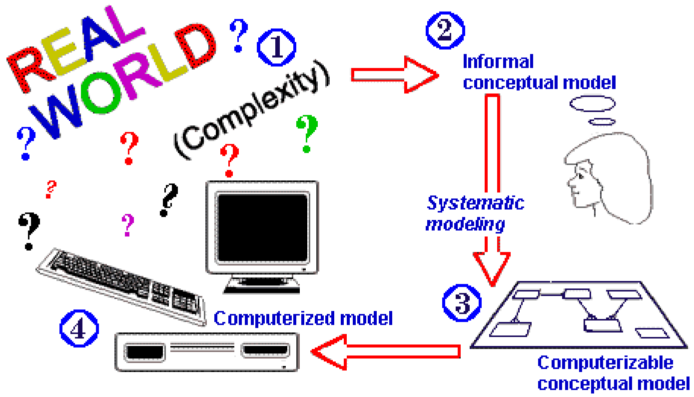
Chapter 9

Numerical Models for Mixing in Rivers and Estuaries



Chapter 9
Numerical Models for Mixing in Rivers and Estuaries

Contents

Chapter 9
Numerical Models for Mixing in Rivers and Estuaries

Objectives

- Think about the definition of model

- Introduce procedure of modeling

- Study various types of numerical schemes

9.1 Modeling Mixing in Rivers and Estuaries

9.1.1 Introduction

- Definition of Model
- What is a model?
  - a deliberate misrepresentation of reality
  - simplification (approximation) of real system
- Reason: convenience
- Purpose:
  - gain understanding
  - predict an outcome
- Constraints:
  - degree of accuracy depends on degree of simplification

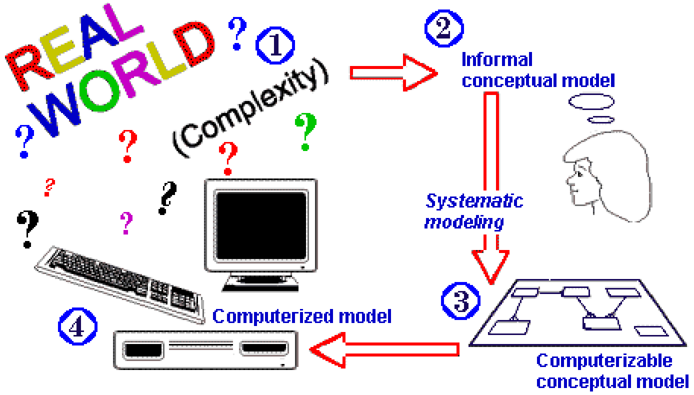
9.1 Modeling Mixing in Rivers and Estuaries

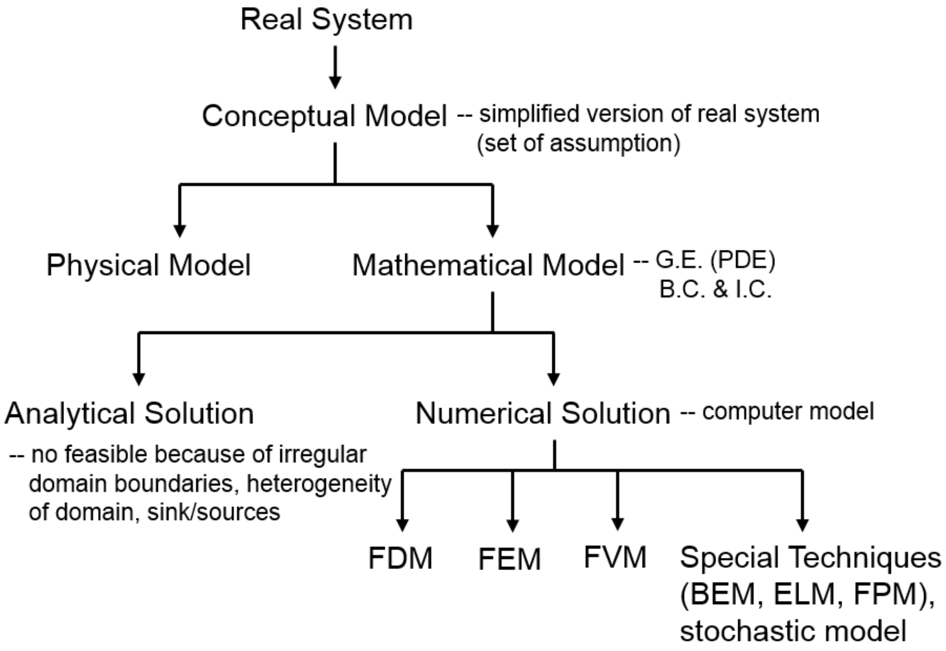
- River model

Describe the real system of river dynamics using physical or mathematical approach

- Purpose

Understanding and prediction of river dynamics




Real System

Conceptual Model -- simplified version of real system
(set of assumption)

Physical Model

Mathematical Model -- G.E. (PDE)
B.C. & I.C.

Analytical Solution
-- no feasible because of irregular domain boundaries, heterogeneity of domain, sink/sources

Numerical Solution -- computer model

FDM

FEM

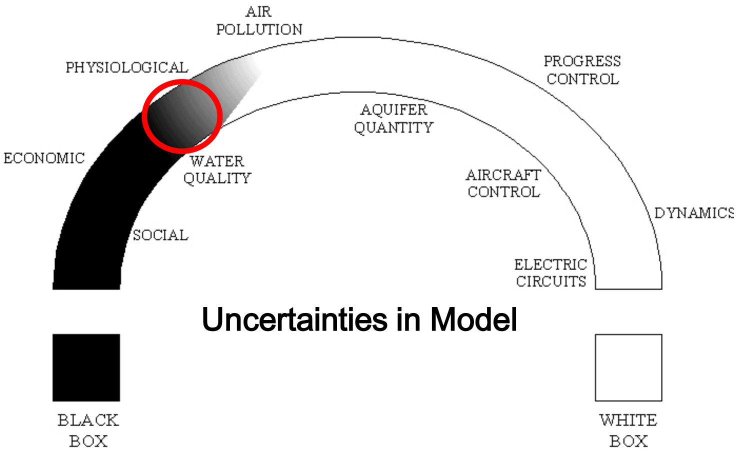
FVM

Special Techniques (BEM, ELM, FPM), stochastic model

9.1 Modeling Mixing in Rivers and Estuaries

- Uncertainty

Most models are intermediate forms between physical-based models and empirical models.



Uncertainties in Model

- Parameter

Model have its own parameters to represent their characteristics.

- Calibration

Comparison of model output with observations to tune the model parameters

→ The calibrated models can be called empirical models

- Validation

Comparison of output from the calibrated models with observations to evaluate validity of the calibrated models.

9.1 Modeling Mixing in Rivers and Estuaries

9.1.2 Selection of Model

Code	Name	Description
1A	One-dimensional tidally averaged	A numerical solution of 1-D tidally averaged dispersion equation [Eq.8.38] • steady state model: coefficients are constant in time. • unsteady model: flow parameters and dispersion coefficient vary between tidal cycles.
1T	One-dimensional tidally varying	A numerical solution of Eq. (8.46) - Tidal evaluation, velocity and dispersion coefficient vary during tidal cycle.

9.1 Modeling Mixing in Rivers and Estuaries

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. • 2VA: horizontally averaged model → reservoir, lake • 2HA: vertically averaged model → river, estuary
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

9.1 Modeling Mixing in Rivers and Estuaries

3T	Three-dimensional tidally varying	
P	Physical model	A small-scale physical replica of the prototype geometry with provisions of generating tidal and river flow
NP	Hybrid numerical physical	A combination of a physical and a numerical model, using one model to generate input information for the other

9.1 Modeling Mixing in Rivers and Estuaries

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.

9.1 Modeling Mixing in Rivers and Estuaries

Tidal pumping	2HT physical model	Accuracy of 2HT may be difficult to establish.
Shear flow dispersion	2HT 2VT	
Wind effects	2HT 3T	
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

9.1 Modeling Mixing in Rivers and Estuaries

9.1.3 Modeling Procedure

- Model parameters

\- Model parameters exist only in context of model.

\- Model coefficients

- Model calibration

\- Parameter tuning to fit observed data to predicted data

\- To estimate parameters of model from available information

\- Model becomes less mechanistic (more empirical)

\- Parameter identification problem

9.1 Modeling Mixing in Rivers and Estuaries

- Procedure of Calibration and Verification

	Data Set I	Data Set II
Input	I_1	I_2
Output	O_1	O_2
Parameter	?	P

i) Calibration

$I_1 \longrightarrow$ Model(?) $\longrightarrow \tilde{O}_1$ Fit $\tilde{O}_1$ to O_1

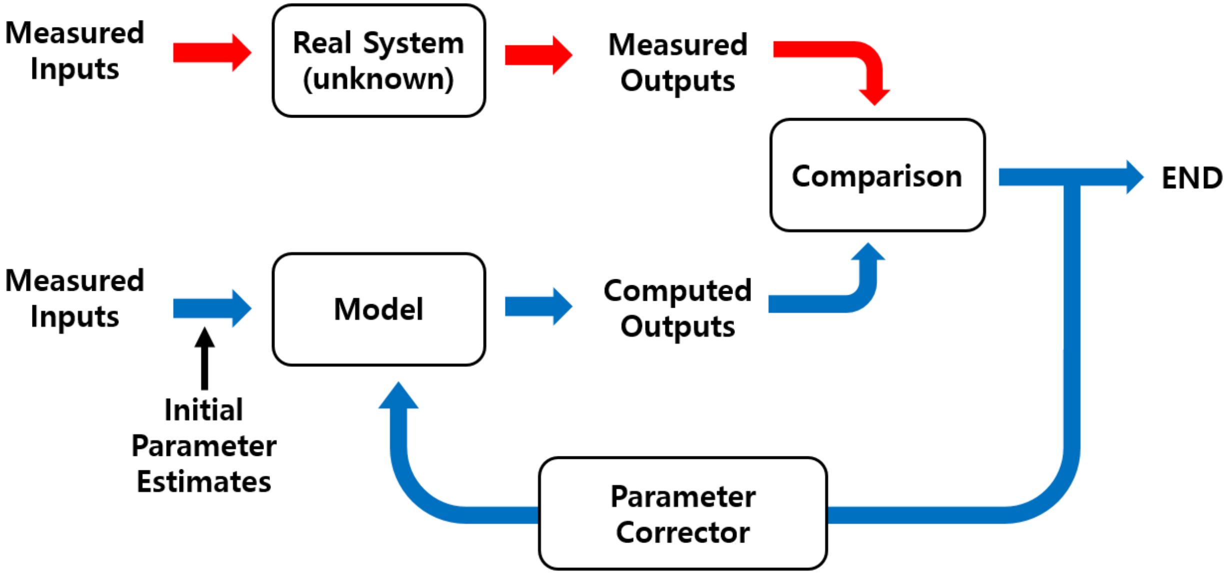
Find P (set of values of parameters(coefficients))

ii) Verification

$I_2 \longrightarrow$ Model(P) $\longrightarrow \tilde{O}_2$ Predict $\tilde{O}_2$ with calibrated parameter P

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

9.1 Modeling Mixing in Rivers and Estuaries



- Best fit

~ techniques for <u>determining the "best", or "optimal" values </u>of the model coefficients

i.e., values that make the predicted values and the measured ones sufficiently close to each other

9.1 Modeling Mixing in Rivers and Estuaries

9.1.4 Numerical Solutions

- Analytical Solution

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

- easier to use than a numerical model

- Numerical Solution

- The complex water body geometry and flow fields and nonlinearities of the source and sink terms make it impossible to obtain analytical solutions to the differential equation

- solve using numerical techniques

9.1 Modeling Mixing in Rivers and Estuaries

- Numerical techniques

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

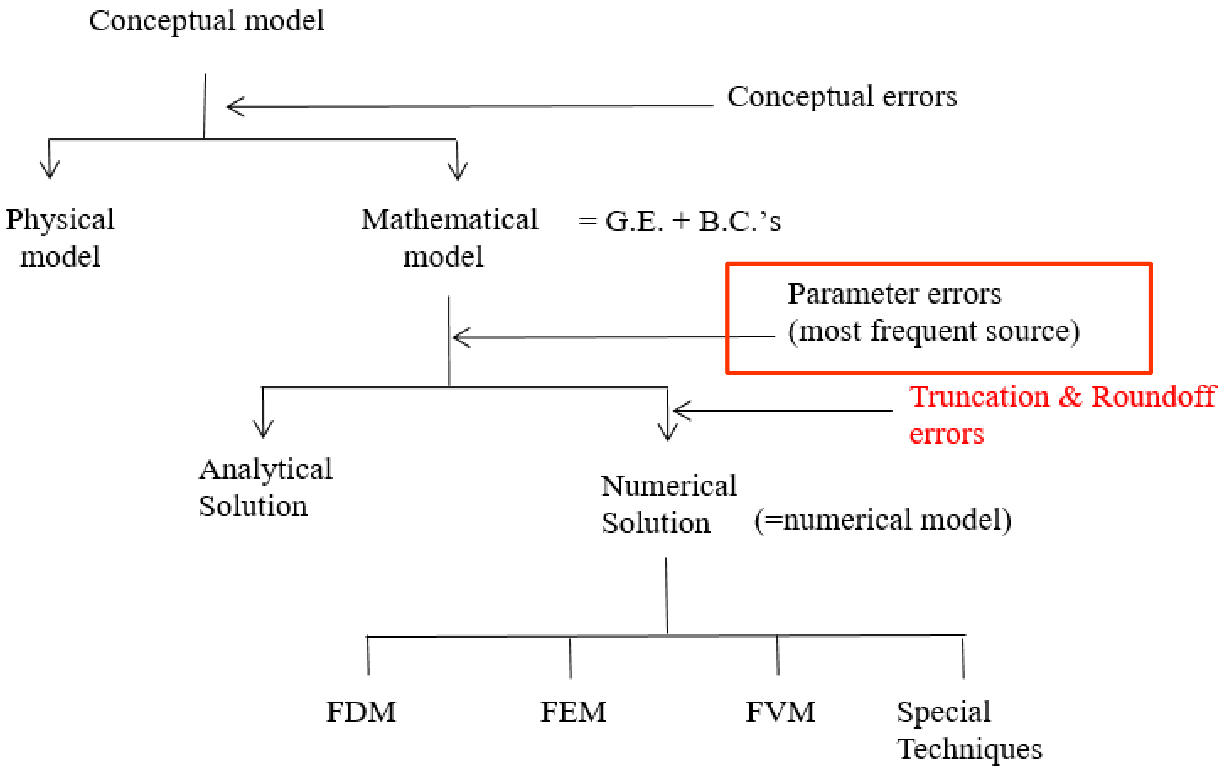
- matrix-inversion methods

- Types of numerical techniques

  1) FDM (Finite Difference Method)
  2) FEM (Finite Element Method)
  3) FVM (Finite Volume Method)
  4) FPM (Finite Particle Method)

