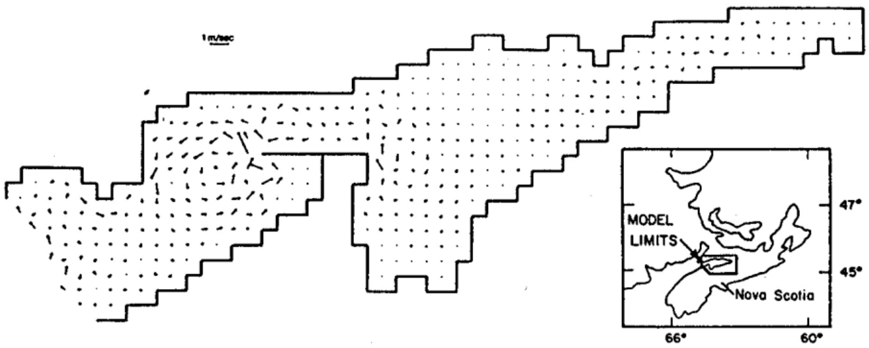


Figure 8.6a The tide-driven residual circulation in the Minas Basin, Nova Scotia, according to Tee's (1976) numerical model. [After Tee (1977).]

8.1.3 Physical models

8.1.3.1 Introduction

• Physical model - physical representation at small scale

• Useful to the engineer, lay public, and political decision maker

◎ Distorted model to contain the model in a building of reasonable size

horizontal scale for river and estuary	1/1000
vertical scale	1/100

typical estuarine depth	5～30 m
model depth	5～30 cm

• Flow would be dominated by viscous and surface tension effects if model depth is less than 5cm.

→ The vertical exaggeration converts a typically wide and shallow cross section into the more canyonlike cross section

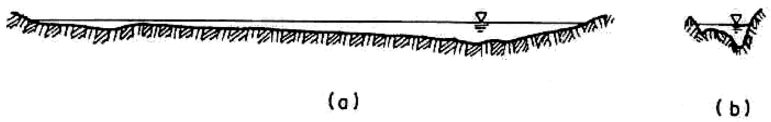


Figure 8.7 (a) A typical estuarine cross section (b) the transformed shape of the same cross section in a 10 to 1 distorted model.

→ The conversion serves the essential purpose of making the model flow turbulent, but it also changes the longitudinal slope of the channels and distorts rates of vertical and transverse mixing.

→ The tendency of the model flow to be too fast, because of the increased slope, must be resisted by adding friction to the channels.

→ The vertical copper strips are arrayed over the entire channel to provide the extra friction needed to counteract the distorted channel and water surface slopes.

→ During the construction process most models are calibrated against prototype observations of tidal elevation and currents in the main channels.

→ These calibrations do not assure that mixing will be modeled correctly.

8.1.3.2 Model Laws and Scaling Ratios

• Fixed bed estuary models

$$L_r = \text{length ratio} = \frac{L_p}{L_m}$$

$$d_r = \text{depth ratio} = \frac{d_p}{d_m}$$

Once the length and depth ratios have been selected, the ratios of all other quantities are established by physical laws.

(1) Froude law

A frictionless small amplitude wave propagates at the correct velocity.

wave velocity $c = \sqrt{gd}$

$$\frac{c_m}{c_p} = \sqrt{\frac{gd_m}{gd_p}} = \sqrt{\frac{d_m}{d_p}}$$

$$c_r = d_r^{1/2} \quad (8.\ 12)$$

time required for wave to propagate a distance L

$$t = L / c$$

$$t_r = \frac{L_r}{c_r} = L_r d_r^{-1/2} \tag{8. 13}$$

velocity ratio, $u_r = L_r / t_r = \frac{L_r}{L_r / c_r} = c_r = d_r^{1/2}$ (8. 14)

Froude number, $F_r = \frac{u_r}{g d_r^{1/2}} = 1$

$$F_r = \frac{\text{inertial force}}{\text{gravitational force}}$$

• The propagation of tidal and flood waves depends on gravitational, inertial, and frictionless forces.

→ Froude law scaling assures the proper ratio of gravitational forces.

→ The copper strips are used to obtain the proper ratio of frictional forces.

• Density stratified flows

- The internal Froude number should be the same in the model and in the prototype to obtain the correct ratio for internal wave velocities.

$$F_i = u \left(\frac{\Delta \rho}{\rho} g d \right)^{-\frac{1}{2}}$$

$$\therefore \left(\frac{\Delta \rho}{\rho} \right)_r = 1$$

• Other important ratios

slope ratio $s_r = d_r / L_r$

width ratio $W_r = L_r$

cross sectional area ratio $A_r = W_r d_r = L_r d_r$

discharge ratio $Q_r = A_r u_r = L_r d_r d_r^{1/2} = L_r d_r^{3/2}$

• Shear velocity ratio

$$u_r^* = (gds)_r^{1/2} = d_r / L_r^{1/2}$$

• Mixing coefficient ratio

$$\varepsilon_r = \sigma_r^2 / t_r$$

$$\varepsilon_{vr} = d_r^2 / t_r = d_r^{5/2} / L_r \qquad (8.15\text{ a})$$

$$\varepsilon_{tr} = L_r^2 / t_r = L_r d_r^{1/2} \qquad (8.15\text{ b})$$

cf) $\varepsilon = \ \propto du^*$

$$\therefore \varepsilon_r = \left(du^*\right)_r = dr^2 / Lr^{1/2} \qquad (8.15\text{ c})$$

Eqs. (8.15 a, b) and (8.15 c) are quite different.

→ The turbulent mixing may not be modeled correctly.

<Example> The model of San Francisco Bay :

$L_r = 1000$ $d_r = 100$

$u_r = 10$ $Q_r = 1{,}000{,}000$

$t_r = 100$ $u_r^* = 3.13$

$$S_r = 1/10 \qquad \left(du^*\right)_r = 313$$

• The model operator controls only the discharge ratio for the tributary inflows, the height ratio and time ratio for the ocean tides, and the salinity ratio in the ocean.

• The actual elevations, currents, and salinities occurring throughout the model are determined by the frictional characteristics of the model channels and the distribution of the copper strips.

8.2 Model Building and Use

8.2.1 Definition of Model

○ What is a model?

Model = a deliberate misrepresentation of reality

(simplification) (real system)

approximation

Reason = convenience

Purpose = understanding (gain understanding)

prediction (predict an outcome)

Constraints = degree of simplification

degree of accuracy

• Real System

↓ Simplification

Conceptual Model = set of assumptions

Physical Model

Mathematical Model = Compact form of a set of equations

Governing Equation (Eq. of mass balance, flux eqs, kinetic eq.)

+ Initial & Boundary conditions

+ Domain Geometry

+ Model Parameters

Analytical model

Numerical model

① irregular shape of the domain's boundaries

② heterogeneity of the domain (coefficient)

③ irregular temporal and spatial distributions of various inputs

④ source and sink

8.2.2 Model Mechanisticity (Karplus (1976))

← Empirical (Black Box)			Air Pollution (Gray Box)		Mechanistic → (White Box)
Social	Econometric Model	Standard Watershed Model	Deterministic Water Quality Model	Process Control	Models of Computers

* Karplus, W.J. (1976) The future of mathematical models of water resources systems.
In "System Simulation in Water Resources", pp11-18 North Holland Publishing Company

~ No model is either completely mechanistic or empirical.

~ All models are somewhere in between.

8.2.3 Modeling Procedure

◎ Models and Parameters

→ Model Parameters exist only in context of model. (Model Coefficients)

◎ Model Calibration = parameter tuning to fit observed data to predicted data.

Model becomes less mechanistic (more empirical)

= Parameter Identification Problem

Inputs (Excitation) → Model (Parameter) → Outputs (Responses)

√	√	?	Prediction Problem (Forecasting)
√	?	√	Parameter Identification (Estimation or Inverse)
?	√	√	Signal Identification

○ Verification

= Establishment of the model validity by comparison between observed and predicted data.

○ Calibration and verification should be done with two separate (different) data sets

○ Procedure of Calibration and Verification

	Data Set I	Data Set II
Input	I_1	I_2
Output	O_1	O_1
Parameter	?	P

(i) Calibration

$I_1 \rightarrow$ [Model(?)] $\rightarrow \tilde{O}_1$

Fit $\tilde{O}_1$ to O_1

Find P (set of values of parameters (coefficients))

(ii) Verification

$I_2 \rightarrow$ [Model (P)] $\rightarrow \tilde{O}_2$

Predict $\tilde{O}_2$ with calibrated parameter P

Compare $\tilde{O}_2$ to O_2 to see if $\tilde{O}_2 = O_2$

◎ Dimensionless Coefficients

E (Dispersion Coefficient) p126 Fischer et al

		E/du^*
$= 0.1 \sim 0.4\ \mathrm{m}^2/\mathrm{s}$	Lab channel	180~400
0.76~1500		8.6~7500

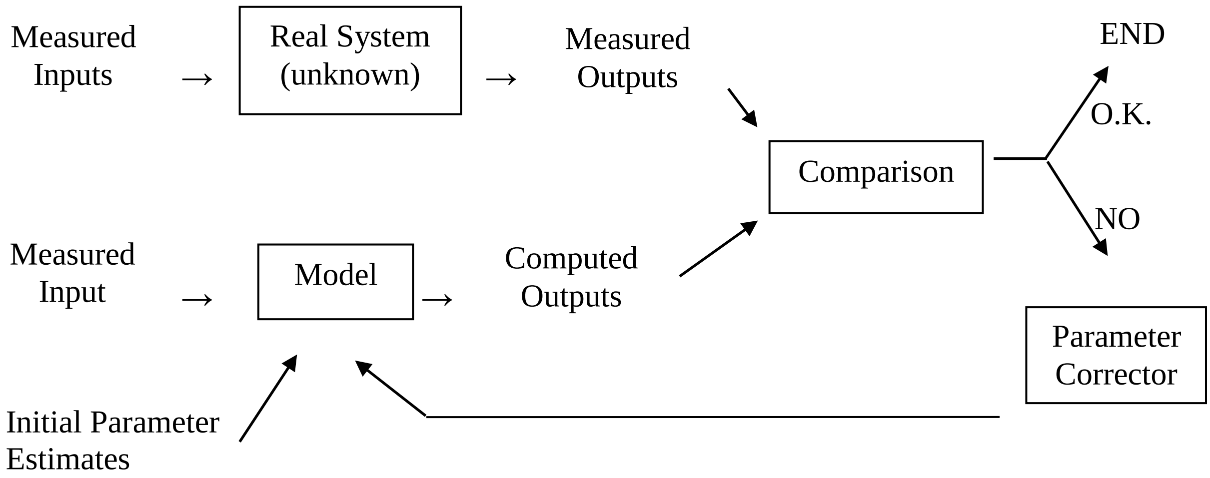
See paper by Seo (1991)

◎ Best fit

~ techniques for determining the "best", or "optimal" values of the model coefficients, i.e., values that make the predicted values and the measured ones sufficiently close to each other.

◎ Calibration

~ to estimate parameters of model from available information



8.3 Finite Difference Method

8.3.1 Errors

Analytical Solution

= closed-form algebraic expression for temporal and spatial distribution of the constituent

~ easier to use than a numerical model

Numerical Solutions

Complex water body geometry and flow fields
Nonlinearities of the source / sink terms }

→ make it impossible to obtain analytical solutions to the differential equation

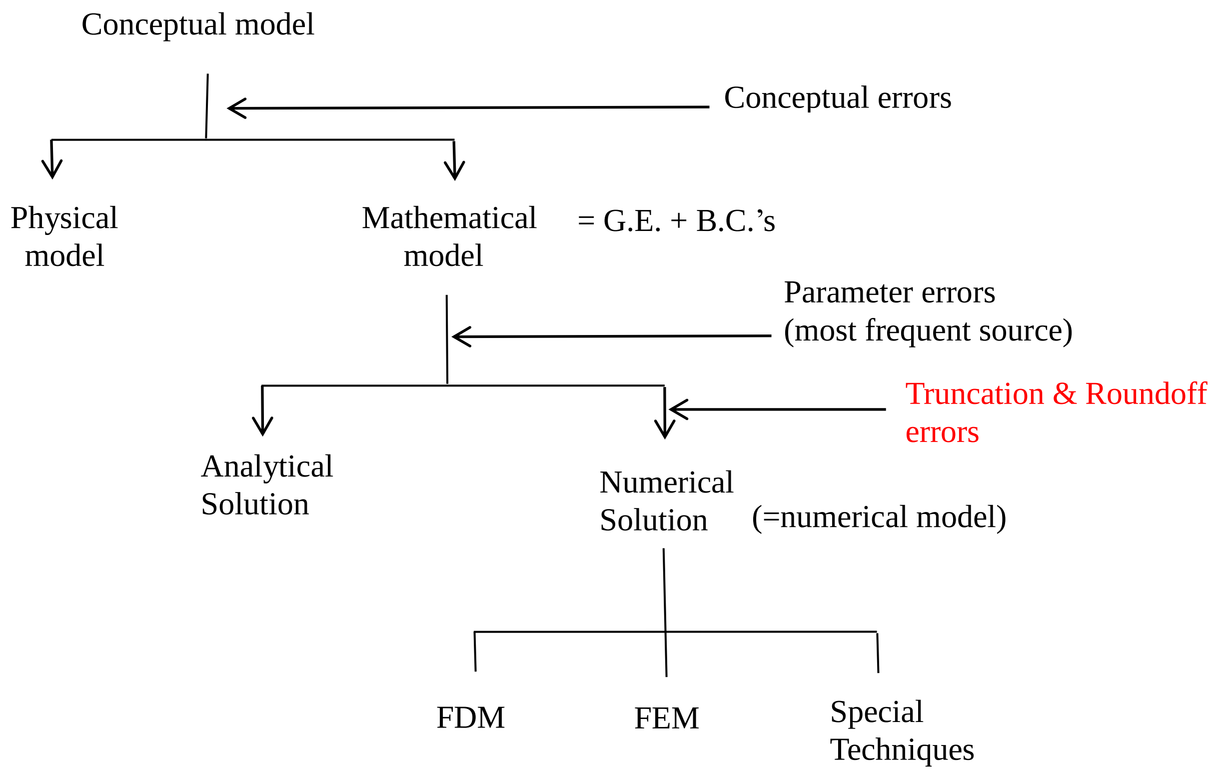
→ solve using numerical techniques

○ Numerical techniques

~ simultaneous solution of a series of mass balances on a number of small fluid elements

~ matrix-inversion methods

◎ Source of error

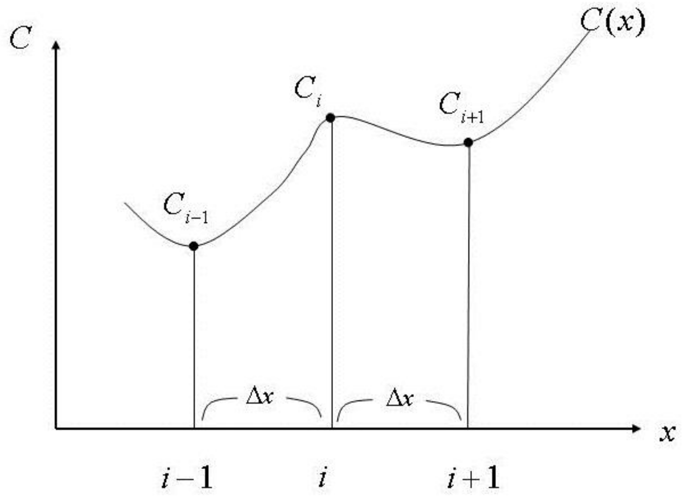


• Truncation error = discretization error

• Round-off error = error occurred in the arithmetic operations needed to solve FDE

8.3.2 Finite-Difference Methods

• Basic Relationships



①Break $x\ (y \,\&\, z)$ into finite segments of Δx in length

②Subscript all variables and constants, C_i, U_i, A_i, E_i,… etc.,

such that i subscript indicates the value of variable or parameter at point i

③Apply Taylor Series expansions

$$C_{i+1} = C_i + \Delta x \frac{\partial C_i}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 C_i}{\partial x^2} + \frac{\Delta x^3}{3!}\frac{\partial^3 C_i}{\partial x^3} + \mathrm{O}\Delta x^4 \qquad \text{(a)}$$

$$C_{i-1} = C_i - \Delta x \frac{\partial C_i}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 C_i}{\partial x^2} - \frac{\Delta x^3}{3!}\frac{\partial^3 C_i}{\partial x^3} + \mathrm{O}\Delta x^4 \qquad \text{(b)}$$

$$\frac{\partial C_i}{\partial x} \equiv \left.\frac{\partial C}{\partial x}\right|_{x=i}$$

$$\Delta x^2 = \left(\Delta x\right)^2$$

$$\mathrm{O}\Delta x^4 = \text{order of } (\Delta x^4) \text{ and smaller}$$

(i) Forward-difference

(a): $$\frac{\partial C_i}{\partial x} \cong \frac{C_{i+1} - C_i}{\Delta x} \underbrace{- \frac{\Delta x}{2}\frac{\partial^2 C_i}{\partial x^2} - \frac{\Delta x^2}{3!}\frac{\partial^3 C_i}{\partial x^3} - \mathrm{O}\Delta x^3}_{\mathrm{O}\Delta x \ \sim \text{ first-order error}}$$

