

# Tentative program

8.15 – 8.30	Group work – Discuss questions and prepare a talk of definitions Question :10 to 18
8.30 – 8.45	Group wise presentation
8.45 – 10.00	Numerical modelling and formulation of finite difference equations
10.00 – 10.30	Break
10.30 – 11.00	Numerical modelling and formulation of finite difference equations
11.00 – 13.00	Exercises 2
13.00 – 14.00	Implementation of boundary conditions
14.00 – 16.00	Exercise 2

# Questions

1. How is the saturated zone defined
2. What is an aquifer?
3. What is an aquitard?
4. What is an unconfined aquifer?
5. What is a confined aquifer?
6. What is a conceptual model?
7. How is specific storage defined ?
8. How is specific yield defined?
9. How is storage coefficient defined?
10. What is hydraulic conductivity?
11. What is the difference between hydraulic conductivity and permeability ?
12. What is transmissivity?
13. What is the typical range for hydraulic conductivity for sand?
14. What is the typical range for hydraulic conductivity for clay?
15. How is hydraulic head defined?
16. What is the Darcy velocity?
17. What is the pore water velocity?
18. Which two equations is joined in the governing equation for groundwater flow?

# Mathematical basis for groundwater flow

The equation of continuity equation combined with the Darcy equation

$$K_x \frac{\partial^2 h}{\partial x^2} + K_y \frac{\partial^2 h}{\partial y^2} + K_z \frac{\partial^2 h}{\partial z^2} - R = S_s \frac{\partial h}{\partial t}$$

