Advection, diffusion and dispersion

Advection

- Transport with pore water (plug flow)

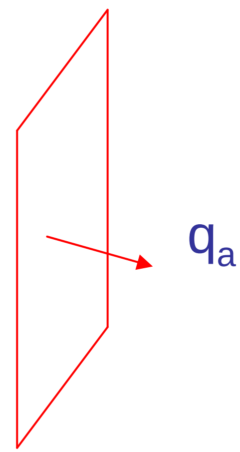
Darcy flux

Effective porosity

$$q_a = qC = v_a C \theta_{eff}$$

Pore water velocity

Concentration



Advection, diffusion and dispersion

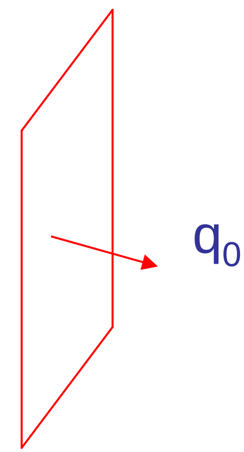
Diffusion

- Spreading due to gradient in concentrations

$$q_0 = -D_0 \frac{\partial c}{\partial x}$$

Concentration gradient

Diffusion coefficient



Advection, diffusion and dispersion

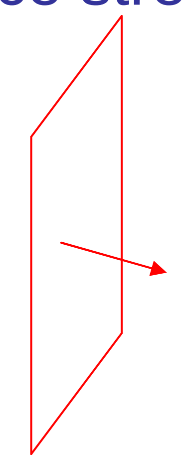
Dispersion

- Spreading due to:
  - pore to pore variation in velocity
  - velocity variation within the pores
  - spreading due to incomplete knowledge regarding geological heterogeneities, source strength, source location, locale flow pattern, etc.