(ii) Backward-difference = upwind difference

(b): $$\frac{\partial C_i}{\partial x} \cong \frac{C_i - C_{i-1}}{\Delta x} \underbrace{+ \frac{\Delta x}{2}\frac{\partial^2 C_i}{\partial x^2} - \frac{\Delta x^2}{3!}\frac{\partial^3 C_i}{\partial x^3} - \mathrm{O}\Delta x^3}_{\mathrm{O}\Delta x}$$

(iii) Central-difference

Subtract (b) from (a)

$$\frac{\partial C_i}{\partial x} \cong \frac{C_{i+1} - C_i}{2\Delta x} \underbrace{+ \frac{1}{3}\Delta x^2 \frac{\partial^3 C_i}{\partial x^3} - \mathrm{O}(\Delta x^4)}_{\mathrm{O}\Delta x^2 \ \sim \text{ 2nd-order error}}$$

(iv) Central-difference for 2nd derivative

Add (a) and (b)

$$\frac{\partial^2 C_i}{\partial x^2} \cong \frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2} - Q(\Delta x^2)$$

<u>Assembling a model</u>

A. 1-D transient transport w/ dispersion, Conservative

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \frac{1}{A}\left(\frac{\partial}{\partial x} EA \frac{\partial C}{\partial x}\right)$$

$$A, E, U = f_n(x)$$

(1) Explicit Solutions

Superscript n - time step

Subscript i - distance step

(a) Formulation a

Forward-difference for time derivative → explicit

Forward-difference for 1st derivative in x

$$\frac{\partial C}{\partial t} \approx \frac{C_i^{n+1} - C_i^n}{\Delta t}$$

$$\frac{\partial C}{\partial x} \approx \frac{C_{i+1}^n - C_i^n}{\Delta t}$$

$$\frac{1}{A}\left(\frac{\partial}{\partial x} EA \frac{\partial C}{\partial x}\right) \approx \frac{E_i A_i (C_{i+1}^n - C_i^n) - E_{i-1} A_{i-1} (C_i^n - C_{i-1}^n)}{A_i \Delta x^2}$$

Substituting & rearranging

$$C_i^{n+1} = C_i^n - \frac{\Delta t}{\Delta x} u_i (C_{i+1}^n - C_i^n) + \frac{E_i \Delta t}{\Delta x^2}(C_{i+1}^n - C_i^n) - \frac{E_{i-1} A_{i-1}}{A_i} \frac{\Delta t}{\Delta x^2}\left(C_i^n - C_{i-1}^n\right)$$

Rearranging Further

$$C_i^{n+1} = \left(1 + \frac{u_i \Delta t}{\Delta x} - \frac{E_i \Delta t}{\Delta x^2} - \frac{E_{i-1} A_{i-1}}{A_i} \frac{\Delta t}{\Delta x^2}\right) C_i^n$$

$$+ \left(\frac{E_i \Delta t}{\Delta x^2} - \frac{u_i \Delta t}{\Delta x}\right) C_{i+1}^n + \frac{E_{i-1} A_{i-1}}{A_i} \frac{\Delta t}{\Delta x^2} C_{i-1}^n$$

Let

$$\frac{u_i \Delta t}{\Delta x} = a_i \quad \rightarrow \text{Courant No.}$$

$$\frac{E_i \Delta t}{\Delta x^2} = b_i$$

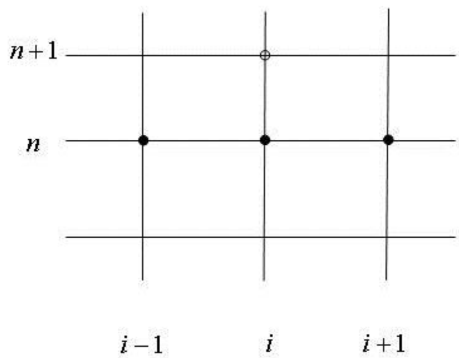
$$\frac{E_{i-1} A_{i-1}}{A_i} \frac{\Delta t}{\Delta x^2} = d_i$$

b_i, d_i → Peclet No.

a_i, b_i, d_i: dimensionless numbers

Then

$$C_i^{n+1} = d_i C_{i-1}^n + \left(1 + a_i - b_i - d_i\right) C_i^n + \left(b_i - a_i\right) C_{i+1}^n$$



Note that

$$\cancel{d_i} + (1 + \cancel{a}_i - \cancel{b}_i - \cancel{d}_i) + (\cancel{b}_i - \cancel{a_i}) = 1$$

∴ C_i^{n+1} is weighted average of C_{i-1}^n, C_i^n and C_{i+1}^n

<u>Solution</u>

Boundary conditions :
① C known for all x @ $t = 0$
② C known for all t @ $x = 0$

Procedure : ① Use equation to get $C_1^1, C_2^1, C_3^1,$ etc.

② Then get $C_1^2,\ C_2^2,\ C_3^2$ on the basis of $C_1^1,\ C_2^1,$ etc.

③ Continue as far in time as desired

(b) Formulation b

- Forward difference for time derivative
- Backward difference for spatial derivative

$$\frac{\partial C}{\partial t} \approx \frac{C_i^{n+1} - C_i^n}{\Delta t}$$

$$\frac{\partial C}{\partial x} \approx \frac{C_i^n - C_{i-1}^n}{\Delta x}$$

$$\frac{1}{A}\left(\frac{\partial}{\partial x} EA \frac{\partial C}{\partial x}\right) \approx \frac{E_{i+1}A_{i+1}(C_{i+1}^n - C_i^n) - E_i A_i (C_i^n - C_{i-1}^n)}{A_i \Delta x^2}$$

Let's include the source/sink term in this time

$$S_i = f\left(c\right)$$

Substituting and rearranging

$$C_i^{n+1} = C_i^n - \frac{u_i \Delta t}{\Delta x}(C_i^n - C_{i-1}^n) + \frac{E_i A_{i+1}}{A_i}\frac{\Delta t}{\Delta x^2}(C_{i+1}^n - C_i^n)$$

$$- \frac{E_i \Delta t}{\Delta x^2}(C_i^n - C_{i-1}^n) + f\left(C_i^n\right)\Delta t$$

$$= \left(1 - \frac{u_i \Delta t}{\Delta x} - \frac{E_i A_{i+1}}{A_i}\frac{\Delta t}{\Delta x^2} - \frac{E_i \Delta t}{\Delta x^2}\right) C_i^n + \left(\frac{u_i \Delta t}{\Delta x} + \frac{E_i \Delta t}{\Delta x^2}\right) C_{i-1}^n$$

$$+\frac{E_i \Delta t}{\Delta x^2}\frac{A_{i+1}}{A_i}C_{i+1}^n + f(C_i^n)\Delta t$$

Let $\quad \dfrac{E_{i+1}A_{i+1}}{A_i}\dfrac{\Delta t}{\Delta x^2} = d_i$

$$C_i^{n+1} = (a_i + b_i)C_{i-1}^n + d_i C_{i+1}^n + \left(1 - a_i - b_i - d_i\right)C_i^n + f(C_i^n)\Delta t$$

Assume first-order decay

$$S = f\left(c\right) = -kc$$

$$\therefore f(C_i^n)\Delta t = -k_i \Delta t C_i^n$$

$$\therefore C_i^{n+1} = \left(a_i + b_i\right)C_{i-1}^n + \left(1 - a_i - b_i - d_i - k_i \Delta t\right)C_i^n + d_i C_{i+1}^n$$

Note that now $\quad \sum Coeffs \neq 1$

<u>Stability Problem</u> → cause problem to explicit scheme only

<u>Convergence</u>

The numerical scheme is convergent

If for any fixed time $T = n\Delta t$ and fixed location

$$X = i\Delta t, \qquad C(X,T) \to \overline{C}\left(X,T\right) \qquad (or \left|C\left(X,T\right) - \overline{C}\left(X,T\right)\right| = 0)$$

as $\Delta t \to 0$ and $\Delta t \to 0$

in which $\quad C\left(X, T\right) =$ computed value at the fixed point X, T of the FDE

$\bar{C}(X,T) =$ exact solution to the PDE

Consistency

The FDE is consistent with the PDE if the local truncation error goes to zero as $\Delta x \to 0$ and $\Delta t \to 0$

Stability

The numerical scheme is stable if E_i^n remains bounded as $n \to \infty$ for fixed Δt ($t \to \infty$ or as computation proceeds)

in which $E_i^n =$ roundoff errors

$$= \tilde{C}(x,t) - C(x,t)$$

$C(x,t) =$ computed value of FDE by computer

$\tilde{C}(x,t) =$ exact solution to the FDE

◎ Lax Equivalence Theorem

Consistency + Stability → Convergence

◎ Analysis of Stability

- Von Neumann Method
- Matrix Method

◎ Source of Errors

Mathematical Model	PDE	$\bar{C}$
↓	↓ ←	Truncation Error
Numerical Model	FDE	$\tilde{C}$
	↓ ←	Roundoff Error
	Solution to FDE	$\tilde{C}$

◎ Errors in machine computations   Kuo (1970)   p 313

Roundoff error = stem from a finite number of digits in a computer word
or from initial data

Truncation error = due to finite approximations of limiting processes

◎ Roundoff Errors

(i) Decimal-binary conversion error

~ computer converts decimal number to its binary equivalent

~ conversion error may be introduced because of
finite word length of computer particularly
if there is not exact binary equivalent

(ii) Non decimal-binary conversion error

~ if calculation requires more digits than available digits through a machine
(decimal computer)

(Examples)

(i) $0.625 = \left(\frac{1}{2}\right)^1 + \left(\frac{1}{2}\right)^3 = .101$

$0.626 = \left(\frac{1}{2}\right)^1 + \left(\frac{1}{2}\right)^3 + \left(\frac{1}{2}\right)^{10} + \left(\frac{1}{2}\right)^{16} + \left(\frac{1}{2}\right)^{17} + \left(\frac{1}{2}\right)^{21} + \cdots$ (infinite series)

$= .101000....$

if binary machine has 20 bits available binary-decimal reconversion to a decimal equivalent with 8-digit accuracy

→ 0.62599945 without rounding
 0.62600040 with rounding

(ii) if decimal computer of capacity of 8 significant digits

0.33333333	0.33333333
+ 0.33333333	+0.33333333
add 3000 times	+0.33333333
Expected value = 999.99999	+0.33333333
Rounded-off value= 999.99091	1.33333332 → 1.3333333
Roundoff error = 0.00908	8digit
	True value Truncated to
	Error = 0.00000002

◎ Stability Problem

○ Explicit Solutions

~ accurate & easy

~ may be unstable

→ need a stability criterion

○ Let $C_i^n = T_i^n + e_i^n$ (1)

$C_i^n =$ computed value of FDE by computer

$T_i^n =$ true (exact) value to FDE at the x and t associated with i and $n = \tilde{C}$

$e_i^n =$ error at that point

Substitute this into formulation a)

$$e_i^{n+1} = \underline{(1+a_i-b_i-d_i)e_i^n + (b_i-a_i)e_{i+1}^n + d_i e_{i+1}^n} \quad ①$$

$$\underline{-T_i^{n+1} + (1+a_i-b_i-a_i)T_i^n + (b_i-a_i)T_{i+1}^n + d_i T_{i-1}^n} \quad ② \qquad (2)$$

→ error for newly-calculated concentration depends not only on true concentration (exact solution to FDE) (T-terms) but also on other errors (e-terms)

~ Part ② may not be zero because of truncated terms in formulating FDE out of PDE

PDE ⟶ FDE ⟶ Solution

↑ Truncation error | T-terms (PDE → FDE)

↑ roundoff error | e-terms (FDE → Solution)

But assume truncation error is zero, and worry only about the e-terms or propagation (magnification) of roundoff errors.

To insure stability (to prevent magnification of errors)

$$\left|e_i^{n+1}\right| \le \max\left[\left|e_{i-1}^n\right|, \left|e_i^n\right|, \left|e_{i+1}^n\right|\right] \tag{3}$$

For Formulation a)

$$\left|e_i^{n+1}\right| \le \left\{\left|1+a_i-b_i-d_i\right| + \left|b_i-a_i\right| + \left|d_i\right|\right\}\left|e_i^n\right|$$

$$\left|1+a_i-b_i-d_i\right| + \left|b_i-a_i\right| + \left|d_i\right| \le 1 \tag{4}$$

Absolute values of the coefficients should add to less than one.

Now, since $a_i, b_i, d_i \ge 0$, there are 4 possibilities.

α) $if \quad 1+a_i-b_i-d_i > 0 \;\&\; b_i - a_i > 0$

then $1 + \not{a}_i - \not{b}_i - \not{d}_i + \not{b}_i - \not{a}_i + \not{d}_i = 1 \quad \le 1$

which is satisfied for all values of a_i, b_i, and d_i which meet these conditions.

β) $if \quad 1+a_i-b_i-d_i > 0 \;\&\; b_i - a_i \le 0$

$$1 + a_i - b_i - \not{d}_i - b_i + a_i + \not{d}_i \le 1$$

$$2a_i \le 2b_i$$

$$\underline{a_i \le b_i}$$

γ) *if* $1 + a_i - b_i - d_i < 0 \;\; \& \;\; b_i - a_i > 0$

$$-1 - a_i + b_i + d_i + b_i - a_i + d_i \le 1$$

$$2d_i + 2b_i - 2a_i \le 2$$

$$\underline{d_i + b_i - a_i \le 1}$$

if $d_i = b_i$

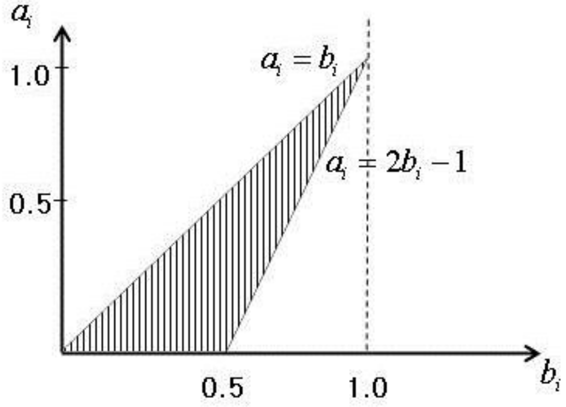
then $\underline{2b_i \le 1 + a_i}$

δ) *if* $1 + a_i - b_i - d_i < 0 \quad \& \quad b_i - a_i \le 0$

$$-1 - \cancel{a_i} + \cancel{b_i} + d_i - \cancel{b_i} + \cancel{a_i} + d_i \le 1$$

$$2d_i \le 2$$

$d_i \le 1$ *or* $b_i \le 1$ *if* $b_i = d_i$



○ Restrictions on Δx and Δt

$$a \le b$$

$$\frac{u\Delta t}{\Delta x} \le \frac{E\Delta t}{\Delta x^2} \quad \rightarrow \quad \Delta x \le \frac{E}{u} \qquad ①$$

$$2b \le 1 + a$$

$$2\frac{E\Delta t}{\Delta x^2} \le 1 + \frac{u\Delta t}{\Delta x} \quad \rightarrow \quad \frac{1}{\Delta t} \ge \frac{2E}{\Delta x^2} - \frac{u}{\Delta x}$$

$$\rightarrow \quad \Delta t \le \frac{1}{\frac{2E}{\Delta x^2} - \frac{u}{\Delta x}} \qquad ②$$

Substitute ① into ②

$$\Delta t < \frac{1}{\frac{2E}{\left(\frac{E}{u}\right)^2} - \frac{u}{\left(\frac{E}{u}\right)}}$$

$$\Delta t < \frac{1}{\frac{2u^2}{E} - \frac{u^2}{E}} = \frac{1}{\frac{u^2}{E}} = \frac{E}{u^2}$$

$$\Delta t < \frac{E}{u^2} \qquad ③$$

$$\therefore \begin{cases} \Delta x \le \frac{E}{u} \\ \Delta t < \frac{E}{u^2} \\ \Delta t \le \frac{1}{\frac{2E}{\Delta x^2} - \frac{u}{\Delta x}} \end{cases}$$

○ Stability Criterion for Formulation (b) w/o decay term

$$|1-a_i-b_i-d_i|+|a_i+b_i|+|d_i|\le 1$$

there are only 2 cases to be considered

α) *if* $1-a_i-b_i-d_i \ge 0$

$$1-\cancel{a_i}-\cancel{b_i}-\cancel{d_i}+\cancel{a_i}+\cancel{b_i}+\cancel{d_i}\le 1$$

$$1\le 1$$

Satisfied for any values of a_i, b_i, and d_i

β) *if* $1-a_i-b_i-d_i \le 0$

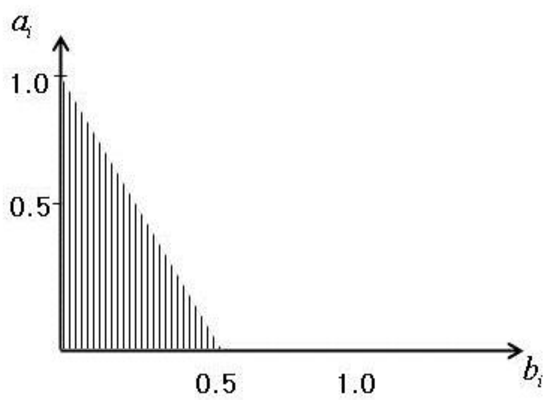
$$-1+a_i+b_i+d_i+a_i+b_i+d_i\le 1$$

$$2(a_i+b_i+d_i)\le 2$$

$$a_i+b_i+d_i\le 1$$

if $b_i = d_i$

$\underline{a_i+2b_i\le 1}$ $\qquad a_i \le 1-2b_i$



$$a + 2b \le 1$$

$$\frac{u\Delta t}{\Delta x} + 2\frac{E\Delta t}{\Delta x^2} \le 1$$

$$\Delta t \le \frac{1}{\dfrac{u}{\Delta x} + \dfrac{2E}{\Delta x^2}}$$

γ) Formulation EXCD

- Central difference for spatial derivative
- Forward difference for time derivative

$$\frac{\partial C}{\partial x} \approx \frac{C_{i+1}^{n} - C_{i-1}^{n}}{2\Delta x}$$

$$\frac{\partial C}{\partial x} \approx \frac{C_{i}^{n+1} - C_{i}^{n}}{\Delta t}$$