9.1 Modeling Mixing in Rivers and Estuaries

- Errors in numerical solutions



- Truncation error: discretization error
- Round-off error: error occurred in the arithmetic operations needed to solve FDE

9.2 Finite Difference Model

9.2.1 Explicit Finite-Difference Methods

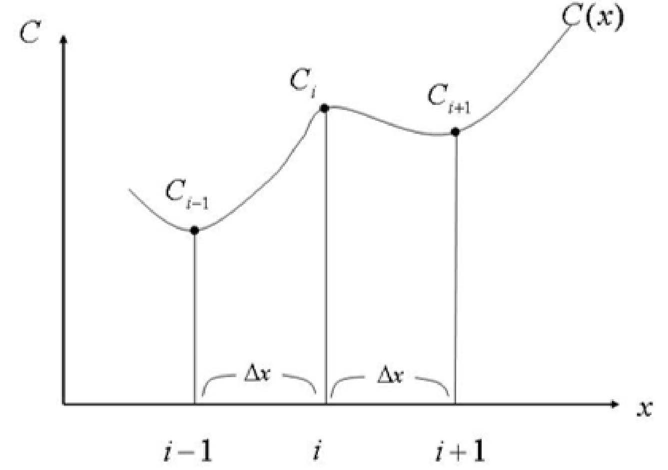
- Procedure of finite difference scheme

a. Break x into finite segments of Δx in length

b. Subscript 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

c. Apply Taylor series expansions to approximate the differentials



9.2 Finite Difference Model

- *Taylor Series expansions*

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

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

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

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

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

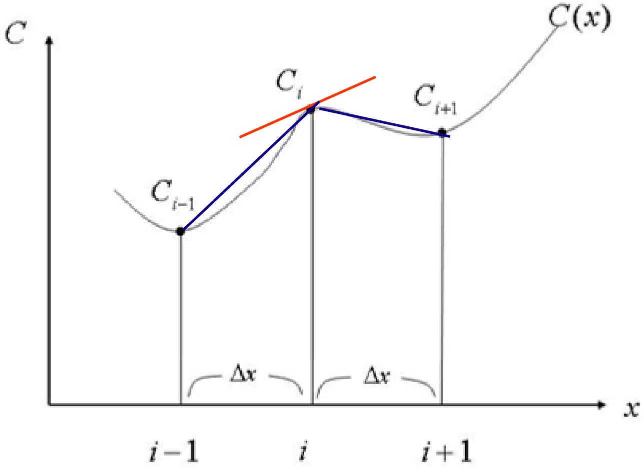
9.2 Finite Difference Model

1) Forward-difference ← (a)

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

2) Backward-difference (Upwind difference) ← (b)

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



9.2 Finite Difference Model

3) Central-difference

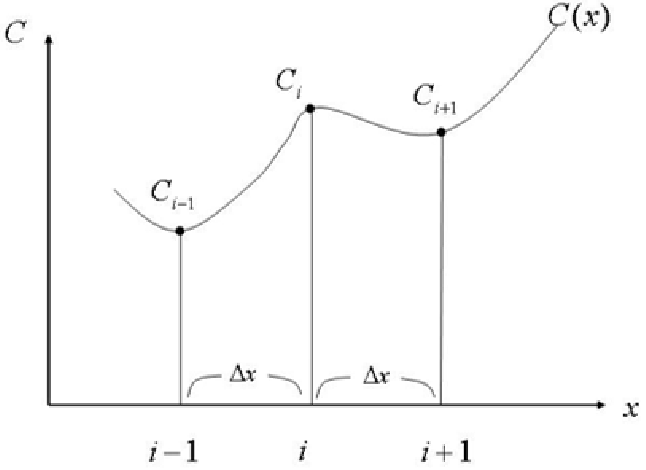
Subtract (b) from (a)

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

4) Central-difference for 2nd derivative

Add (a) and (b)

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



9.2 Finite Difference Model

9.2.2 Model Assembling for Explicit Scheme

1D advection-dispersion equation for conservative pollutant is

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

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

1) **Formulation** ***Ex-a***

- Explicit solution ***Ex-a***:

① Forward-difference for time derivative → explicit method

② Forward-difference for 1st derivative in x

9.2 Finite Difference Model

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

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

Superscript *n* - time step

Subscript *i* - distance step

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

← Combination of FD and BD

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

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

9.2 Finite Difference Model

Let

$$\frac{u_i \Delta t}{\Delta x} = a_i$$ -> Courant No. → stability

$$\frac{E_i \Delta t}{\Delta x^2} = b_i$$ -> Peclet No. → numerical dispersion

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

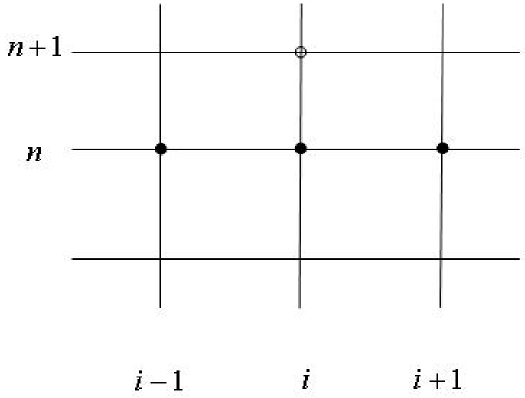
Then

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

9.2 Finite Difference Model

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

$$\therefore\ C_i^{n+1} \text{ is weighted average of } \quad C_{i-1}^n, C_i^n, and\, C_{i+1}^n$$



Solution

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

② C known for all $t\ @\ x = 0$

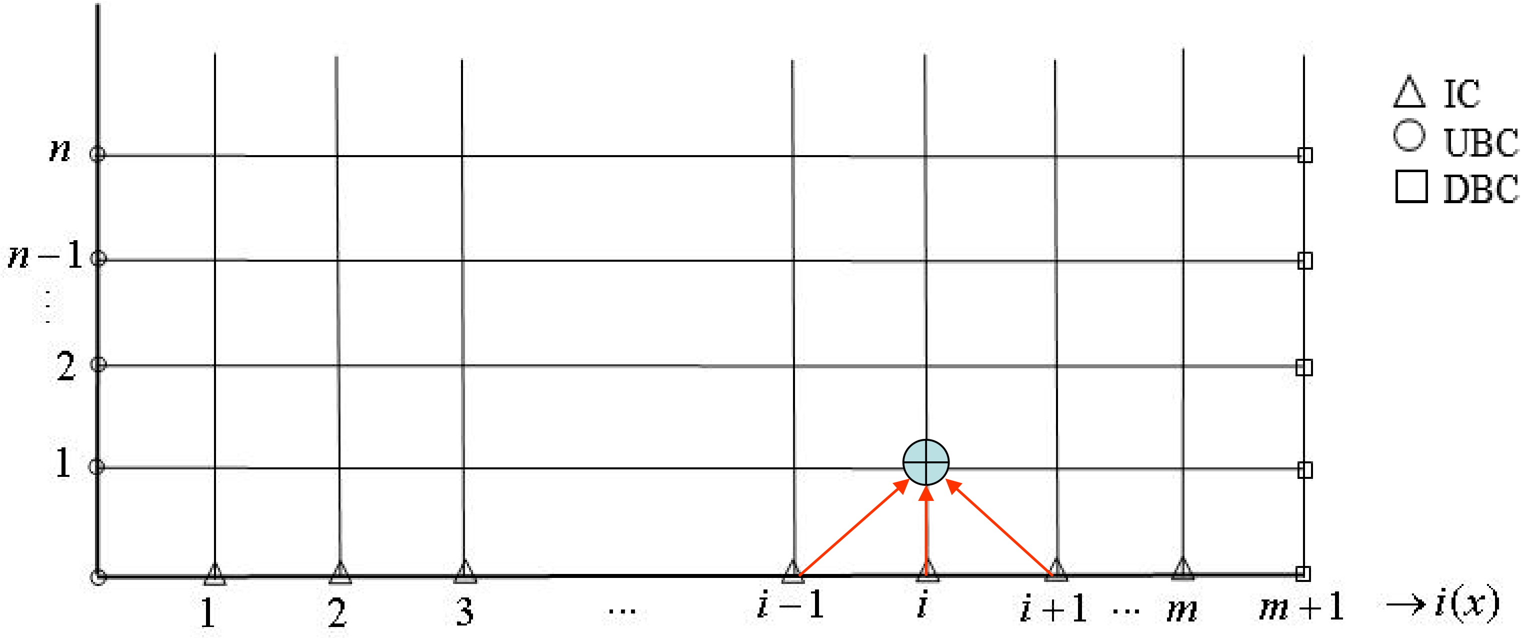
Procedure:

① Use Eq. (1) 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

9.2 Finite Difference Model



9.2 Finite Difference Model

2) **Formulation *Ex-b***

① Forward difference for time derivative → explicit scheme

② 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

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

9.2 Finite Difference Model

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

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

9.2 Finite Difference Model

Assume first-order decay

$$S = f\left(C\right) = -kC$$

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

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

Note that now

$$\sum Coeffs \neq 1$$

9.2 Finite Difference Model

3) **Formulation** ***Ex-cd***

Forward difference for time derivative→ explicit method

Central difference for spatial derivatives, 1st and 2nd derivatives

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

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

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

9.2 Finite Difference Model

Substitute these into 1-D transport equation

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

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

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

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

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

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

9.2 Finite Difference Model

9.2.3 Error Analysis

(1) **Source of Errors**

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

- Errors in machine computations

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

9.2 Finite Difference Model

- Roundoff Error

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

$0.626 = \left(\frac{1}{2}\right)^1 + \left(\frac{1}{2}\right)^3 + \left(\frac{1}{2}\right)^{10} + \left(\frac{1}{2}\right)^{16} + \left(\frac{1}{2}\right)^{17} + \left(\frac{1}{2}\right)^{21} + \cdots \Rightarrow .101000$ (infinite series)

9.2 Finite Difference Model

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

$$\rightarrow \begin{cases} 0.62599945 \text{ without rounding} \\ 0.62600040 \text{ with rounding} \end{cases}$$

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

0.33333333
+ 0.33333333
add 3,000 times
Expected value = 999.99999
Rounded-off value= 999.99091
Roundoff error = 0.00908

0.33333333
+0.33333333
+0.33333333
+0.33333333
1.33333332 → 1.3333333
True value　Truncated to　8digit
Error = 0.00000002

9.2 Finite Difference Model

(2) **Lax Equivalence Theorem**

Consistency + Stability → Convergence

- ***Convergence***

The numerical scheme is convergent if for any fixed time $T = n\Delta t$

and fixed location $X = i\Delta x$,

$$C(X,T) \rightarrow \bar{C}(X,T) \qquad (or \left| C(X,T) - \bar{C}(X,T) \right| = 0) \qquad as\, \Delta x \rightarrow 0\; and\; \Delta t \rightarrow 0$$

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

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

9.2 Finite Difference Model

- ***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

9.2 Finite Difference Model

(3) **Analysis of Stability**

Von Neumann Method

Matrix Method

- Explicit solutions

~ accurate & easy

~ may be unstable → need a stability criterion

1) Formulation ***Ex-a***

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

$e_i^n =$ error at that point

9.2 Finite Difference Model

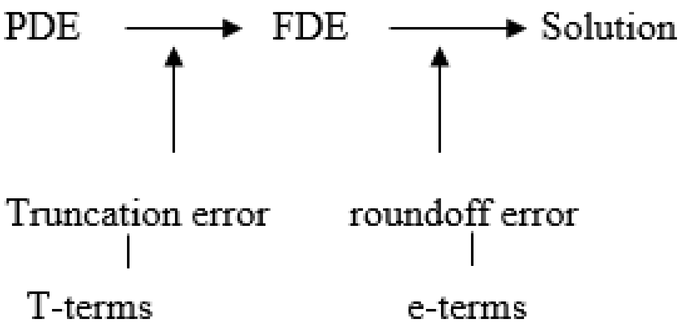
Substitute this into Formulation *a)*

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

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

→ 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

roundoff error | e-terms

9.2 Finite Difference Model

But, we 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)

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

For Formulation *a*

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

$$\left|1+a_i-b_i-d_i\right| + \left|b_i-a_i\right| + \left|d_i\right| \le 1 \qquad (4)$$

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.

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

then $1+\cancel{a}_i-\cancel{b_i}-\cancel{d_i}+\cancel{b_i}-\cancel{a_i}+\cancel{d}_i=1 \quad \le 1$

9.2 Finite Difference Model

which is satisfied for all values of and which meet these conditions.

