'MODELLING FOR GEOCHEMISTS' EVERYTHING YOU ALWAYS WANTED TO KNOW ABOUT MODELLING, BUT WERE AFRAID TO ASK!

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INTRODUCTION

During previous SWIM's, we noted some of the modellers lacked the knowledge to fully appreciate the papers of the chemists and the other way round. To make the papers of the other 'root' of our work better understandable, the 17th SWIM included two parallel lectures. In this one, the practise of modelling will be explained to those usually concerned with chemistry. The other course explains the basics of hydrogeochemical studies to the modellers.

This is not a 'regular' paper. Instead of writing text, I preferred to hand in my presentation sheets as a paper. This paper should give a refreshing view on the subject. In my opinion, this time sheets are better than words. No bullshit and to the (power)point !! I hope anyone who reads this, will know the ins and outs of groundwater modelling.

Modelling for Chemists

Everything you always wanted to know about modelling, but were afraid to ask!

- Modelling protocol
- Discretisation Partial Differential Equation (PDE)
- Groundwater flow: MODFLOW
- Solute transport: MOC3D

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Modelling for Chemists

- Difficult to determine target group for this lecture
- No density differences considered
- I like equations, so don't be shocked by the PDEs
- 45 min.: not enough to understand it all completely
- These sheets will be available

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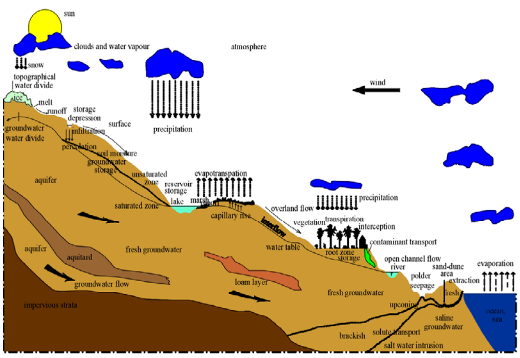
The Hydrological Circle



Ten steps of the Modelling Protocol

1. Problem definition
2. Purpose definition
3. Conceptualisation
4. Selection computer code
5. Model design
6. Calibration
7. Verification
8. Simulation
9. Presentation
10. Postaudit

MODELLING PROTOCOL

IMPORTANT

Modelling protocol

Why numerical modelling?

+:
- cheaper than scale models
- analysis of very complex systems is possible
- a model can be used as a database

-:
- simplification of the reality
- only a tool, no purpose on itself
- garbage in=garbage out: (field)data important
- perfect fit measurement and simulation is suspicious

IMPORTANT

Modelling protocol

3. Conceptualisation (I)

Model is only a schematisation of the reality

Which hydro(geo)logical processes are relevant?

Which processes can be neglected?

Boundary conditions

Variables and parameters:
- subsoil parameters
- fluxes in and out
- initial conditions
- geochemical data

Mathematical equations

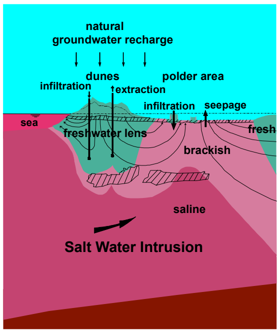
Modelling protocol

3. Concept (II): example of salt water intrusion

Relevant processes:
- groundwater flow in a heterogeneous porous medium
- solute transport
- variable density flow
- natural recharge
- extraction of groundwater

Negligible processes:
- heat flow
- swelling of clayey aquitard
- non-steady groundwater flow

Boundary conditions
- no flow at bottom
- flux in dune area
- constant head in polder area



4. Selection computer code

There are numerous good groundwater computer codes!

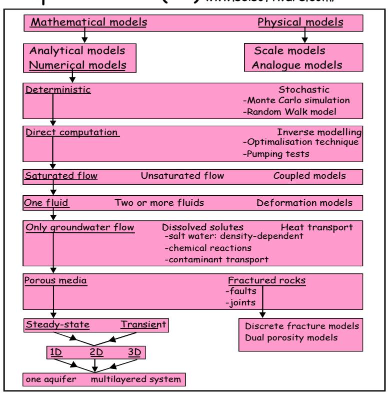
See internet, e.g.:

USGS: water.usgs.gov/nrp/gwsoftware/
Scientific Software Group: www.scisoftware.com/

4. Selection computer code (II)

water.usgs.gov/nrp/gwsoftware/
www.scisoftware.com/

Groundwater computer codes



Modelling protocol

5. Model design (I)

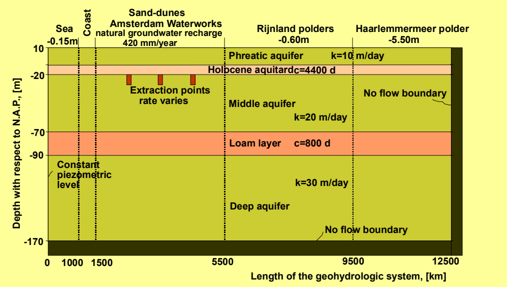
Choice grid Δx:
- depends on natural variation in the groundwater system
- concept model
- data collection

Choice time step Δt

Conditions:
- initial conditions
- boundary conditions:
  1. Dirichlet: head
  2. Neumann: flux, e.g., no flow
  3. Cauchy: mixed boundary condition

5. Model design (II): example

Geometry, subsoil parameters, boundary conditions



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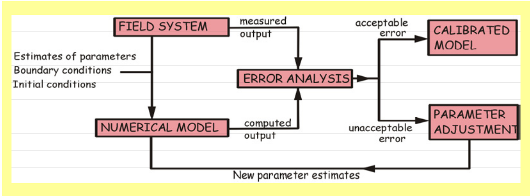
6. Calibration (I)

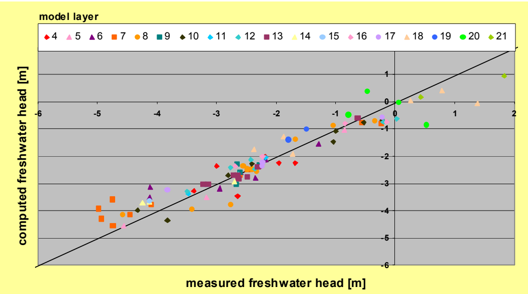
Fitting the groundwater model: is your model okay?

