# Numerical simulation of soil water dynamics: transient flow

The relation between $\psi_m$ and the unsaturated hydraulic conductivity $k(\psi_m)$ or the differential soil water capacity $C(\psi_m)$ causes the differential equation (DE) to be strongly non-linear!

➔ There are no analytical solutions available to solve the DE for initial and boundary conditions found under **field conditions**.

➔ So: numerical solutions will be needed to solve the DE:

- finite difference solutions of the DE
- finite element solutions of the DE

There are different methods to solve the non-linear DE, example 1D-vertical:

1. Use time steps $\Delta t$ and depth compartments $\Delta z$ small enough so $k(\psi_m)$ and $C(\psi_m)$ can be assumed constant during the time step $\Delta t$ (explicit and implicit numerical solutions)

# Finite-difference methods

partial differential equations

$$\frac{\delta\theta}{\delta t} = \frac{-\delta q}{\delta z} = \frac{\delta}{\delta z}\left(k(\theta)\cdot\left(\frac{\delta\psi}{\delta z}+1\right)\right) - S$$

$$\frac{\delta\psi}{\delta t} = \frac{1}{C(\psi)}\cdot\frac{\delta}{\delta z}\left(k(\psi)\cdot\left(\frac{\delta\psi}{\delta z}+1\right)\right) - S$$

➔ Transform into finite-difference equations

Time and space discretisation: time steps $\Delta t$ and depth compartments $\Delta z$

Approximate terms in ◯

Taylor theorem:

$$\psi(t+\Delta t) = \psi(t) + \Delta t \cdot \psi'(t) + \frac{1}{2}\Delta t^2 \cdot \psi''(t) + \ldots$$

$$\theta(t+\Delta t) = \theta(t) + \Delta t \cdot \theta'(t) + \frac{1}{2}\Delta t^2 \cdot \theta''(t) + \ldots$$

Forward finite-difference quotient ψ

$$\frac{\delta\psi}{\delta t} \approx \frac{\psi(t+\Delta t) - \psi(t)}{\Delta t} \qquad O(\Delta t)$$

Forward finite-difference quotient θ

$$\frac{\delta\theta}{\delta t} \approx \frac{\theta(t+\Delta t) - \theta(t)}{\Delta t} \qquad O(\Delta t)$$

- assuming second and higher powers of Δt can be neglected ➔ errors are of order O(Δt )
- thus : numerical solutions are an approximation of the true solution due to the neglection of rest-terms

Central differential quotient:

$$\psi(z+\Delta z)=\psi(z)+\Delta z\cdot\psi'(z)+\frac{1}{2}\Delta z^{2}\cdot\psi''(z)+\ldots \qquad (\mathbf{1})$$

$$\psi(z-\Delta z)=\psi(z)-\Delta z\cdot\psi'(z)+\frac{1}{2}\Delta z^{2}\cdot\psi''(z)-\ldots \qquad (\mathbf{2})$$

<u>(**1**) - (**2**):</u>

$$\psi'(z)=\frac{\delta\psi}{\delta z}\approx\frac{\psi(z+\Delta z)-\psi(z-\Delta z)}{2\Delta z}$$

$O(\Delta z^{2})$
(= error)

<u>(**1**) + (**2**):</u>

$$\psi''(z)=\frac{\delta^{2}\psi}{\delta z^{2}}\approx\frac{\psi(z+\Delta z)-2\psi(z)+\psi(z-\Delta z)}{\Delta z^{2}}$$

$O(\Delta z^{3})$
(= error)