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{C_{i+1}^{n} - 2C_{i}^{n} + C_{i-1}^{n}}{\Delta x^2}$$

Substitute these into 1-D transport equation

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = E\frac{\partial^2 C}{\partial x^2}$$

$$\frac{C_{i}^{n+1} - C_{i}^{n}}{\Delta x} + u\frac{C_{i+1}^{n} - C_{i-1}^{n}}{2\Delta x} = E\frac{C_{i+1}^{n} - 2C_{i}^{n} + C_{i-1}^{n}}{\Delta x^2}$$

$$C_{i}^{n+1} = \left(1 - 2\frac{E\Delta t}{\Delta x^2}\right)C_{i}^{n} + \left(\frac{E\Delta t}{\Delta x^2} - \frac{u\Delta t}{2\Delta x}\right)C_{i+1}^{n} + \left(\frac{E\Delta t}{\Delta x^2} + \frac{u\Delta t}{2\Delta x}\right)C_{i-1}^{n}$$

$$C_i^{n+1} = \left(\frac{a}{2} + b\right) C_{i-1}^n + (1-2b) C_{i+1}^n + \left(b - \frac{a}{2}\right) C_{i+1}^n$$

$$a = \frac{u\Delta t}{\Delta x}$$

$$b = \frac{E\Delta t}{\Delta x^2}$$

• Stability Criterion

$$|1-2b| + \left|\frac{a}{2} + b\right| + \left|b - \frac{a}{2}\right| \le 1$$

α) if $\quad 1-2b > 0 \quad \& \quad b - \frac{a}{2} > 0$

$$1 - \cancel{2b} + \cancel{\frac{a}{2}} + \cancel{b} + \cancel{b} - \cancel{\frac{a}{2}} \le 1$$

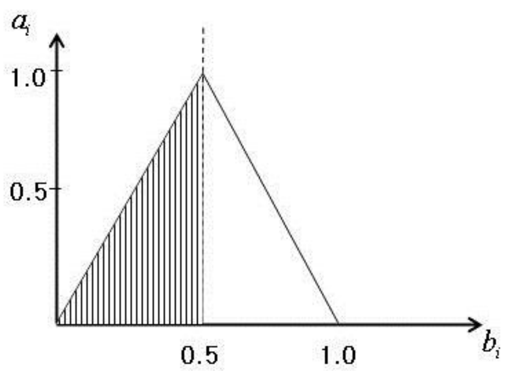
$$1 \le 1$$

β) if $\quad 1-2b > 0 \quad \& \quad b - \frac{a}{2} < 0$

$$1 - 2b + \frac{a}{2} + \cancel{b} - \cancel{b} + \frac{a}{2} \le 1$$

$$a - 2b \le 0$$

$$a \le 2b$$



γ) if $\quad 1-2b < 0 \quad \& \quad b - \frac{a}{2} > 0$

$$-1-2b+\frac{a}{2}+b+b-\frac{a}{2}\le 1$$

$$4b\le 2 \quad b\le\frac{1}{2}$$

δ) if $\;1-2b<0 \quad \& \quad b-\frac{a}{2}<0$

$$-1+2b+\frac{a}{2}+\cancel{b}-\cancel{b}+\frac{a}{2}\le 1$$

$$2b+a\le 2$$

$$b+\frac{a}{2}\le 1$$

$$a\le 2b$$

$$\frac{u\Delta t}{\Delta x}\le 2\frac{E\Delta t}{\Delta x^2}$$

$$\Delta x\le 2\frac{E}{u}$$

$$b\le\frac{1}{2}$$

$$\frac{E\Delta t}{\Delta x^2}\le\frac{1}{2}$$

$$\Delta t\le\frac{\Delta x^2}{2E}$$

◎ Numerical Dispersion

Taylor series expansion

$$\frac{\partial C}{\partial x} = \frac{C_{i+1}^{n} - C_{i-1}^{n}}{2\Delta x} + \overbrace{\frac{\Delta x^2}{3!}\frac{\partial^3 C}{\partial x^3}}^{O\Delta x^2} + O\Delta x^3 \qquad (\alpha) \text{ cential}$$

$$\frac{\partial C}{\partial t} = \frac{C_{i}^{n+1} - C_{i}^{n}}{\Delta t} - \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} - O\Delta x^2 \qquad (\beta) \text{ forward}$$

By the way think about 1-D transport equation w/o dispersion term (pure advection)

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} \qquad ①$$

differentiate w.r.t x

$$\frac{\partial^2 C}{\partial x \partial t} = -u\frac{\partial^2 C}{\partial x^2} \qquad ②$$

differentiate ① w.r.t. t

$$\frac{\partial^2 C}{\partial t^2} = -u\frac{\partial^2 C}{\partial t \partial x} \qquad ③$$

② $$\frac{\partial^2 C}{\partial x \partial t} = -u\frac{\partial^2 C}{\partial x^2}$$

③ $$\frac{\partial^2 C}{\partial t \partial x} = -\frac{1}{u}\frac{\partial^2 C}{\partial t^2}$$

$$\therefore \; -u\frac{\partial^2 C}{\partial x^2} = -\frac{1}{u}\frac{\partial^2 C}{\partial t^2}$$

$$\therefore \therefore \; \frac{\partial^2 C}{\partial t^2} = u^2\frac{\partial^2 C}{\partial x^2} \qquad ④$$

Formulate ① with $(\alpha)\,\&\,(\beta)$

$$\frac{C_i^{n+1}-C_i^n}{\Delta t}-\frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2}=-u\left(\frac{C_{i+1}^n-C_{i-1}^n}{2\Delta t}\right)+\mathrm{O}(\Delta t^2,\Delta x^2)$$

Substitute ④

$$\frac{C_i^{n+1}-C_i^n}{\Delta t}=-u\left(\frac{C_{i+1}^n-C_{i-1}^n}{2\Delta t}\right)+\underbrace{\frac{\Delta t}{2}u^2\frac{\partial^2 C}{\partial x^2}}_{\text{numerical dispersion term}}+\mathrm{O}(\Delta t^2,\Delta x^2)$$

Let $E_n=\dfrac{\Delta t}{2}u^2=\dfrac{u\Delta x}{2}a$ $\left(a=\dfrac{u\Delta t}{\Delta x}=\text{Courant No}\right)$

= numerical dispersion coeff

Then

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}-E_n\frac{\partial^2 C}{\partial x^2}+\mathrm{O}(\Delta t^2,\Delta x^2)=0$$

So, add E_n to physical dispersion coeff. E

$$E_f=E+E_n$$

for numerical dispersion correction

2. Implicit Solutions

(1) Formulation (c)

Backward difference for $\frac{\partial C}{\partial t}$

Forward difference for $\frac{\partial C}{\partial x}$

$$\frac{\partial C}{\partial t} \approx \frac{C_i^n - C_i^{n-1}}{\Delta t}$$

$$\frac{\partial C}{\partial x} \approx \frac{C_{i+1}^n - C_i^n}{\Delta x}$$

$$\frac{1}{A}\frac{\partial}{\partial x}(EA\frac{\partial C}{\partial x}) \approx \frac{1}{A_i \Delta x^2}\left\{E_i A_i (C_{i+1}^n - C_i^n) - E_{i-1}A_{i-1}(C_i^n - C_{i-1}^n)\right\}$$

Substituting and rearranging

$$C_i^n - C_i^{n-1} = -\frac{u_i \Delta t}{\Delta x}(C_{i+1}^n - C_i^n) + \frac{E_i \Delta t}{\Delta x^2}(C_{i+1}^n - C_i^n) - \frac{E_{i-1}A_{i-1}\Delta t}{A_i \Delta x^2}(C_i^n - C_{i-1}^n)$$

$$(1 - \frac{u_i \Delta t}{\Delta x} + \frac{E_i \Delta t}{\Delta x^2} + \frac{E_{i-1}A_{i-1}\Delta t}{A_i \Delta x^2})C_i^n + (\frac{u_i \Delta t}{\Delta x} - \frac{E_i \Delta t}{\Delta x^2})C_{i+1}^n$$

$$-\frac{E_{i-1}A_{i-1}\Delta t}{A_i \Delta x^2}C_{i-1}^n = C_i^{n-1}$$

let $a_i = \frac{u_i \Delta t}{\Delta x}$

$$b_i = \frac{E_i \Delta t}{\Delta x^2}$$

$$d_i = \frac{E_{i-1}A_{i-1}\Delta t}{A_i \Delta x^2}$$

$$(1-a_i+b_i+d_i)C_i^n+(a_i-b_i)C_{i+1}^n-d_iC_{i-1}^n=C_i^{n-1}$$

$\rightarrow$ $C_i^{n-1}=$ weighted average of $C_i^n, C_{i+1}^n,$ and C_{i-1}^n

We need I.C., UBC, and DBC to solve system of algebraic equation

$\rightarrow$ See Fig. in next page.

◎ let $L_i=-d_i$; $M_i=1-a_i+b_i+d_i$, $U_i=a_i-b_i$

then $L_iC_{i-1}^n+M_iC_i^n+U_iC_{i+1}^n=C_i^{n-1}$

(i) If C known @ $\begin{pmatrix} x=0 & (i=0) \\ x=\infty & (i=m+1) \end{pmatrix}$ $\quad C(0), C(m+1)$

$\rightarrow$ Dirichlet (first kind) type B.C.

$$i=1:\ L_1C_0^n+M_1C_1^n+U_1C_2^n=C_1^{n-1}$$

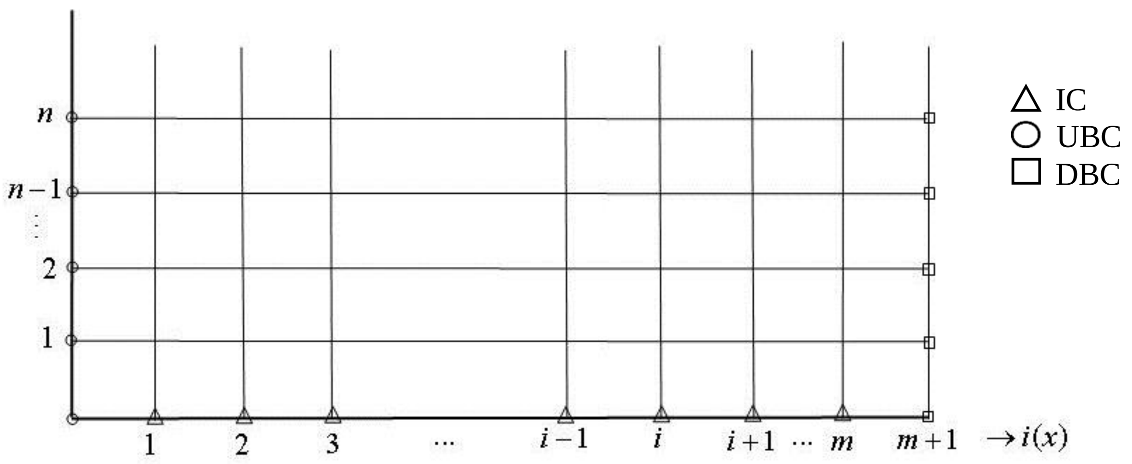
$$\rightarrow M_1C_1^n+U_1C_2^n=\underbrace{C_1^{n-1}-L_1C_0^n}_{Known}$$

$$i=2:\ L_2C_1^n+M_2C_2^n+U_2C_3^n=C_2^{n-1}$$

$$i=m:\ L_mC_{m-1}^n+M_mC_m^n+U_mC_{m+1}^n=C_m^{n-1}$$

$$\rightarrow L_mC_{m-1}^n+M_mC_m^n=\underbrace{C_m^{n-1}-U_mC_{m+1}^n}_{Known}$$

$$\begin{bmatrix} M_1 & U_1 & 0 & . & \cdots & . & 0 \\ L_2 & M_2 & U_2 & 0 & & \cdots & 0 \\ 0 & L_3 & M_3 & U_3 & 0 & \cdots & 0 \\ 0 & & & & & & \\ & & & & L_{m-1} & M_{m-1} & U_{m-1} \\ & & & & & L_m & M_m \end{bmatrix} \begin{Bmatrix} C_1^n \\ C_2^n \\ C_3^n \\ \\ C_{m-1}^n \\ C_m^n \end{Bmatrix} = \begin{bmatrix} C_1^{n-1} - L_1 C_0^n \\ C_2^{n-1} \\ C_3^{n-1} \\ . \\ . \\ C_{m-1}^{n-1} \\ C_m^{n-1} - U_m C_{m+1}^n \end{bmatrix}$$



→ All concentrations for one value of n are solved for simultaneously, and the solution marches in time.

→ Implicit Solution

• Tridiagonal matrix → Gaussian elimination

Thomas Algorithm

(ii) If C known @ x=0 (i=0) → Dirichet

And $\dfrac{\partial C}{\partial x}$ known @ $x = \infty \, (i = m+1)$ → Neumann(2nd kind)

◎ No flux @ boundary → $\left.\frac{\partial C}{\partial x}\right|_{m+1}^{n} = 0$

$$\left.\frac{\partial C}{\partial x}\right|_{m+1}^{n} \approx \frac{C_{m+1}^{n} - C_{m}^{n}}{\Delta x} = 0 \qquad \text{Backward difference}$$

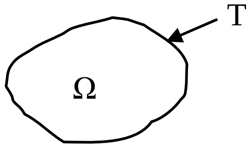
$$\therefore\ C_{m+1}^{n} = C_{m}^{n}$$

$$i = m:\ L_m C_{m-1}^{n} + M_m C_m^{n} + U_m C_{m+1}^{n} = C_m^{n-1}$$

$$\therefore\ L_m C_{m-1}^{n} + (M_m + U_m) C_m^{n} = C_m^{n-1}$$

$$\begin{bmatrix} M_1 & U_1 & 0 & & & \\ L_2 & M_2 & U_2 & 0 & & \\ & & & & & \\ & & & & & \\ & & & L_{m-1} & M_{m-1} & U_{m-1} \\ & & & 0 & L_m & M_m + U_m \end{bmatrix} \begin{Bmatrix} C_1 \\ C_2 \\ \cdot \\ \cdot \\ C_{m-1} \\ C_m \end{Bmatrix}^{n} = \begin{bmatrix} C_1^{n-1} - L_1 C_0^{n} \\ C_2^{n-1} \\ \cdot \\ \cdot \\ C_{m-1}^{n-1} \\ C_m^{n-1} \end{bmatrix}$$

8.3.3 Boundary Conditions



Dirichlet (1st Type) $C(x,y) = f_1(x,y)$ on T_1

Neumann (2nd Type) $\frac{\partial C}{\partial n} = f_2(x,y)$ $on \ T_2$

$\frac{\partial C}{\partial n} =$ derivative normal to a boundary = $\frac{\partial C}{\partial x} \ or \ \frac{\partial C}{\partial y}$

Mixed (3rd Type) $a\frac{\partial C}{\partial n} + bC = f_3(x,y)$ $on \ T_3$

(2) Formulation d ~ most commonly used formulation

Backward difference for $\frac{\partial C}{\partial t}$

Backward difference for $\frac{\partial C}{\partial x}$

$$\frac{\partial C}{\partial t} \approx \frac{C_i^n - C_i^{n-1}}{\Delta t}$$

$$\frac{\partial C}{\partial x} \approx \frac{C_i^n - C_{i-1}^n}{\Delta x}$$

$$\frac{1}{A}(\frac{\partial}{\partial x} EA \frac{\partial C}{\partial x}) \approx \frac{1}{A_i \Delta x^2}\left[E_{i+1}A_{i+1}(C_{n+1}^n - C_i^n) - E_i A_i (C_i^n - C_{i-1}^n)\right]$$

Substituting and rearranging

$$(1+a_i+b_i+d_i)C_i^n-(a_i+b_i)C_{i-1}^n-d_iC_{i+1}^n=C_i^{n-1}$$

where $d_i=\frac{E_{i+1}A_{i+1}}{A_i}\frac{\Delta t}{\Delta x^2}$

let $L_i=-(a_i+b_i)$

$$M_i=(1+a_i+b_i+d_i)$$

$$U_i=-d_i$$

then $L_iC_{i-1}^n+M_iC_i^n+U_iC_{i+1}^n=C_i^{n-1}$

(3) Formulation Im-Cd

Backward difference for $\frac{\partial C}{\partial t}$

Central difference for $\frac{\partial C}{\partial x}$

$$\frac{\partial C}{\partial t}\approx\frac{C_i^n-C_i^{n-1}}{\Delta t}$$

$$\frac{\partial C}{\partial x}\approx\frac{C_{i+1}^n-C_{i-1}^n}{2\Delta x}$$

Final discretized equation results in

$$U_i C_{i-1}^n + M_i C_i^n + U_i C_{i+1}^n = C_i^{n-1}$$

where $U_i = -\dfrac{a_i}{2} - b_i$

$$M_i = 1 + 2b_i$$

$$U_i = \frac{a_i}{2} - b_i$$

$$b_i = \frac{E_i \Delta t}{\Delta x^2}$$

◎ Numerical Dispersion

= artificial viscosity, numerical dissipation

= smearing of concentration fronts due to excessive damping

= Taylor's series truncation error

<Ref>

Lantz, R.B., "Quantitative evaluation of numerical diffusion (truncation error)," Soc. Pet. Engr. J., pp.315-320, Sept., 1971.