- trial and error
- automatic parameter estimation/inverse modelling (PEST, UCODE)



6. Calibration (II): example

Measured and computed freshwater heads



IMPORTANT

6. Calibration: errors during modelling protocol

•Wrong model concept

•Incomplete equations

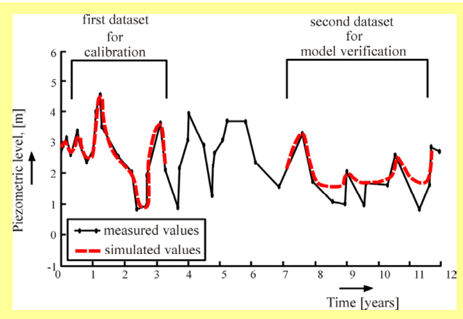
•Inaccurate parameters and variables

•Errors in computer code

•Numerical inaccuracies

IMPORTANT

7. Verification: testing the calibrated model



'*verification problem*': there is always a lack of data

8. Simulation

Simulation of scenarios

Computation time depends on:

- computer speed
- size model
- efficiency compiler
- output format

9. Presentation

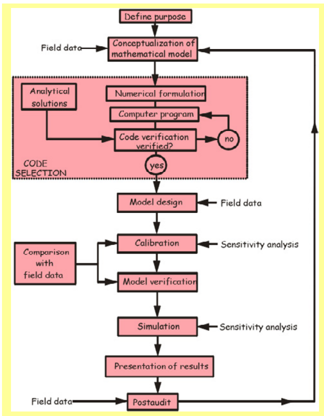
10. Postaudit

Postaudit:
analysing model results after a long time

Anderson & Woessner('92):
four postaudits from the 1960's

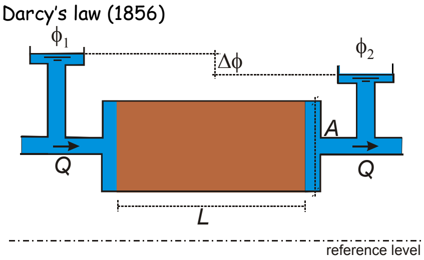
Errors in model results are mainly caused by:
•wrong concept
•wrong scenarios

Modelling scheme



DISCRETIZATION PDE

I. Darcy's law (1856)



$Q \propto \phi_1 - \phi_2 \quad Q \propto \frac{1}{L} \quad Q \propto A$ gives $Q \propto A\frac{\phi_1 - \phi_2}{L}$

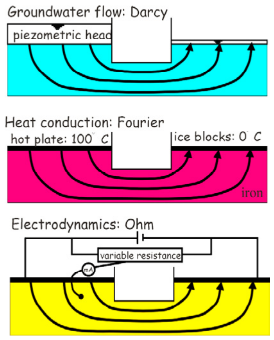
$Q = KA\frac{\phi_1 - \phi_2}{L}$ where K= hydraulic conductivity [L/T]

II. Darcy's Law

$$q_x = -k_x\frac{\partial\phi}{\partial x} \qquad q_y = -k_y\frac{\partial\phi}{\partial y} \qquad q_z = -k_z\frac{\partial\phi}{\partial z}$$

q=Darcian specific discharge [L/T]
ϕ=piezometric head [L]
k_i=hydraulic conductivity [L/T]

Analogy physical processes

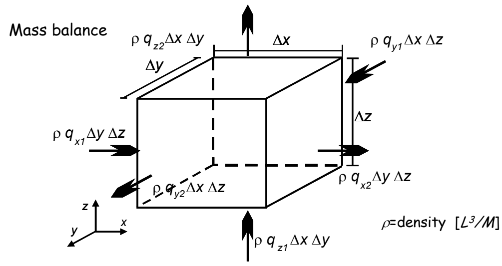


$$q = -k\frac{\partial\phi}{\partial x}$$

$$h = -\lambda\frac{\partial T}{\partial x}$$

$$i = -\sigma\frac{\partial V}{\partial x}$$

Continuity equation: steady state



ρ=density [L^3/M]

$$\frac{\partial\rho q_x}{\partial x} + \frac{\partial\rho q_y}{\partial y} + \frac{\partial\rho q_z}{\partial z} = 0$$

IMPORTANT

Steady state groundwater flow equation (PDE=Partial Differential Equation)

Flow equation (Darcy's Law) $\quad q_x = -k_x\frac{\partial\phi}{\partial x} \quad q_y = -k_y\frac{\partial\phi}{\partial y} \quad q_z = -k_z\frac{\partial\phi}{\partial z}$

+

Continuity equation $\quad \frac{\partial\rho q_x}{\partial x} + \frac{\partial\rho q_y}{\partial y} + \frac{\partial\rho q_z}{\partial z} = 0$

=

Groundwater flow equation

$$\frac{\partial\rho\left(-k_x\frac{\partial\phi}{\partial x}\right)}{\partial x} + \frac{\partial\rho\left(-k_y\frac{\partial\phi}{\partial y}\right)}{\partial y} + \frac{\partial\rho\left(-k_z\frac{\partial\phi}{\partial z}\right)}{\partial z} = 0$$

If k_i=constant and ρ=constant then:

$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2} = 0$ Laplace equation

$\nabla^2\phi = 0$

IMPORTANT

Taylor series development (I)