$K_x, K_y, K_z$  - hydraulic conductivity

$h$  - *total head*

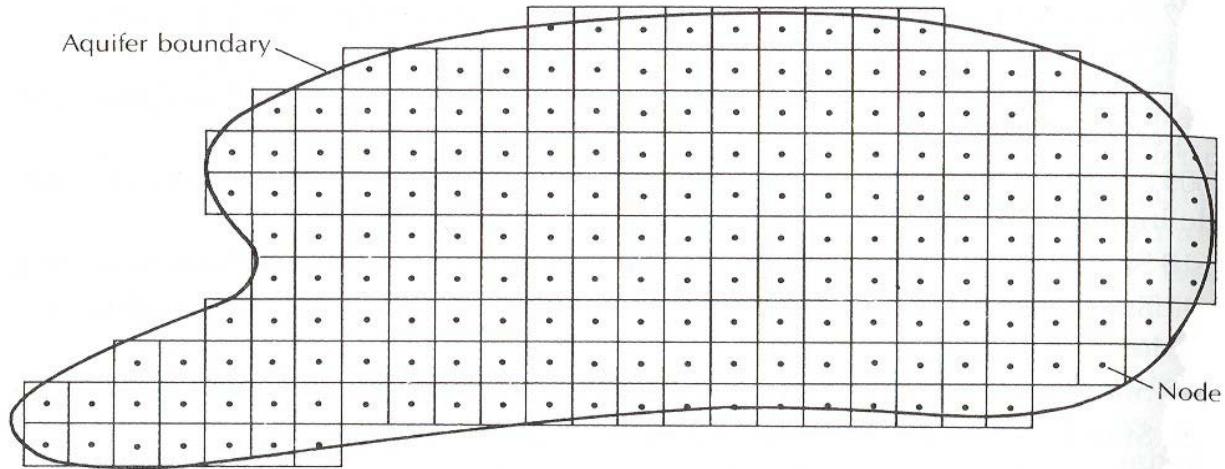
$R$  - *Sink/source term*

$S_s$  - *Specific storage*

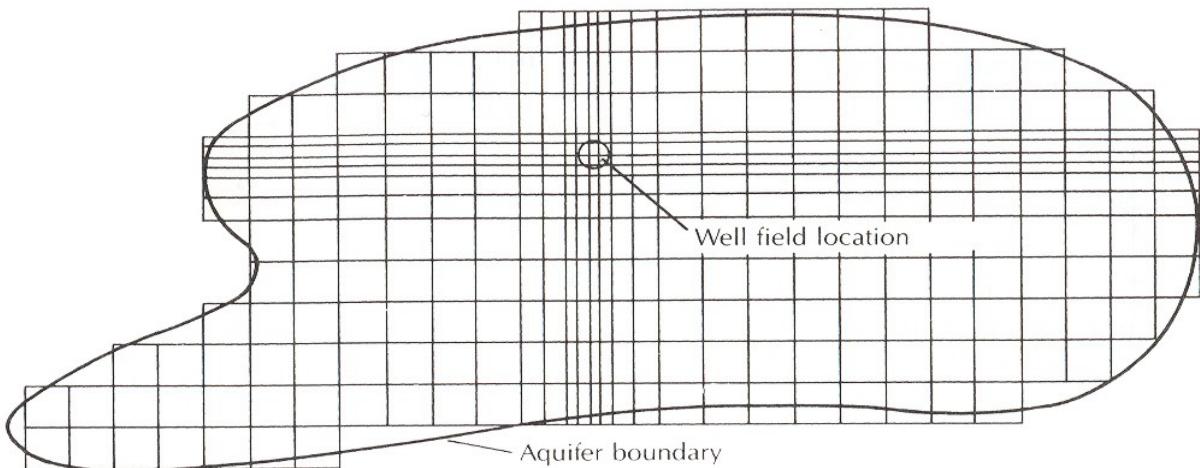
# Numerical models

Finite difference modeller:

square cells

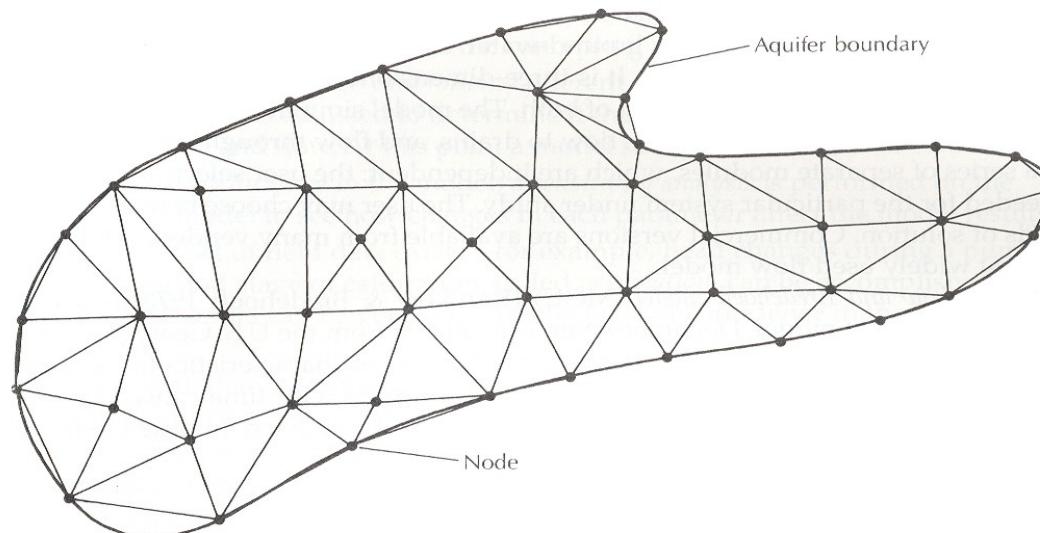


rectangular cells



# Numerical models

## Finite element models:



# Numerical models

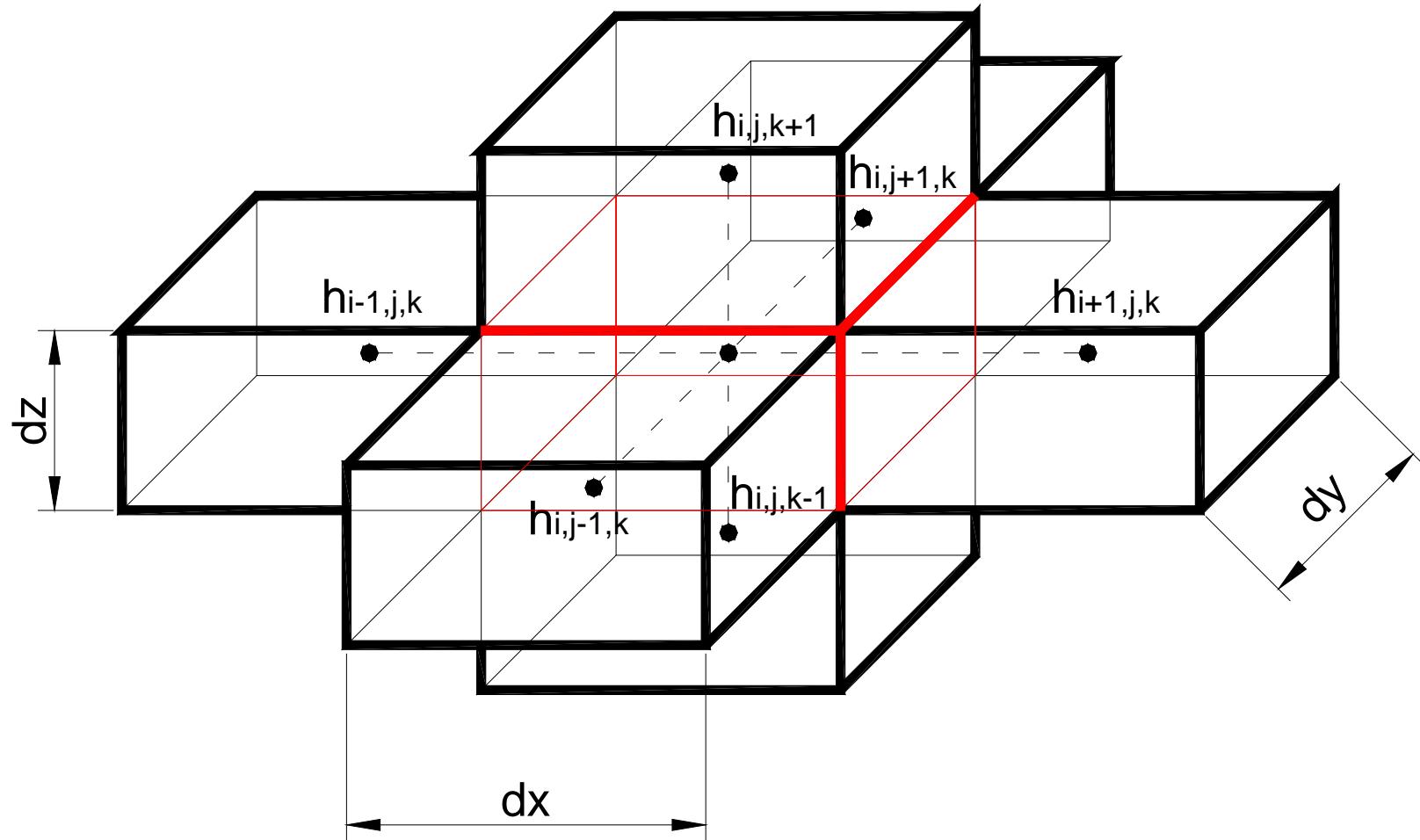
## Spatial discretisation - consider:

- Purpose of modelling
- Variations in hydraulic head (Near well fields, rivers, faults, etc.)
- Geological layers
- Locations of well fields
- Exchange with rivers
- Computational resources
- ...

## Discretisation in time - consider:

- Purpose of modelling
- Head/flow variation at boundaries
- Timescale of involved processes
- ....

# Description of Finite Difference equations for 3D groundwater flow



# Description of Finite Difference equations for 3D groundwater flow

Equation of continuity:

$$\text{in} - \text{out} = \Delta sto$$

$$\Delta t (Q_x^- - Q_x^+ + Q_y^- - Q_y^+ + Q_z^- - Q_z^+ - R) = \Delta sto$$

The Darcy equation:

$$Q_x^- = -\frac{h_{i,j,k}^{n+1} - h_{i-1,j,k}^{n+1}}{\Delta x} Kx_{i-\frac{1}{2},j,k} \Delta y \Delta z$$

$$Q_y^- = -\frac{h_{i,j,k}^{n+1} - h_{i,j-1,k}^{n+1}}{\Delta y} Ky_{i,j-\frac{1}{2},k} \Delta x \Delta z$$

$$Q_z^- = -\frac{h_{i,j,k}^{n+1} - h_{i,j,k-1}^{n+1}}{\Delta z} Kz_{i,j,k-\frac{1}{2}} \Delta x \Delta y$$

$$Q_x^+ = -\frac{h_{i+1,j,k}^{n+1} - h_{i,j,k}^{n+1}}{\Delta x} Kx_{i+\frac{1}{2},j,k} \Delta y \Delta z$$

$$Q_y^+ = -\frac{h_{i,j+1,k}^{n+1} - h_{i,j,k}^{n+1}}{\Delta y} Ky_{i,j+\frac{1}{2},k} \Delta x \Delta z$$

$$Q_z^+ = -\frac{h_{i,j,k+1}^{n+1} - h_{i,j,k}^{n+1}}{\Delta z} Kz_{i,j,k+\frac{1}{2}} \Delta x \Delta y$$