◎ Formulation b

Taylor series expansion in *x* direction

$$C_{i-1}^n = C_i^n - \Delta x \frac{\partial C_i}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 C_i}{\partial x^2} - O(\Delta x^3)$$

$$(C_{i+1}^n = C_i^n + \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 C_i}{\partial x^2} + O(\Delta x^3))$$

$$\frac{C_i^n - C_{i-1}^n}{\Delta x} = \frac{\partial C_i}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 C_i}{\partial x^2} - O(\Delta x^2) \qquad ①$$

$$C_i^{n+1} = C_i^n + \Delta t \frac{\partial C}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 C}{\partial t^2} + O(\Delta t^3)$$

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \frac{\partial C}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 C}{\partial x^2} + O(\Delta t^2) \qquad ②$$

Consider the 1-D transport equation with no dispersion term (pure advection)

$$\frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x}$$

Formulation b $\dfrac{C_i^{n+1} - C_i^n}{\Delta t} = -u \dfrac{C_i^n - C_{i-1}^n}{\Delta x}$ ③

$$Ex\ a \quad \frac{C_{i+1}^n - C_i^n}{\Delta x} = \frac{\partial C_i}{\partial x} + \frac{\Delta x}{2}\frac{\partial^2 C_i}{\partial x^2} + O(\Delta x^2)$$

$$Ex\ b \quad \frac{C_i^n - C_{i-1}^n}{\Delta x} = \frac{\partial C_0}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 C_0}{\partial x^2} - O(\Delta x^2)$$

$$Ex\ c \quad \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x} = \frac{\partial C_i}{\partial x} - \frac{\Delta x^2}{3}\frac{\partial^3 C}{\partial x^3} - O(\Delta x^4)$$

Im a

$$C_{i-1}^{n} = C_i^n - \Delta t \frac{\partial C}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 C_i}{\partial t^2} - \mathrm{O}(\Delta t^3)$$

$$\frac{C_i^n - C_i^{n-1}}{\Delta t} = \frac{\partial C}{\partial t} - \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} + \mathrm{O}(\Delta t^3)$$

differentiating ③ w.r.t. t

$$\frac{\partial^2 C}{\partial t^2} = -u \frac{\partial^2 C}{\partial t \partial x} \quad ④$$

differentiating ③ w.r,t x

$$\frac{\partial^2 C}{\partial x \partial t} = -u \frac{\partial^2 C}{\partial x^2} \quad ⑤$$

$$\left.\begin{array}{l} \dfrac{\partial^2 C}{\partial t \partial x} = -\dfrac{1}{u}\dfrac{\partial^2 C}{\partial t^2} \\ \dfrac{\partial^2 C}{\partial x \partial t} = \dfrac{\partial^2 C}{\partial t \partial x} = -u \dfrac{\partial^2 C}{\partial x^2} \end{array}\right\} -\frac{1}{u}\frac{\partial^2 C}{\partial t^2} = -u \frac{\partial^2 C}{\partial x^2}$$

$$\therefore \frac{\partial^2 C}{\partial t^2} = u^2 \frac{\partial^2 C}{\partial x^2} \quad ⑥$$

Substituting ① and ② into ③

$$* \quad \frac{\partial C}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} = -u\left\{\frac{\partial C}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2}\right\} + \mathrm{O}(\Delta t^2 + \Delta x^2)$$

Substituting ⑥

$$\underbrace{\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x}}_{PDE} + \underbrace{\underbrace{\left\{\frac{u\Delta x}{2} - \frac{\Delta t}{2}u^2\right\}\frac{\partial^2 C}{\partial x^2}}_{Numerical\ dispersion} + \underbrace{O(\Delta t^2 + \Delta x^2)}_{Truncation\ error}}_{Total\ error}$$

Define numerical dispersion coefficient

$$E_n = \frac{u\Delta x}{2}(1 - \frac{u\Delta t}{\Delta x}) = \frac{u\Delta x}{2}(1-a)$$

$$a = \frac{u\Delta t}{\Delta x} = Courant\ No$$

Then $\dfrac{\partial C}{\partial t} = -u\dfrac{\partial C}{\partial x} + E_n\dfrac{\partial^2 C}{\partial x^2}$

If we include real dispersion term

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \underbrace{(E + E_n)}_{E_c = Computed\ dispersion}\frac{\partial^2 C}{\partial x^2}$$

◎ How to remove E_n

(i) Choose and Δt and Δx such that $E_n = 0$

$$E_n = \frac{u\Delta t}{2}(1-a) = 0$$

$$\therefore a = \frac{u\Delta t}{\Delta x} = 1 \qquad ①$$

However, stability criterion for Formulation b is

$$\frac{u\Delta t}{\Delta x}+\frac{2E\Delta t}{\Delta x^2}\le 1 \quad ②$$

If we make $\frac{u\Delta t}{\Delta x}=1$

then ② becomes

$$\frac{E\Delta t}{\Delta x^2}\le 0 \quad ③$$

Therefore we have to choose and Δt and Δx

Satisfying both ① & ③ → impossible

<Example>

$$u=1$$

$$\Delta x=2,\ \Delta t=1$$

$$a=\frac{1\cdot 1}{2}=\frac{1}{2} \qquad E_n=\frac{1(2)}{2}\left(1-\frac{1}{2}\right)=\frac{1}{2}$$

$$\frac{1}{2}+\frac{2(1)}{(2)^2}E=\frac{1}{2}+\frac{E}{2}\le 1$$

$$\frac{E}{2}\le\frac{1}{2}$$

$$E\le\frac{1}{4}$$

(ii) Dispersion correction technique

$\rightarrow$ make $E_c = E$

For Formulation b, subtract E_n from E_c

$$\therefore E_c' = E + E_n - E_n = E$$

(iii) make Δx and Δt small

◎ $E_c = E + E_n$

Formulation		Numerical dispersion, E_n	Effective solution to ND
E_x	a	$-\frac{u\Delta x}{2}(1+a)$	$Add(-E_n)$
E_x	b	$\frac{u\Delta x}{2}(1-a)$	$Subtract\ E_n(Be\ careful\ when\ E < E_n)$
E_x	cd	$-\frac{u^2}{2}\Delta t$ $(No\ numerical\ dispersion\ due\ to\ advection)$	$Add(-E_n)$
I_m	c	$\frac{u\Delta x}{2}(1-a)$	$Make\ a = 1$
I_m	d	$\frac{u\Delta x}{2}(1+a)$	$Subtract\ E_n$
I_m	cd	$\frac{u^2}{2}\Delta t$	$Subtract\ E_n$

◎ Lagrangian Formulations

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \frac{1}{A}\left(\frac{\partial}{\partial x}EA\frac{\partial C}{\partial x}\right) + S$$

(1) Formulation e -explicit

Forward difference formula at the i+1 grid point for $\frac{\partial C}{\partial t}$

$$\frac{\partial C}{\partial t} \approx \frac{C_{i+1}^{n+1} - C_{i+1}^{n}}{\Delta t}$$

Forward difference formula for $\frac{\partial C}{\partial x}$

$$\frac{\partial C}{\partial x} \approx \frac{C_{i+1}^{n} - C_{i}^{n}}{\Delta x}$$

Eulerian formulation for second derivative

$$\frac{1}{A}\left(\frac{\partial}{\partial x} EA \frac{\partial C}{\partial x}\right) \approx \frac{1}{A_i \Delta x^2}\left[E_i A_i \left(C_{i+1}^{n} - C_{i}^{n}\right) - E_{i-1} A_{i-1}\left(C_{i}^{n} - C_{i-1}^{n}\right)\right]$$

Substituting into Governing eq.

$$C_{i+1}^{n+1} = C_{i+1}^{n} - \frac{u_i \Delta t}{\Delta x}\left(C_{i+1}^{n} - C_{i}^{n}\right) + \frac{E_i \Delta t}{\Delta x^2}\left(C_{i+1}^{n} - C_{i}^{n}\right)$$

$$- \frac{E_{i-1} A_{i-1} \Delta t}{A_i \Delta x^2}\left(C_{i}^{n} - C_{i-1}^{n}\right) + S_i \Delta t$$

Rearranging further

$$C_{i+1}^{n+1} = \left(1 - \frac{u_i \Delta t}{\Delta x} - \frac{E_i \Delta t}{\Delta x^2}\right) C_{i+1}^{n} + \left(\frac{u_i \Delta t}{\Delta x} - \frac{E_i \Delta t}{\Delta x^2} - \frac{E_{i-1} A_{i-1} \Delta t}{A_i \Delta x^2}\right) C_{i}^{n}$$

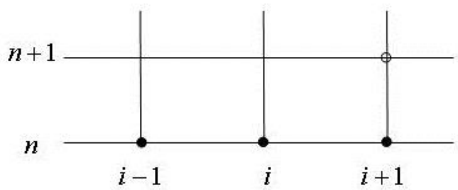
$$+ \frac{E_{i-1} A_{i-1} \Delta t}{A_i \Delta x^2} C_{i-1}^{n} + S_i \Delta t$$

Let $a_i = \dfrac{u_i \Delta t}{\Delta x}$

$$b_i = \frac{E_i \Delta t}{\Delta x^2}$$

$$d_i = \frac{E_{i-1} A_{i-1} \Delta t}{A_i \Delta x^2}$$

then $\underline{C_{i+1}^{n+1} = (1 - a_i + b_i) C_{i+1}^n + (a_i - b_i - d_i) C_i^n + d_i C_{i-1}^n + S_i \Delta t}$



• We need 2 UBC and IC, need no DBC

◎ Numerical Dispersion

Pure Advection Problem

$$\frac{C_{i+1}^{n+1} - C_{i+1}^n}{\Delta t} = -u \frac{C_{i+1}^n - C_i^n}{\Delta x}$$ ① Formulation e

Taylor Series Expansion in t direction

$$C_{i+1}^{n+1} = C_{i+1}^n + \Delta t \frac{\partial C}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 C}{\partial t^2} + O(\Delta t^3)$$

$$\rightarrow \frac{C_{i+1}^{n+1} - C_{i+1}^n}{\Delta t} = \frac{\partial C}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 C}{\partial t^2} + O(\Delta t^2)$$ ②

Taylor Series Expansion in x direction

$$C_{i+1}^n = C_i^n + \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2} + O(\Delta x^3)$$

$$\rightarrow \frac{C_{i+1}^n - C_i^n}{\Delta x} = \frac{\partial C}{\partial x} + \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} + O(\Delta x^2) \qquad ③$$

Substitute ② & ③ into ①

$$\frac{\partial C}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} + O(\Delta t^2) = -u\left\{\frac{\partial C}{\partial x} + \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} + O(\Delta x^2)\right\}$$

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - \frac{\Delta t}{2}\underbrace{\frac{\partial^2 C}{\partial t^2}}_{u^2\frac{\partial^2 C}{\partial x^2}} - u\frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} + O(\Delta x^2 + \Delta t^2)$$

$$\therefore \frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - \underbrace{\frac{u}{2}\Delta x(1+a)}_{E_n}\frac{\partial^2 C}{\partial x^2} + O(\Delta x^2 + \Delta t^2)$$

$$\therefore E_n = \underline{-\frac{u\Delta x}{2}(1+a)}$$

◎ Stability Criteria

$$1 - a_i + b_i \geq 0 \;\; \& \;\; a - b_i - d_i \geq 0$$

$$\downarrow \qquad\qquad \downarrow$$

$$\Delta t \leq \frac{\Delta x^2}{u\Delta x - E} \qquad \Delta x \geq \frac{2E}{u}$$

(2) Formulation f - Implicit

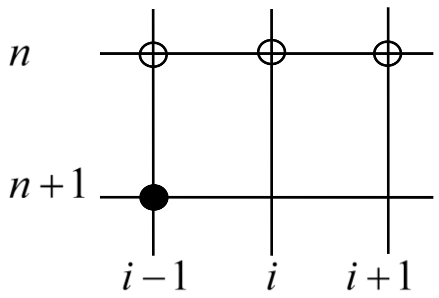
Backward difference for $\frac{\partial C}{\partial t}$ at the i-l grid point

Backward difference for $\frac{\partial C}{\partial x}$

$$\frac{\partial C}{\partial t} \approx \frac{C_{i-1}^{n} - C_{i-1}^{n-1}}{\Delta t}$$

$$\frac{\partial C}{\partial x} \approx \frac{C_{i}^{n} - C_{i-1}^{n}}{\Delta x}$$

$$\left(a_i + d_i - 1\right)C_{i-1}^{n} + \left(-a_i - b_i - d_i\right)C_i^n + b_i C_{i+1}^{n} + S_i \Delta t = C_{i-1}^{n-1}$$



We need 1 IC &
2 DBC

No UBC

◎ Numerical Dispersion

$$E_n = \frac{u\Delta x}{2}(1+a) \qquad \sim \quad \mathrm{I}_m \quad d$$

◎ "Two-Step" techniques

~ Advection is "tracked" to a new set of grid points and dispersion follows separately

◎ Lagrangian approach (Bella & Dobbins, 1968)

~ Observer is traveling at the same speed as the parcel of water under observation

• Two-step explicit method → Two processes are assumed to occur sequentially rather than simultaneously as in the prototype.

(1) 1st step (advection process) : to advect the pollutant downstream for one-time step

→ Eulerian Frame $C_i^n = C_i^{n+1}$

$$C_0^n = C_0^{n+1}$$

(2) 2nd step (dispersion process) : to calculate new values on the n+1 row using only the dispersion

→ Lagrangian Frame $\dfrac{C_i^{n+1} - C_i^n}{\Delta t} = \dfrac{E}{\Delta x^2}(C_{i-1}^n - 2C_i^n + C_{i+1}^n)$

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

◎ Crank-Nicholson Scheme

(1) Upwind (Backward) → Formulation CN-b

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = -\frac{u}{\Delta x}\underbrace{(C_i^\varepsilon - C_{i-1}^\varepsilon)}_{B.D.} + \frac{E}{\Delta x^2}(C_{i+1}^\varepsilon - 2C_i^\varepsilon + C_{i-1}^\varepsilon)$$

$\varepsilon = n$ → Explicit

$\varepsilon = n+1$ → Implicit

(Explicit and Implicit: 4Point scheme)

$\varepsilon = n + \dfrac{1}{2}$ → Crank-Nicholson

$$C_i^{n+\frac{1}{2}} = \frac{1}{2}(C_i^n + C_i^{n+1})$$

$$\therefore \frac{C_i^{n+1} - C_i^n}{\Delta t} = -\frac{u}{\Delta x}\left\{\frac{1}{2}(C_i^n + C_i^{n+1}) - \frac{1}{2}(C_{i-1}^n + C_{i-1}^{n+1})\right\}$$

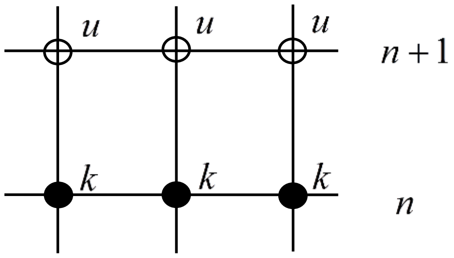
$$+\frac{E}{\Delta x^2}\left\{\frac{1}{2}(C_{i+1}^n + C_{i+1}^{n+1}) - \frac{1}{2}\cdot 2(C_i^n + C_i^{n+1}) + \frac{1}{2}(C_{i-1}^n + C_{i-1}^{n+1})\right\}$$

$$\left(\frac{E\Delta t}{2\Delta x^2} - \frac{u\Delta t}{2\Delta x}\right)C_{i-1}^{n+1} + (1 + \frac{u\Delta t}{2\Delta x} + \frac{E\Delta t}{\Delta x^2})C_i^{n+1} - \frac{E\Delta t}{2\Delta x^2}C_{i+1}^{n+1}$$

$$= \left(\frac{E\Delta t}{2\Delta x^2} + \frac{u\Delta t}{2\Delta x}\right)C_{i-1}^n + (1 - \frac{u\Delta t}{2\Delta x} - \frac{E\Delta t}{\Delta x^2})C_i^n + \frac{E\Delta t}{2\Delta x^2}C_{i+1}^n$$

$$[A]\{C\}^{n+1} = [B]\{C\}^n + \{b\}$$

$[A],[B]$ $\rightarrow$ Tridiagonal Method



6 Point scheme

- 3 knowns @ time level n
- 3 unknowns @ time level n+1

C-N method $\rightarrow O(\Delta x + \Delta t^2)$

Fully Implicit $\rightarrow O(\Delta x + \Delta t)$

(2) Central difference for $\dfrac{\partial C}{\partial x}$ $\rightarrow$ Formulation CN-cd

$$C_i^{n+1} - C_i^n = -\frac{u\Delta t}{2\Delta x}\underbrace{(C_{i+1}^{\varepsilon} - C_{i-1}^{\varepsilon})}_{C.D} + \frac{E\Delta t}{\Delta x^2}(C_{i+1}^{\varepsilon} - 2C_i^{\varepsilon} + C_{i-1}^{\varepsilon})$$

