Numerical groundwater modelling
Finite difference method (FD)

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Contents

• **Finite difference method** for 3D flow equation

• **When 2D, when 3D?**

• **2.5 D**: Layer oriented discretization in the vertical direction

• **Steps from concept to numerical model**
Solution methods

- **Analytical** (very limited)
  - Evaluation of pumping tests
- **Numerical** (requires discretisation)
  - Finite differences
  - Finite volumes
  - Finite elements
Discretisation methods

Finite differences
- Balance of box

Finite elements
- Balance over patch

Finite volumes
- Balance over FV
Prototype: Finite Differences, 2D

**Steps** (transient case):

- **Discretise** space in rectangular boxes \((i,j)\)
- **Establish water balance for each box** and time interval \([t, t+\Delta t]\)
- **Express balance equation** by unknown heads at nodes and neighbouring nodes using Darcy’s law
- **Apply boundary conditions** in boxes at boundary
- **Establish equation system** for unknowns \(h_{ij}(t+\Delta t)\)
- **Solve equation system**
- **Make results the initial condition of next time step**
In images: Implicit method

Use boundary conditions for $i=1, i=N_x, j=1, j=N_y$

Initial conditions

$$\alpha h^{t+\Delta t}(i-1, j) + \beta h^{t+\Delta t}(i+1, j) + \gamma h^{t+\Delta t}(i, j) +$$
$$\delta h^{t+\Delta t}(i, j-1) + \varepsilon h^{t+\Delta t}(i, j+1) = \eta(h^t(k, l))$$

Solution $h_{i,j}(t+\Delta t)$
2D or 3D?

2D - modelling (horizontal)

Regional flow:
- Thickness much smaller than horizontal dimensions
- No separation into layers by aquitards, completely screened wells
- Vertical Darcy-velocities much smaller than horizontal ones

Regional transport: in addition
- Vertical mixing strong, small groundwater recharge
- No density effects

3D- modelling: if above restrictions are not fulfilled, e.g.:
- Small scale analysis (e.g., remediation or transport)
- Only partially screened wells in aquifers of large thickness
- Separation of layers by aquitards, density effects
- Vertical Darcy-velocities in the same order of magn. as horizontal
Finite differences in 3D

Analogous.

**Main difference:** More flow terms per cell. Therefore larger bandwidth of matrix. Details later!

\[
\begin{bmatrix}
    a_{m,l} \\
    \vdots
\end{bmatrix}
\begin{bmatrix}
    h_l
\end{bmatrix}
= 
\begin{bmatrix}
    b_m
\end{bmatrix}
\]

$a_{ml}$ non-zero for all cells $l$, which are directly linked with cell $m$ via face
In images: Implicit method, isotropic case

\[ \alpha h^{t+\Delta t}(i-1, j, k) + \beta h^{t+\Delta t}(i+1, j, k) + \gamma h^{t+\Delta t}(i, j, k) + \delta h^{t+\Delta t}(i, j-1, k) + \varepsilon h^{t+\Delta t}(i, j+1, k) + \\
\zeta h^{t+\Delta t}(i, j, k-1) + \theta h^{t+\Delta t}(i, j, k+1) = \eta(h^t(l, m, n)) \]

Use boundary conditions for \( i=1, \ i=N_x, \ j=1, \ j=N_y, \ k=1, \ k=N_z \)

\[ \sum_l \left( a_{m,l(i,j,k)} \right) \left( h_{l(i,j,k)}(t+\Delta t) \right) = (b_m) \]

Initial conditions

Solution \( h_{i,j,k}(t+\Delta t) \)
3D-discretisation example FD

Explanation

--- Aquifer Boundary

• Active Cell

○ Inactive Cell

$\Delta r_J$ Dimension of Cell Along the Row Direction. Subscript (J) Indicates the Number of the Column

$\Delta c_I$ Dimension of Cell Along the Column Direction. Subscript (I) Indicates the Number of the Row

$\Delta v_K$ Dimension of the Cell Along the Vertical Direction. Subscript (K) Indicates the Number of the Layer
FD discretisation in 2D