# Description of Finite Difference equations for 3D groundwater flow

Effective conductivity on the cell edges :

$$Kx_{i-\frac{1}{2},j,k} = \frac{2}{\frac{1}{Kx_{i-1,j,k}} + \frac{1}{Kx_{i,j,k}}}, \quad Kx_{i+\frac{1}{2},j,k} = \frac{2}{\frac{1}{Kx_{i+1,j,k}} + \frac{1}{Kx_{i,j,k}}}$$

$$Ky_{i,j-\frac{1}{2},k} = \frac{2}{\frac{1}{Ky_{i,j-1,k}} + \frac{1}{Ky_{i,j,k}}}, \quad Ky_{i,j+\frac{1}{2},k} = \frac{2}{\frac{1}{Ky_{i,j+1,k}} + \frac{1}{Ky_{i,j,k}}}$$

$$Kz_{i,j,k-\frac{1}{2}} = \frac{dz_{i,j,k-1} + dz_{i,j,k}}{\frac{dz_{i,j,k-1}}{Kz_{i,j,k-1}} + \frac{dz_{i,j,k}}{Kz_{i,j,k}}}, \quad Kz_{i,j,k+\frac{1}{2}} = \frac{dz_{i,j,k+1} + dz_{i,j,k}}{\frac{dz_{i,j,k+1}}{Kz_{i,j,k+1}} + \frac{dz_{i,j,k}}{Kz_{i,j,k}}}$$

Storage:

$$\Delta sto = \frac{h_{i,j,k}^{n+1} - h_{i,j,k}^n}{\Delta t} S \Delta x \Delta y = \frac{h_{i,j,k}^{n+1} - h_{i,j,k}^n}{\Delta t} S_s \Delta z \Delta x \Delta y$$

# Description of Finite Difference equations for 3D groundwater flow

## Equation of continuity and the Darcy equation

$$\begin{aligned}
 & -\frac{h_{i,j,k}^{n+1} - h_{i-1,j,k}^{n+1}}{\Delta x} Kx_{i-\frac{1}{2},j,k} \Delta y \Delta z + \frac{h_{i+1,j,k}^{n+1} - h_{i,j,k}^{n+1}}{\Delta x} Kx_{i+\frac{1}{2},j,k} \Delta y \Delta z - \frac{h_{i,j,k}^{n+1} - h_{i,j-1,k}^{n+1}}{\Delta y} Ky_{i,j-\frac{1}{2},k} \Delta x \Delta z + \frac{h_{i,j+1,k}^{n+1} - h_{i,j,k}^{n+1}}{\Delta y} Ky_{i,j+\frac{1}{2},k} \Delta x \Delta z \\
 & -\frac{h_{i,j,k}^{n+1} - h_{i,j,k-1}^{n+1}}{\Delta z} Kz_{i,j,k-\frac{1}{2}} \Delta x \Delta y + \frac{h_{i,j,k+1}^{n+1} - h_{i,j,k}^{n+1}}{\Delta z} Kz_{i,j,k+\frac{1}{2}} \Delta x \Delta y - R = \frac{h_{i,j,k}^{n+1} - h_{i,j,k}^n}{\Delta t} S_s \Delta x \Delta y \Delta z
 \end{aligned}$$

↓

$$\begin{aligned}
 & \left( Kx_{i+\frac{1}{2},j,k} \frac{\Delta y \Delta z}{\Delta x} \right) h_{i+1,j,k}^{n+1} + \left( Kx_{i-\frac{1}{2},j,k} \frac{\Delta y \Delta z}{\Delta x} \right) h_{i-1,j,k}^{n+1} + \left( Ky_{i,j+\frac{1}{2},k} \frac{\Delta x \Delta z}{\Delta y} \right) h_{i,j+1,k}^{n+1} + \left( Ky_{i,j-\frac{1}{2},k} \frac{\Delta x \Delta z}{\Delta y} \right) h_{i,j-1,k}^{n+1} \\
 & + \left( Kz_{i,j,k+\frac{1}{2}} \frac{\Delta x \Delta y}{\Delta z} \right) h_{i,j,k+1}^{n+1} + \left( Kz_{i,j,k-\frac{1}{2}} \frac{\Delta x \Delta y}{\Delta z} \right) h_{i,j,k-1}^{n+1} \\
 & + \left( -Kx_{i-\frac{1}{2},j,k} \frac{\Delta y \Delta z}{\Delta x} - Kx_{i+\frac{1}{2},j,k} \frac{\Delta y \Delta z}{\Delta x} - Ky_{i,j-\frac{1}{2},k} \frac{\Delta x \Delta z}{\Delta y} - Ky_{i,j+\frac{1}{2},k} \frac{\Delta x \Delta z}{\Delta y} - Kz_{i,j,k-\frac{1}{2}} \frac{\Delta x \Delta y}{\Delta z} - Kz_{i,j,k+\frac{1}{2}} \frac{\Delta x \Delta y}{\Delta z} - \frac{S_s \Delta x \Delta y \Delta z}{\Delta t} \right) h_{i,j,k}^{n+1} \\
 & = R - \frac{h_{i,j,k}^n}{\Delta t} S_s \Delta x \Delta y \Delta z
 \end{aligned}$$