Best estimate of ϕ_{i+1} is based on ϕ_i

$$\phi_{i+1} = \phi_i + \Delta x\frac{\partial\phi_i}{\partial x} + \frac{1}{2}\Delta x^2\frac{\partial^2\phi_i}{\partial x^2} + \frac{1}{6}\Delta x^3\frac{\partial^3\phi_i}{\partial x^3} + \frac{1}{24}\Delta x^4\frac{\partial^4\phi_i}{\partial x^4} + \text{K}$$

$$\phi_{i-1} = \phi_i - \Delta x\frac{\partial\phi_i}{\partial x} + \frac{1}{2}\Delta x^2\frac{\partial^2\phi_i}{\partial x^2} - \frac{1}{6}\Delta x^3\frac{\partial^3\phi_i}{\partial x^3} + \frac{1}{24}\Delta x^4\frac{\partial^4\phi_i}{\partial x^4} + \text{K}$$

−

$$\phi_{i+1} - \phi_{i-1} = 2\Delta x\frac{\partial\phi_i}{\partial x} + \frac{1}{3}\Delta x^3\frac{\partial^3\phi_i}{\partial x^3} + \text{K}$$

$$\frac{\partial\phi_i}{\partial x} = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} + \text{O}\left(-\frac{1}{6}\Delta x^2\frac{\partial^3\phi_i}{\partial x^3} + \text{K}\right)$$

IMPORTANT

Discretisation PDE

Taylor series development (II)

$$\phi_{i+1} = \phi_i + \Delta x \frac{\partial \phi_i}{\partial x} + \frac{1}{2}\Delta x^2 \frac{\partial^2 \phi_i}{\partial x^2} + \frac{1}{6}\Delta x^3 \frac{\partial^3 \phi_i}{\partial x^3} + \frac{1}{24}\Delta x^4 \frac{\partial^4 \phi_i}{\partial x^4} + K$$

$$\phi_{i-1} = \phi_i - \Delta x \frac{\partial \phi_i}{\partial x} + \frac{1}{2}\Delta x^2 \frac{\partial^2 \phi_i}{\partial x^2} - \frac{1}{6}\Delta x^3 \frac{\partial^3 \phi_i}{\partial x^3} + \frac{1}{24}\Delta x^4 \frac{\partial^4 \phi_i}{\partial x^4} + K$$

+

$$\phi_{i+1} + \phi_{i-1} = 2\phi_i + \Delta x^2 \frac{\partial^2 \phi_i}{\partial x^2} + \frac{1}{12}\Delta x^4 \frac{\partial^4 \phi_i}{\partial x^4} + K$$

$$\frac{\partial^2 \phi_i}{\partial x^2} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} + O\left(-\frac{1}{12}\Delta x^2 \frac{\partial^4 \phi_i}{\partial x^4} + K\right)$$

IMPORTANT

Discretisation PDE

Laplace equation in 2D

$$\nabla^2 \phi = 0 \Leftrightarrow \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$$

Discretisation in *x*-direction (*i*): $\frac{\partial^2 \phi_{i,j}}{\partial x^2} = \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta x^2}$

Discretisation in *y*-direction (*j*): $\frac{\partial^2 \phi_{i,j}}{\partial y^2} = \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{\Delta y^2}$

$$\frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta x^2} + \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{\Delta y^2} = 0$$

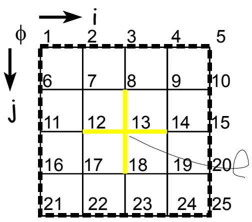
If $\Delta x = \Delta y$ then: $\phi_{i+1,j} + \phi_{i-1,j} - 4\phi_{i,j} + \phi_{i,j+1} + \phi_{i,j-1} = 0$

$$\phi_{i,j} = \frac{\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1}}{4}$$ 'Fivepoint operator'

Discretisation PDE

Fivepoint operator: constant head example (I)

$$\phi_{i,j} = \frac{\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1}}{4}$$

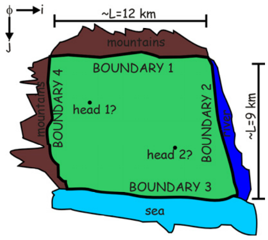


Constant head boundary

$$\phi_{13} = \frac{\phi_{14} + \phi_{12} + \phi_{18} + \phi_{8}}{4}$$

Discretisation PDE

Fivepoint operator: example (II)



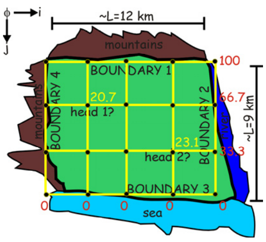
$$\phi_{i,j} = \frac{\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1}}{4}$$

Characteristics:
Hydraulic conductivity k=10 m/dag
Groundwater recharge N=0 mm/dag
Thickness aquifer D=50m

Boundary conditions
BOUNDARY 1: no-flow near the mountains
BOUNDARY 2: linear from 100 m (near mountains) to 0 m (near sea)
BOUNDARY 3: constant seawater level of 0 m
BOUNDARY 4: no-flow

Discretisation PDE

Fivepoint operator: example (III)



$$\phi_{i,j} = \frac{\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1}}{4}$$

On BOUNDARY 1:

$$\phi_{i,j} = \frac{\phi_{i+1,j} + \phi_{i-1,j} + 2\phi_{i,j+1}}{4}$$

On BOUNDARY 4:

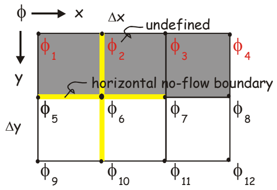
$$\phi_{i,j} = \frac{2\phi_{i+1,j} + \phi_{i,j+1} + \phi_{i,j-1}}{4}$$

- Initial estimate head=50m
- Convergence-criterion=0.01m
- Number of iterations=74

Discretisation PDE

Fivepoint operator: No-flow example (I)