$$q_M = -D_M \frac{\partial c}{\partial x}$$

Concentration gradient

Mechanical dispersion coefficient



$$D_M = \alpha \cdot v_a$$

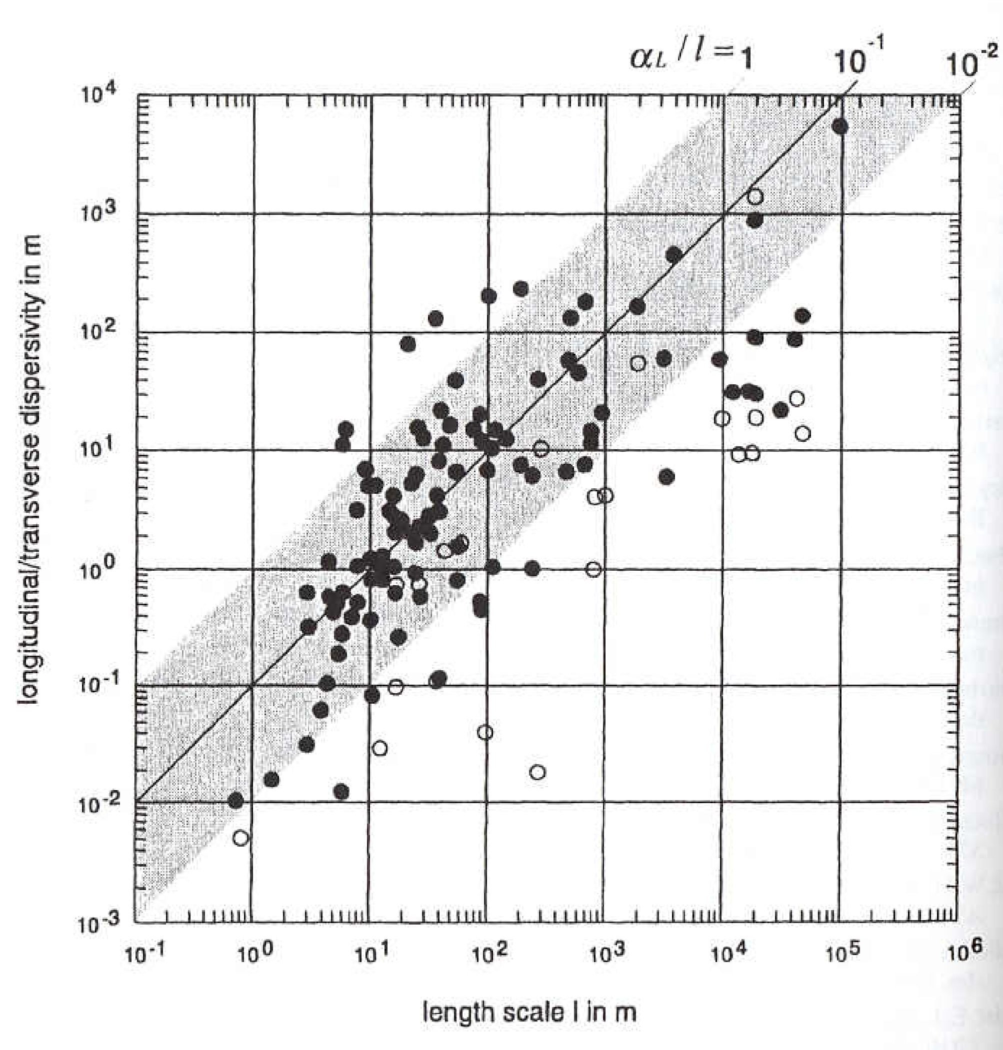
Pore velocity

Dispersivity

See a list of field-scale dispersivities in appendix D.3

Field dispersivity

$$\alpha_L \approx \frac{1}{10}\,\text{travel distance}$$



(Travel length)

See a list of field-scale dispersivities in appendix D.3

Solution of the 3D advection-dispersion equation

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - v_{a,i}\frac{\partial C}{\partial x_i} + S_n = \frac{\partial C}{\partial t}$$

Dispersion and diffusion

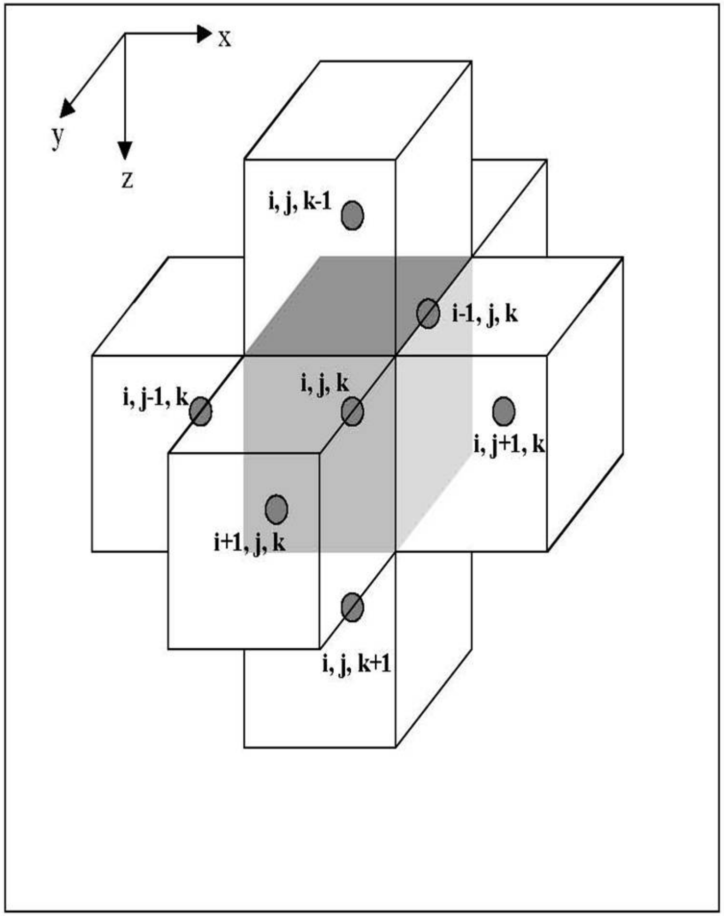
Advective in/outflow

Source/sink (decay, sorption, etc.)