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

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

$$2a_i\le 2b_i$$

$$a_i\le b_i$$

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

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

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

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

$$if \quad d_i=b_i$$

$$then \quad 2b_i\le 1+a_i$$

9.2 Finite Difference Model

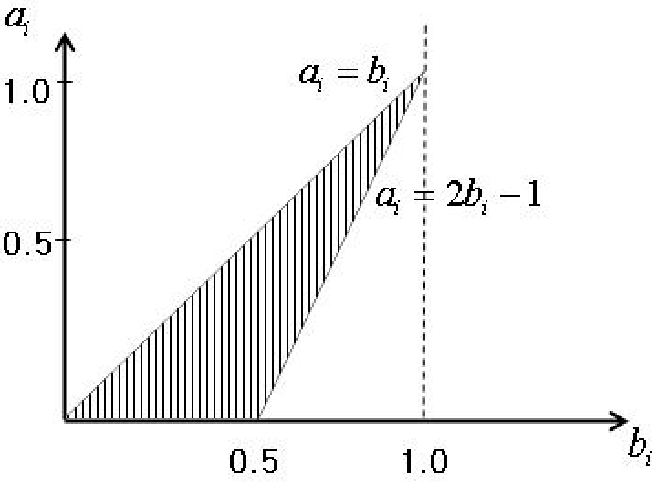
$$iv)\quad if \quad 1 + a_i - b_i - d_i < 0 \quad \& \quad b_i - a_i \le 0$$

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

$$2d_i \le 2$$

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

Combine these conditions



9.2 Finite Difference Model

- Restrictions on Δx and Δt

$$ii)\, a \le b$$

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

$$iii)\, 2b \le 1 + a$$

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

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

9.2 Finite Difference Model

Substitute (1) into (2)

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

$$\Delta t < \frac{E}{u^2} \qquad (3)$$

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

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

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

9.2 Finite Difference Model

2) **Formulation** ***Ex-b***

Consider formulation w/o decay term

$$\left|1-a_i-b_i-d_i\right|+\left|a_i+b_i\right|+\left|d_i\right|\leq 1$$

There are only 2 cases to be considered

$$i)\ \ if\ \ 1-a_i-b_i-d_i\geq 0$$

$$1-\cancel{a}_i-\cancel{b}_i-\cancel{d}_i+\cancel{a}_i+\cancel{b}_i+\cancel{d}_i\leq 1$$

$$1\leq 1$$

$$Satisfied\ \ for\ \ any\ \ values\ \ of\ \ a_i,\ b_i, and\ \ d_i$$

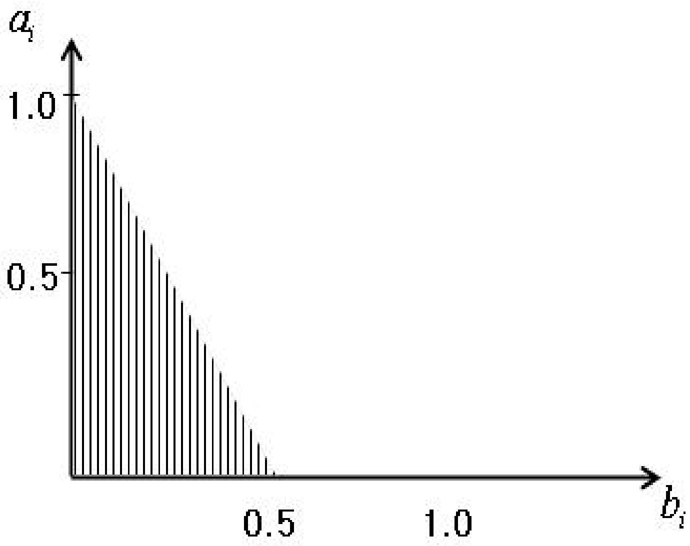
$$ii)\ if\ \ 1-a_i-b_i-d_i\leq 0$$

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

$$2\left(a_i+b_i+d_i\right)\leq 2$$

$$a_i+b_i+d_i\leq 1 \qquad if\quad b_i=d_i$$

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



9.2 Finite Difference Model

$$a + 2b \leq 1$$

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

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

9.2 Finite Difference Model

3) **Formulation *Ex-cd***

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

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

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

$$1\le 1$$

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

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

$$a-2b\le 0$$

$$a\le 2b$$

9.2 Finite Difference Model

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

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

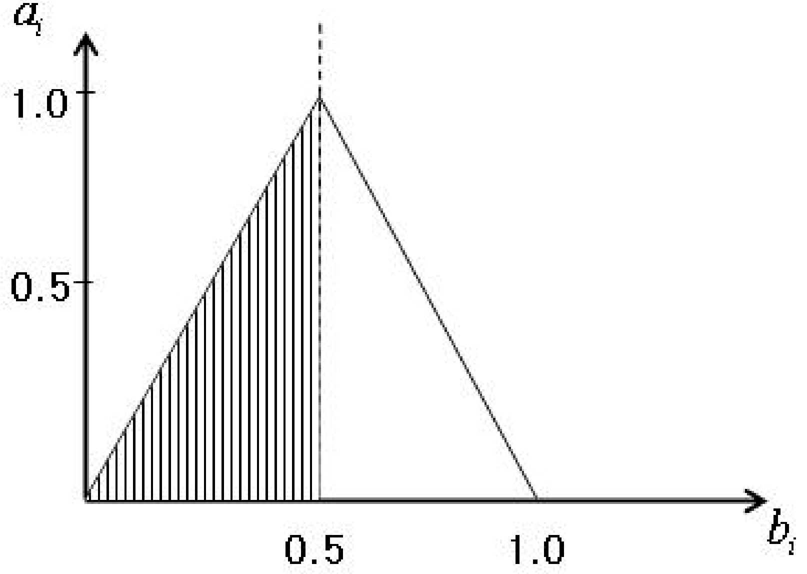
$$b\le\frac{1}{2}$$

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

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

$$2b+a\le 2$$

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



9.2 Finite Difference Model

$$a \le 2b$$

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

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

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

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

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

9.2 Finite Difference Model

9.2.4 Implicit Finite-Difference Methods

1) **Formulation *Im-c***

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

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

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

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

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

9.2 Finite Difference Model

Substituting and rearranging yields

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

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

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

let $a_i = \frac{u_i \Delta t}{\Delta x}$ $\quad b_i = \frac{E_i \Delta t}{\Delta x^2}$ $\quad d_i = \frac{E_{i-1} A_{i-1} \Delta t}{A_i \Delta x^2}$

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

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

9.2 Finite Difference Model

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

Let $L_i = -d_i; \quad M_i = 1 - a_i + b_i + d_i, \quad U_i = a_i - b_i$

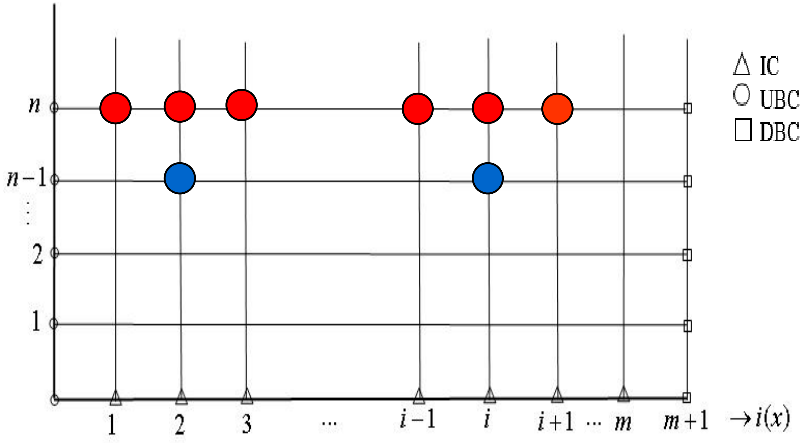
Then $L_i C_{i-1}^n + M_i C_i^n + U_i C_{i+1}^n = C_i^{n-1}$

(i) If C is known $@\left(\begin{array}{ll} x = 0 & (i = 0) \\ x = \infty & (i = m+1) \end{array}\right.$ $C(0), C(m+1)$

→ Dirichlet (The 1st kind) type B.C.

$$i = 1: \; L_1 C_0^n + M_1 C_1^n + U_1 C_2^n = C_1^{n-1}$$

$$\rightarrow M_1 C_1^n + U_1 C_2^n = \underbrace{C_1^{n-1} - L_1 C_0^n}_{Known}$$



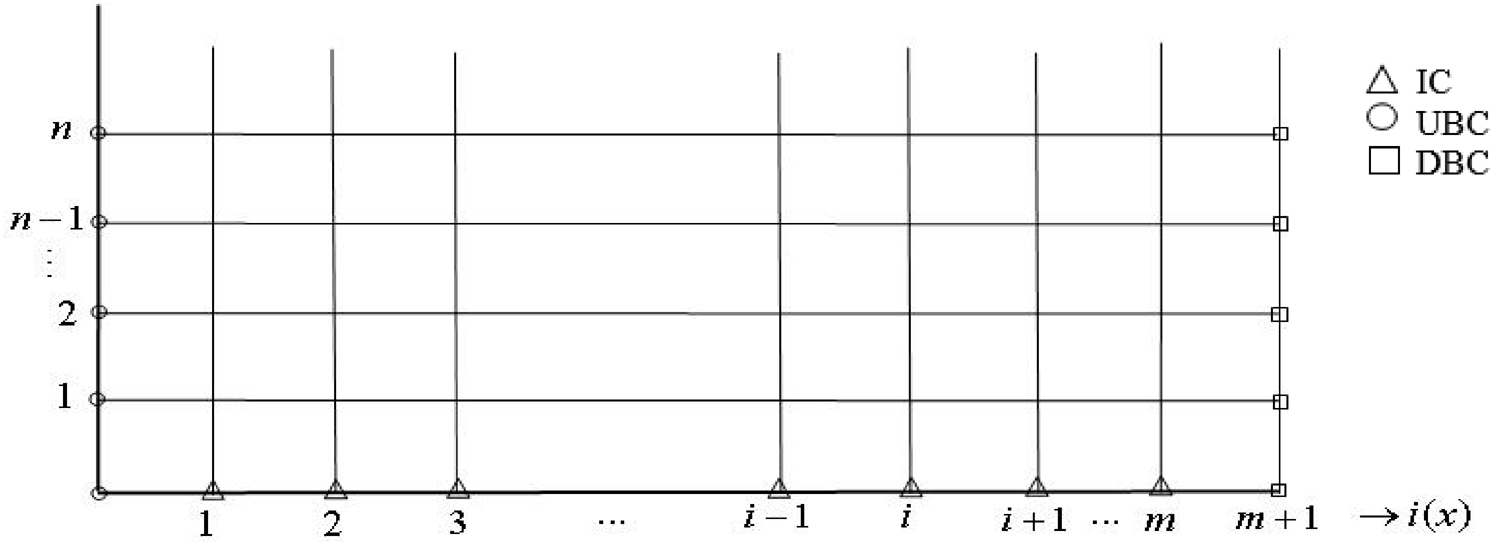
$$i = 2: \; L_2 C_1^n + M_2 C_2^n + U_2 C_3^n = C_2^{n-1}$$

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

$$\rightarrow L_m C_{m-1}^n + M_m C_m^n = \underbrace{C_m^{n-1} - U_m C_{m+1}^n}_{Known}$$

9.2 Finite Difference Model

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



9.2 Finite Difference Model

→ 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 (Stone and Brian, 1963)

[Ref] Stone, H.L., and Brian, P.L.T., “Numerical Solutions of Convective Transport Problems,” AIChE. Jour. (1963) Vol.9, No.5, pp. 681-688.

(ii) If C known $@\ x = 0\,(i = 0)$ → Dirichlet

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

9.2 Finite Difference Model

Suppose no flux @ boundary → $\left.\dfrac{\partial C}{\partial x}\right|_{m+1}^{n} = 0$ → Reflecting boundary

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

Backward difference

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

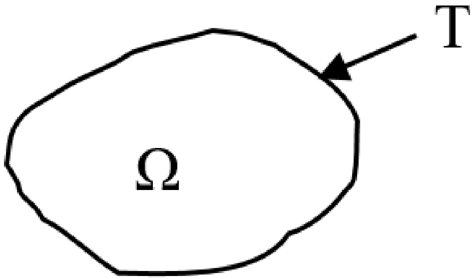
$$i = m : \; L_m C_{m-1}^{n} + M_m C_{m}^{n} + U_m C_{m+1}^{n} = C_{m}^{n-1}$$

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

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

9.2 Finite Difference Model

[Re] Boundary Conditions



Boundary Conditions

- Dirichlet (1st type): $C(x,y) = f_1(x,y) \quad \text{on} \quad T_1$
- Neumann (2nd type): $\frac{\partial C}{\partial n} = f_2(x,y) \quad on \quad T_2$

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

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

9.2 Finite Difference Model

2) Formulation *Im-d*

~ most commonly used formulation

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

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

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

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

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

9.2 Finite Difference Model

Substituting and rearranging yields

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

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

9.2 Finite Difference Model

3) Formulation *Im-cd*

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

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

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

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

Final discretized equation is given as

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

$$L_i = -\frac{a_i}{2} - b_i \qquad M_i = 1 + 2b_i \qquad U_i = \frac{a_i}{2} - b_i \qquad a_i = \frac{u_i \Delta t}{\Delta x} \qquad b_i = \frac{E_i \Delta t}{\Delta x^2}$$

9.2 Finite Difference Model

9.2.5 Numerical Dispersion for Finite-Difference Methods

- Numerical Dispersion

~ Truncation error of Taylor's series in converting PDE of diffusion equation into FDE

~ artificial viscosity, numerical dissipation

~ smearing of concentration fronts due to excessive damping

<Ref>

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

9.2 Finite Difference Model

- **Numerical dispersion of *Ex-cd***

From Taylor series expansion, we get

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

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

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

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

differentiate w.r.t *x*

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

9.2 Finite Difference Model

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

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

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

9.2 Finite Difference Model

Formulate (1) with (a) and (b)

$$\frac{C_i^{n+1}-C_i^{n}}{\Delta t}\boxed{-\frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2}}=-u\left(\frac{C_{i+1}^{n}-C_{i-1}^{n}}{2\Delta x}\right)+\mathrm{O}(\Delta t^2,\Delta x^2) \qquad (5)$$

Substitute (4) into (5)

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

Let E_n= <u>numerical dispersion coefficient</u>

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

$$\boxed{\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=E_n\frac{\partial^2 C}{\partial x^2}+\mathrm{O}(\Delta t^2,\Delta x^2)} \qquad (6)$$

9.2 Finite Difference Model

- Numerical dispersion of *lm-c*

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

$$\frac{C_i^n - C_i^{n-1}}{\Delta t} = \frac{\partial C}{\partial t} - \frac{\Delta t}{2} \frac{\partial^2 C}{\partial t^2} + \mathrm{O}(\Delta t^2) \qquad (c) \quad \text{backward}$$

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

$$\frac{C_{i+1}^n - C_i^n}{\Delta x} = \frac{\partial C_i}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 C_i}{\partial x^2} + \mathrm{O}(\Delta x^2) \qquad (d) \quad \text{forward}$$

9.2 Finite Difference Model

Substituting (c) and (d) into (1)

$$\frac{\partial C}{\partial t}+\frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2}=-u\left\{\frac{\partial C}{\partial x}-\frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2}\right\}+\mathrm{O}(\Delta t^2+\Delta x^2) \qquad (7)$$