↓

$$Ah_{i+1,j,k}^{n+1} + Bh_{i-1,j,k}^{n+1} + Ch_{i,j+1,k}^{n+1} + Dh_{i,j-1,k}^{n+1} + Eh_{i,j,k+1}^{n+1} + Fh_{i,j,k-1}^{n+1} + Gh_{i,j,k}^{n+1} = H$$

# Description of Finite Difference equations for 1D groundwater flow

## Equation of continuity and the Darcy equation

$$-\frac{h_i^{n+1} - h_{i-1}^{n+1}}{\Delta x} Kx_{i-\frac{1}{2}} \Delta y \Delta z + \frac{h_{i+1}^{n+1} - h_i^{n+1}}{\Delta x} Kx_{i+\frac{1}{2}} \Delta y \Delta z - R = \frac{h_i^{n+1} - h_i^n}{\Delta t} S_s \Delta x \Delta y \Delta z$$

↓

$$-(h_i^{n+1} - h_{i-1}^{n+1})Kx_{i-\frac{1}{2}} + (h_{i+1}^{n+1} - h_i^{n+1})Kx_{i+\frac{1}{2}} - \frac{\Delta x R}{\Delta y \Delta z} = \frac{h_i^{n+1} - h_i^n}{\Delta t} S_s \Delta x \Delta x$$

↓

$$(Kx_{i+\frac{1}{2}})h_{i+1}^{n+1} + (Kx_{i-\frac{1}{2}})h_{i-1}^{n+1} + \left( -Kx_{i-\frac{1}{2}} - Kx_{i+\frac{1}{2}} - \frac{S_s \Delta x \Delta x}{\Delta t} \right) h_i^{n+1}$$

$$= R \frac{\Delta x}{\Delta y \Delta z} - \frac{h_i^n}{\Delta t} S \Delta x \Delta x$$

↓

$$A_i h_{i-1}^{n+1} + B_i h_i^{n+1} + C_i h_{i+1}^{n+1} = D_i$$

# Description of Finite Difference equations for 1D groundwater flow

The  $n$  finite difference equations:

$$\begin{array}{cccccc} B_1 & C_1 & & \cdots & h_1 & D_1 \\ A_2 & B_2 & C_2 & & h_2 & D_2 \\ \vdots & & \ddots & & \vdots & \vdots \\ & & & A_{n-1} & B_{n-1} & C_{n-1} \\ & & & A_n & B_n & h_n \end{array} = \begin{array}{c} D_{n-1} \\ D_n \end{array}$$

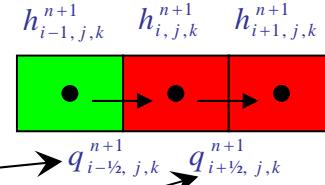


$$h_{i-1,j,k}^{n+1} = \text{constant}$$

## Implementation of boundary conditions

Prescribed head or Dirichlet's condition  
(surface water body, measured groundwater head)

### 1D FD equations



$$-\frac{h_{i,j,k}^{n+1} - h_{i-1,j,k}^{n+1}}{\Delta x} Kx_{i-\frac{1}{2},j,k} \Delta y \Delta z + \frac{h_{i+1,j,k}^{n+1} - h_{i,j,k}^{n+1}}{\Delta x} Kx_{i+\frac{1}{2},j,k} \Delta y \Delta z - R = \frac{h_{i,j}^{n+1} - h_{i,j}^n}{\Delta t} S_s \Delta x \Delta y \Delta z$$

$$\Downarrow \bullet \Delta x \quad \text{and} \quad /(\Delta y \Delta z)$$

$$-(h_{i,j,k}^{n+1} - h_{i-1,j,k}^{n+1}) Kx_{i-\frac{1}{2},j,k} + (h_{i+1,j,k}^{n+1} - h_{i,j,k}^{n+1}) Kx_{i+\frac{1}{2},j,k} - \frac{\Delta x R}{\Delta y \Delta z} = \frac{h_{i,j}^{n+1} - h_{i,j}^n}{\Delta t} S_s \Delta x \Delta x$$

$\Downarrow$

$$(Kx_{i+\frac{1}{2},j,k}) h_{i+1,j,k}^{n+1} + \left( -Kx_{i-\frac{1}{2},j,k} - Kx_{i+\frac{1}{2},j,k} - \frac{S_s \Delta x \Delta x}{\Delta t} \right) h_{i,j,k}^{n+1}$$

$$= R \frac{\Delta x}{\Delta y \Delta z} - \frac{h_{i,j,k}^n}{\Delta t} S \Delta x \Delta x - (Kx_{i-\frac{1}{2},j,k}) h_{i-1,j,k}^{n+1}$$