$\varepsilon = n$ Explicit

$\varepsilon = n+1$ Implicit

$\varepsilon = n + \dfrac{1}{2}$ C-N

$$C_i^{n+1} - C_i^n = -\frac{u\Delta t}{2\Delta x}\left\{\frac{1}{2}(C_{i+1}^n + C_{i+1}^{n+1}) - \frac{1}{2}(C_{i-1}^n + C_{i-1}^{n+1})\right\}$$

$$+\frac{E}{\Delta x^2}\left\{\frac{1}{2}(C_{i+1}^n + C_{i+1}^{n+1}) - \frac{1}{2}\cdot 2(C_i^n + C_i^{n+1}) + \frac{1}{2}(C_{i-1}^n + C_{i-1}^{n+1})\right\}$$

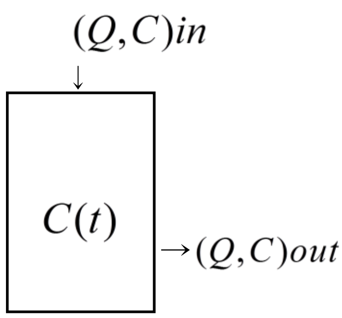
$$\left(\frac{E\Delta t}{2\Delta x^2} - \frac{u\Delta t}{4\Delta x}\right)C_{i-1}^{n+1} + \left(1 + \frac{E\Delta t}{\Delta x^2}\right)C_i^{n+1} + \left(\frac{u\Delta t}{4\Delta x} - \frac{E\Delta t}{2\Delta x^2}\right)C_{i+1}^{n+1}$$

$$= \left(\frac{E\Delta t}{2\Delta x^2} + \frac{u\Delta t}{4\Delta x}\right)C_{i-1}^n + \left(1 - \frac{E\Delta t}{\Delta x^2}\right)C_i^n + \left(\frac{E\Delta t}{2\Delta x^2} - \frac{u\Delta t}{4\Delta x}\right)C_{i+1}^n$$

◎ Models based on Solutions to Ordinary Differential Equations

Consider transient zero dimensional problems (Box model)

$$\frac{dc}{dt} = S + Q(C_{in} - C_{out})$$



→ Initial value problem

→ Solution marches forward in time

(1) Euler Method (Explicit method)

$$\frac{dc}{dt} \approx \frac{C^{n+1} - C^{n}}{\Delta t} \qquad \sigma(\Delta t)$$

then

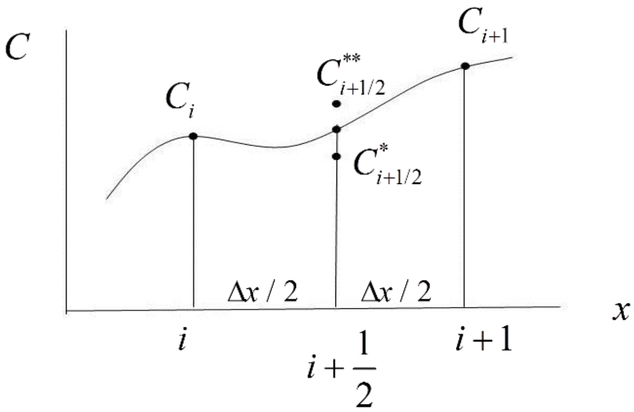
$$C^{n+1} = C^{n} + \Delta t\left[S + Q(C_{in} - C_{out})\right]$$

in which $S = S(C^{n})$

$\therefore$ Choose Δt, march forward in time

(2) Runge-Kutta Method

- 2nd order RK
- 4th order RK → most popular
- 5th order RK



Given $\dfrac{dc}{dx} = f(x,c)$

$$C_{i+1} = C + \Delta C_i$$

Calculate in order

$$C^{*}_{i+\frac{1}{2}} = C_i + \frac{\Delta x}{2} f\left(C_i, X_i\right)$$

$$C^{**}_{i+\frac{1}{2}} = C_i + \frac{\Delta x}{2} f\left(C^{*}_{i+1/2}, X_{i+\frac{1}{2}}\right)$$

$$C^{*}_{i+1} = C_i + \frac{\Delta x}{2} f\left(C^{**}_{i+1/2}, X_{i+\frac{1}{2}}\right)$$

Then

$$C_{i+1} = C_i + \Delta x\left[\frac{1}{6} f(C_i, X_i) + \frac{1}{3} f\left(C^{*}_{i+1/2}, X_{i+\frac{1}{2}}\right) + \frac{1}{3} f\left(C^{**}_{i+1/2}, X_{i+\frac{1}{2}}\right) + \frac{1}{6} f\left(C^{*}_{i+1} + X_{i+1}\right)\right]$$

$$\sim \mathrm{O}\left(\Delta x^4\right)$$

◎ 4th R-K with Runge's coefficient

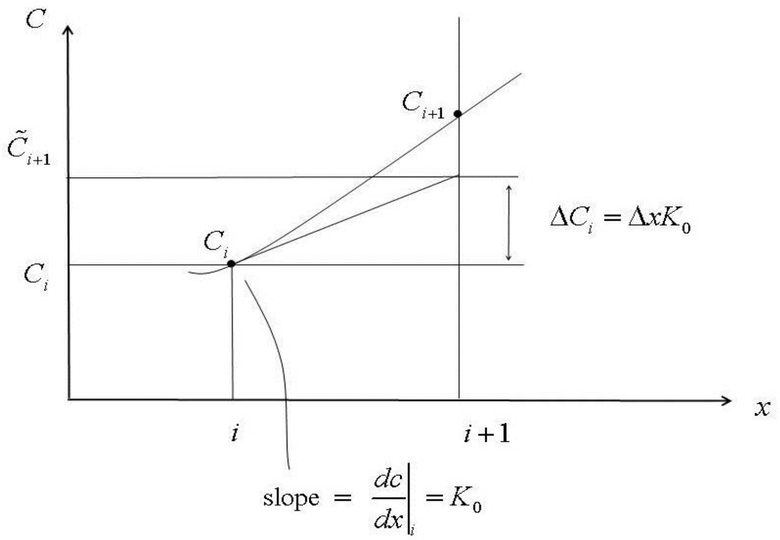
○ Euler's Method

$$\frac{dc}{dx} = f(x,c) \quad \rightarrow \left| C_{i+1} = C_i + \Delta x f(x,c) + \mathrm{O}(\Delta x) \right.$$

$$C_{i+1} = C_i + \Delta C_i$$

$$\Delta C_i = \frac{\Delta x}{6}\left[K_0 + 2K_1 + 2K_2 + K_3\right] \sim \mathrm{O}\left(\Delta x^4\right)$$

~ weighted average of slopes



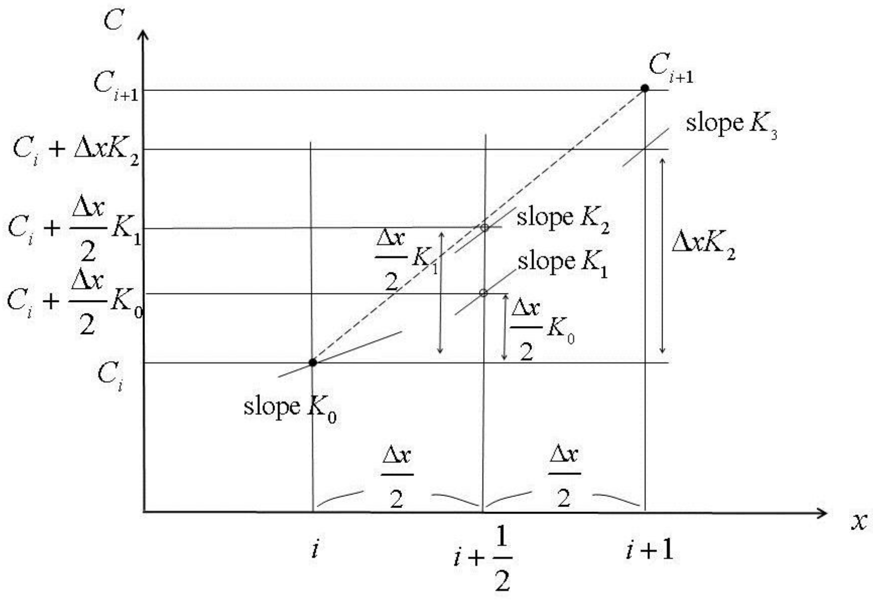
in which

$$K_0 = f\left(x_i, c_i\right)$$

$$K_1 = f\left(x_i + \frac{\Delta x}{2}, C_i + \frac{K_0}{2}\Delta x\right)$$

$$K_2 = f\left(x_i + \frac{\Delta x}{2}, C_i + \frac{K_1}{2}\Delta x\right)$$

$$K_3 = f\left(x_i + \Delta x, C_i + K_2 \Delta x\right)$$



○ Derivation by Taylor series expansion

→ see "Computer Applications of Numerical Methods", S. Kuo (1972) p.137

◎ R-K formula with Kutta coefficient

$$C_{i+1} = C_i + \Delta C_i$$

$$\Delta C_i = \frac{\Delta x}{8}\left(K_0 + 3K_1 + 3K_2 + K_3\right)$$

$$K_0 = f\left(X_i, C_i\right)$$

$$K_1 = f\left(x_i + \frac{\Delta x}{3}, C_i + \frac{K_0}{3}\Delta x\right)$$

$$K_2 = f\left[x_i + \frac{2\Delta x}{3}, C_i + (\frac{-K_0 + K_1}{3})\Delta x\right]$$

$$K_3 = f\left[x_i + \Delta x, C_i + (K_0 - K_1 + K_2)\Delta x\right]$$

◎ Simpson rule

~ Special case of R-K with Runge coefficients

If $\dfrac{dc}{dx} = f(only\, x)$ independent of C

Then $C_{i+1} = C_i + \Delta C_i$

$$\Delta C_i = \frac{\Delta x}{6}\left(K_0 + 2K_1 + 2K_2 + K_3\right)$$

$$K_0 = f\left(x_i\right),$$

$$K_1 = f\left(x_i + \frac{\Delta x}{2}\right),$$

$$K_2 = f\left(x_i + \frac{\Delta x}{2}\right),$$

$$K_3 = f\left(x_i + \Delta x\right)$$

$$\therefore \Delta C_i = \frac{\Delta x}{6}\left[f(x_i) + 4f\left(x_i + \frac{\Delta x}{2}\right) + f\left(x_i + \Delta x\right)\right]$$

◎ 1-D Steady-state Problem

$$u\frac{dc}{dx} = E\frac{d^2c}{dx^2} - kC$$ ① 2nd order ODE

Let $Z = \dfrac{dc}{dx}$

then ① becomes coupled 1st-order ODE

$$uz = E\frac{dz}{dx} - kC$$ ②

$$Z = \frac{dc}{dx} \qquad ③$$

Boundary conditions (Initial Conditions)

(i) Initial Value Problems

$$c(0) = c_0 \qquad @ \;\; x = 0$$

$$\frac{dc}{dx}\Big|_0 = z_0 \qquad @ \;\; x = 0$$

Solve simultaneously by using either Euler or R-K method

② : $$\frac{dz}{dx} = \frac{u}{E} z + \frac{k}{E} e = f_1(z, c, x)$$

③ : $$\frac{dc}{dx} = z = f_2(z, c, x)$$

$$c^*_{i+\frac{1}{2}} = c_i + \frac{\Delta x}{2} z_i$$

$$z^*_{i+\frac{1}{2}} = z_i + \frac{\Delta x}{2}\left(\frac{u}{E} z_i + \frac{k}{E} c_i\right)$$

$$c^{**}_{i+\frac{1}{2}} = c_i + \frac{\Delta x}{2} z^*_{i+\frac{1}{2}} = c_i + \frac{\Delta x}{2} f_2\left(z^*_{i+\frac{1}{2}}, c^*_{i+\frac{1}{2}}, x_{i+\frac{1}{2}}\right)$$

$$z^{**}_{i+\frac{1}{2}} = z_i + \frac{\Delta x}{2} f_1\left(z^{*}_{i+\frac{1}{2}}, c^{*}_{i+\frac{1}{2}}, x_{i+\frac{1}{2}} \right) = z_i + \frac{\Delta x}{2}\left(\frac{u}{E} z^{*}_{i+\frac{1}{2}} + \frac{k}{E} c^{*}_{i+\frac{1}{2}} \right)$$

$$c^{*}_{i+1} = c_i + \Delta x f_2\left(z^{**}_{i+\frac{1}{2}}, c^{**}_{i+\frac{1}{2}}, x^{**}_{i+\frac{1}{2}} \right)$$

$$= c_i + \Delta x\, z^{**}_{i\frac{1}{2}}$$

$$z^{**}_{i+1} = z_i + \Delta x\left(\frac{u}{E} z^{**}_{i+\frac{1}{2}} + \frac{k}{E} c^{**}_{i+\frac{1}{2}} \right)$$

$$\therefore \quad c_{i+1} = c_i + \frac{\Delta x}{6}\left[z_i + 2z^{*}_{i+\frac{1}{2}} + 2z^{**}_{i+\frac{1}{2}} + z^{*}_{i+1} \right]$$

$$z_{i+1} = z_i + \frac{\Delta x}{6}\left[\left(\frac{u}{E} z_i + \frac{k}{E} c_i \right) + 2\left(\frac{u}{E} z^{*}_{i+\frac{1}{2}} + \frac{k}{E} c^{*}_{i+\frac{1}{2}} \right) \right.$$

$$\left. + 2\left(\frac{u}{E} z^{**}_{i+\frac{1}{2}} + \frac{k}{E} c^{**}_{i+\frac{1}{2}} \right) + \left(\frac{u}{E} z^{*}_{i+1} + \frac{k}{E} c^{*}_{i+1} \right) \right]$$

(ii) Boundary value problems

$$c = c_0 \qquad @ \quad x = 0$$

$$c = c_L \qquad @ \quad x = L$$

→ use "Shooting method"

Guess z_0 @ $x = 0$

Solve ② and ③ simultaneously by using $R-K$

check $c_L^j = c_L$

Vary z_0 such that target = c_L is hit

→ "Shooting method"

• Iteration rules for Shooting method

let $z_0^j = j th$ estimate of $\frac{dc}{dx}\Big|_{x=0}$

$z_0^{j+1} = j+1 th$ estimate of $\frac{dc}{dx}\Big|_{x=0}$

By interpolation

$$z_0^{j+1} = z_0^j - \frac{c_L^j - c_L}{c_L^j - c_L^{j-1}}(z_0^j - z_0^{j-1})$$

<Ref.>

1. Pinder, G. and W. Gray, Finite Element Simulation in Surface and Subsurface Hydrology, Academic Press, New York, 1977

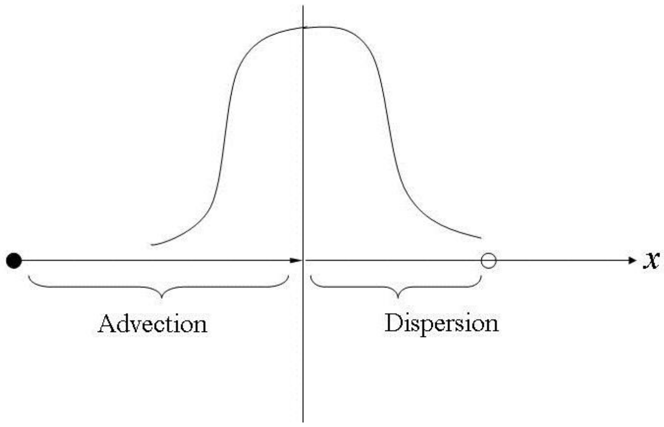
2. Ames, W.F. , Numerical Methods for Partial Differential Equations, Academic Press, New York, 1977

3. Richtmyer, R.D. and K.W. Morton, Difference Methods for Initial-Value Problems, Interscience Publishers, 1967.

4. Lapidus, L. and G.F. Pinder, Numerical Solution of Partial Differential Equations in Science and Engineering, A Wiley-Interscience Publication, 1982.

8.4 Finite Particle ("Random Walk") Model

~ based an the concept that dispersion is a random process



New position = Old position + Advection + Dispersion

~ In the computer code, enough particles are included (released) so that their locations and density are adequate to describe the distribution of the dissolved constituent of interest

→ "Giant Molecule" method

~ release a number of particles, each representing a finite mass of solute, at a rate proportional to the strength of each source.