Substituting (4) into (7) yields

$$\underbrace{\frac{\partial C}{\partial t}=-u\frac{\partial C}{\partial x}}_{PDE}+\underbrace{\left\{\frac{u\Delta x}{2}-\frac{\Delta t}{2}u^2\right\}\frac{\partial^2 C}{\partial x^2}}_{Numerical\ dispersion\,(TE1)}+\underbrace{\mathrm{O}(\Delta t^2+\Delta x^2)}_{Truncation\ error\,2}$$

Define numerical dispersion coefficient as

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

Then

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

If we include real dispersion term

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=\boxed{\underbrace{(E+E_n)}_{E_c\,=\,Computed\ dispersion}}\frac{\partial^2 C}{\partial x^2} \qquad (8)$$

9.2 Finite Difference Model

- How to remove E_n

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

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

$$\boxed{\therefore a = \frac{u\Delta t}{\Delta x} = 1} \qquad (9)$$

However, stability criterion for Formulation *Ex-b* is

$$\frac{u\Delta t}{\Delta x} + \frac{2E\Delta t}{\Delta x^2} \le 1 \qquad (10)$$

If we make $\frac{u\Delta t}{\Delta x} = 1$ then (10) becomes

$$\frac{E\Delta t}{\Delta x^2} \le 0 \qquad (11)$$

Therefore we have to choose Δt and Δx satisfying both (9) & (11) → impossible

9.2 Finite Difference Model

<Example> For *Ex-b*

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

$$a = \frac{1 \cdot 1}{2} = \frac{1}{2}$$

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

$$SC\ \ for\ Ex - b : \frac{1}{2} + \frac{2(1)}{(2)^2} E = \frac{1}{2} + \frac{E}{2} \le 1$$

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

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

9.2 Finite Difference Model

(ii) Dispersion correction technique

→ make $E_c = E$

For Formulation *Ex-b*, subtract E_n from E_c

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

(iii) make Δx and Δt small

→ make E_n small

9.2 Finite Difference Model

- *Summary*

Formulation	Numerical dispersion, E_n	measure to ND
$Ex-a$	$-\dfrac{u\Delta x}{2}(1+a)$	$Add(-E_n)$
$Ex-b$	$\dfrac{u\Delta x}{2}(1-a)$	$Subtract\ E_n(Be\ careful$ $when\, E < E_n)$
$Ex-cd$	$\dfrac{u^2}{2}\Delta t$	$Subtract\, E_n$
$\mathrm{Im}-c$	$\dfrac{u\Delta x}{2}(1-a)$	$Make\ \ a=1$
$\mathrm{Im}-d$	$\dfrac{u\Delta x}{2}(1+a)$	$Subtract\ E_n$
$\mathrm{Im}-cd$	$\dfrac{u^2}{2}\Delta t$	$Subtract\ E_n$

9.2 Finite Difference Model

9.2.6 Lagrangian Formulations

- **Lagrangian approach**

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

• Two-step explicit method (Bella & Dobbins, 1968)

→ Two processes of the advection-diffusion equation are assumed to occur sequentially rather than simultaneously as in the prototype

1) **1st step (advection process)**

~ to translate the pollutant downstream for one-time step in Eulerian frame

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

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

9.2 Finite Difference Model

2) **2nd step (dispersion process)**

~ to calculate new values on the *n*+1 row using only the dispersion in Lagrangian frame

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

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

9.2 Finite Difference Model

1) Formulation ***La-e***

~ explicit

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

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

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

9.2 Finite Difference Model

Substituting this into Governing Eq. yields

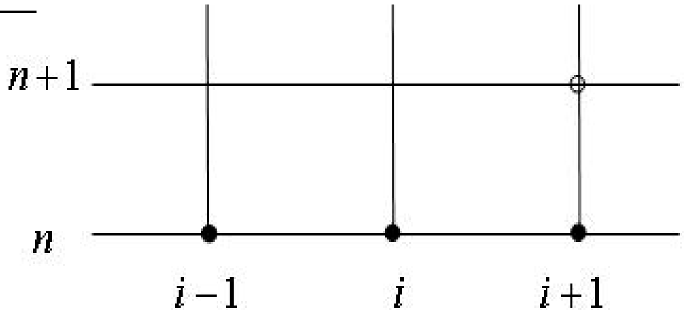
$$C_{i+1}^{n+1} = C_{i+1}^{n} - \frac{u_i\Delta t}{\Delta x}\left(C_{i+1}^{n} - C_i^n\right) + \frac{E_i\Delta t}{\Delta x^2}\left(C_{i+1}^n - C_i^n\right) - \frac{E_{i-1}A_{i-1}\Delta t}{A_i\Delta x^2}\left(C_i^n - C_{i-1}^n\right) + S_i\Delta t$$

Rearranging further gives

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

Let $a_i = \frac{u_i\Delta t}{\Delta x}$ $b_i = \frac{E_i\Delta t}{\Delta x^2}$ $d_i = \frac{E_{i-1}A_{i-1}\Delta t}{A_i\Delta x^2}$

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



→ We need 2 UBC and IC, need no DBC

9.2 Finite Difference Model

- Numerical Dispersion of Formulation *La-e*

Pure Advection Problem

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

Taylor Series expansion in t direction

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

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

Taylor Series expansion in x direction

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

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

9.2 Finite Difference Model

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**

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

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

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

9.2 Finite Difference Model

2) Formulation ***La-f***

~ implicit method

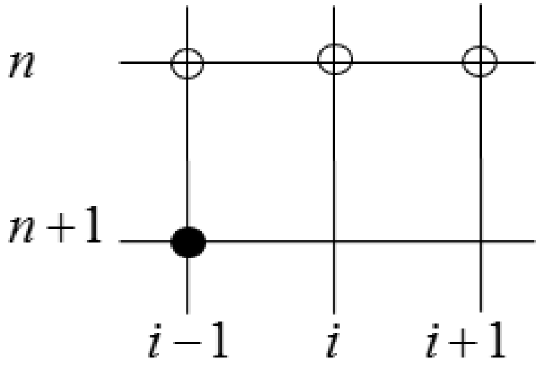
Backward difference for $\frac{\partial C}{\partial t}$ at the *i*-l grid point

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

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

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

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



- Numerical Dispersion

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

9.2 Finite Difference Model

9.2.7 Crank-Nicholson Scheme

1) Formulation *CN-b*

~ Upwind (Backward) difference for $\dfrac{\partial C}{\partial x}$

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

$\varepsilon = n$ → Explicit

$\varepsilon = n+1$ → Implicit

$\left.\right]$ → 4 point scheme

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

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

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

$$+\frac{E}{\Delta x^2}\left\{\frac{1}{2}(\overset{\diamond}{C_{i+1}^n}+\boxed{C_{i+1}^{n+1}}) - \frac{1}{2}\cdot 2(\boxed{C_i^n}+\overset{\bigcirc}{C_i^{n+1}}) + \frac{1}{2}(\overset{\triangledown}{C_{i-1}^n}+\overset{\triangle}{C_{i-1}^{n+1}})\right\}$$

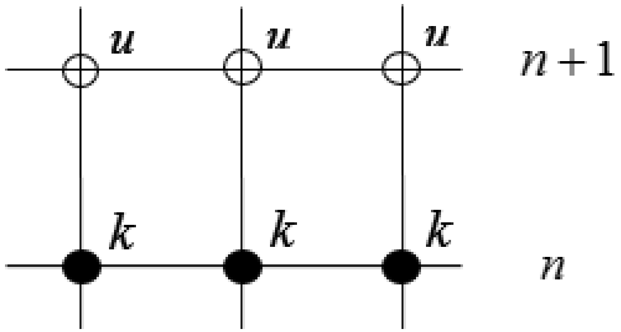
9.2 Finite Difference Model

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

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

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

$[A],[B]$ → Tridiagonal method



6 Point scheme

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

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

Fully Implicit $\rightarrow \mathrm{O}\left(\Delta x+\Delta t\right)$

9.2 Finite Difference Model

2) Formulation *CN-cd*

~ Central difference for $\dfrac{\partial C}{\partial x}$

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

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

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

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

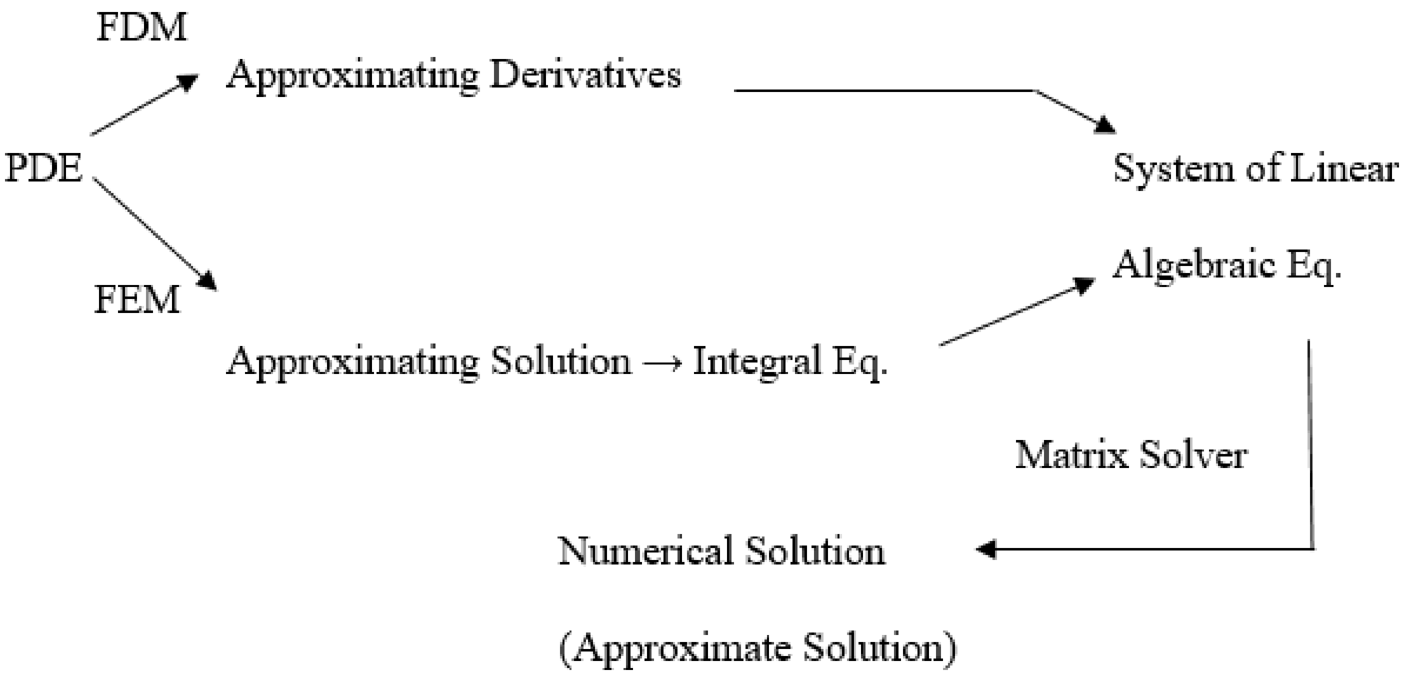
$$= \left(\frac{E\Delta t}{2\Delta x^2} + \frac{u\Delta t}{4\Delta x}\right)C_{i-1}^{n} + \left(1 - \frac{E\Delta t}{\Delta x^2}\right)C_i^{n} + \left(\frac{E\Delta t}{2\Delta x^2} - \frac{u\Delta t}{4\Delta x}\right)C_{i+1}^{n}$$

9.3 Finite Element Model

9.3.1 Introduction

- Difference between FDM and FEM solutions to PDE

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left(E\frac{\partial C}{\partial x}-uC\right) \qquad ①$$



PDE

FDM

Approximating Derivatives

FEM

Approximating Solution → Integral Eq.

System of Linear

Algebraic Eq.

Matrix Solver

Numerical Solution

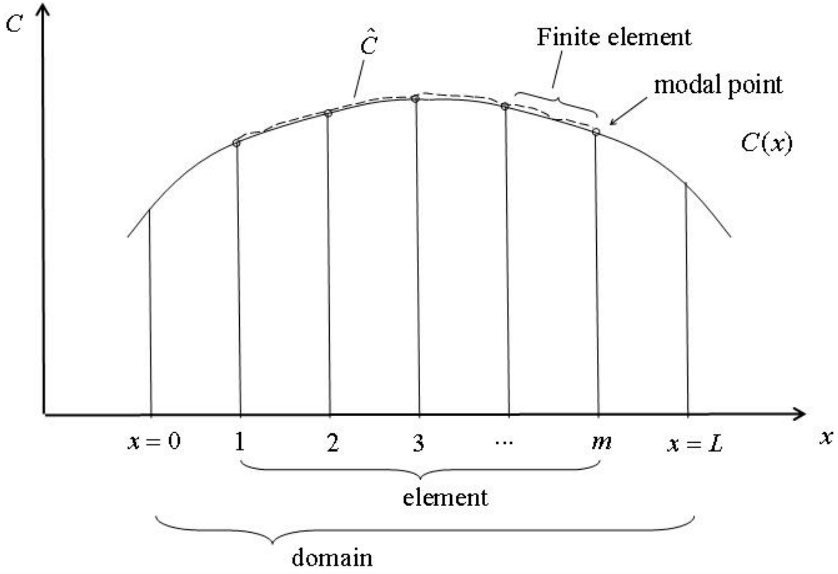
(Approximate Solution)

9.3 Finite Element Model

9.3.1 Introduction

FDM: A domain of interest is replaced by a set of discrete points. Then, the function of *C* is represented by an approximate function using Taylor series.