Nodes on the edges of an element



$$q = -k\frac{\partial \phi}{\partial y} = 0$$

$$\frac{\partial \phi}{\partial y} = \frac{\phi_{10} - \phi_2}{2\Delta y} \Leftrightarrow \phi_{10} = \phi_2$$

$$\phi_6 = \frac{\phi_7 + \phi_5 + \phi_{10} + \phi_2}{4}$$

$$\phi_6 = \frac{\phi_7 + \phi_5 + 2\phi_{10}}{4}$$

Discretisation PDE

Non steady state groundwater flow equation

Flow equation (Darcy's Law) $q_x = -k\frac{\partial \phi}{\partial x}$ $q_y = -k\frac{\partial \phi}{\partial y}$ $q_z = -k\frac{\partial \phi}{\partial z}$

+

Non steady state continuity equation $\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = S_s\frac{\partial \phi}{\partial t} + W'$

=

Groundwater flow equation

S_s=specific storage coefficient [1/L]
W'=source-term

$$\frac{\partial\left(-k\frac{\partial \phi}{\partial x}\right)}{\partial x} + \frac{\partial\left(-k\frac{\partial \phi}{\partial y}\right)}{\partial y} + \frac{\partial\left(-k\frac{\partial \phi}{\partial z}\right)}{\partial z} = S_s\frac{\partial \phi}{\partial t} + W'$$

Multiply with constant thickness D of the aquifer gives:

$$T\frac{\partial^2 \phi}{\partial x^2} + T\frac{\partial^2 \phi}{\partial y^2} + T\frac{\partial^2 \phi}{\partial z^2} = S\frac{\partial \phi}{\partial t} + W$$

S=elastic storage coefficient [-]
T=kD= transmissivity [L^2/T]

Discretisation PDE

Explicit numerical 1D solution

One-dimensional non steady state groundwater flow equation:

$$S\frac{\partial \phi}{\partial t} = T\frac{\partial^2 \phi}{\partial x^2} + N$$

Explicit ('forwards in space'):

$$\frac{\partial^2 \phi_i}{\partial x^2} \approx \frac{\phi_{i+1}^t - 2\phi_i^t + \phi_{i-1}^t}{\Delta x^2} \qquad \frac{\partial \phi_i}{\partial t} \approx \frac{\phi_i^{t+\Delta t} - \phi_i^t}{\Delta t}$$

$$\phi_i^{t+\Delta t} = \phi_i^t + \frac{N\Delta t}{S} + \frac{T\Delta t}{S\Delta x^2}\left(\phi_{i+1}^t - 2\phi_i^t + \phi_{i-1}^t\right)$$

Properties:
- Direct solution
- Can be numerical instable

MODFLOW

MODFLOW

IMPORTANT

MODFLOW

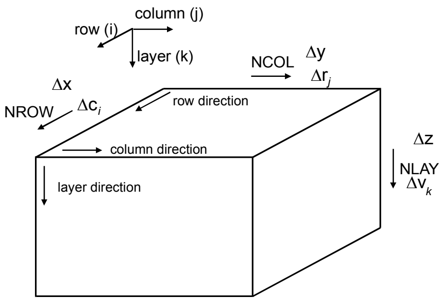
a modular 3D finite-difference ground-water flow model

(M.G. McDonald & A.W. Harbaugh, from 1983 on)

- USGS, 'public domain'
- non steady state
- heterogeneous porous medium
- anisotropy
- coupled to reactive solute transport
  - MOC3 (Konikow *et al*, 1996)
  - MT3D, MT3DMS (Zheng, 1990)
  - RT3D
- easy to use due to numerous Graphical User Interfaces (GUI's)
  - PMWIN, GMS, Visual Modflow, Argus One, Groundwater Vistas, etc.

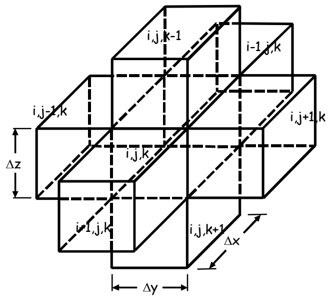
MODFLOW

Nomenclature MODFLOW element



MODFLOW

MODFLOW: start with water balance of one element [i,j,k]



IMPORTANT

MODFLOW

Continuity equation (I)

In - Out = Storage

$$\frac{\partial}{\partial x}\left(k_{xx}\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_{yy}\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_{zz}\frac{\partial\phi}{\partial z}\right)-W=S_s\frac{\partial\phi}{\partial t}$$

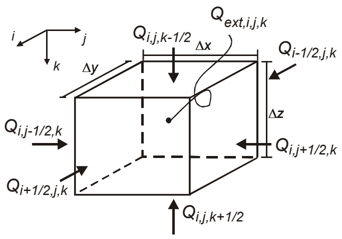
$$\sum Q_i = S_s\frac{\Delta\phi}{\Delta t}\Delta V$$

MODFLOW

Continuity equation (II)

$$\sum Q_i = S_s\frac{\Delta\phi}{\Delta t}\Delta V$$

In = positive

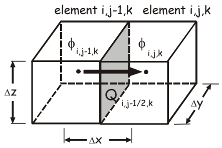


$$Q_{i,j-1/2,k}+Q_{i,j+1/2,k}+Q_{i-1/2,j,k}+Q_{i+1/2,j,k}+Q_{i,j,k-1/2}+Q_{i,j,k+1/2}+Q_{ext,i,j,k}$$
$$=SS_{i,j,k}\frac{\phi^{t}_{i,j,k}-\phi^{t+\Delta t}_{i,j,k}}{\Delta t}\Delta V$$

IMPORTANT

MODFLOW

Flow equation (Darcy's Law)



$$Q = surface * q = surface * k\frac{\partial\phi}{\partial x}$$

$$Q_{i,j-1/2,k} = k_{i,j-1/2,k}\,\Delta y\,\Delta z\,\frac{\phi_{i,j-1,k}-\phi_{i,j,k}}{\Delta x}$$