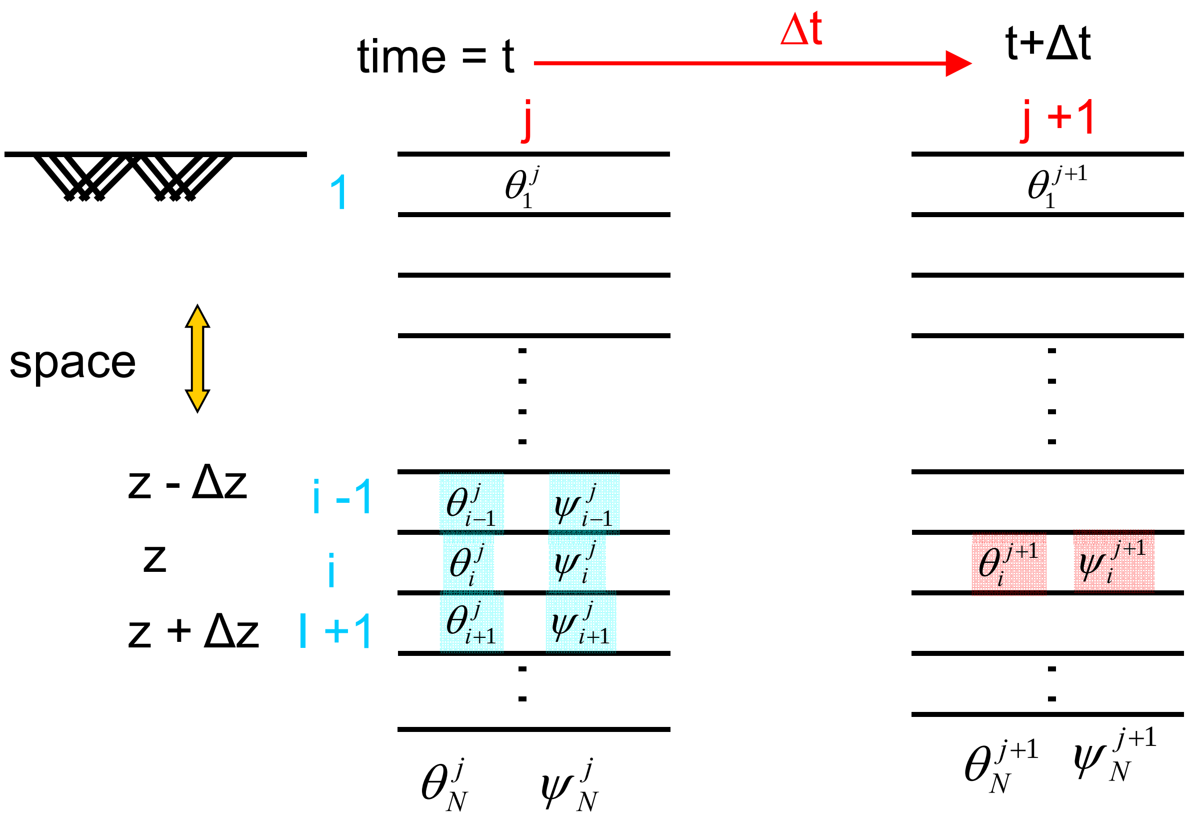
Error: - order O of the approximation
- approximation in time and space due to discretisation

Explicit and implicit  Finite-Difference Methods
Notation:

$$\psi(z) = \psi_i \qquad \psi(t) = \psi^j$$

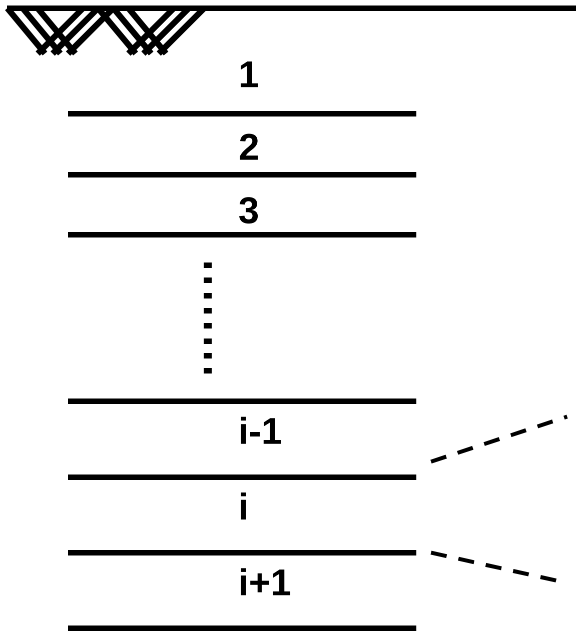
$$\psi^{j+1}_{i+1}$$

$$\psi(z+\Delta z) = \psi_{i+1} \qquad \psi(t+\Delta t) = \psi^{j+1}$$



Explicit scheme with explicit linearization:

Spatial discretization:




$$q^j_{i-\frac{1}{2}} = -k^j_{i-\frac{1}{2}}\left(\frac{\psi^j_{i-1} - \psi^j_i}{\Delta z} + 1\right)$$

$$\psi = \psi_m$$

$$q^j_{i+\frac{1}{2}} = -k^j_{i+\frac{1}{2}}\left(\frac{\psi^j_i - \psi^j_{i+1}}{\Delta z} + 1\right)$$

$$\frac{\delta\theta}{\delta t} = -\frac{\delta q}{\delta z} = \frac{\delta}{\delta z}\left[k(\psi)\cdot\left(\frac{\delta\psi_m}{\delta z} + 1\right)\right]$$

$$\frac{\theta^{j+1}_i - \theta^j_i}{\Delta t} = \frac{1}{\Delta z}\left[k^j_{i-\frac{1}{2}}\cdot\frac{(\psi^j_{i-1} - \psi^j_i)}{\Delta z} + k^j_{i-\frac{1}{2}}\right] - \frac{1}{\Delta z}\left[k^j_{i+\frac{1}{2}}\cdot\frac{(\psi^j_i - \psi^j_{i+1})}{\Delta z} + k^j_{i+\frac{1}{2}}\right]$$

rearrange:

$$\theta_i^{j+1} = \theta_i^j + \frac{\Delta t}{\Delta z}\left[k^j_{i-\frac{1}{2}} \cdot \frac{(\psi^j_{i-1} - \psi^j_i)}{\Delta z} + k^j_{i-\frac{1}{2}}\right] - \frac{\Delta t}{\Delta z}\left[k^j_{i+\frac{1}{2}} \cdot \frac{(\psi^j_i - \psi^j_{i+1})}{\Delta z} + k^j_{i+\frac{1}{2}}\right]$$

$$\left.\begin{aligned} k^j_{i-\frac{1}{2}} &= \sqrt{k(\psi^j_{i-1}) \cdot k(\psi^j_i)} \\ k^j_{i+\frac{1}{2}} &= \sqrt{k(\psi^j_i) \cdot k(\psi^j_{i+1})} \end{aligned}\right\} \text{geometrical mean}$$

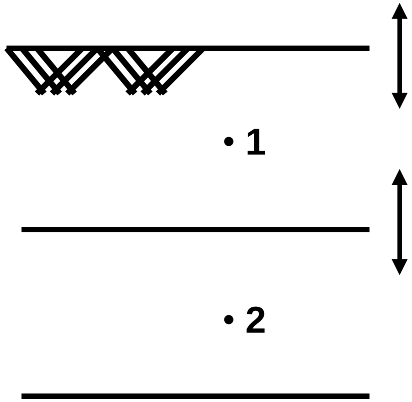
Boundary conditions:

- at the top → flux $q_0$ < infiltration / evaporation

- at the bottom → groundwater table $\psi_m = 0$

→ prescribe $\psi_m$ e.g. $\psi_m = -50\text{cm}$

## The solution of the top nodal point:




$$q_0$$

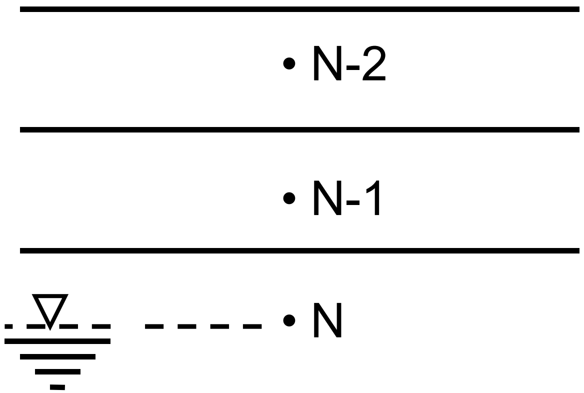
$$q^{j}_{1\frac{1}{2}} = -k^{j}_{1\frac{1}{2}}\left(\frac{\psi^{j}_{1} - \psi^{j}_{2}}{\Delta z} + 1\right)$$