FEM: A domain is divided into subdomains (finite elements). Then, the unknown function C is represented by an interpolating polynomials within each element



9.3 Finite Element Model

- Procedure (Summary) of FEM

i) Discretize domain into elements

ii) Select basis functions

iii) Derive an integral equation based on Method of Weighted Residuals (MWR)

iv) Compute element matrix and vectors

v) Assemble global matrix and vectors

vi) Incorporate boundary conditions

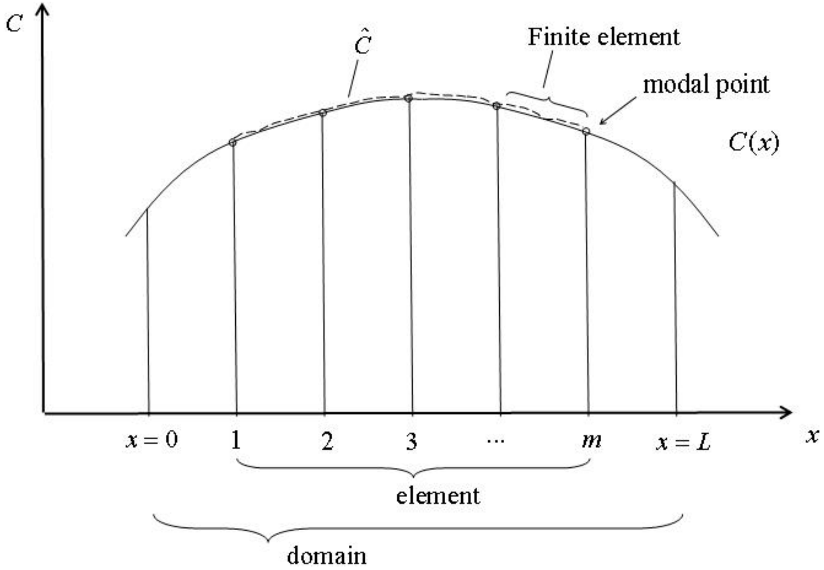
vii) Use a finite difference for time discretization

viii) Solve a system of simultaneous linear algebraic equation

9.3 Finite Element Model

9.3.2 FEM Formulation

(1) Domain Discretization



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

continuous function of x

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

piecewise continuous function

9.3 Finite Element Model

We may approximate the true solution by a polynomial

$$\boxed{\hat{C}^e(x) = \sum_{j=1}^{m} C_j \phi_j^e(x)} \qquad ②$$

in which

ϕ_j = basis function (shape, approximate) function

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

9.3 Finite Element Model

(2) Selection of Basis Function

1) Lagrangian interpolating polynomials

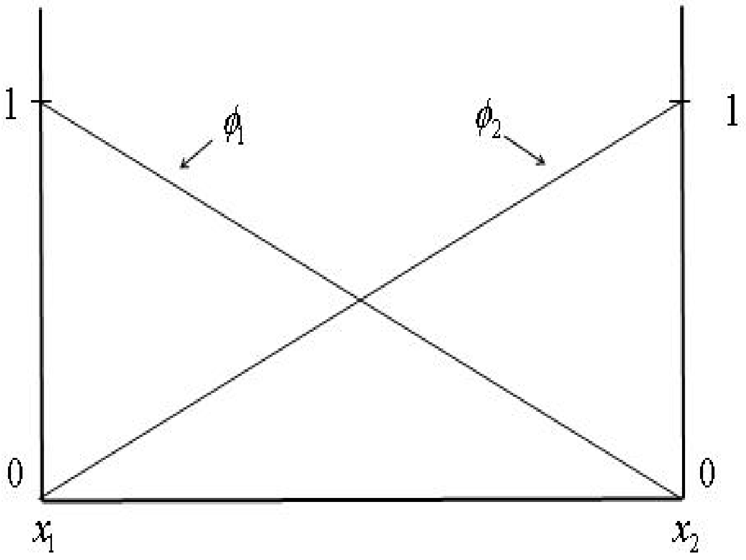
$$\boxed{\phi_j(x) = \prod_{\substack{k=1 \\ k\neq j}}^{m} \frac{x - x_k}{x_j - x_k}}$$

i) Linear function: m =2

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

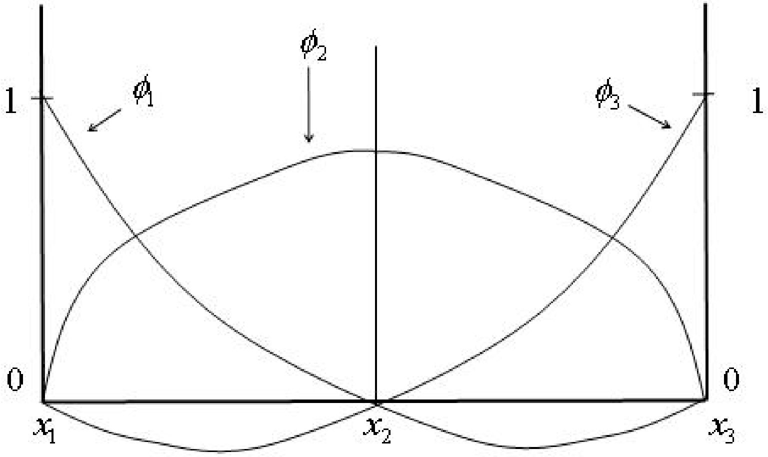
$$\phi_2(x) = \frac{x - x_1}{x_2 - x_1}$$

$$\therefore \hat{C}^e(x) = C_1\phi_1(x) + C_2\phi_2(x)$$



9.3 Finite Element Model

ii) Quadratic function: $m = 3$



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

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

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

$$\therefore \hat{C}^e(x) = C_1\phi_1(x) + C_2\phi_2(x) + C_3\phi_3(x)$$

2) Hermitian interpolating polynomials

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

$$\hat{C}^e(x) = \sum_{j=1}^{m}\left[C_j\phi_j^{(0)} + \left(\frac{dC}{dx}\right)_j \phi_j^{(1)}\right]$$

9.3 Finite Element Model

(3) Method of Weighted Residuals

- Formulation of approximating integral equation

$\left\{ \begin{array}{l} \text{Variational Method} \\ \text{Method of Weighted Residuals (MWR)} \end{array} \right.$

Select MWR

Substitute ② into ①

$$\boxed{\frac{\partial \hat{C}}{\partial t} - \frac{\partial}{\partial x}\left(E\frac{\partial \hat{C}}{\partial x} - u\hat{C} \right) \neq 0 = R(x,t) \rightarrow \text{Residual}} \quad ③$$

If $\hat{C} = C$ then $R\left(x,t\right) = 0$

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

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

9.3 Finite Element Model

Let's set the weighted integrals of the residual to zero → MWR

$$\int_{\Omega^e} R(x,t)\omega_i\left(x\right)d\Omega = 0, \qquad i = 1,2,\ldots.M \rightarrow \text{Integral Eq.} \quad ④$$

$$\boxed{\int \left\{ \frac{\partial \hat{C}}{\partial t} - \frac{\partial}{\partial x}\left(E\frac{\partial \hat{C}}{\partial x} - u\hat{C} \right) \right\} \omega_i\left(x\right)dx = 0} \quad ⑤$$

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

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

9.3 Finite Element Model

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

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

4) Least Squares Method

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

p(x) = arbitrary positive function

minimize the integrated square residual w.r.t a_i

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

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

9.3 Finite Element Model

[Re] Basis function vs Weighting function

The unknown function C is represented by an interpolating polynomials within each element

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

$u_j =$ undetermined coefficient

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

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

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

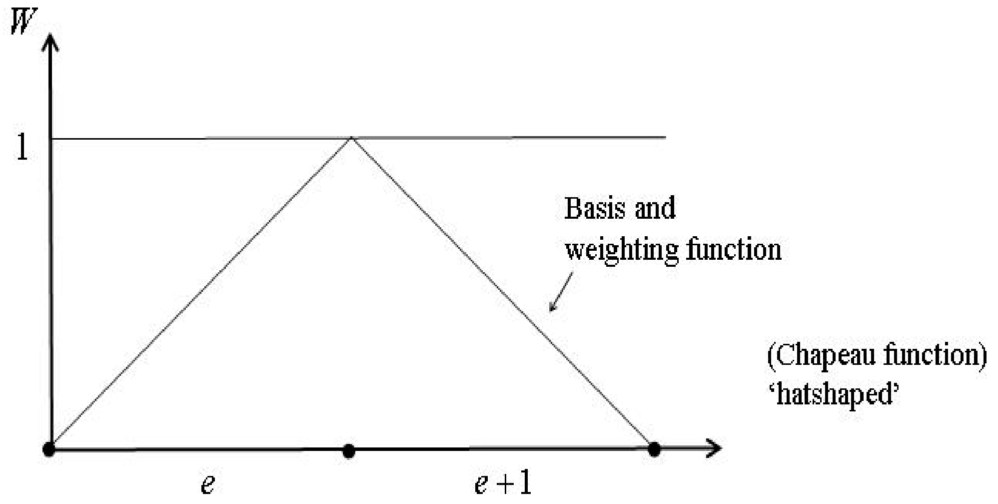
$\omega_j(\cdot) =$ weighting function

9.3 Finite Element Model

- **Galerkin Method**

Weighting function is chosen to be the basis function

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



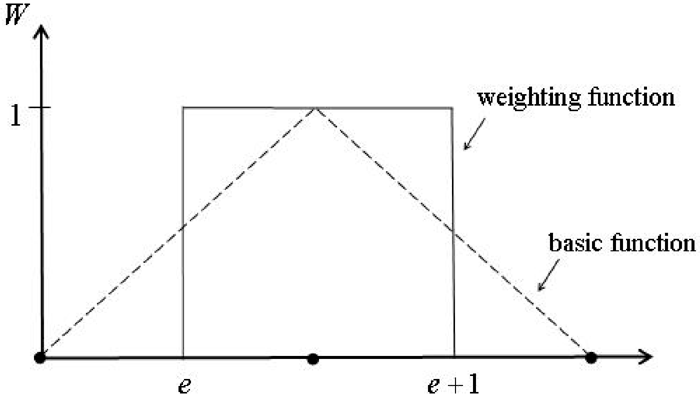
9.3 Finite Element Model

- **Subdomain Method**

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

where

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



Subdomain Method

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

9.3 Finite Element Model

- **Collocation Method**

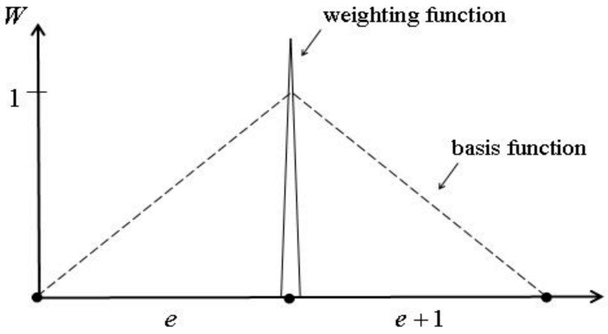
Weighting function is chosen to be the Dirac delta

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

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

~ Calculate the value of residual at the selected points

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



9.3 Finite Element Model

[Example]

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

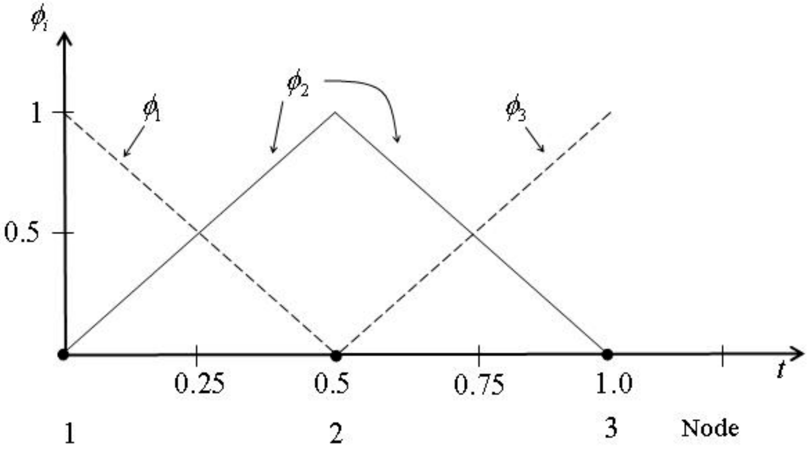
$$0 \le t \le 1$$

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

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

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

$i =$ nodal points



9.3 Finite Element Model

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

ii) $$\int_t R(t) w_i (t) dt = 0, \qquad i = 1, 2, 3$$

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

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

Apply Galerkin method

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

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

9.3 Finite Element Model

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

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

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

$$\phi_1\phi_3=0$$

9.3 Finite Element Model

iv) Expansion yields the following matrix equation

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

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

9.3 Finite Element Model

- Basis functions (Interpolation)

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

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

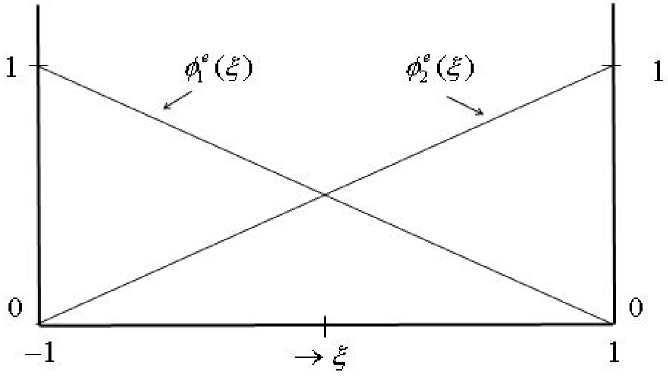
- Natural coordinate system for element basis function

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

i) Linear

$$\phi_1^e(\xi) = \frac{1}{2}(1-\xi) \qquad \phi_2^e(\xi) = \frac{1}{2}(1+\xi)$$

$$\frac{d\phi_1^e}{d\xi} = -\frac{1}{2} \qquad \frac{d\phi_2^e}{d\xi} = \frac{1}{2}$$



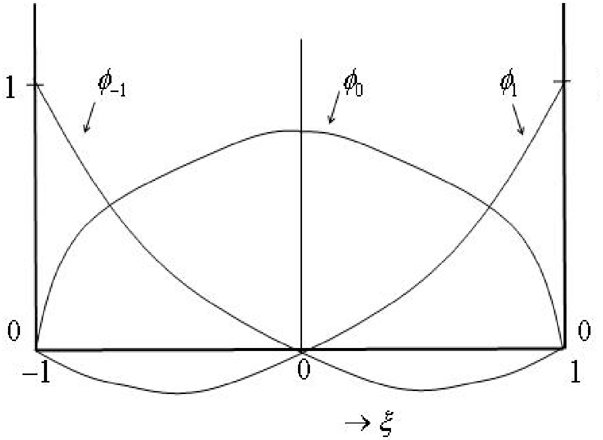
9.3 Finite Element Model

ii) Quadratic

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

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

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



9.3 Finite Element Model

- Galerkin method

Select the basis functions as the weighting functions

$$\omega_i = \phi_i$$

Thus the weighted integral equation of the residuals becomes

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

$$\underbrace{\int_{\Omega^e} \frac{\partial \hat{C}}{\partial t}\phi_i^e dx}_{A} - \underbrace{\int_{\Omega^e} \underbrace{\frac{\partial}{\partial x}\left(E\frac{\partial \hat{C}}{\partial x} - u\hat{C}\right)}_{d\upsilon} \underbrace{\phi_i^e}_{u} dx}_{B} = 0 \qquad \text{⑥}$$