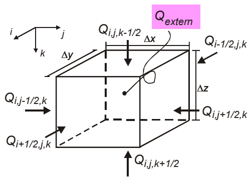
$$Q_{i,j-1/2,k} = CR_{i,j-1/2,k}\left(\phi_{i,j-1,k}-\phi_{i,j,k}\right)$$

where $CR_{i,j-1/2,k}=\frac{k_{i,j-1/2,k}\,\Delta y\,\Delta z}{\Delta x}$ is the conductance [L²/T]

MODFLOW

Groundwater flow equation

$$Q_{i,j-1/2,k}=CR_{i,j-1/2,k}\left(\phi_{i,j-1,k}-\phi_{i,j,k}\right)$$
$$Q_{i,j+1/2,k}=CR_{i,j+1/2,k}\left(\phi_{i,j+1,k}-\phi_{i,j,k}\right)$$
$$Q_{i-1/2,j,k}=CC_{i-1/2,j,k}\left(\phi_{i-1,j,k}-\phi_{i,j,k}\right)$$
$$Q_{i+1/2,j,k}=CC_{i+1/2,j,k}\left(\phi_{i+1,j,k}-\phi_{i,j,k}\right)$$
$$Q_{i,j,k-1/2}=CV_{i,j,k-1/2}\left(\phi_{i,j,k-1}-\phi_{i,j,k}\right)$$
$$Q_{i,j,k+1/2}=CV_{i,j,k+1/2}\left(\phi_{i,j,k+1}-\phi_{i,j,k}\right)$$



$$Q_{i,j-1/2,k}+Q_{i,j+1/2,k}+Q_{i-1/2,j,k}+Q_{i+1/2,j,k}+Q_{i,j,k-1/2}+Q_{i,j,k+1/2}+Q_{ext,i,j,k}=SS_{i,j,k}\frac{\phi^{t}_{i,j,k}-\phi^{t+\Delta t}_{i,j,k}}{\Delta t}\Delta V$$

IMPORTANT

MODFLOW

Thé MODFLOW Groundwater flow equation

$$Q_{i,j-1/2,k}+Q_{i,j+1/2,k}+Q_{i-1/2,j,k}+Q_{i+1/2,j,k}+Q_{i,j,k-1/2}+Q_{i,j,k+1/2}+Q_{ext,i,j,k}=SS_{i,j,k}\frac{\phi^{t}_{i,j,k}-\phi^{t+\Delta t}_{i,j,k}}{\Delta t}\Delta V$$

and:

$$Q_{ext,i,j,k}=P_{i,j,k}\phi^{t+\Delta t}_{i,j,k}+Q'_{i,j,k}$$

gives:

$$CV_{i,j,k-1/2}\phi^{t+\Delta t}_{i,j,k-1}+CC_{i-1/2,j,k}\phi^{t+\Delta t}_{i-1,j,k}+CR_{i,j-1/2,k}\phi^{t+\Delta t}_{i,j-1,k}$$
$$+\left(-CV_{i,j,k-1/2}-CC_{i-1/2,j,k}-CR_{i,j-1/2,k}-CR_{i,j+1/2,k}-CC_{i+1/2,j,k}-CV_{i,j,k+1/2}+HCOF_{i,j,k}\right)\phi^{t+\Delta t}_{i,j,k}$$
$$+CR_{i,j+1/2,k}\phi^{t+\Delta t}_{i,j+1,k}+CC_{i+1/2,j,k}\phi^{t+\Delta t}_{i+1,j,k}+CV_{i,j,k+1/2}\phi^{t+\Delta t}_{i,j,k+1}=RHS_{i,j,k}$$

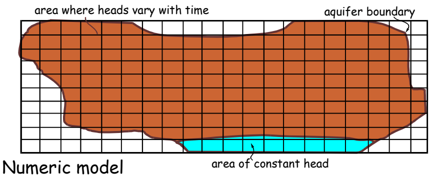
with:

$$HCOF_{i,j,k}=P_{i,j,k}-SC1_{i,j,k}/(\Delta t)$$
$$RHS_{i,j,k}=-Q'_{i,j,k}-SC1_{i,j,k}\phi^{t}_{i,j,k}/(\Delta t)$$
$$SC1_{i,j,k}=SS_{i,j,k}\Delta V$$

MODFLOW

Boundary conditions in MODFLOW (I)

Example of a system with three types of boundary conditions



Numeric model

0	1	1	1	1	1	0	0	0	0	0	0	0	1	1	1	1	1	0	0
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0
0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0
0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0
0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0
0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	1	0	0
0	0	0	0	0	0	0	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	0	0	0

MODFLOW

Boundary conditions in MODFLOW (II)

For a constant head condition: IBOUND<0
For a no flow condition: IBOUND=0
For a variable head: IBOUND>0

IMPORTANT

MODFLOW

Packages in MODFLOW

1. Well package
2. River package
3. Recharge package
4. Drain package
5. Evaporation package
6. General head package

MODFLOW

1. Well package

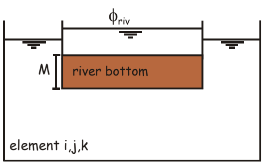
$$Q_{well}=Q_{i,j,k}$$

Example: an extraction of 10 m^3 per day should be inserted in an element as $Q_{ext,i,j,k}=-10$ (in = positive)

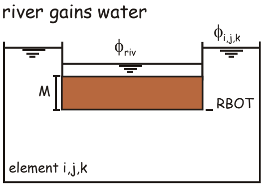
MODFLOW

2. River package (I)

river loses water



river gains water



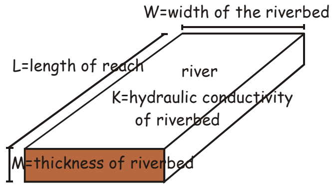
$$Q_{riv}=KLW\left(\frac{\phi_{riv}-\phi_{i,j,k}}{M}\right)$$

$$Q_{riv}=\frac{KLW}{M}\left(\phi_{riv}-\phi_{i,j,k}\right)\quad\Leftrightarrow\quad Q_{riv}=C_{riv}\left(\phi_{riv}-\phi_{i,j,k}\right)$$