$\Downarrow$

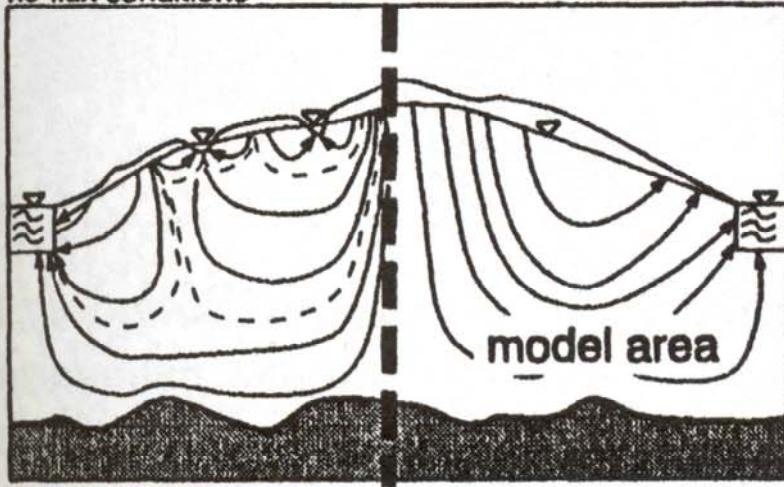
$$A h_{i+1,j,k}^{n+1} + C h_{i,j,k}^{n+1} = D - B h_{i-1,j,k}^{n+1}$$

All known terms

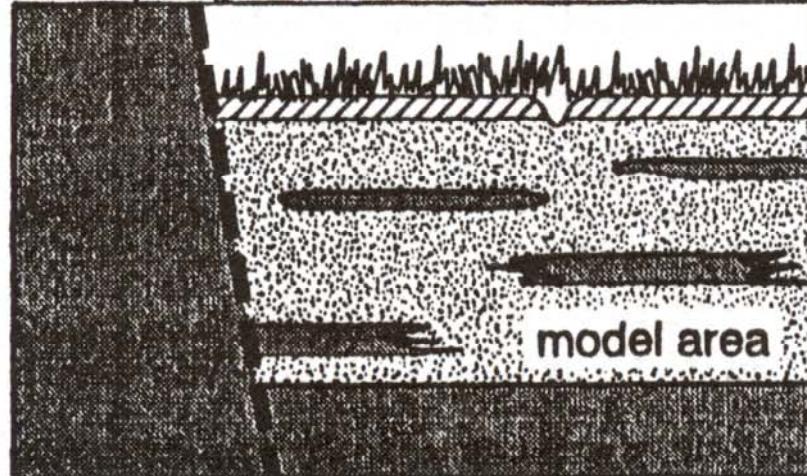
# Boundary conditions

## PRESCRIBED FLUX OR SECOND KIND OR NEUMANN'S CONDITION

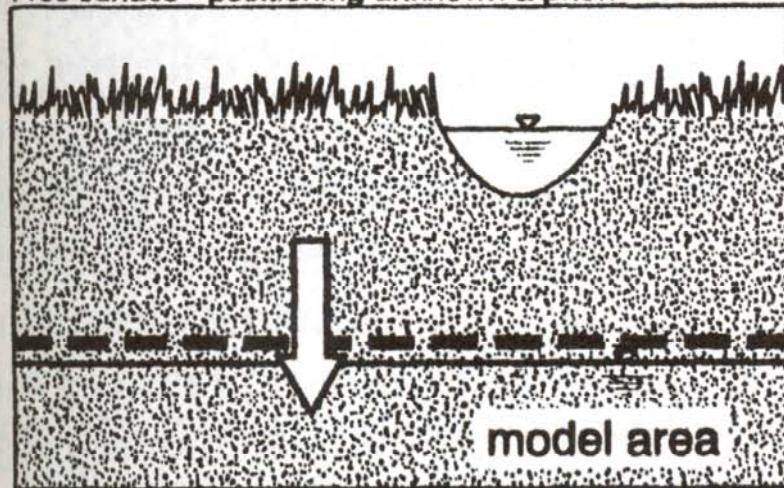
Groundwater divide or streamlines imposing  
no-flux conditions