The particles are then "tracked" in space and time. → "Particle Tracking" method

Ref. Prickett et al. (1981)

○ Distribution of concentration of solute

~ represented by the distribution of a finite number of discrete particles

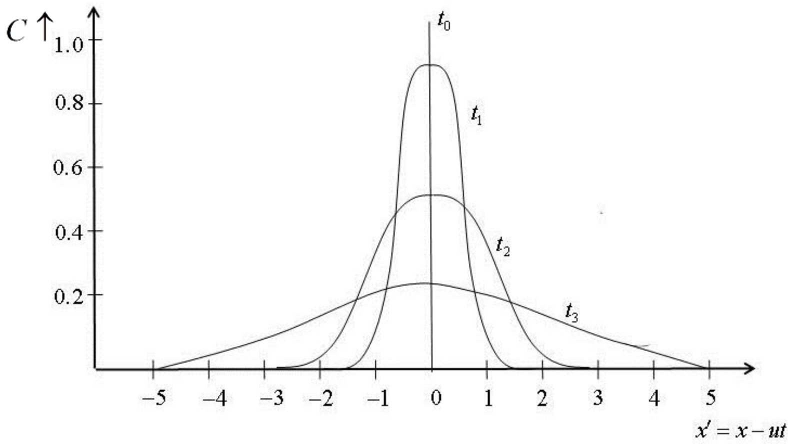
~ each particle is moved by flow and is assigned a mass which represents a fraction of the total mass of chemical constituent.

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = E\frac{\partial^2 c}{\partial x^2} \qquad (-kc) \tag{1}$$

If a unit slug of solute placed initially at $x = 0$

then analytical solution is

$$c(x,t) = \frac{1}{\sqrt{4\pi Et}} \exp\left[-\frac{(x-ut)^2}{4Et} \right] \qquad (2)$$



◎ Statistics

○ Random variable x if said to be normally distributed if its density function, $n(x)$ is given by

$$n(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2} \right] \qquad (3)$$

$\sigma =$ standard deviation

$\mu =$ mean

Now, if we let

$$\sigma = \sqrt{2Et} \qquad (4)$$

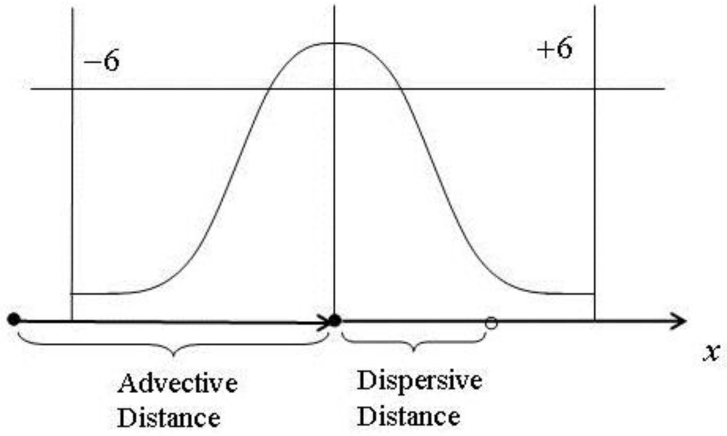
$$\mu = ut \qquad (5)$$

$$n(x) = c(x,t) \qquad (6)$$

Then Eqs (2) and (3) are equivalent.

So, the key to solute transport is the realization that dispersion can be considered a random process, tending to the normal distribution.

○ Random walk modeling



Advective distance $= u\,\Delta t$ (7)

Δt = time increment

Dispersive distance $= \pm 6\sigma$

$$= \sqrt{2E\Delta t}\ \text{ANORM}(0) \quad (8)$$

in which $\pm 6\sigma =$ Probable locations of particles out to 6 standard deviations either side of the mean (> 99.9%)

ANORM (0) = a random number between -6 and +6, drawn from a normal distribution of numbers having a standard deviation of 1 and a mean of zero.

∴ New position of the particle

$$= \text{Old position} + u\Delta t + \sqrt{2E\Delta t}\ \text{ANORM(0)} \tag{9}$$

◎ Repeat for numerous particles, all having the same initial position and advection term.

→ Create a map of the new positions of the particles having the discrete density function.

$$c(x,t) \rightarrow n(x) \rightarrow \frac{N}{\Delta x}$$

$$= \frac{N_0}{\sqrt{2\pi}\sqrt{2\Delta x E \Delta t}} \exp\left[-\frac{(x-u\Delta t)^2}{4\Delta x E \Delta t}\right] \tag{10}$$

in which Δx = incremental distance over which N particles are found

N_o = total number of particles in the experiment

◎ The distribution of particles around the mean position, $u\Delta t$, is made to be normally distributed via the function ANORM(0)

○ Generation of ANORM(0) in computer code.

(1) Summation of Random function

$$\text{ANORM(0)} = \sum_{i=1}^{12} \underbrace{RF(0,1)}_{||} - 6$$

In LOTUS or EXCEL (RAND())

use @RAND function to generate a uniform random number between 0 and 1 = $U(0,1)$

(2) Multiply Random function

$$\text{ANORM(0)} = \underbrace{RF(0,1)}_{RAND()} \times 12 - 6$$

◎ Numerical Recipes

ANORM(0)= GASDEV (IDUM)

RAND() = RAN1(IDUM)

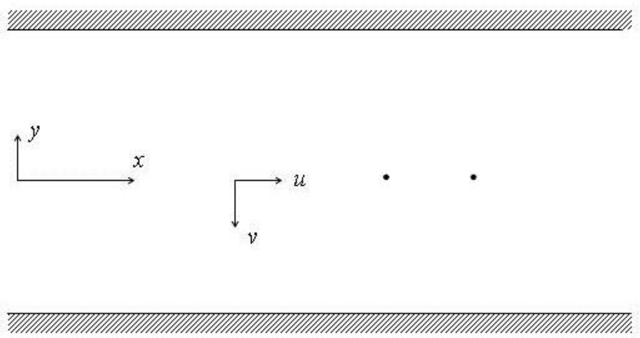
◎ Advantages of the Random-walk technique

1. There is no numerical dispersion, despite the use of an Eulerian framework.
2. Computer CPU time is drastically reduced. Solutions are additive. If not enough particles are included for adequate definition in one run, subsequent runs may be made and the results of these may be superimposed upon the first.
3. This method is particularly suited to time-sharing systems where velocity fields can be stored.

◎ Disadvantages

1. It may require a large number of particles to obtain meaningful results.
2. It doesn't easily accommodate nonlinear kinetic expressions.

◎ 2-D Model : Depth-averaged



$$\frac{\partial c}{\partial t}+u(x,y)\frac{\partial c}{\partial x}+\upsilon(x,y)\frac{\partial c}{\partial y}=\frac{\partial}{\partial x}\left(\varepsilon_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(\varepsilon_y\frac{\partial c}{\partial y}\right)+S$$

in which

$$\varepsilon_x = 5.93du_*$$

$$\varepsilon_y = 0.6du_*$$

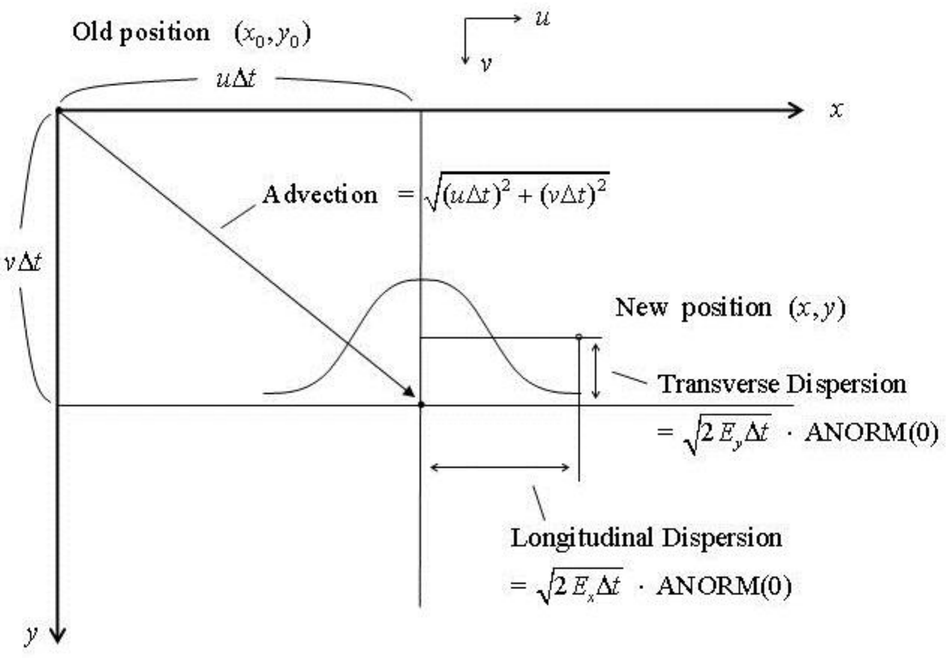
$$u_* = \sqrt{gds}$$

cf) 1-D Model : Depth & Width-averaged

(Cross-sectional)

$$\frac{\partial c}{\partial t}+U\frac{\partial c}{\partial x}=\frac{\partial}{\partial x}(D_L\frac{\partial c}{\partial x})$$

◎ 2-D Advection-Dispersion Model



○ Longitudinal and transverse dispersion take place simultaneously

$$x = x_0 + u\Delta t + \sqrt{2E_x\Delta t} \quad \text{ANORM (0)}$$

$$y = y_0 + \upsilon\Delta t + \sqrt{2E_y\Delta t} \quad \text{ANORM (0)}$$

○ In natural rivers

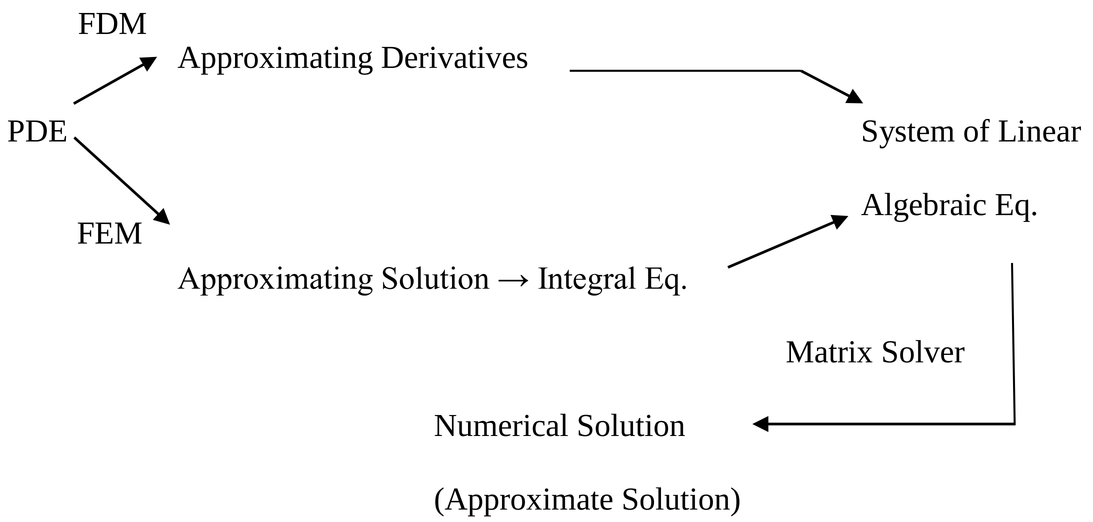
$$E_Y = 5.93\, dU_*$$

$$E_y = 0.6\, dU_*$$

8.5 Finite Element Method

$$G.E.: \quad \frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(E\frac{\partial c}{\partial x} - uc \right) \qquad \text{PDE} \qquad ①$$

○ Numerical solutions to PDE



8.5.1 Procedure (Summary) of FEM

1. Discretize domain into elements.

2. Select Basis Functions.

3. Derive an Integral equation based on. Method of Weighted Residuals (MWR).

4. Compute element matrix and vectors.

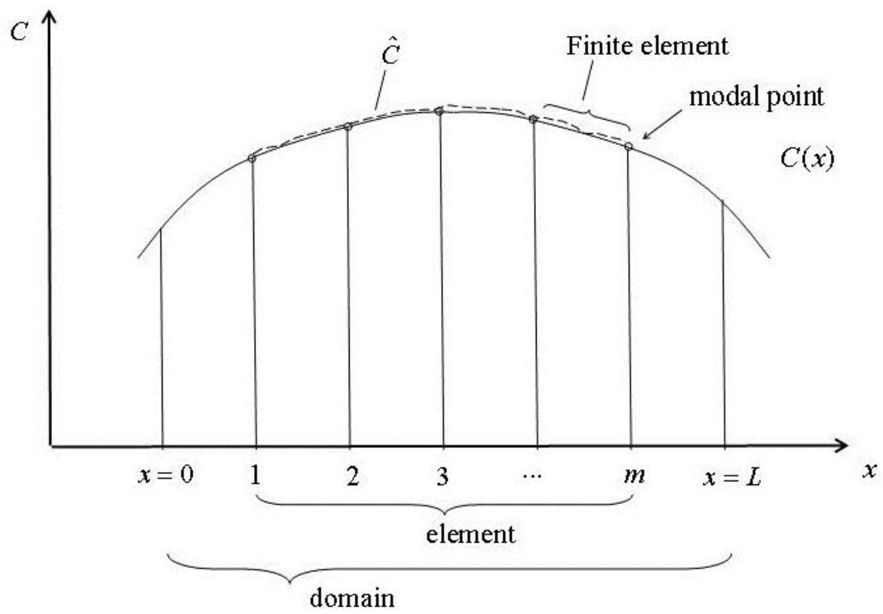
5. Assemble global matrix and vectors.

6. Incorporate boundary conditions.

7. Use a finite difference for time discretization.

8. Solve a system of simultaneous linear algebraic eg.

A. Domain Discretization



$c(x) =$ true(and unknown) solution to PDE

continuous function of x

$\hat{c}(x) =$ approximate solution

piecewise continuous function

We may approximate the true solution by a polynomial

$$\hat{c}^e(x) = \sum_{j=1}^{m} c_j \phi_j^{\,e}(x) \qquad ②$$

in which

ϕ_j = basis function (shape, approximate) functions

Now, we are seeking the "best" value of the c_j to give us the best values for $\hat{c}^e(x)$

B. Basis functions

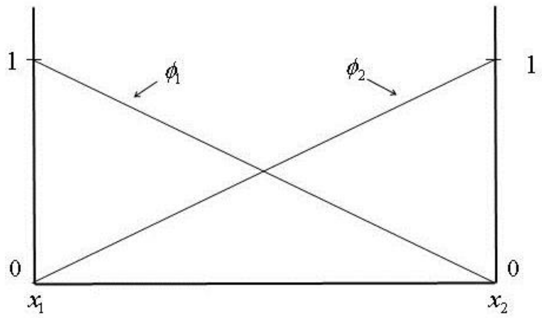
(1) Lagrangian Interpolating Polynomials

$$\phi_j(x) = \prod_{\substack{k=1 \\ k \neq j}}^{m} \frac{x - x_k}{x_j - x_k}$$

(i) linear ; m=2

$$\phi_1(x) = \frac{x - x_2}{x_1 - x_2}$$

$$\phi_2(x) = \frac{x - x_1}{x_2 - x_1}$$



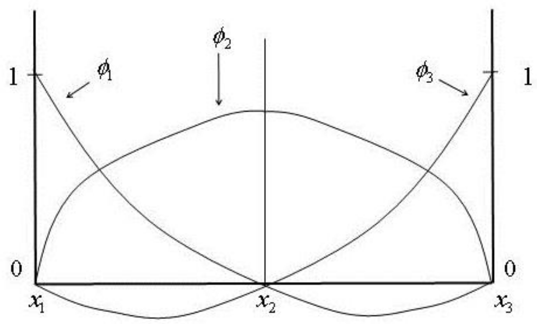
$$\therefore \hat{c}^e(x) = c_1\phi_1(x) + c_2\phi_2(x)$$

(ii) quadratic ; m=3

$$\phi_1(x) = \frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)}$$

$$\phi_2(x) = \frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)}$$

$$\phi_3(x) = \frac{(x - x_1)(x - x_2)}{(x_3 - x_1)(x_3 - x_2)}$$



$$\therefore \hat{c}^e(x) = c_1\phi_1(x) + c_2\phi_2(x) + c_3\phi_3(x)$$

(2) Hermitian Interpolating Polynomials

~ interpolate $c(x_i)$ and $\left.\frac{dc}{dx}\right|_{x_i}$ (function and slope)

$$c(x) \approx \sum_{j=1}^{m}\left[c_j\phi_j^{(0)} + \left(\frac{dc}{dx}\right)_j \phi_j^{(1)}\right]$$

C. Method of Weighted Residuals

◎ Formulation of approximating integral equation

{ Variational method
Method of Weighted Residuals (MWR)

MWR :

Substitute ② into ①

$$\frac{\partial \hat{c}}{\partial t} - \frac{\partial}{\partial x}\left(E\frac{\partial \hat{c}}{\partial x} - u\hat{c}\right) \neq 0 = R(x,t) \qquad \text{......residual} \qquad ③$$

If $\hat{c} = c$ then $R(x,t) = 0$

But $\hat{c} \neq c$ $R(x,t) \neq 0$

So, in the MWR, an attempt is made force this residual to zero through selection of the constant $c_j\,(j = 1, 2, ...M)$.