MODFLOW

2. River package (II)

Determine the conductance of the river in one element:

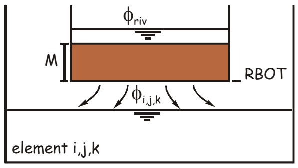


where $C_{riv}=\frac{KLW}{M}$ is the conductance [L^2/T] of the river

MODFLOW

2. River package (III)

Leakage to the groundwater system

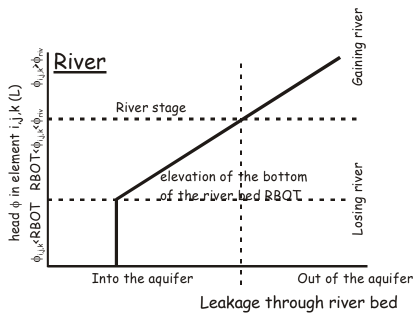


Special case:

if $\phi_{i,j,k}$<RBOT, then $Q_{riv} = C_{riv}(\phi_{riv} - RBOT)$

MODFLOW

2. River package (IV)



MODFLOW

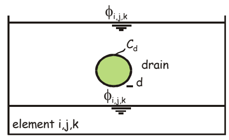
3. Recharge package

$$Q_{rec} = I\Delta x \Delta y$$

MODFLOW

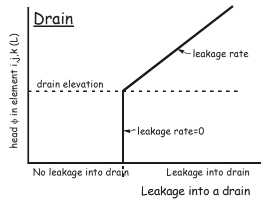
4. Drain package

$$Q_{drn} = C_{drn}(\phi_{i,j,k} - d)$$



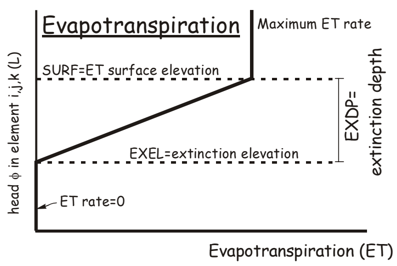
Special case:

if $\phi_{i,j,k}$ < d than $Q_{drn} = 0$



MODFLOW

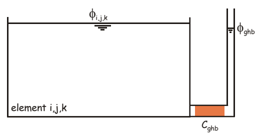
5. Evapotranspiration package

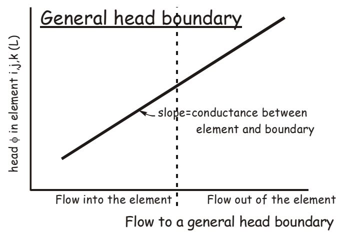


MODFLOW

6. General head boundary package

$$Q_{ghb} = C_{ghb}(\phi_{ghb} - \phi_{i,j,k})$$





MODFLOW

Time indication MODFLOW

ITMUNI=1: seconde
ITMUNI=2: minute
ITMUNI=3: hour
ITMUNI=4: day
ITMUNI=5: year

MOC3D

MOC3D

Solute transport equation

Partial differential equation (PDE):

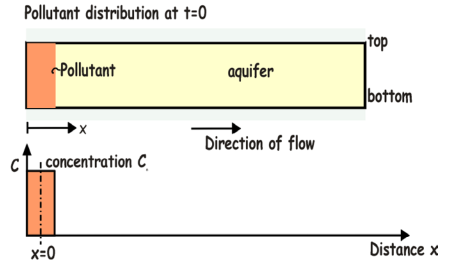
$$R_d \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(CV_i) + \frac{(C-C')W}{n_e} - R_d \lambda C$$

change in concentration | dispersion diffusion | advection | source/sink | decay

D_{ij}=hydrodynamic dispersion [$L^2 T^{-1}$]
R_d=retardation factor [-]
λ=decay-term [T^{-1}]

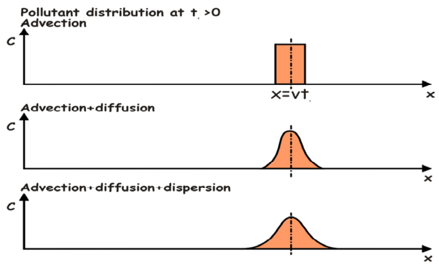
MOC3D

Solute transport equation: column test (I):



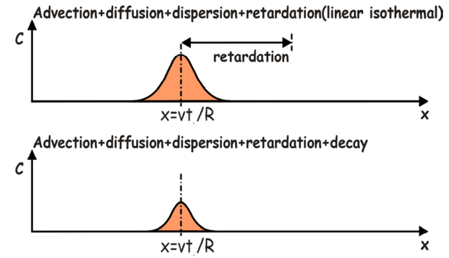
MOC3D

Solute transport equation: column test (II):



MOC3D

Solute transport equation: column test (III):



MOC3D

Hydrodynamic dispersion

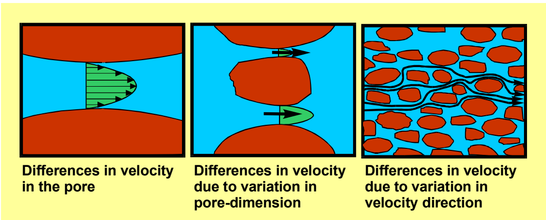
hydrodynamic dispersion
=
mechanical dispersion+ diffusion

mechanical dispersion:
- tensor
- velocity dependant

diffusion:
- molecular process
- solutes spread due to concentration differences

MOC3D

Mechanical dispersion



IMPORTANT

MOC3D

Method of Characteristics (MOC)

Solve the advection-dispersion equation (ADE) with the Method of Characteristics

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(CV_i) + \frac{(C - C')W}{n_e}$$

Lagrangian approach:

Splitting up the advection part and the dispersion/source part:

- advection by means of a particle tracking technique
- dispersion/source by means of the finite difference method

MOC3D

Advantage of the approach of MOC?