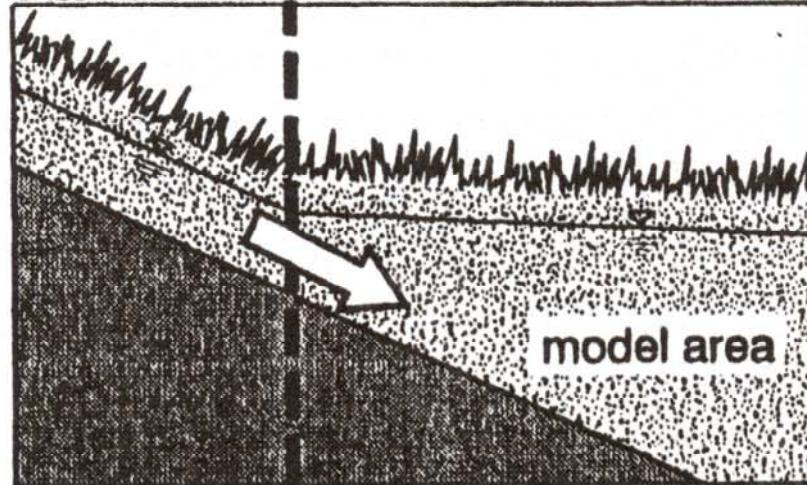
Fault imposing no-flux or fixed flux conditions



Free surface - positioning unknown a priori



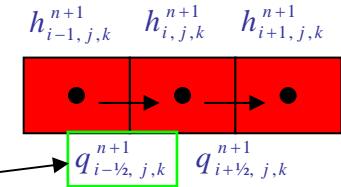
Subsurface inflow or outflow



# Boundary conditions

Prescribed flux or Neumann's condition  
 (Groundwater divide, subsurface inflow/outflow, etc.)

$$q_{i-\frac{1}{2},j,k} = \frac{h_{i,j,k}^{n+1} - h_{i-1,j,k}^{n+1}}{\Delta x} Kx_{i-\frac{1}{2},j,k} \Delta y \Delta z = \text{constant}$$



## 1D FD equations

$$q_{i-\frac{1}{2},j,k} + \frac{h_{i+1,j,k}^{n+1} - h_{i,j,k}^{n+1}}{\Delta x} Kx_{i+\frac{1}{2},j,k} \Delta y \Delta z - R = \frac{h_{i,j}^{n+1} - h_{i,j}^n}{\Delta t} S_s \Delta x \Delta y \Delta z$$

↓

$$(Kx_{i+\frac{1}{2},j,k})h_{i+1,j,k}^{n+1} - (Kx_{i-\frac{1}{2},j,k})h_{i,j,k}^{n+1} = R \frac{\Delta x}{\Delta y \Delta z} - \frac{h_{i,j,k}^n}{\Delta t} S \Delta x \Delta x - q_{i-\frac{1}{2},j,k}$$

↓

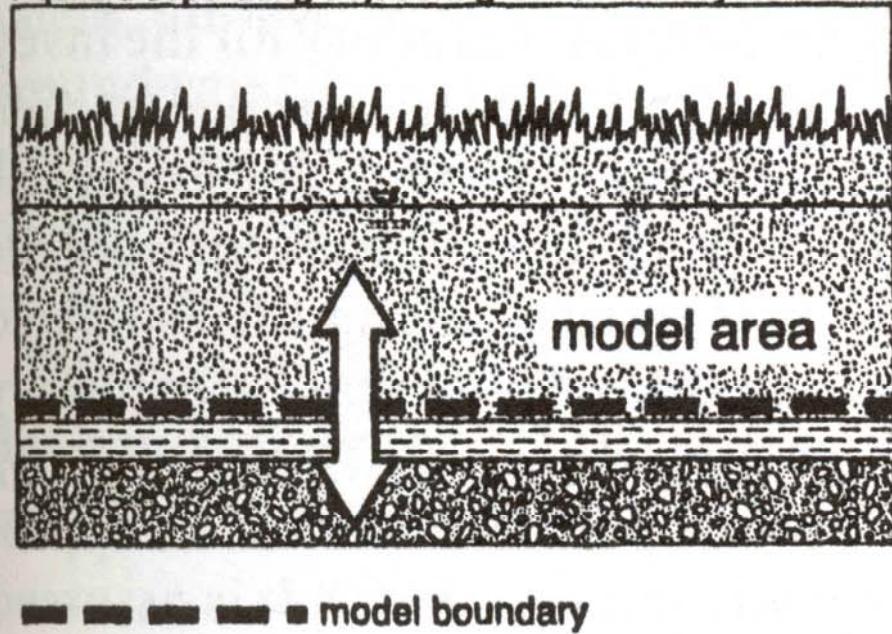
$$Ah_{i+1,j,k}^{n+1} + Ch_{i,j,k}^{n+1} = D - q_{i-\frac{1}{2},j,k}$$