9.3 Finite Element Model

Term A: 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 $\int udv = uv - \int vdu$

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

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

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

9.3 Finite Element Model

∴ Eq ⑥ :

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

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

⑦

Let

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

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

9.3 Finite Element Model

(4) Element matrix equation

The 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

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

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

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

9.3 Finite Element Model

By the way

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

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

$$m_{ij}^e = \int_{\Omega^e} \phi_j(x) \phi_i(x) dx = \int_{-1}^{1} \phi_j(\xi) \phi_i(\xi) d\xi \frac{dx}{d\xi} = \int_{-1}^{1} \phi_j \phi_i \, d\xi \frac{\Delta x}{2}$$

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

$$[A]^e = \begin{bmatrix} \frac{E}{\Delta x} - \frac{u}{2} & -\frac{E}{\Delta x} + \frac{u}{2} \\ -\frac{E}{\Delta x} - \frac{u}{2} & \frac{E}{\Delta x} + \frac{u}{2} \end{bmatrix} \quad [M]^e = \frac{\Delta x}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \quad \{B\}^e = \begin{Bmatrix} \left(E \frac{\partial \hat{C}}{\partial x} - u\hat{C} \right)_{x_1} \\ -\left(E \frac{\partial \hat{C}}{\partial x} - u\hat{C} \right)_{x_2} \end{Bmatrix}$$

9.3 Finite Element Model

(5) Assemble global matrix equations

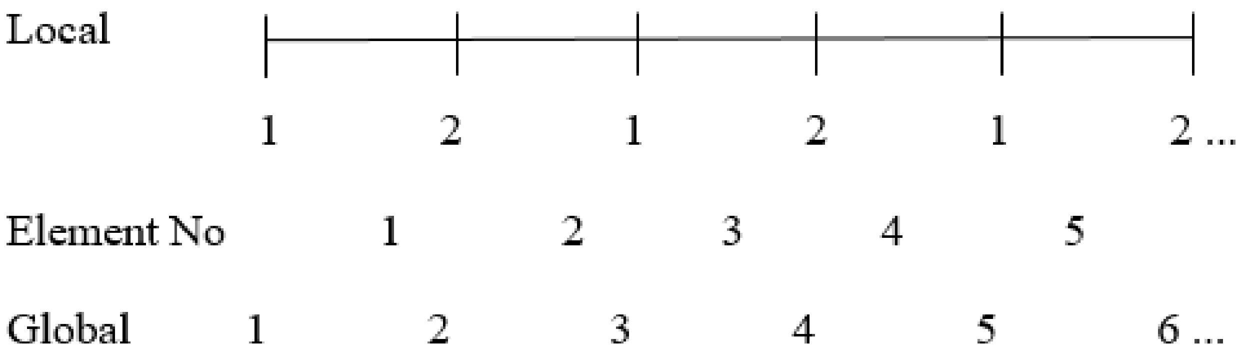
Combining element equations

For each element, apply

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

$[M]^e \& [A]^e$ ~ 2×2 matrices

- Numbering Systems



Local 1 2 1 2 1 2 ...

Element No 1 2 3 4 5

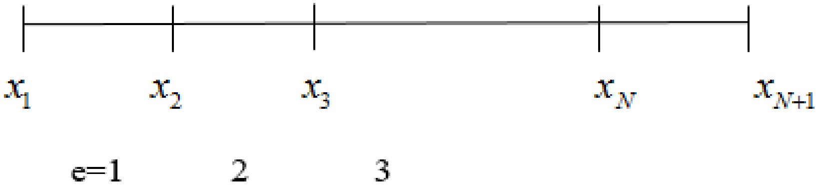
Global 1 2 3 4 5 6 ...

9.3 Finite Element Model

Let N (= number of element) = 30

number of nodes = 31

Then



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

9.3 Finite Element Model

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

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

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

- Boundary Conditions

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

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

9.3 Finite Element Model

(6) Time discretization

1) Fully Implicit

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

$$\left(\frac{[M]}{\Delta t}+[A]\right)\{\tilde{C}\}^{k+1}=\frac{[M]}{\Delta t}\{\hat{C}\}^{k}-\{B\}^{k+1} \qquad ⑩$$

$$[R]\{\hat{C}\}^{k+1}=[S]\{\hat{C}\}^{k}-\{B\} \qquad ⑪$$

In which

$$[R]=\frac{[M]}{\Delta t}+[A] \qquad [S]=\frac{[M]}{\Delta t}$$

9.3 Finite Element Model

(2) Crank-Nicholson scheme

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

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

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

$$\therefore\ [P]\{\hat{C}\}^{k+1}=[Q]\{\hat{C}\}^{k}-\{B\} \qquad ⑫$$

9.4 Finite Volume Model

9.4.1 FVM for one-dimensional diffusion

- Finite Difference Method:

A domain of interest is replaced by a set of discrete points. Then, the function of *C* is represented by an approximate function using Taylor series.

- Finite Volume Method:

A domain is divided into the discrete control volumes. Then, the governing equation is integrated over a control volume to yield a discretized equation at a nodal point.

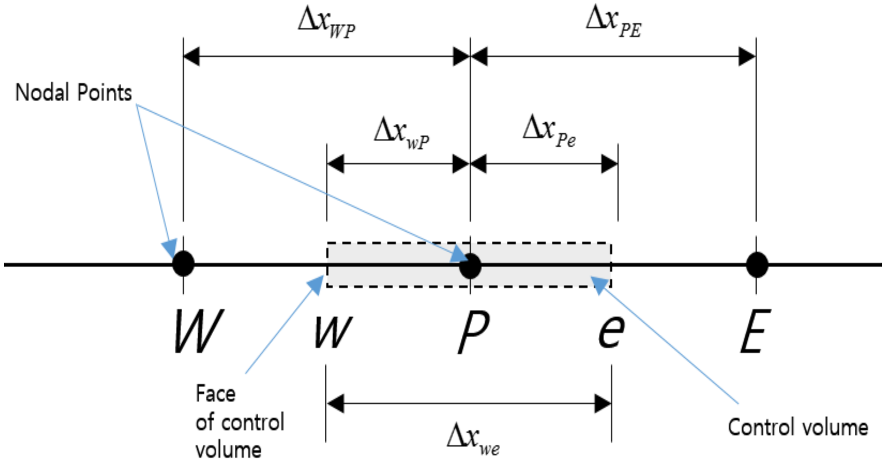
Consider the steady state diffusion of a concentration, C in a one-dimensional domain

$$\frac{d}{dx}\left(D\frac{dC}{dx}\right)+S=0$$

9.4 Finite Volume Model

- Grid generation

~ divide the domain into discrete control volumes



P : Nodal point

W and *E* : Neighbor nodes to west and east respectively

w and *e* : west and east side of face of control volume

The faces of control volumes are positioned mid-way between adjacent nodes.

→ each node is surrounded by a control volume (cell)

9.4 Finite Volume Model

- Discretization

The integration of the governing equation over a control volume to yield a discretized equation at its nodal point *P*

$$\int_{\Delta V} \frac{d}{dx}\left(D\frac{dC}{dx}\right)dV + \int_{\Delta V} S\,dV = \left(DA\frac{dC}{dx}\right)_e - \left(DA\frac{dC}{dx}\right)_w + \overline{S}\Delta V = 0 \qquad ①$$

where *A* : the cross-sectional area of the control volume face.

ΔV : the volume of the control volume.

$\overline{S}$: the average value of source *S* over the control volume.

9.4 Finite Volume Model

The diffusion coefficient, *D* and the gradient, $\dfrac{dC}{dx}$ at east(*e*) and west(*w*) faces are required in order to derive the discretized equations.

→ use Linear approximation (Central differencing)

$$\left(DA\frac{dC}{dx}\right)_e = D_e A_e\left(\frac{C_E - C_P}{\Delta x_{PE}}\right) \quad ②$$

$$\left(DA\frac{dC}{dx}\right)_w = D_w A_w\left(\frac{C_P - C_W}{\Delta x_{WP}}\right) \quad ③$$

If the source term is approximated by means of a linear form,

$$\overline{S}\Delta V = S_u + S_p C_p \quad ④$$

Substituting equations ②, ③ and ④ into equation ① gives

$$D_e A_e\left(\frac{C_E - C_P}{\Delta x_{PE}}\right) - D_w A_w\left(\frac{C_P - C_W}{\Delta x_{WP}}\right) + \left(S_u + S_p C_p\right) = 0 \quad ⑤$$

9.4 Finite Volume Model

Equation ⑤ can be rearranged as

$$\left(\frac{D_e}{\Delta x_{PE}}A_e+\frac{D_w}{\Delta x_{WP}}A_w-S_p\right)C_P=\left(\frac{D_w}{\Delta x_{WP}}A_w\right)C_W+\left(\frac{D_e}{\Delta x_{PE}}A_e\right)C_E+S_u$$

↓

$$a_pC_p=a_WC_W+a_EC_E+S_u \qquad ⑥$$

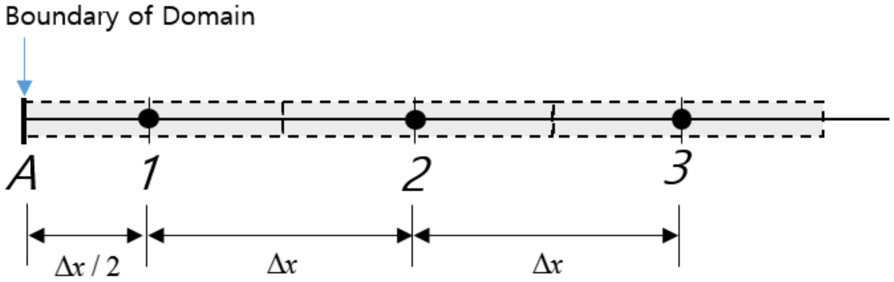
where

a_W	a_E	a_p
$\frac{D_w}{\Delta x_{WP}}A_w$	$\frac{D_e}{\Delta x_{PE}}A_e$	$a_W+a_E-S_p$

Discretized equation ⑥ must be set up at each of the nodal points. For control volume that are adjacent to the domain boundaries, the general discretized equation ⑥ is modified to incorporate boundary conditions.

9.4 Finite Volume Model

○ Treatment of the node adjacent to boundary



Treatment of the node adjacent to boundary

Node 1 that is located adjacent to boundary can be treated in same manner of derivation of discretized equation ⑥

Integration of governing equation at Node 1,

$$D_e A_e \left(\frac{C_E - C_p}{\Delta x} \right) - D_A A_A \left(\frac{C_p - C_A}{\Delta x / 2} \right) + \bar{S} \Delta V = 0$$

$$\downarrow$$

$$a_p C_p = a_W C_W + a_E C_E + S_u$$

9.4 Finite Volume Model

Where

a_W	a_E	a_p	S_p	S_u
0	$\frac{D_e}{\Delta x} A_e$	$a_W + a_E - S_p$	$-\frac{2D_A}{\Delta x} A_A$	$\bar{S}\Delta V + \frac{2D_A A_A}{\Delta x} C_A$

9.4 Finite Volume Model

9.4.2 FVM for two-dimensional diffusion

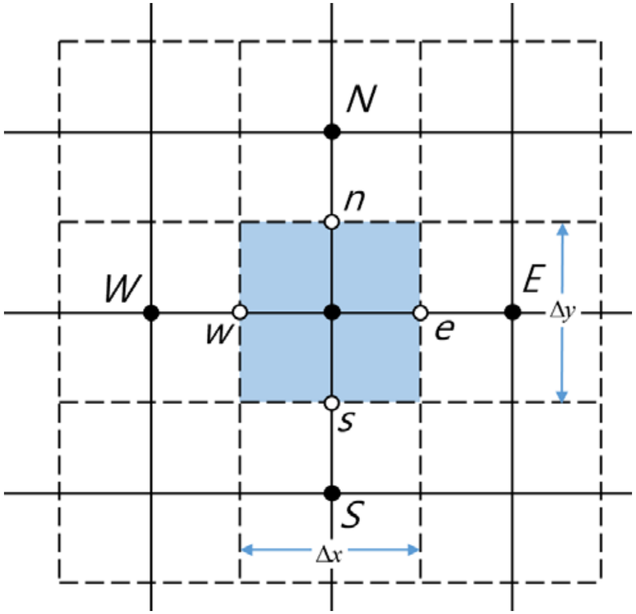
Two-dimensional steady state diffusion equation is given by

$$\frac{d}{dx}\left(D\frac{dC}{dx}\right)+\frac{d}{dy}\left(D\frac{dC}{dy}\right)+S=0$$

9.4 Finite Volume Model

○ Grid generation

~divide the domain into discrete control volumes



Grid generation

Upper case letter (*E, W, N, W*): Neighbor nodes

Lower case letter (*e, w, n, w*): control volume faces

9.4 Finite Volume Model

○ Discretization

~integrate governing equation over control volume (cell)

$$\int_{\Delta V}\frac{d}{dx}\left(D\frac{dC}{dx}\right)dx\cdot dy+\int_{\Delta V}\frac{d}{dy}\left(D\frac{dC}{dy}\right)dx\cdot dy+\int_{\Delta V}S\,dV=0$$

Noting that $A_e = A_w = \Delta y$ and , $A_n = A_s = \Delta x$ we obtain

$$\left[D_eA_e\left(\frac{\partial C}{\partial x}\right)_e-D_wA_w\left(\frac{\partial C}{\partial x}\right)_w\right]+\left[D_nA_n\left(\frac{\partial C}{\partial y}\right)_n-D_sA_s\left(\frac{\partial C}{\partial x}\right)_s\right]+\overline{S}\Delta V=0$$

→ The balance of the generation of *C* in a control volume and the fluxes through its cell faces.