Change in storage

- Standard finite difference methods
- Particle based methods (MOC, MMOC, HMOC)
- High order FD or FV methods (TVD)

Standard finite difference methods

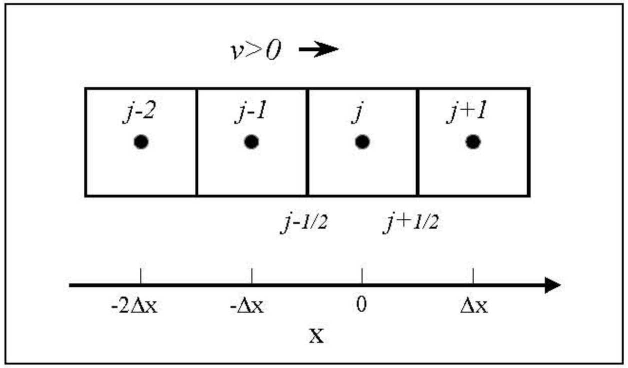


$$R\theta \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(\theta v_x C) - \frac{\partial}{\partial y}(\theta v_y C) - \frac{\partial}{\partial z}(\theta v_z C) + L(C)$$

storage — advection — dispersion

Only good for transport problems not dominated by advection

High order FD or FV methods (TVD)



$$C(0,0) = C_j, \; at \; x = 0$$

$$C(-2\Delta x,0) = C_{j-2}, \; at \; x = -2\Delta x$$

$$C(-\Delta x,0) = C_{j-1}, \; at \; x = -\Delta x$$

$$C(\Delta x,0) = C_{j+1}, \; at \; x = \Delta x$$

Third-order polynomial

$$C(x,0) = a + bx + cx^2 + dx^3$$

where

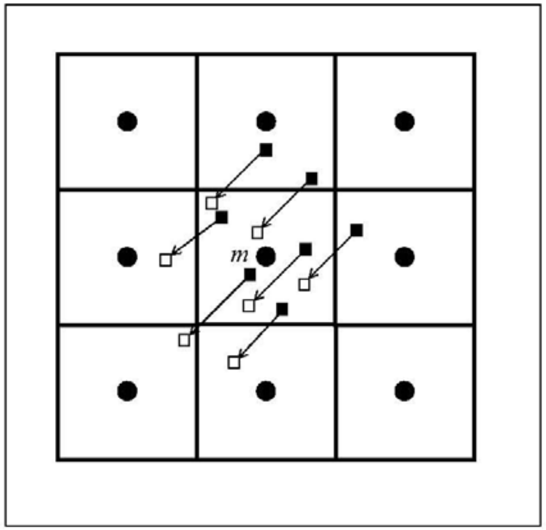
$$a = C_j$$

$$b = \frac{1}{\Delta x}\left(\frac{C_{j+1}}{3} + \frac{C_j}{2} - C_{j-1} + \frac{C_{j-2}}{6}\right)$$

$$c = \frac{1}{2(\Delta x)^2}\left(C_{j+1} - 2C_j + C_{j-1}\right)$$

$$d = \frac{1}{6(\Delta x)^3}\left(C_{j+1} - 3C_j + 3C_{j-1} - C_{j-2}\right)$$

Methods of characteristics (MOC)