It is difficult to solve the whole advection-dispersion equation in one step, because the so-called Peclet-number is high in most groundwater flow/solute transport problems.

(hyperbolic form of the equation is dominant)

The Peclet number stands for the ratio between advection and dispersion

IMPORTANT

MOC3D

Procedure of MOC: advective transport by particle tracking

- Place a number of particles in each element
- Determine the effective velocity of each particle by (bi)linear interpolation of the velocity field which is derived from MODFLOW
- Move particles during one solute time step Δt_{solute}
- Average values of all particles in an element to one node value
- Calculate the change in concentration in all nodes due to advective transport
- Add this result to dispersive/source changes of solute transport

MOC3D

Steps in MOC-procedure

1. Determine concentration gradients at old timestep k-1
2. Move particles to model advective transport
3. Concentration of particles to concentration in element node
4. Determine concentration gradients on new timestep k*
5. Determine concentration in element node after advective, dispersive/source transport on timestep k

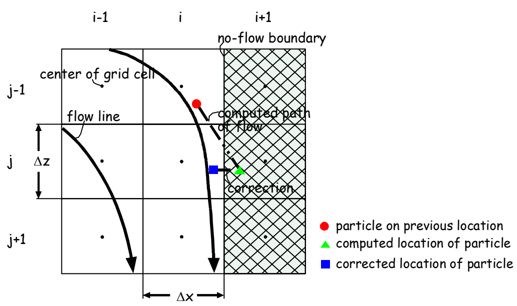
MOC3D

Causes of errors in MOC-procedure

1. Concentration gradients
2. Average from particles to node element, and visa versa
3. Concentration of sources/sinks to entire element
4. Empty elements
5. No-flow boundary: reflection in boundary

MOC3D

Reflection in boundary



MOC3D

Stability criteria (I)

Stability criteria are necessary because the ADE is solved explicitly

1. Neumann criterion:

$$\frac{D_{xx}\Delta t_s}{\Delta x^2} + \frac{D_{yy}\Delta t_s}{\Delta y^2} + \frac{D_{zz}\Delta t_s}{\Delta z^2} \le 0.5$$

$$\Delta t_s \le \frac{0.5}{\frac{D_{xx}}{\Delta x^2} + \frac{D_{yy}}{\Delta y^2} + \frac{D_{zz}}{\Delta z^2}}$$

MOC3D

Stability criteria (II)

2. Mixing criterion

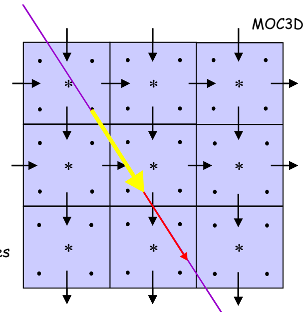
Change in concentration in element is not allowed to larger than the difference between the present concentration in the element and the concentration in the source

$$\Delta t_s \le \frac{n_e b^k_{i,j,k}}{Q'_{i,j,k}}$$

MOC3D

Stability criteria (III)

3. Courant criterium



* Node element
· Particle

Velocity direction

Movement particles

$0 < \xi <= \sim 1$

$$\Delta t_s \le \frac{\xi \Delta x}{V_{x,\max}} \qquad \Delta t_s \le \frac{\xi \Delta y}{V_{y,\max}} \qquad \Delta t_s \le \frac{\xi \Delta z}{V_{z,\max}}$$

FILES

MODFLOW

Files in MODFLOW: infile.nam file

```
INFILE.NAM
list    16      ext.lst
bas     95      ext.bas
bcf     11      ext.bcf
sip     19      ext.sip
wel     12      ext.wel
conc    33      ext_moc.nam
```

Additional information (good documentation):
MODFLOW: *http://water.usgs.gov/nrp/gwsoftware/modflow.html*
MOC3D: *http://water.usgs.gov/nrp/gwsoftware/moc3d/moc3d.html*

Files in MODFLOW: *.bas file

MODFLOW

```
EXT.BAS
Groundwater extraction
     NLAY      NROW      NCOL      NPER     ITMUNI
        1        19        19         1          1
FREE
        0         1     ; IAPART,ISTRT
       95         1(19I3)                              3   ; IBOUND1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
     0.00                                        ; HNOFLO
       95       1.0(19F5.0)                  1   ; HEAD1
  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  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  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  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  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  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  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  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  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  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  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  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  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  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  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  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  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  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  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
  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  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  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  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  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  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  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  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  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
  86400.0        20       1.0    ; PERLEN,NSTP,TSMULT
end
```

MODFLOW

Files in MODFLOW: *.bcf file

```
EXT.BCF
         0          0 0.0 0 0.0 0 0    ISS,IBCFBD      BCF Input
         0 LAYCON
         0          1.0      TRPY
         0         50.0      DELR
         0         50.0      DELC
         0     0.00075       Sf1
         0      0.0023       TRAN1
```

Files in MODFLOW: *.wel file

```
EXT.WEL
         1        0     AUXILIARY CONC CBCALLOCATE MXWELL,IWELBD
         1              ITMP (NWELLS)
         1       10        10     -0.004     2.5E3 ; k i j q c
        -1
         1              ITMP (NWELLS)
         1        8         7     -0.004     2.5E3 ; k i j q c
```

Files in MODFLOW: *.sip file

```
EXT.SIP
      500         5     ; MXITER,NPARM          SIP Input
       1.    0.0001        0     0.001 0 ; ACCL,HCLOSE,IPCALC,WSEED,IPRSIP
```