9.4 Finite Volume Model

Flux across the west face $= D_w A_w \left(\frac{\partial C}{\partial x} \right)_w = D_w A_w \frac{C_p - C_W}{\Delta x}$

Flux across the east face $= D_e A_e \left(\frac{\partial C}{\partial x} \right)_e = D_e A_e \frac{C_E - C_p}{\Delta x}$

Flux across the south face $= D_s A_s \left(\frac{\partial C}{\partial x} \right)_s = D_s A_s \frac{C_p - C_S}{\Delta y}$

Flux across the north face $= D_n A_n \left(\frac{\partial C}{\partial x} \right)_n = D_n A_n \frac{C_N - C_p}{\Delta y}$

Substituting the above expressions into equation

$$D_e A_e \frac{C_E - C_p}{\Delta x} - D_w A_w \frac{C_p - C_W}{\Delta x} + D_n A_n \frac{C_N - C_p}{\Delta y} - D_s A_s \frac{C_p - C_S}{\Delta y} + \bar{S} \Delta V = 0$$

9.4 Finite Volume Model

Assuming the source term in linearized form is $\overline{S}\Delta V = S_u + S_p C_p$ and rearranging

$$\left(\frac{D_w A_w}{\Delta x} + \frac{D_e A_e}{\Delta x} + \frac{D_s A_s}{\Delta y} + \frac{D_n A_n}{\Delta y} - S_p\right) C_p$$

$$= \left(\frac{D_w A_w}{\Delta x}\right) C_W + \left(\frac{D_e A_e}{\Delta x}\right) C_E + \left(\frac{D_s A_s}{\Delta y}\right) C_S + \left(\frac{D_n A_n}{\Delta y}\right) C_N + S_u$$

The general discretized equation form is

$$a_p C_p = a_W C_W + a_E C_E + a_S C_S + a_N C_N + S_u$$

Where

a_W	a_E	a_S	a_N	a_p
$\frac{D_w A_w}{\Delta x}$	$\frac{D_e A_e}{\Delta x}$	$\frac{D_s A_s}{\Delta y}$	$\frac{D_n A_n}{\Delta y}$	$a_W + a_E + a_S + a_N - S_p$

At the boundary where the concentration are known, the discretized equations are modified to incorporate boundary conditions in the manner demonstrated in one-dimensional problem.

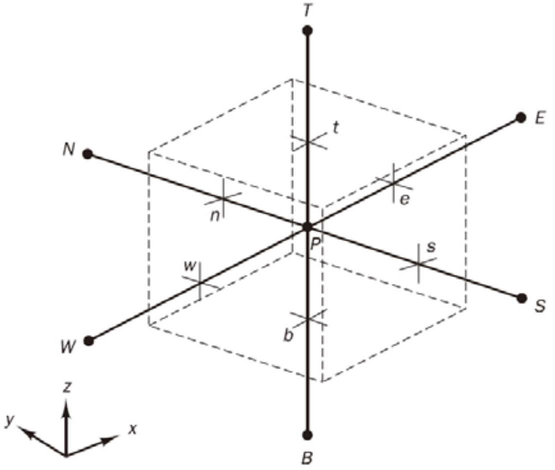
9.4 Finite Volume Model

9.4.3 FVM for three-dimensional diffusion

Steady state diffusion in a three-dimensional situation is governed by

$$\frac{d}{dx}\left(D\frac{dC}{dx}\right)+\frac{d}{dy}\left(D\frac{dC}{dy}\right)+\frac{d}{dz}\left(D\frac{dC}{dz}\right)+S=0$$

○ Grid generation



A cell contacting node P has six neighboring nodes identified as west, east, south, north, bottom and top *(W, E, S, N, B, T)*.

The notation *w, e, s, n, b* and *t* is used to refer to the west, east, south, north, bottom and top cell faces.

9.4 Finite Volume Model

○ Discretization

~integrate governing equation over control volume (cell)

$$\left[D_e A_e\left(\frac{\partial C}{\partial x}\right)_e - D_w A_w\left(\frac{\partial C}{\partial x}\right)_w\right] + \left[D_n A_n\left(\frac{\partial C}{\partial y}\right)_n - D_s A_s\left(\frac{\partial C}{\partial x}\right)_s\right]$$

$$+\left[D_t A_t\left(\frac{\partial C}{\partial z}\right)_t - D_b A_b\left(\frac{\partial C}{\partial x}\right)_b\right] + \overline{S}\Delta V = 0$$

~ Follow the procedure developed for one- and two-dimensional cases the discretized form of equation is obtained:

$$\left[D_e A_e \frac{C_E - C_p}{\Delta x} - D_w A_w \frac{C_p - C_W}{\Delta x}\right] + \left[D_n A_n \frac{C_N - C_p}{\Delta y} - D_s A_s \frac{C_p - C_S}{\Delta y}\right]$$

$$+\left[D_t A_t \frac{C_T - C_p}{\Delta z} - D_b A_b \frac{C_p - C_B}{\Delta z}\right] + \left(S_u + S_p C_p\right) = 0$$

9.4 Finite Volume Model

The general discretized equation form is

$$a_p C_p = a_W C_W + a_E C_E + a_S C_S + a_N C_N + a_B C_B + a_T C_T + S_u$$

Where

a_W	a_E	a_S	a_N	a_B	a_T	a_p
$\frac{D_w A_w}{\Delta x}$	$\frac{D_e A_e}{\Delta x}$	$\frac{D_s A_s}{\Delta y}$	$\frac{D_n A_n}{\Delta y}$	$\frac{D_b A_b}{\Delta z}$	$\frac{D_t A_t}{\Delta z}$	$a_W + a_E + a_S + a_N + a_B + a_T - S_p$

9.4 Finite Volume Model

9.4.4 FVM for advection-dispersion

Steady advection and dispersion of concentration C in a given one-dimensional flow field U is governed by

$$\frac{d}{dx}\left(\rho UC\right)=\frac{d}{dx}\left(K\frac{dC}{dx}\right)$$

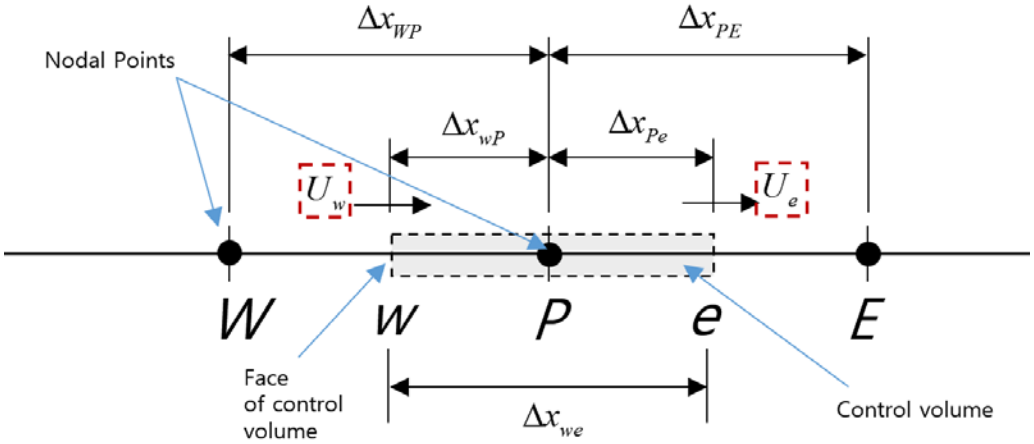
The flow must also satisfy continuity equation.

$$\frac{d}{dx}\left(\rho U\right)=0$$

9.4 Finite Volume Model

○ Grid generation

~divide the domain into discrete control volumes.



Grid generation

The same notation as in the one-dimensional diffusion problem is used.

U_w and U_e are cross-sectional average velocity on the faces of control volume.

9.4 Finite Volume Model

○ Discretization

Integration of transport equation over the control volume

$$\left(\rho UAC\right)_e-\left(\rho UAC\right)_w=\left(KA\frac{dC}{dx}\right)_e-\left(KA\frac{dC}{dx}\right)_w$$

Integration of continuity equation over the control volume

$$\left(\rho UA\right)_e-\left(\rho UA\right)_w=0$$

For convenience, convective mass flux unit area and dispersion term are replaced to: $F=\rho U \quad , \quad D=\dfrac{K}{\Delta x}$

The cell face values of the F and D can be written as

$$F_w=\left(\rho U\right)_w \quad , \quad F_e=\left(\rho U\right)_e$$

$$D_w=\frac{K_w}{\Delta x} \quad , \quad D_e=\frac{K_e}{\Delta x}$$

9.4 Finite Volume Model

Assuming that $A_w = A_e = A$, the integrated advection-dispersion equation can be written as

$$F_e C_e - F_w C_w = D_e \left(C_E - C_p\right) - D_w \left(C_p - C_W\right)$$

And the integrated continuity equation as

$$F_e - F_w = 0$$

When we have one-dimensional flow field U, F_e and F_w can be calculated.

~ need to know the transported concentration C at the e and w faces

(1) Central differencing scheme for advection

For a uniform grid, the cell face values of concentration C as

$$C_e = \left(C_p + C_E\right)/2$$

$$C_w = \left(C_W + C_p\right)/2$$

Substitution of the above expressions into the advection term

$$\frac{F_e}{2}\left(C_p + C_E\right) - \frac{F_w}{2}\left(C_W + C_p\right) = D_e \left(C_E - C_p\right) - D_w \left(C_p - C_W\right)$$

9.4 Finite Volume Model

This can be rearrange to give

$$\left[\left(D_w+\frac{F_w}{2}\right)+\left(D_e-\frac{F_e}{2}\right)+\left(F_e-F_w\right)\right]C_p=\left(D_w+\frac{F_w}{2}\right)C_W+\left(D_e-\frac{F_e}{2}\right)C_E$$

Central differencing expressions for the discretized advection-dispersion equation are

$$a_p C_p = a_W C_W + a_E C_E$$

where

a_W	a_E	a_p
$D_w+\frac{F_w}{2}$	$D_e-\frac{F_e}{2}$	$a_W+a_E+\left(F_e-F_w\right)$

9.4 Finite Volume Model

(2) Upwind differencing scheme for advection

In a strongly convective flow, the cell face should receive much stronger influencing from upstream node.

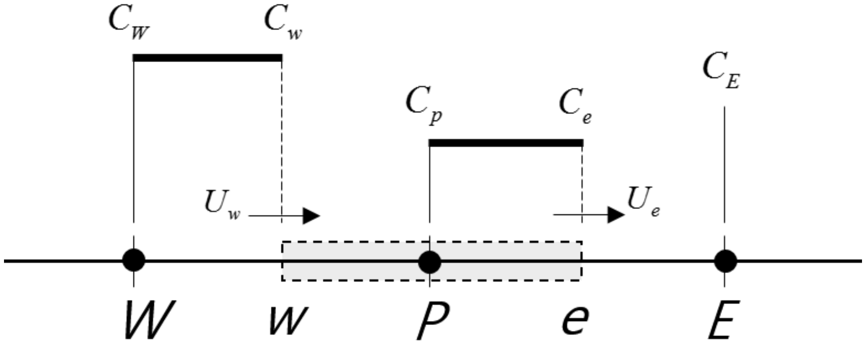
~ UDS takes into account the flow direction when determining the value at a cell face

~ The transported value of C at a cell face is taken to be equal to the value at the upstream node.

○ Flow in the positive direction

$$u_w > 0 \ , \ u_e > 0$$

$C_w = C_W$ and $C_e = C_p$



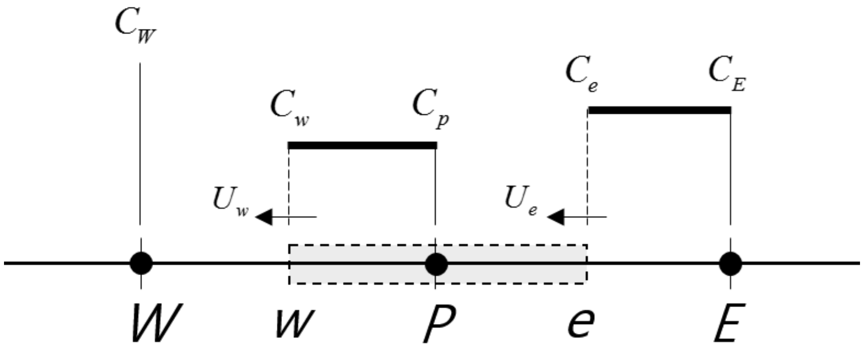
9.4 Finite Volume Model

The discretized equation becomes

$$F_eC_p - F_wC_W = D_e\left(C_E - C_p\right) - D_w\left(C_p - C_W\right)$$

This can be rearrange as

$$\left[\left(D_w + F_w\right) + D_e + \left(F_e - F_w\right)\right]C_p = \left(D_w + F_w\right)C_W + D_eC_E$$



- ○ Flow in the negative direction

$$u_w < 0 \ , \ u_e < 0$$

$C_w = C_p$ and $C_e = C_E$

The discretized equation becomes

$$F_eC_E - F_wC_p = D_e\left(C_E - C_p\right) - D_w\left(C_p - C_W\right)$$

This can be rearrange as

$$\left[D_w + \left(D_e - F_e\right) + \left(F_e - F_w\right)\right]C_p = D_wC_W + \left(D_e - F_e\right)C_E$$

9.4 Finite Volume Model

Upwind differencing expressions for the discretized advection-dispersion equation are $a_p C_p = a_W C_W + a_E C_E$

Where

	a_W	a_E	a_p
$F_w > 0,\ F_e > 0$	$D_w + F_w$	D_e	$a_W + a_E + (F_e - F_w)$
$F_w < 0,\ F_e < 0$	D_w	$D_e - F_w$	

(3) Hybrid differencing scheme for advection

~ based on a combination of central and upwind differencing schemes.

~central differencing scheme is employed for small Peclet number ($Pe<2$)

~upwind differencing scheme is employed for large Peclet number ($Pe \geq 2$)

~Peclet number is evaluated at the face of the control volume.

9.4 Finite Volume Model

For west face of control volume

$$Pe_w = \frac{F_w}{D_w} = \frac{(\rho U)_w}{K_w / \Delta x}$$

The hybrid differencing formula for the net flux per unit area though the west face is

$$q_w = F_w \left[\frac{1}{2}\left(1 + \frac{2}{Pe_w}\right) C_W + \frac{1}{2}\left(1 - \frac{2}{Pe_w}\right) C_p \right] \qquad \text{For} \quad -2 < Pe_w < 2$$

$$q_w = F_w C_W \qquad \text{For} \quad Pe_w \geq 2$$

$$q_w = F_w C_p \qquad \text{For} \quad Pe_w \leq -2$$

East face of control volume also follow the same manner.