Let's set the weighted integrals of the residual to zero, i.e., →MWR

$$\int_{\Omega^e} R(x,t)\omega_i(x)\,d\Omega = 0, \qquad i = 1, 2, ...M \qquad ④$$

→ Integral Eq.

$$\int\left\{\frac{\partial\hat{c}}{\partial t}-\frac{\partial}{\partial x}\left(E\frac{\partial\hat{c}}{\partial x}-u\hat{c}\right)\right\}\cdot\omega_i\left(x\right)dx=0 \qquad ⑤$$

There are several MWRs which is distinguished by the choice of weighting function ω_i

(1) Galerkin method : $\omega_i=\phi_i\left(x\right)$

(2) Subdomain method

divide domain B into M subdomains B_i

$$\omega_j=\left[\begin{array}{l}1,\ x\ in\ B_i\\ 0,\ x\ not\ in\ B_i\end{array}\right.$$

(3) Collocation method

M point x_i (collocation points) are specified in B and weighting functions are Dirac delta functions

$$\omega_i=\delta(x-x_i)$$

which have the property that

$$\int_B R\left(x\right)\omega_i dx=R\left(x_i\right)=0$$

(4) Least Squares Method

$$\omega_i=p\left(x\right)\frac{\partial R}{\partial a_i}$$

p(x) = arbitrary positive function

minimize the integrated square residual w.r.t a_i

$$I = \int p(x) R^2(x) dx$$

$$\therefore \frac{\partial I}{\partial a_i} = 0 \quad (i = 1, 2, ..., M)$$

FDM ~ domain of interest is replaced by a set of discrete points

FEM ~ domain is divided into subdomains (finite elements) unknown function C is represented by an interpolating polynomials within each element

$$u(\cdot) \approx \hat{u}(\cdot) = \sum_{j=1}^{N} u_j \phi_j(\cdot), \quad j = 1, 2, ..., N$$

$u_j =$ undetermined coefficient

$\phi_j(\cdot) =$ function over both time and space

$\phi_j(\cdot) =$ Basis (shape, interpolation) function

~ chosen to be polynomials that satisfy certain boundary conditions imposed on the problem

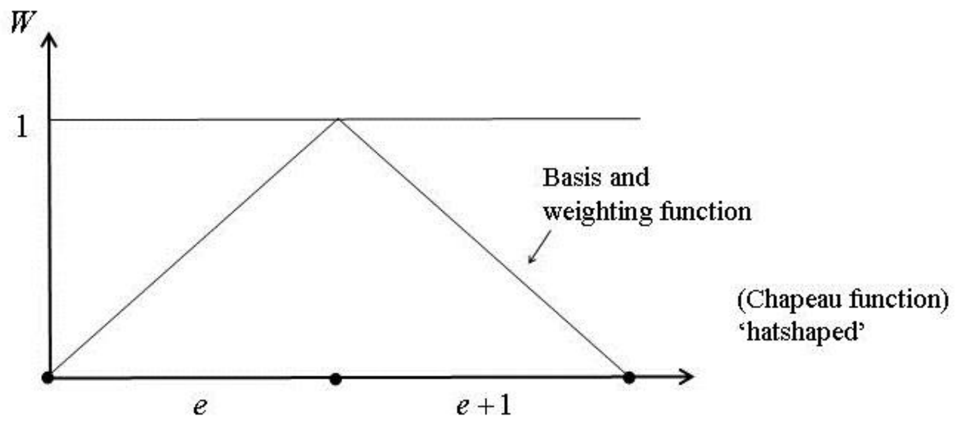
PDE : $Lu - f = 0$

$L\hat{u}(\cdot) - f = R(\cdot) =$ residual

The objective is to select the undetermined coefficients u_j such that this residual is minimized in some sense.

$$\int_t \int_v R(\cdot) \omega_i(\cdot) dv dt = 0, \qquad i = 1, 2, ..., N$$

(1) Galerkin Method



~ Weighting function is chosen to be the basis function

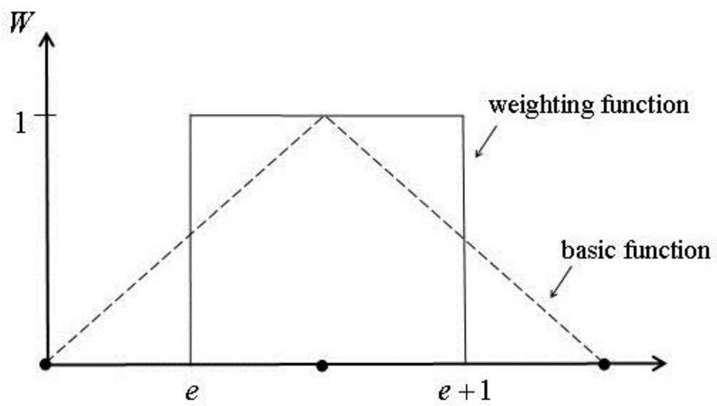
$$\int_t \int_v R(\cdot)\phi_i(\cdot)\,dv\,dt = 0, \qquad i = 1, 2, ..., N$$

(2) Subdomain Method

$$\int_v R(x)\,\omega_i\,dv = 0, \qquad i = 1, 2, ..., N$$

where

$$\omega_i = \begin{cases} 1, & (x, y, z) \ in \ v_i^* \\ 0, & (x, y, z) \ not \ in \ v_i^* \end{cases}$$



~ integrations are less tedious than those in Galerkin's method

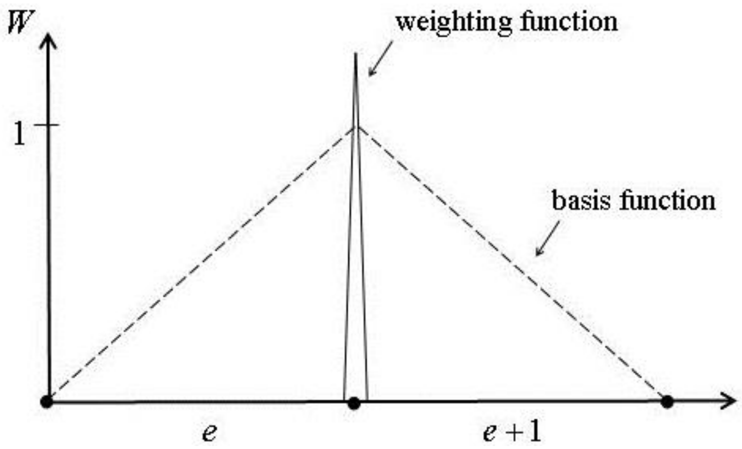
(3) Collocation Method

~ Weighting function is chosen to be the Dirac delta

$$\omega_i = \delta(x - x_i)$$

$$\int_t \int_v R(\cdot)\delta_i(\cdot)\,dvdt = 0, \qquad i = 1, 2, 3, \ldots, N$$

~ Calculate the value of residual at the selected points



$$\int_t \int_v a(\cdot)\delta_i(x - x_i, y - y_i, z - z_i, t - t_i)\,dvdt \equiv a\Big|_{x_i, y_i, z_i, t_i}$$

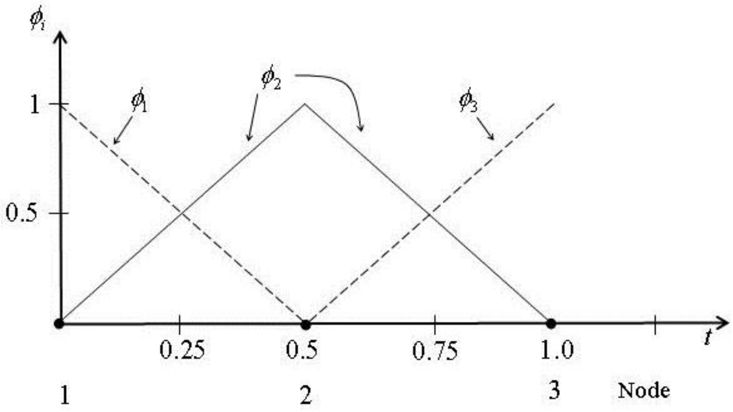
<Example>

$$\frac{dT}{dt} + k(T - T_e) = 0$$

$$0 \le t \le 1$$

$$T(t = 0) = 1$$

$$k = 2 \quad ; \quad T_e = \frac{1}{2}$$



$$\phi_i = \begin{cases} \dfrac{t - t_{i-1}}{t_i - t_{i-1}}, & t_{i-1} \le t \le t_i \\ \dfrac{t_{i+1} - t}{t_{i+1} - t_i}, & t_i \le t \le t_{i+1} \end{cases}$$

i = nodal points

1. $T \approx \hat{T} = \sum_{j=1}^{3} T_j \phi_j(t)$

2. $\int_t R(t)\, w_i(t)\, dt = 0, \quad i = 1,$

$$\int_t \left\{ \frac{d\hat{T}}{dt} + k(\hat{T} - T_e) \right\} w_i(t)\, dt = 0$$

$$\int_t \left\{ \sum_{j=1}^{3} T_j \left(\frac{d\phi_j}{dt} + k\phi_j \right) - kT_e \right\} w_i(t)\, dt = 0, \quad i = 1,2,3$$

3. Galerkin

$$\sum_{j=1}^{3} T_j \int_0^1 \left\{ \frac{d\phi_j}{dt} + k\phi_j \right\} \phi_i\, dt = \int_0^1 kT_e \phi_i\, dt, \qquad i = 1,2,3$$

$$i = 1 \ : \quad \sum_{j=1}^{3} T_j \int_0^1 \left\{ \frac{d\phi_j}{dt} + k\phi_j \right\} \phi_1\, dt = \int_0^1 kT_e \phi_1\, dt$$

$$i = 1 \qquad T_1 \int_0^1 \left\{ \frac{d\phi_1}{dt} + k\phi_1 \right\} \phi_1\, dt + T_2 \int_0^1 \left\{ \frac{d\phi_2}{dt} + k\phi_2 \right\} \phi_1\, dt + T_3 \int_0^1 \left\{ \frac{d\phi_3}{dt} + k\phi_3 \right\} \phi_1\, dt = \int_0^1 kT_e \phi_1\, dt$$

$$i=2 \qquad T_1\int_0^1\left\{\frac{d\phi_1}{dt}+k\phi_1\right\}\phi_2 dt+T_2\int_0^1\left\{\frac{d\phi_2}{dt}+k\phi_2\right\}\phi_2 dt+T_3\int_0^1\left\{\frac{d\phi_3}{dt}+k\phi_3\right\}\phi_2 dt=\int_0^1 kT_e\phi_2 dt$$

$$i=3 \qquad T_1\int_0^1\left\{\frac{d\phi_1}{dt}+k\phi_1\right\}\phi_3 dt+T_2\int_0^1\left\{\frac{d\phi_2}{dt}+k\phi_2\right\}\phi_3 dt+T_3\int_0^1\left\{\frac{d\phi_3}{dt}+k\phi_3\right\}\phi_3 dt=\int_0^1 kT_e\phi_3 dt$$

$$\phi_1\phi_3=0$$

Expansion yields the following matrix equation

$$\begin{bmatrix} \int_0^{\frac{1}{2}}\left(\frac{d\phi_1}{dt}\phi_1+k\phi_1\phi_1\right)dt & \int_0^{\frac{1}{2}}\left(\frac{d\phi_2}{dt}\phi_1+k\phi_2\phi_1\right)dt & 0 \\ \int_0^{\frac{1}{2}}\left(\frac{d\phi_1}{dt}\phi_2+k\phi_1\phi_2\right)dt & \int_0^1\left(\frac{d\phi_2}{dt}\phi_2+k\phi_2\phi_2\right)dt & \int_{\frac{1}{2}}^1\left(\frac{d\phi_2}{dt}\phi_2+k\phi_3\phi_2\right)dt \\ 0 & \int_{\frac{1}{2}}^1\left(\frac{d\phi_2}{dt}\phi_3+k\phi_2\phi_3\right)dt & \int_{\frac{1}{2}}^1\left(\frac{d\phi_3}{dt}\phi_3+k\phi_3\phi_3\right)dt \end{bmatrix}\begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix}=\begin{bmatrix} \int_0^{\frac{1}{2}}kT_e\phi_1 dt \\ \int_0^1 kT_e\phi_2 dt \\ \int_{\frac{1}{2}}^1 kT_e\phi_3 dt \end{bmatrix}$$

$$\frac{1}{2}\begin{bmatrix} -1+\frac{k}{3} & 1+\frac{k}{6} & 0 \\ -1+\frac{k}{6} & \frac{2k}{3} & 1+\frac{k}{6} \\ 0 & -1+\frac{k}{6} & 1+\frac{k}{3} \end{bmatrix}\begin{bmatrix} 1 \\ T_2 \\ T_3 \end{bmatrix}=\frac{1}{2}\begin{bmatrix} k\frac{T_e}{2} \\ kT_e \\ \frac{kT_e}{2} \end{bmatrix}$$

○ Basis functions (Interpolation)

$$c(x,t)\approx\hat{c}(x,t)=\sum_{j=1}^{m}\hat{c}_j(t)\phi_j^e(x,t)$$

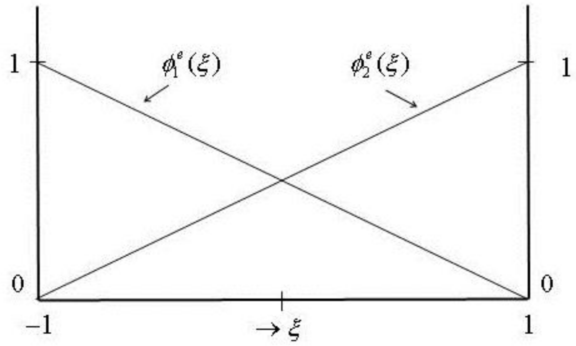
$$=\sum_{j=1}^{m}\hat{c}_j(t)\phi_j^e(x)$$

$$\frac{\partial\hat{C}}{\partial t}=\sum_{j=1}^{m}C_j\frac{\partial\phi_j}{\partial x}$$

$$\frac{\partial \hat{C}}{\partial t} = \sum_{j=1}^{m} \frac{dc}{dt} \phi_j(x)$$

○ Natural Coordinate System for element basis function

(Dimensionless ξ coordinate system where $-1 \le \xi \le 1$)



(1)Linear

$$\phi_1^e(\xi) = \frac{1}{2}(1-\xi)$$

$$\phi_2^e(\xi) = \frac{1}{2}(1+\xi)$$

$$\frac{d\phi_1^e}{d\xi} = -\frac{1}{2}$$

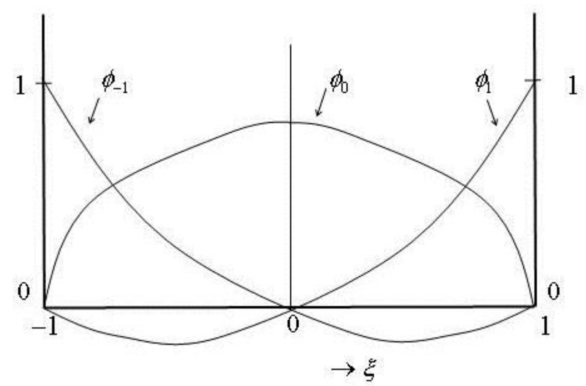
$$\frac{d\phi_2^e}{d\xi} = \frac{1}{2}$$

(2) Quadratic

$$\phi_{-1}(\xi) = -\frac{1}{2}\xi(1-\xi)$$

$$\phi_0(\xi) = 1-\xi^2$$

$$\phi_1(\xi) = \frac{1}{2}\xi(1+\xi)$$



◎ Galerkin method

Select the basis functions as the weighting functions

$$\omega_i = \phi_i$$

Thus the weighted integral equation of the residuals becomes

$$\int_{\Omega^e} \left\{ \frac{\partial \hat{c}}{\partial t} - \frac{\partial}{\partial x}\left(E \frac{\partial \hat{c}}{\partial t} - u\hat{c}\right) \right\} \phi_i dx = 0 \qquad ⑥$$

$$\underbrace{\int_{\Omega^e} \frac{\partial \hat{c}}{\partial t} \phi_i dx}_{A} - \underbrace{\int_{\Omega^e} \underbrace{\frac{\partial}{\partial x}\left(E \frac{\partial \hat{e}}{\partial x} - u\hat{e}\right)}_{d\upsilon} \overset{u}{\phi_i^e} \, dx}_{B} = 0$$

Term A ※ (See 7-1 for basis functions) – use Linear, Basis function

$$\int_{\Omega^e} \frac{\partial \hat{c}}{\partial t} \phi_i dx = \int_{\Omega^e} \sum_{j=1}^{m} \frac{dc_j}{dt} \phi_j^e(x) \phi_i^e dx$$

$$= \sum_{j=1}^{m} \frac{dc_j(t)}{dt} \int_{\Omega^e} \phi_j(x) \phi_i(x) dx$$

Term B : Integration by parts $\int udv = uv - \int vdu$

$$-\int_{\Omega^e} \frac{\partial \phi_i^e(x)}{\partial x}\left(E \frac{\partial \hat{c}}{\partial x} - u\hat{c}\right) + \left[\phi_i^e(x)\left(E \frac{\partial \hat{c}}{\partial x} - u\hat{c}\right) \right]_{x_1}^{x_m}$$

$$= -\frac{\partial \phi_i^e(x)}{\partial x} \left\{ E \sum_{j=1}^{m} C_j(t) \frac{\partial \phi_j^e(x)}{\partial x} - u \sum_{j=1}^{m} C_j(t) \phi_j^e(x) \right\} dx + \left[\phi_i^e(x)\left(E \frac{\partial \hat{c}}{\partial x} - u\hat{c}\right) \right]_{x_1}^{x_m}$$

$$=+\sum_{j=1}^{m} C_j(t)\left\{\int_{\Omega^e} E\frac{\partial\phi_j^e(x)}{\partial x}\ \frac{\partial\phi_j^e}{\partial x}dx - \int_{\Omega^e} u\phi_j^e(x)\frac{\partial\phi_i}{\partial x}dx\right\} - \left[\phi_i^e(x)(E\frac{\partial\hat{c}}{\partial x} - u\hat{c})\right]_{x_1}^{x_m}$$