Advection ➔ particle-tracking techniques

Dispersion ➔ finite-difference techniques

Advection

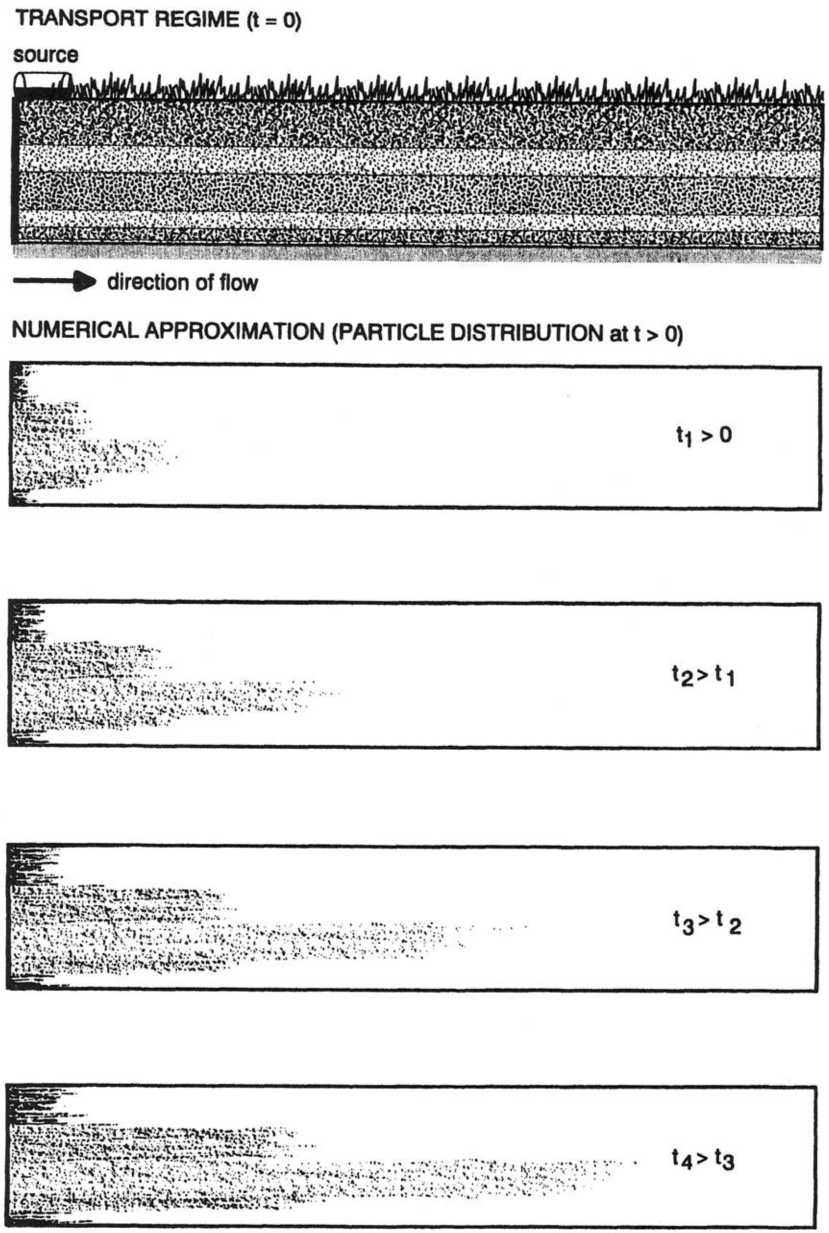
Number of particles within cell m

$$C_m^{n*} = \frac{1}{NP_m} \sum_{p=1}^{NP_m} C_p^n \quad if \quad NP_m > 0$$

Concentration of the p^{th} particle at the old time level *n*

Concentration in cell m at the new time level *n**

Particle tracking



Advective transport

$$\Delta x = v_{xa} \Delta t$$

$$\Delta y = v_{ya} \Delta t$$

Dispersive transport in flow direction

$$P_L = \pm Z_1 \sqrt{2 D_L \Delta t}$$

Dispersive transport transverse to the flow direction

$$P_T = \pm Z_2 \sqrt{2 D_T \Delta t}$$

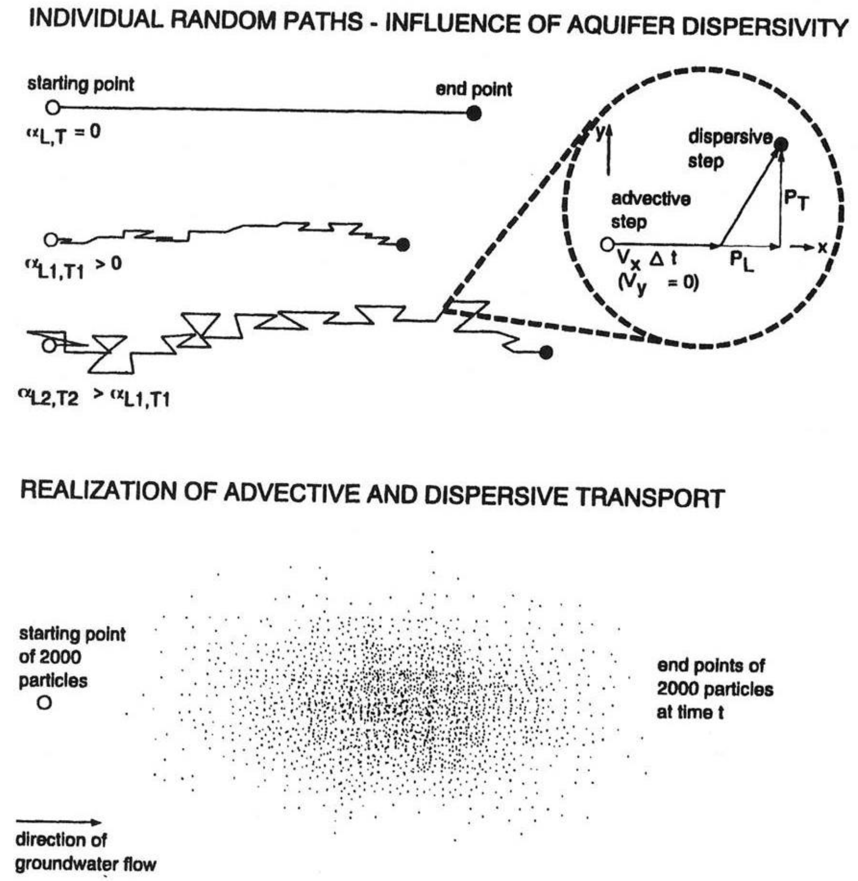
where

D_L = longitudinal dispersion coef. [L^2/T]

D_L = transverse dispersion coef. [L^2/T]

$Z_{1,2}$ = independent unit Gaussian random numbers [-]

Particle tracking



PARTICLE DISTRIBUTION COUNTED ON A RECTANGULAR GRID AT TIME t

				0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
				0	0	0	1	0	0	1	2	0	0	0	1	1	0	0	0	0	0	0	0	0
				0	0	1	0	0	1	2	3	1	1	2	4	1	1	2	3	1	1	0	0	0
				0	2	2	3	2	3	4	11	14	16	9	11	10	5	2	4	2	3	1	0	0
				0	1	3	8	4	11	14	16	14	33	19	27	32	12	9	8	6	4	2	0	0
				0	1	2	5	13	14	24	27	30	54	50	49	46	33	29	20	7	5	3	1	0
O				0	1	5	3	9	20	21	42	53	57	60	54	45	33	23	25	8	4	2	0	0
				0	2	3	7	6	16	19	35	28	43	44	56	41	31	13	16	11	6	3	1	0
				0	1	1	2	4	9	12	20	22	24	21	33	27	22	13	5	2	4	0	2	0
				0	1	2	0	1	3	5	6	14	10	9	8	12	7	5	4	1	2	0	0	0
				0	0	0	0	0	0	2	1	5	2	1	1	1	3	2	3	2	1	0	0	0
				0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	1	0	0	0	0	0
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Solution options