All known terms

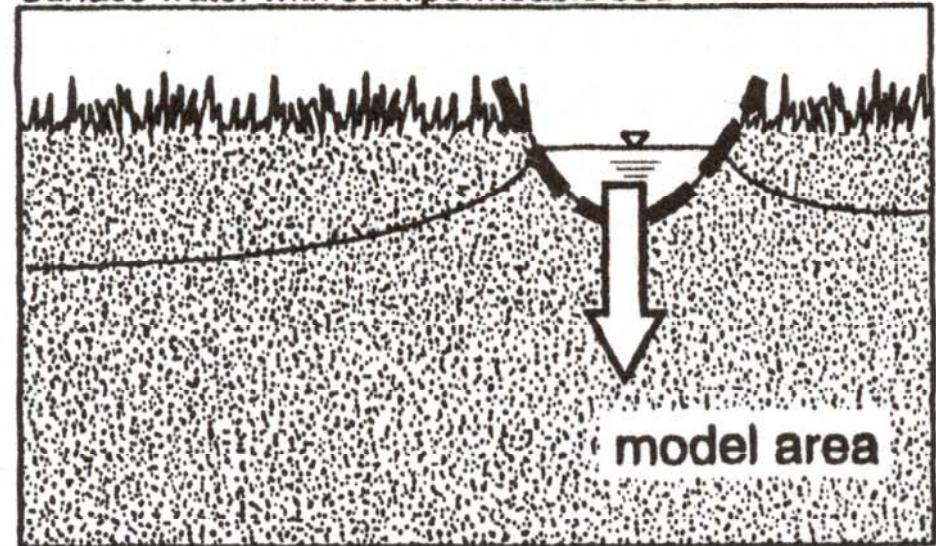
# Boundary conditions

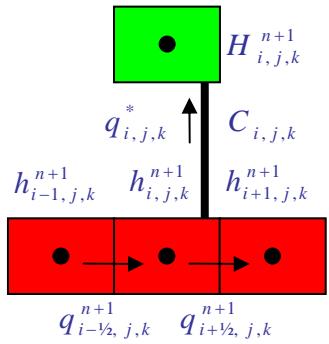
## SEMPERMEABLE OR THIRD KIND OR CAUCHY'S CONDITION

Aquitard separating adjacent groundwater systems



Surface water with semipermeable bed





## Boundary conditions

Semipermeable or Cauchy's condition

(Leakage between aquifers, surface water – groundwater flow, etc.)

$$q_{i,j,k}^* = (h_{i,j,k}^{n+1} - H_{i,j,k}^{n+1})C_{i,j,k}$$

Surface water elevation  
Leakage coefficient

## 1D FD equations

$$-\frac{h_i^{n+1} - h_{i-1}^{n+1}}{\Delta x} Kx_{i-\frac{1}{2}} \Delta y \Delta z + \frac{h_{i+1}^{n+1} - h_i^{n+1}}{\Delta x} Kx_{i+\frac{1}{2}} \Delta y \Delta z - R - \boxed{C(h_i^{n+1} - H_i^{n+1}) \Delta x \Delta y} = \frac{h_i^{n+1} - h_i^n}{\Delta t} S_s \Delta x \Delta y \Delta z$$

↓

$$-(h_i^{n+1} - h_{i-1}^{n+1})Kx_{i-\frac{1}{2}} + (h_{i+1}^{n+1} - h_i^{n+1})Kx_{i+\frac{1}{2}} - \frac{\Delta x R}{\Delta y \Delta z} - \boxed{C(h_i^{n+1} - H_i^{n+1}) \frac{\Delta x \Delta x}{\Delta z}} = \frac{h_i^{n+1} - h_i^n}{\Delta t} S_s \Delta x \Delta x$$

↓

$$(Kx_{i+\frac{1}{2}})h_{i+1}^{n+1} + (Kx_{i-\frac{1}{2}})h_{i-1}^{n+1} + \left( -Kx_{i-\frac{1}{2}} - Kx_{i+\frac{1}{2}} + \boxed{C \frac{\Delta x \Delta x}{\Delta z}} - \frac{S_s \Delta x \Delta x}{\Delta t} \right) h_i^{n+1}$$

$$= R \frac{\Delta x}{\Delta y \Delta z} - \boxed{CH_i^{n+1} \frac{\Delta x \Delta x}{\Delta z}} - \frac{h_i^n}{\Delta t} S \Delta x \Delta x$$

All known terms

↓

$$A h_{i+1,j,k}^{n+1} + B h_{i-1,j,k}^{n+1} + C h_{i,j,k}^{n+1} = D$$