∴ Eq ⑥ :

$$\sum_{J=1}^{M}\frac{d\hat{c}_j(t)}{dt}\int_{\Omega^e}\phi_j(x)\phi_i(x)dx + \sum_{j=1}^{m} c_j(t)\left\{\int_{\Omega^e} E\frac{\partial\phi_j^e(x)}{\partial x}\ \frac{\partial\phi_i^e(x)}{\partial x}dx\right.$$

$$\left.-\int_{\Omega^e} E\frac{\partial\phi_j^e(x)}{\partial x}\ \frac{\partial\phi_i^e(x)}{\partial x}dx\right\} - \left[\phi_i^e(x)(E\frac{\partial\hat{c}}{\partial x} - u\hat{c})\right]_{x_1}^{x_m} = 0 \qquad ⑦$$

Let

$$a_{ij}^e = \int_{\Omega^e} E\frac{\partial\phi_j^e(x)}{\partial x}\ \frac{\partial\phi_i^e}{\partial x}dx - \int_{\Omega^e} u\phi_j^e(x)\frac{\partial\phi_i}{\partial x}dx \quad , \quad i=1,\dots,m$$

$$m_{ij}^e = \int_{\Omega^e}\phi_j(x)\phi_i(x)dx \quad , \quad \{B\}^e = \begin{Bmatrix} \phi_1^e(x)(E\frac{\partial\hat{c}}{\partial x} - u\hat{c})_{x_1} \\ \cdot \\ \cdot \\ \phi_m^e(x)(E\frac{\partial\hat{c}}{\partial x} - u\hat{c})_{x_m} \end{Bmatrix}$$

D. Element matrix equation

~ Element matrix equation results in

$$[A]^e\{\hat{c}\} + [M]^e\left\{\frac{d\hat{c}}{dt}\right\} + \{B\}^e = 0 \qquad ⑧$$

Use Linear Basis function

$$a_{ij}^e = \int_{\Omega^e} E\frac{\partial\phi_j^e(x)}{\partial x}\ \frac{\partial\phi_i^e}{\partial x}dx - \int_{\Omega^e} u\phi_j^e(x)\frac{\partial\phi_i}{\partial x}dx$$

$$=\int_{-1}^{1} E \frac{\partial \phi_j}{\partial \xi} \frac{\partial \xi}{\partial x} \frac{\partial \phi_j}{\partial \xi} \frac{\partial \xi}{\partial x} d\xi \frac{dx}{d\xi} - \int_{-1}^{1} u\phi_j \frac{\partial \phi_j}{\partial \xi} \frac{\partial \xi}{\partial x} d\xi \frac{dx}{d\xi}$$

$$=\int_{-1}^{1} E \frac{\partial \phi_j}{\partial \xi} \frac{\partial \phi_i}{\partial \xi} d\xi \frac{d\xi}{dx} - \int_{-1}^{1} u\phi_j \frac{\partial \phi_i}{\partial \xi} d\xi$$

By the way

$$\frac{dx}{d\xi} = x_j \sum_{j=1}^{2} \frac{d\phi_j^e(\xi)}{d\xi} = x_1 \frac{d\phi_1^e}{d\xi} + x_2 \frac{d\phi_2^e}{d\xi}$$

$$= x_1(-\frac{1}{2}) + x_2(\frac{1}{2}) = \frac{1}{2}(x_2 - x_1) = \frac{\Delta x}{2}$$

$$a_{ij}^e = \int_{-1}^{1} E \frac{\partial \phi_j}{\partial \xi} \frac{\partial \phi_i}{\partial \xi} d\xi \left(\frac{2}{\Delta x}\right) - \int_{-1}^{1} u\phi_j \frac{\partial \phi_i}{\partial \xi} d\xi$$

$$m_{ij}^e = \int_{\Omega^e} \phi_j(x)\phi_i(x)\,dx = \int_{-1}^{1} \phi_j(\xi)\phi_i(\xi)\,d\xi \frac{dx}{d\xi}$$

$$= \int_{-1}^{1} \phi_j \phi_i \, d\xi \frac{\Delta x}{2}$$

$$B_i^e = -\left[\phi_i^e(x)\left(E\frac{\partial \hat{c}}{\partial x} - u\hat{c}\right)\right]_{x_1}^{x_2}$$

$$[A]^e = \begin{bmatrix} \frac{E}{\Delta x} - \frac{u}{2} & -\frac{E}{\Delta x} + \frac{u}{2} \\ -\frac{E}{\Delta x} - \frac{u}{2} & \frac{E}{\Delta x} + \frac{u}{2} \end{bmatrix}$$

$$[M]^e = \frac{\Delta x}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

$$\{B\}^e = \begin{Bmatrix} \left(E\dfrac{\partial \hat{c}}{\partial x} - u\hat{c} \right)_{x_1} \\ -\left(E\dfrac{\partial \hat{c}}{\partial x} - u\hat{c} \right)_{x_2} \end{Bmatrix}$$

E. Assemble global matrix equations

Combining element equations

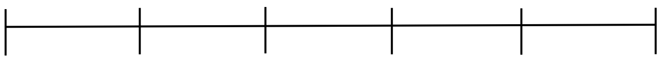
For each element, apply

$$[M]^e \left\{ \frac{dc}{dt} \right\} + [A]^e \{\hat{c}\} + \{B\}^e = 0$$

$[M]^e \,\&\, [A]^e$ ~ 2×2 matrices

○ Numbering Systems

Local



1 2 1 2 1 2 ...

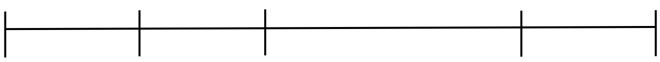
Element No 1 2 3 4 5

Global 1 2 3 4 5 6 ...

Let N (= number of element) = 30

number of nodes = 31

Then



x_1 x_2 x_3 x_N x_{N+1}

e=1 2 3

$$\underset{31\times 31}{[A]} = \sum_{e=1}^{30} [A]^e = \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & & & & \\ a_{21}^{(1)} & a_{22}^{(1)} + a_{11}^{(2)} & a_{12}^{(2)} & & 0 & \\ & a_{21}^{(2)} & a_{22}^{(2)} + a_{11}^{(3)} & & & \\ & & & \ddots & & \\ & 0 & & & a_{22}^{(29)} + a_{11}^{(30)} & a_{12}^{(30)} \\ & & & & a_{21}^{(30)} & a_{22}^{(30)} \end{bmatrix}$$

$$\underset{31\times 31}{[M]} = \sum_{e=1}^{30} [M]^e \qquad \sim \quad same \ \ as \ \ [A]$$

$$\underset{31\times 1}{[B]} = \sum_{e=1}^{30} \{B\}^e = \begin{Bmatrix} B_1^{(1)} \\ B_2^{(1)} + B_1^{(2)} \\ B_2^{(2)} + B_1^{(3)} \\ \cdot \\ \cdot \\ \cdot \\ B_2^{(29)} + B_1^{(30)} \\ B_2^{(30)} \end{Bmatrix} = \begin{Bmatrix} B_1^{(1)} \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ B_2^{(30)} \end{Bmatrix}$$

Since $q_u^e + q_L^{e+1} = 0$

◎ Boundary Conditions

$$At \quad x = x_1 \;\; ; u\hat{c} - E\frac{\partial \hat{c}}{\partial x} = uc_o$$

$$At \quad x = x_N \;\; ; u\hat{c} - E\frac{\partial \hat{c}}{\partial x} = uc_N$$

F. Time discretization

(1) Fully Implicit

$$[M]\frac{\{\hat{C}\}^{k+1} - \{\hat{e}\}^{k}}{\Delta t} + [A]\{\hat{C}\}^{k+1} + \{B\}^{k+1} = 0 \qquad ⑨$$

$$\left(\frac{[M]}{\Delta t} + [A]\right)\left\{\tilde{C}\right\}^{k+1} = \frac{[M]}{\Delta t}\left\{\hat{C}\right\}^{k} - \{B\}^{k+1}$$

$$[R]\left\{\hat{C}\right\}^{k+1} = [S]\left\{\hat{C}\right\}^{k} - \{B\} \qquad ⑩$$

In which $[R] = \frac{[M]}{\Delta t} + [A]$

$$[S] = \frac{[M]}{\Delta t}$$

(2) Crank - Nicholson scheme

$$[M]\frac{\{C\}^{k+1} - \{C\}^{k}}{\Delta t} + [A]\{C\}^{k+\frac{1}{2}} + \{B\}^{k+\frac{1}{2}} = 0$$

$$[M]\frac{\{C\}^{k+1} - \{C\}^{k}}{\Delta t} + [A]\left(\frac{\{C\}^{k+1} - \{C\}^{k}}{2}\right) + \{B\}^{k+\frac{1}{2}} = 0$$

$$\therefore \underbrace{\left(\frac{[M]}{\Delta t}+\frac{[A]}{2}\right)}_{[P]}\{C\}^{k+1}=\underbrace{\left(\frac{[M]}{\Delta t}-\frac{[A]}{2}\right)}_{[Q]}\{C\}^{k}-\left(\frac{\{B\}^{k+1}+\{B\}^{k}}{2}\right)$$

$$\therefore\ [P]\{C\}^{k+1}=[Q]\{C\}^{k}-\{B\} \qquad ⑪$$

8.6 Kinetic Models

○ S_i term

~ effects of
- biochemical, chemical → changes → Non-conservative Solutes
- physical sources and sinks → lateral input; storage zone solute

○ Fundamental differential form of conservation equation

$$\frac{\partial C_i}{\partial t} = -\nabla J_i + S_i$$

↑ accumulation ↑ flux ↑ generation

$C_i =$ concentration of substance i   scalar, mass/vol

○ Fickian Diffusion

$$\frac{\partial C_i}{\partial t} + \nabla (C_i u_i) = \nabla (D_i \nabla C_i) + S_i$$

○ Turbulent Diffusion

$$\frac{\partial C_i}{\partial t} + \nabla (C_i \bar{u}) = \nabla \left[\left\{ D_i + \varepsilon_i \right\} \nabla C_i \right] + S_i$$

$\varepsilon_i =$

$$\bar{u} = \frac{1}{T} = \int_0^T u dt$$

○ Dispersion

2-D : $\frac{\partial C}{\partial t} + u_x \frac{\partial C}{\partial x} + u_y \frac{\partial C}{\partial y} = \frac{1}{H}\frac{\partial}{\partial x}(H E_x \frac{\partial C}{\partial x}) + \frac{1}{H}\frac{\partial}{\partial y}(H E_y \frac{\partial C}{\partial y}) + S_i$

1-D : $\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x}(AE \frac{\partial C}{\partial x}) + S_i$

E= longitudinal dispersion coefficient

○ Solute Transport

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(\frac{Q}{A}C) + \frac{1}{A}\frac{\partial}{\partial x}(AD\frac{\partial C}{\partial t})$$

Q, A, D = const.

$$\frac{\partial C}{\partial t} = -\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2}$$

○ Groundwater and tributary inputs Q_L, C_L
transient storage zones

$$\frac{\partial C}{\partial t} = -\frac{Q}{A}\frac{\partial C}{\partial x} + \frac{1}{A}\frac{\partial}{\partial x}(AD\frac{\partial C}{\partial x}) + \frac{Q_L}{A}(C_L - C) + \alpha(C_S - C)$$

$$\frac{\partial C_S}{\partial t} = -\alpha\frac{A}{A_S}(C_S - C)$$

Q_L =lateral inflow per unit length of stream

C_L = solute concentration in lateral inputs (assumed to be const)

C_S =solute concentration in transient storage zones

A_S =cross-sectional area of the storage zone

α =coefficient for storage zone exchange

◎ Non-conservative solutes

~ terms to simulate solute transfers

~ variety of forms and complexity

~ depends on type of solute and use of model

○ Uptake of a first-order function

(loss of solute from the water column)

Sol)
$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(\frac{Q}{A}C) + \frac{1}{A}\frac{\partial}{\partial x}(AD\frac{\partial C}{\partial t}) - k_C C$$

$$C(x,t) = \frac{M}{2A\sqrt{\pi KT}}\exp\left[-\frac{(x-Ut)^2}{4kt} - k_e t\right]$$

k_e =overall uptake rate coefficient

○ Single benthic compartment with first-order release

$$\begin{cases} \dfrac{\partial C}{\partial t} = -\dfrac{\partial}{\partial x}(\dfrac{Q}{A}C) + \dfrac{1}{A}\dfrac{\partial}{\partial x}(AD\dfrac{\partial C}{\partial t}) - k_C C + \dfrac{1}{h}k_B C_B \\ \dfrac{\partial C_B}{\partial t} = hk_e C - k_B C_B \end{cases}$$

$C =$ water column solute concentration

$C_B =$ benthic concentration

$h =$ depth

$k_C, k_B =$ first-order exchange rate coefficients

$V_f = hkc$ mass transfer coefficient

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(\frac{Q}{A}C) + \frac{1}{A}\frac{\partial}{\partial x}(AD\frac{\partial C}{\partial t}) - \frac{V_f}{h}C + \frac{1}{h}k_B C_B$$

$$\frac{\partial C_B}{\partial t} = V_f C - k_B C_B$$

○ Non-conservative solute

= nutrients
- -nitrogen
- -phosphorus
- -sulfer
- -dissolved organic carbon
- -trace metals copper

○ Stream transport of copper by incorporating first order mass transfer equations for periphyton and sediment reactions

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(\frac{Q}{A}C) + \frac{1}{A}\frac{\partial}{\partial x}(AD\frac{\partial C}{\partial x}) - P_B\frac{\partial C_B}{\partial t} - P_S\frac{\partial C_S}{\partial t}$$

$$\frac{\partial C_B}{\partial t} = \lambda_B(C_B - Kd_B C)$$

$$\frac{\partial C_S}{\partial t} = \lambda_S (C_S - Kd_S C)$$

in which C_B = periphyton solute concentration

C_S = sediment solute concentration

P_B, P_S = mass of periphyton and sediment

λ_B, λ_S = first-order exchange rate coefficients

k_{dB}, k_{dS} = partition coefficients, expressing equilibrium ratios of periphyton to water column and sediment to water column solute conc.

○ Non-linear uptake function (Kuwabara & Heliker, 1988)

~ Monod (or Michaelis-Menten) → algal uptake

$$\left. \begin{aligned} S &= -\frac{U}{h} \\ U &= \frac{U_{\max} C}{K_S + C} \end{aligned} \right\} \quad S = \frac{\partial C}{\partial t} = -\frac{1}{h} \frac{U_{\max} C}{K_S + C}$$

in which $U_{\max}$ = maximum uptake per unit area of stream bottom

K_S = half-saturation constant

~ solute concentration at which uptake is one-half the maximum

◎ Concepts and method for assessing solute dynamics in stream ecosystems (1990)

◎ Solute dynamics

- transport = advection, dispersion
- transfer (transformation)
  - chemical transformations
  - changes in physical state(phase) = sorption, desorption
  - biological processes

◎ Chemical processes in natural water bodies (Orlob p70)

- oxidation-reduction reactions
- acid-base reactions
- gas-solution processes and outgassing
- coordination reactions of metal ions and ligands
- precipitation and dissolution of solid phases
- adsorption-desorption processes at interfaces

○ Aquatic organisms influence the concentrations of many substances by metabolic uptake, transformation, storage, and release.

◎ Reaction Rates and Reaction Equation (Orlob p79)

○ In simplified water quality modeling, chemical, biochemical, and processes are described by

(1) $\frac{dc}{dt} = KC^n$ ~ irreversible diminish (decay)

- linear
  - $n = 0$
  - $n = 1$ $\rightarrow$ first-order reaction
- nonlinear $n \neq 0, n \neq 1$

(2) $$\frac{dc}{dt} = \frac{K_1 C}{K_2 + C}$$ (Michaelis - Menten)

~ non-linear

~ uptake rate of external nutrient concentration

(3) $$\frac{dc_1}{dt} = K C_2^n$$

$$\frac{dc_1}{dt} = K (C_{2,0} - C_2)^n$$

$C_{2,0} =$ saturation conc

~ reaeration , adsorption

(4) $$\frac{dc_1}{dt} = K_1 C_2^n + K_2 C_1 \quad , \quad n \neq 0$$

~ Streeter-Phelps Eq

~ adsorption - desorption processes

(5) $$\frac{dc_1}{dt} = K (C_{1,0} - C_1) C_2^n - K_2 C_1$$

~ adsorption

(6) $$\frac{dc_1}{dt} = K_1 C_1 \frac{C_2}{K_2 + C_2}$$ (Monod)

~ change of the biomass C_1 of a primary producer

(7) $\frac{dc_1}{dt} = K_1 \frac{dc_2}{dt} - K_2 C_1$

~ very rapid reactions