Table 1
Solution Options Available in the MT3DMS Code

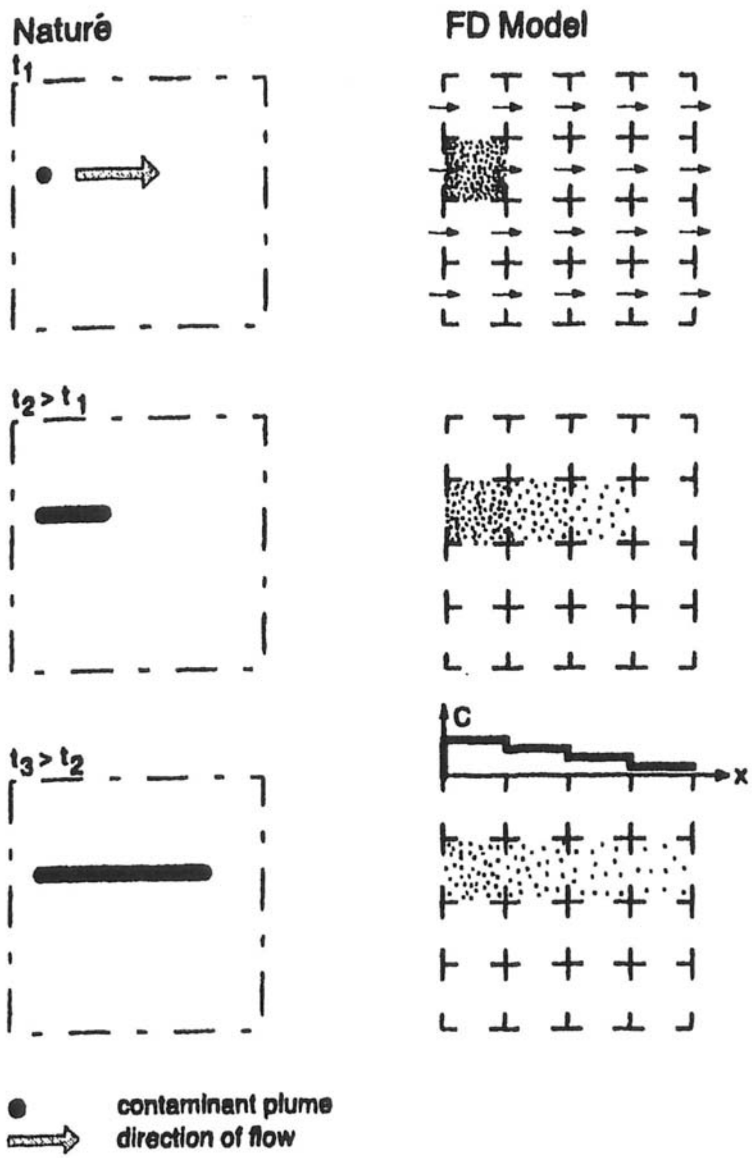
Group	Solution Options for Advection[1]	Solution Options for Dispersion, Sink/Source, and Reaction[1]
A	Particle-tracking-based Eulerian-Lagrangian methods • MOC • MMOC • HMOC	Explicit finite-difference method
B	Particle Tracking Based Eulerian-Lagrangian Methods • MOC • MMOC • HMOC	*Implicit finite-difference method*
C	Explicit Finite-Difference Method • Upstream weighting	Explicit finite-difference method
D	*Implicit Finite-Difference Method* • *Upstream weighting* • *Central-in-space weighting*	*Implicit finite-difference method*
E	*Explicit 3rd-order TVD (ULTIMATE)*	Explicit finite-difference method
F	*Explicit 3rd-order TVD (ULTIMATE)*	*Implicit finite-difference method*

[1] New options are showing in italics.