Files in MOC3D: *.moc file

MODFLOW

```
EXT.MOC
Groundwater extraction
    ISLAY1    ISLAY2    ISROW1    ISROW2    ISCOL1    ISCOL2
         1         1         1        19         1        19
         1       0.0       0.0 ; NODISP, DECAY, DIFFUS
     20000         9           ; NPMAX, NPTPND
       0.5      0.05         2 ; CELDIS, FZERO, INTRPL
 -2 0 0 -1 0 0 0 ; NPNTCL, ICONFM, NPNTVL, IVELFM, NPNTDL, IDSPFM, NPRTPL
   35000.0         ; CNOFLO
        96         1(19F5.0)                    3 ; initial concentration1
  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  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  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  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  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  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  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  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  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  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  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  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  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  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  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  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  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  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  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
  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  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  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  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  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  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  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  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  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
         0                                      ; NZONES to follow
         0         0                            ; IGENPT1
         0       1.0                            ; retardation factor
         0      50.0                            ; thickness1
         0      0.25                            ; porosity1
end
         0   35000.0                            ; C' inflow subgrid
         0     0.001                            ; longitudinal disp.
         0    0.0001                            ; transverse disp. horiz.
         0    0.0001                            ; transverse disp. vert.
```

MODFLOW

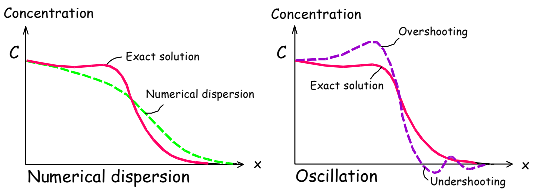
Files in MOC3D: *_moc.nam and *.obs files

```
EXT_MOC.NAM
clst     94       ext.out
moc      96       ext.moc
obs      44       ext.obs
data     45       ext.oba
```

```
EXT.OBS
  3  1             ;NUMOBS  IOBSFL     Observation well data
  1 10 10  45      ;layer, row, column, unit number
  1  8 10          ;layer, row, column
  1  4 10          ;layer, row, column
```

NUMERICAL DISPERSION

Numerical dispersion and oscillation



Derivation of numerical dispersion: 1D (I)

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

Discretisation:
backwards in space
backwards in time

By means of Taylor series development:

$$\frac{C_i^k - C_i^{k-1}}{\Delta t} = D\frac{C_{i+1}^k - 2C_i^k + C_{i-1}^k}{\Delta x^2} - V\frac{C_i^k - C_{i-1}^k}{\Delta x}$$

Derivation of numerical dispersion: 1D (II)

Now Taylor series development with truncation erros!:

$$\frac{C_i^k - C_i^{k-1}}{\Delta t} = \frac{\partial C}{\partial t} - \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} + \frac{\Delta t^2}{6}\frac{\partial^3 C}{\partial t^3} + O(\Delta t^3)$$

$$\frac{C_i^k - C_{i-1}^k}{\Delta x} = \frac{\partial C}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} + \frac{\Delta x^2}{6}\frac{\partial^3 C}{\partial x^3} + O(\Delta x^3)$$

$$\frac{C_{i+1}^k - 2C_i^k + C_{i-1}^k}{\Delta x^2} = \frac{\partial^2 C}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 C}{\partial x^4} + O(\Delta x^4)$$

Derivation of numerical dispersion: 1D (III)

$$\frac{C_i^k - C_i^{k-1}}{\Delta t} = D\frac{C_{i+1}^k - 2C_i^k + C_{i-1}^k}{\Delta x^2} - V\frac{C_i^k - C_{i-1}^k}{\Delta x}$$

$$\frac{\partial C}{\partial t} - \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 C}{\partial x^4}\right) - V\left(\frac{\partial C}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} + \frac{\Delta x^2}{6}\frac{\partial^3 C}{\partial x^3}\right)$$

Neglect 3rd and 4th order terms:

$$\frac{\partial C}{\partial t} - \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} = D\left(\frac{\partial^2 C}{\partial x^2}\right) - V\left(\frac{\partial C}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2}\right)$$

Derivation of numerical dispersion: 1D (IV)

Rewriting term: $\frac{\partial^2 C}{\partial t^2}$

$$\frac{\partial^2 C}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial C}{\partial t}\right) = \frac{\partial}{\partial t}\left(D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x}\right) = D\frac{\partial^2}{\partial x^2}\left(\frac{\partial C}{\partial t}\right) - V\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial t}\right)$$

$$\frac{\partial^2 C}{\partial t^2} = D\frac{\partial^2}{\partial x^2}\left(D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x}\right) - V\frac{\partial}{\partial x}\left(D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x}\right)$$

$$\frac{\partial^2 C}{\partial t^2} = D^2\frac{\partial^4 C}{\partial x^4} - VD\frac{\partial^3 C}{\partial x^3} - VD\frac{\partial^3 C}{\partial x^3} + V^2\frac{\partial^2 C}{\partial x^2}$$

$$\frac{\partial^2 C}{\partial t^2} \approx V^2\frac{\partial^2 C}{\partial x^2}$$

Derivation of numerical dispersion: 1D (V)

Rewrite all extra terms:

$$\frac{\partial C}{\partial t} - \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} = D\left(\frac{\partial^2 C}{\partial x^2}\right) - V\left(\frac{\partial C}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2}\right)$$

$$\frac{\partial^2 C}{\partial t^2} \approx V^2\frac{\partial^2 C}{\partial x^2}$$

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

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

IMPORTANT

Derivation of numerical dispersion: 1D (VI)

Numerical dispersion:

$$D = D_{real} + V\frac{\Delta x}{2} + \frac{\Delta t}{2}V^2$$

Remedy to reduce numerical dispersion:

1. Δx en Δt smaller
2. Use a different numeric scheme (Crank-Nicolson)
3. Use a smaller D_{real}

EVERYTHING YOU ALWAYS WANTED TO KNOW

Modelling for Chemists

1. *Everything you always wanted to know about modelling, and now you know it?*
2. *Everything you always wanted to know about modelling, and now you are definitely afraid to ask?*

Additional information:
Groundwater modelling: ftp://ftp.geo.uu.nl/pub/people/goe/gwm1/gwm1.pdf
Density dependent groundwater flow: ftp://ftp.geo.uu.nl/pub/people/goe/gwm2/gwm2.pdf

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