9.4 Finite Volume Model

The general form of the discretized equation is

$$a_p C_p = a_W C_W + a_E C_E$$

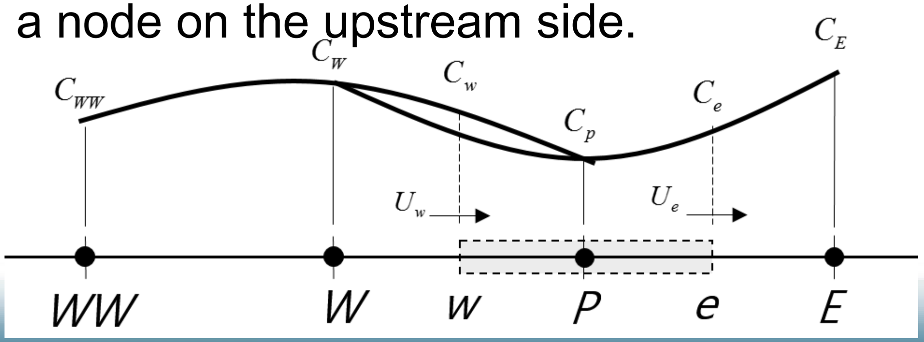
Where

a_W	a_E	a_p
$\max\left[F_w, \left(D_w + \frac{F_w}{2}\right), 0\right]$	$\max\left[-F_e, \left(D_e - \frac{F_e}{2}\right), 0\right]$	$a_W + a_E + \left(F_e - F_w\right)$

(4) Quadratic upwind differencing scheme for advection: the QUICK scheme

~uses a three-point upstream-weighted quadratic interpolation for cell face values.

~The face value of C is obtained from a quadratic function passing through two bracketing nodes and a node on the upstream side.



9.4 Finite Volume Model

For uniform grid the value of C at the cell face between two bracketing nodes i and i-1 and upstream node i-2 is given by:

$$C_{face} = \frac{6}{8}C_{i-1} + \frac{3}{8}C_i - \frac{1}{8}C_{i-2}$$

When $u_w > 0$, the bracketing nodes for the west face w are W and P, the upstream node is WW

$$C_w = \frac{6}{8}C_W + \frac{3}{8}C_p - \frac{1}{8}C_{WW}$$

When $u_e > 0$, the bracketing nodes for the west face e are P and E, the upstream node is W

$$C_e = \frac{6}{8}C_p + \frac{3}{8}C_E - \frac{1}{8}C_W$$

The discretized equation becomes

$$F_e C_e - F_w C_w = D_e\left(C_E - C_p\right) - D_w\left(C_p - C_W\right)$$

$$F_e\left(\frac{6}{8}C_p + \frac{3}{8}C_E - \frac{1}{8}C_W\right) - F_w\left(\frac{6}{8}C_W + \frac{3}{8}C_p - \frac{1}{8}C_{WW}\right) = D_e\left(C_E - C_p\right) - D_w\left(C_p - C_W\right)$$

9.4 Finite Volume Model

This can be rearrange as

$$\left[D_w - \frac{3}{8}F_w + D_e + \frac{6}{8}F_e\right]C_p = \left[D_w + \frac{6}{8}F_w + \frac{1}{8}F_e\right]C_W + \left[D_e - \frac{3}{8}F_e\right]C_E - \frac{1}{8}F_w C_{WW}$$

The general form of the discretized equation is

$$a_p C_p = a_W C_W + a_E C_E + a_{WW} C_{WW} + a_{EE} C_{EE}$$

where

a_W	a_{WW}	a_E	a_{EE}	a_p
$D_w + \frac{6}{8}\alpha_w F_w$ $+\frac{1}{8}\alpha_e F_e$ $+\frac{3}{8}(1-\alpha_w)F_w$	$-\frac{1}{8}\alpha_w F_w$	$D_e - \frac{3}{8}\alpha_e F_e$ $-\frac{6}{8}(1-\alpha_e)F_e$ $-\frac{1}{8}(1-\alpha_w)F_w$	$\frac{1}{8}(1-\alpha_e)F_e$	$a_W + a_E + a_{WW} + a_{EE} + (F_e - F_w)$

Where

$\alpha_w = 1$ for $F_w > 0$ and $\alpha_e = 1$ for $F_e > 0$

$\alpha_w = 0$ for $F_w < 0$ and $\alpha_e = 0$ for $F_e < 0$

9.5 Finite Particle Model

9.5.1 Concepts

- **Finite Particle Model**

A number of particles, each representing a finite mass of solute, are released at a rate proportional to the strength of each source. The particles are then "tracked" in space and time.

→ Particle Tracking Method (Prickett et al., 1981)

→ Giant Molecule Method

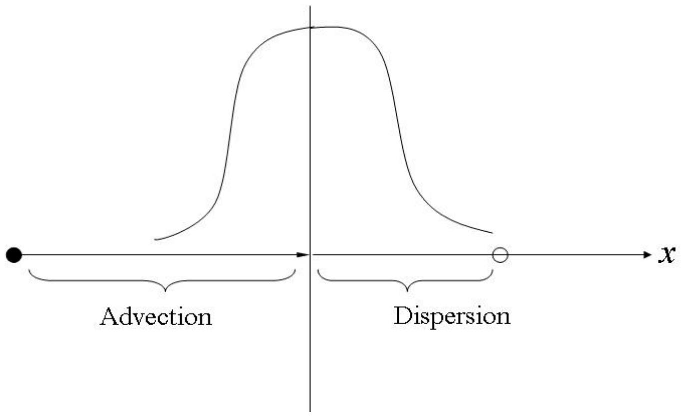
- Distribution of concentration of solute

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

~ each particle which is assigned a mass which represents a fraction of the total mass of chemical constituent, is moved by flow and dispersed by the random mixing

9.5 Finite Particle Model

- In the computer code, enough particles are introduced so that their locations and density are adequate to describe the distribution of the dissolved constituent of interest.
- New position = Old position + Advection + Dispersion
- Dispersion is based on the concept of random process.



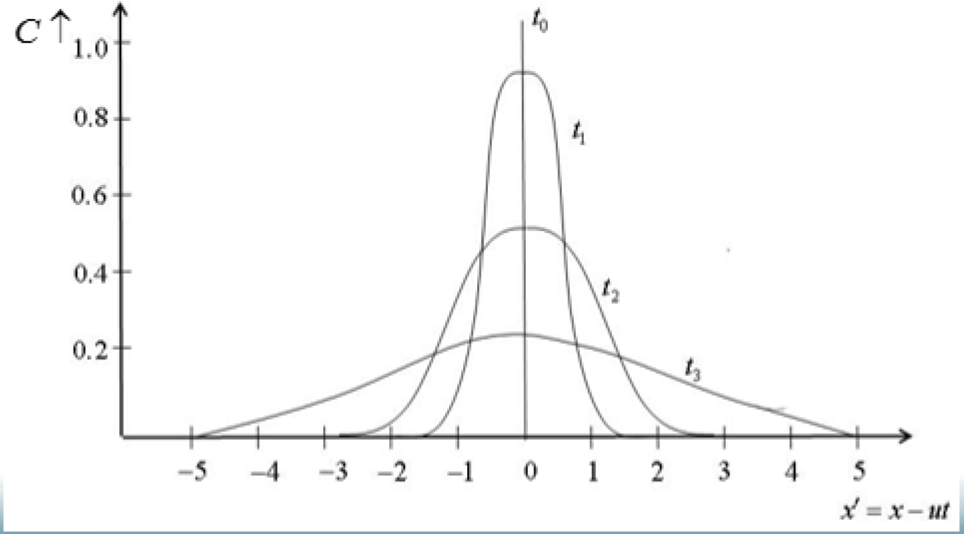
9.5 Finite Particle Model

The advection-dispersion equation is given as

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = E\frac{\partial^2 C}{\partial x^2} - kC \tag{1}$$

The analytical solution for a unit slug of solute placed initially at $x = 0$ is given

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



9.5 Finite Particle Model

- Statistically, a random variable *x* is 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

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

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

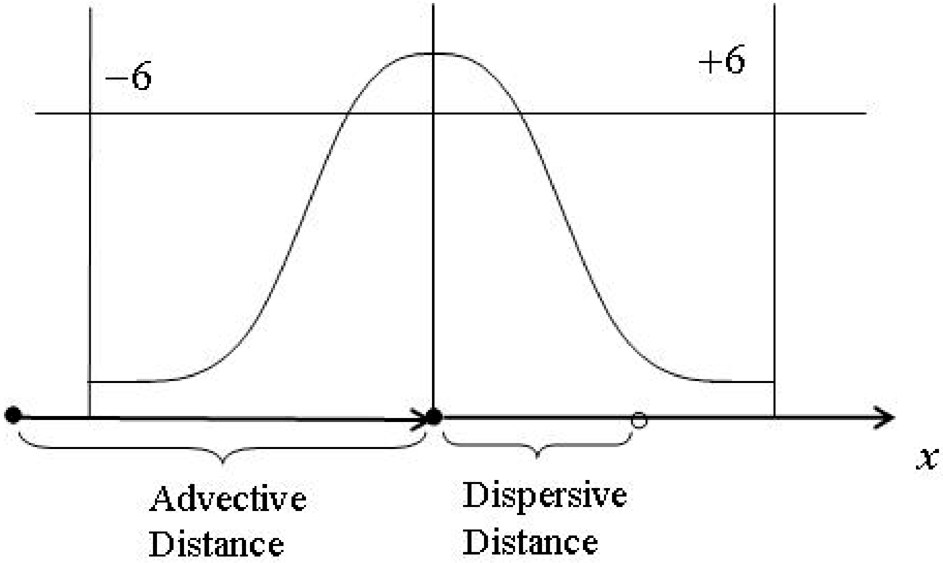
$$n(x) = C(x,t) \qquad (6)$$

9.5 Finite Particle Model

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 Model**



9.5 Finite Particle Model

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

Δt = time increment

Dispersive distance $= \pm 6\sigma$

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

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.

$\therefore$ New position of the particle

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

9.5 Finite Particle Model

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.

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

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

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).

9.5 Finite Particle Model

- Generation of ANORM(0) in computer code.

1) Summation of random function

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

In EXCEL, RAND()

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

2) Multiply random function

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

3) Numerical Recipes

ANORM(0)= GASDEV (IDUM)

RAND() = RAN1(IDUM)

9.5 Finite Particle Model

- Advantages of the Random Walk Model

i) There is no numerical dispersion, despite the use of an Eulerian framework.

ii) Computer CPU time is drastically reduced.

iii) 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 run.

iv) This method is particularly suited to time-sharing systems where velocity fields can be stored.

- Disadvantages

i) It may require a large number of particles to obtain meaningful results.

ii) It doesn't easily accommodate non-linear kinetic expressions.

9.5 Finite Particle Model

9.5.2 2D Random Walk Model

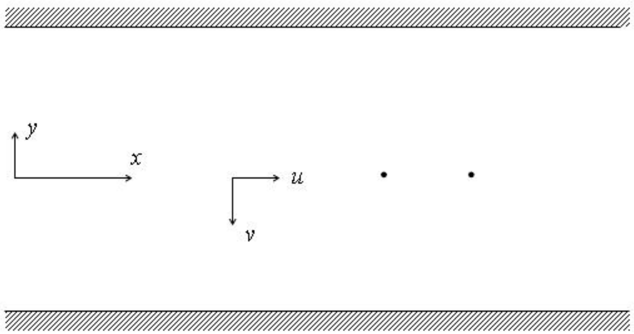
Depth-averaged advection-dispersion equation is

$$\frac{\partial C}{\partial t} + u(x,y)\frac{\partial C}{\partial x} + v(x,y)\frac{\partial C}{\partial y} = \frac{\partial}{\partial x}\left(E_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y\frac{\partial C}{\partial y}\right) + S$$

$$E_x = 5.93du_*$$

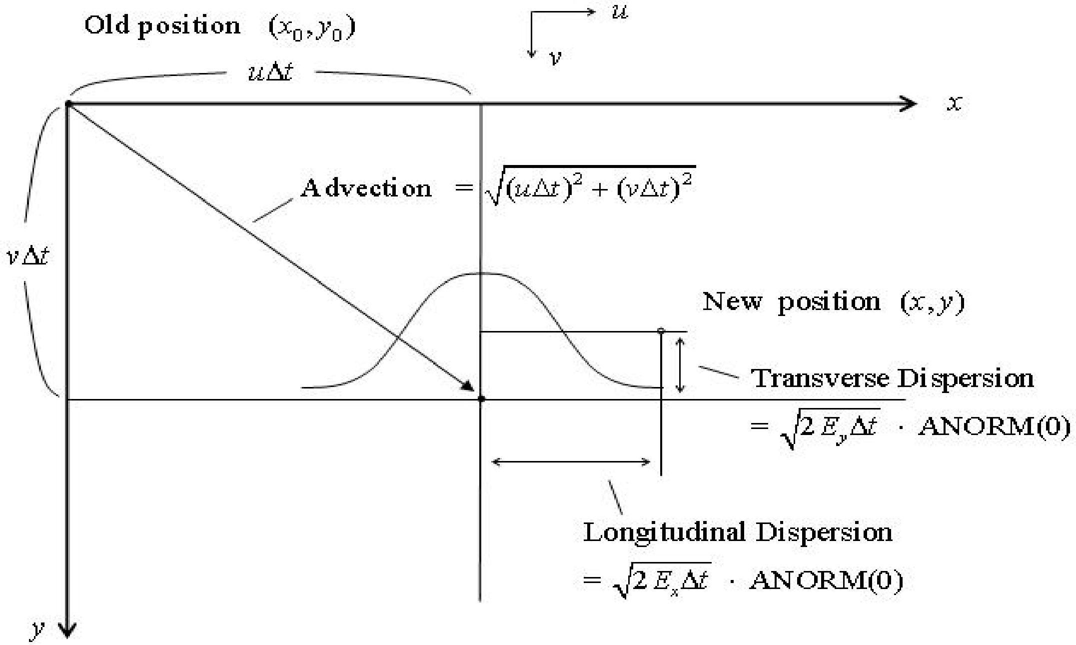
$$E_y = 0.6du_*$$

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



9.5 Finite Particle Model

2D Random Walk Model



9.5 Finite Particle Model

Longitudinal and transverse dispersion take place simultaneously

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

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

In natural rivers

$$E_x = 5.93\, du_*$$

$$E_y = 0.6\, du_*$$