Numerical errors in FD models

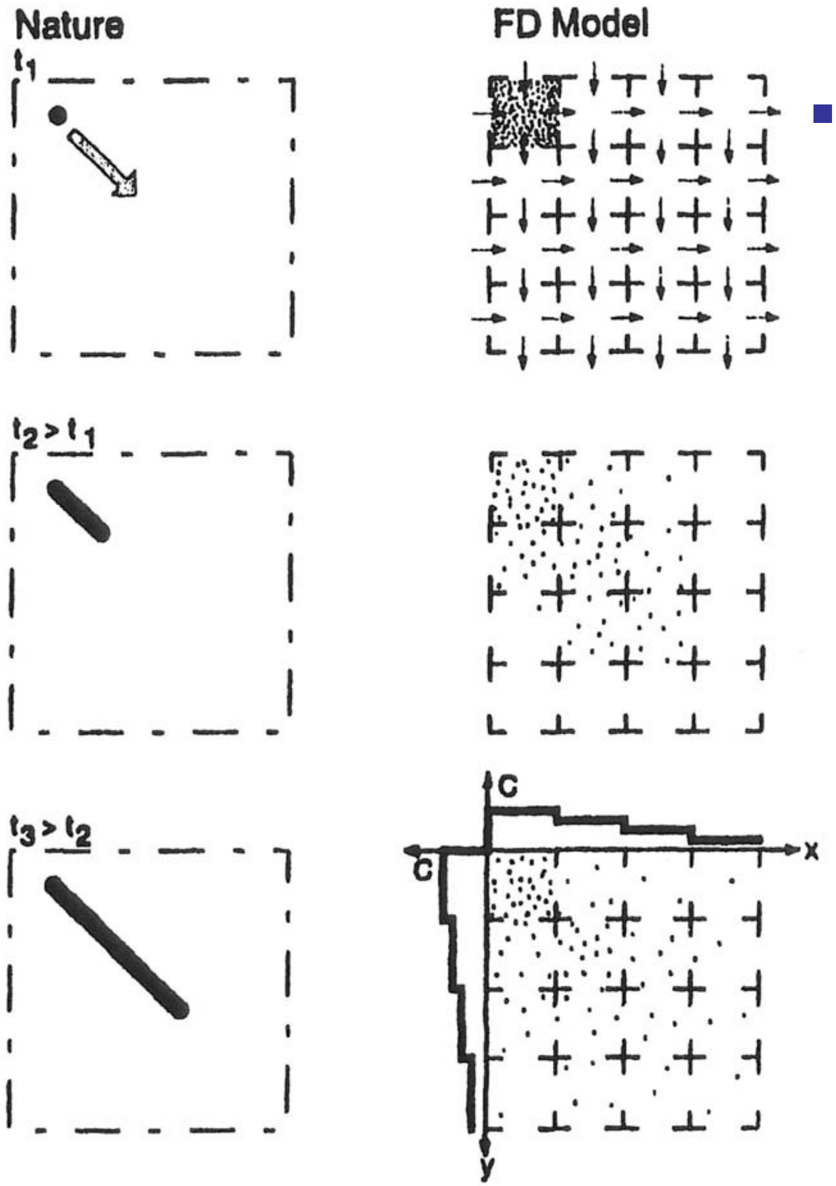
Truncation error:	neglected high order terms in the numerical formulation
Roundoff error:	limitation of the computer to represent digits.
Oscillations:	coarse discretization in time and space in relation to large gradients in concentrations.
Instability:	error will grow as each succeeding step (iteration or time step)
Iteration residual error:	The error that remains when the iteration convergence criteria are fulfilled $\left\| c_i^{k+1} - c_i^k \right\| \leq \varepsilon$

Distance-related numerical dispersion



- The cell size is the smallest resolution of the contaminant concentration – contaminant at a smaller scale will be dissolve on a cell basis
- When the contaminant front has reach the edge of an cell the entire cell is contaminated

Angular-numerical dispersion



- Angular flow is resolved in x,y and z flow-components and since there is an instant dilution of contaminant in the numerical cells we will obtain an artificial spreading´.

Controlling numerical errors

Peclet criterion: controls the spatial discretization *Dx* in respect to porewater velocity, v_a and dispersivity, D_{xx} on a cell basis

$$Pe_{xi} = \frac{v_{a,xi}\Delta x_i}{D_{xxi}} < 1$$

Courant criterion: controls the temporal discretization *Dt* in respect to porewater velocity, v_a and spatial discretization, *Dx* on a cell basis

$$Co_x = \left|\frac{v_{a,x}\Delta t}{\Delta x}\right| \leq 1$$

$$Co_y = \left|\frac{v_{a,y}\Delta t}{\Delta y}\right| \leq 1$$

$$Co_x + Co_y \leq 1$$

Controlling numerical errors

Neumann criterion: restricts the dispersive flux within a time step

$$\frac{D_{xx}\Delta t}{\Delta x^2} + \frac{D_{yy}\Delta t}{\Delta y^2} \leq 0.5$$

Other conditions:

- Orient the grid along main flow direction
- Gentle discretization in time and space
- Refine grid in the plume area
- Decrease time step