Per cell one balance equation, containing
5 unknown heads in the isotropic aquifer ($h_{ij}$ and 4 neighbours)
9 unknown heads in the anisotropic aquifer

Steady state:
$$\sum_{i=1}^{4} Q_i + Q = 0$$

Equation system:
$$[A]\{h\} = \{Q\}$$
FD discretisation in 3D: In analogy to 2D

Per cell one balance equation containing:
7 unknown heads in the isotropic aquifer ($h_{ijk}$ and 6 neighbours)
27 unknown heads in the anisotropic aquifer with a symmetrical difference formulation

Steady state:
$$\sum_{i=1}^{6} Q_i + Q = 0$$

Equation system:
$$[A] \{h\} = \{Q\}$$
Problem: Aquifer structure

Regular grid: Cell may contain a mixture of materials

Layer oriented cell: cell contains material of one geological unit
3D-Modelling

- Very fine discretisation such that cells with more than 1 material are only a small subset of all cells
2.5 D model: Discretisation according to stratigraphy

Is generated from regular grid by displacing top and bottom of each cell according to layering
Discretized equations in 3D and 2.5D

Treatment of $Q_5, Q_6$

**3D**

$$Q_5 = -\Delta x \Delta y K_{zz} \frac{(h_{i,j,k} - h_{i,j,k-1})}{\Delta z}$$

**2.5D**

$$Q_5 = -\Delta x \Delta y l_{k-1,k} \cdot (h_{i,j,k} - h_{i,j,k-1})$$

where $l$ is the leakage factor

$$l = \frac{K_{zz}}{\Delta z}$$
Anisotropy

Horizontal layers

Non-horizontal layers:

Only easily treated in FE-method
Compromise in 2.5 D model

Within layers: $K_{xx}, K_{xy}, K_{yy}$,
Between layers: only $K_{zz}$
2.5 D model: Coupled layers

2.5D model = sequence of 2D-models.

These are coupled by leakage.

2D model layers are unconfined or confined aquifers. A switching from confined to unconfined (and vice versa) according to the position of the piezometric surface is possible.
Aquifer type specified layer by layer

<table>
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$g =$ confined; $f =$ unconfined; $t =$ dry

If **water table declines**, cells of type $g$ can turn into $f$ (unconfined cells) (in MODFLOW: Type of layer “confined-unconfined”)
Problem: Nodes falling dry

![Diagram showing water table levels and node conditions]

When **water table rises**, dry nodes have to be **rewetted** again. They must be made permanently impervious!
Rewetting of cells fallen dry

From the side:

From below:

Iterative procedure, damping necessary to avoid instability
Wells in 2D and 3D

\[ Q \]

\[ Q = \Sigma Q_i \]

\( Q_i \) layerwise prescribed by fraction \( T_i / T_{\text{total}} \), or implementation of one cell containing pump and high vertical hydraulic conductivity to other screened well cells above and below.
Treatment of aquitards in 2.5D model

In Aquifer:
Head contour lines almost vertical, streamlines almost horizontal

In Aquitard:
Head contour lines almost horizontal, streamlines almost vertical

Using the leakage principle aquitard need not be modelled explicitly, gap in vertical discretization (only in flow!)
From geological data to the numerical model

Figure from: Anderson, Woessner, Practical Groundwater Modelling
Figure from: Anderson, Woessner (1991) Practical Groundwater Modelling
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If only piezometric heads are of interest, the absolute position of layers is irrelevant. Only their neighbourhood relationship is important.

Figure from: Anderson, Woessner (1991) Practical Groundwater Modelling
Treatment of pinchout layers

Case 1 -- Confining Bed Pinchout

Arrows show vertical and horizontal connection between nodes. Length of arrows represents amount of hydraulic connection.

Case 2 -- Aquifer Pinchout

Physical Configuration

Model Conceptualization
Data for 3D models and data sources

- **Point data**: Direct measurements
- **Areal data**: Usually by interpolation
- **Time series**
- **Indirect data**: related data from which relevant data can be obtained through correlation or modelling (e.g., environmental tracer data, remote sensing data)

In table: s spatial, t temporal, u unconfined, c confined
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