$q_0 < 0$ infiltration

$q_0 > 0$ evaporation

$$\theta^{j+1}_{1} = \theta^{j}_{1} - \frac{\Delta t}{\Delta z} q_0 - \frac{\Delta t}{\Delta z}\left[k_{1\frac{1}{2}}\left(\frac{\psi^{j}_{1} - \psi^{j}_{2}}{\Delta z} + 1\right)\right]$$

Solution for the bottom boundary condition




$\psi_N$ is known, so N-1 is the last node for which the equation must be solved.

$$\theta_{N-1}^{j+1} = \theta_{N-1}^{j} + \frac{\Delta t}{\Delta z}\left[k^{j}_{N-1\frac{1}{2}}\left(\frac{\psi_{N-2}^{j} - \psi_{N-1}^{j}}{\Delta z} + 1\right)\right] - \frac{\Delta t}{\Delta z}\left[k^{j}_{N-\frac{1}{2}}\left(\frac{\psi_{N-1}^{j} - \psi_{N}}{\Delta z} + 1\right)\right]$$

## Stability and convergence

Explicit linearization means that Δz and Δt should be taken small enough to secure an accurate numerical solution.

- time step Δt : Δt is choosen so, that the water content change Δθ of any compartment in 1 timestep is less than 0.001 (cm³/cm³)

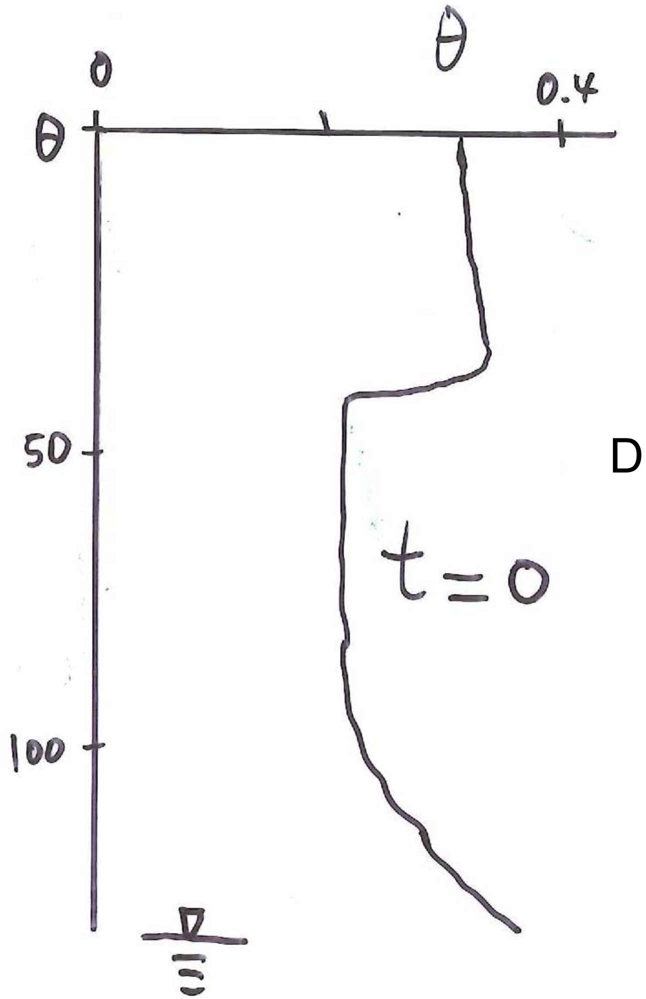
thus: $$\Delta t = \frac{\Delta\theta \cdot \Delta z}{\left|\Delta q_i^n\right|}$$ with $$\left|\Delta q_i^n\right| = \text{netto flux}$$

- space increment Δz : depends on how accurate the solution is wanted. A smaller Δz gives a better resolution and solution

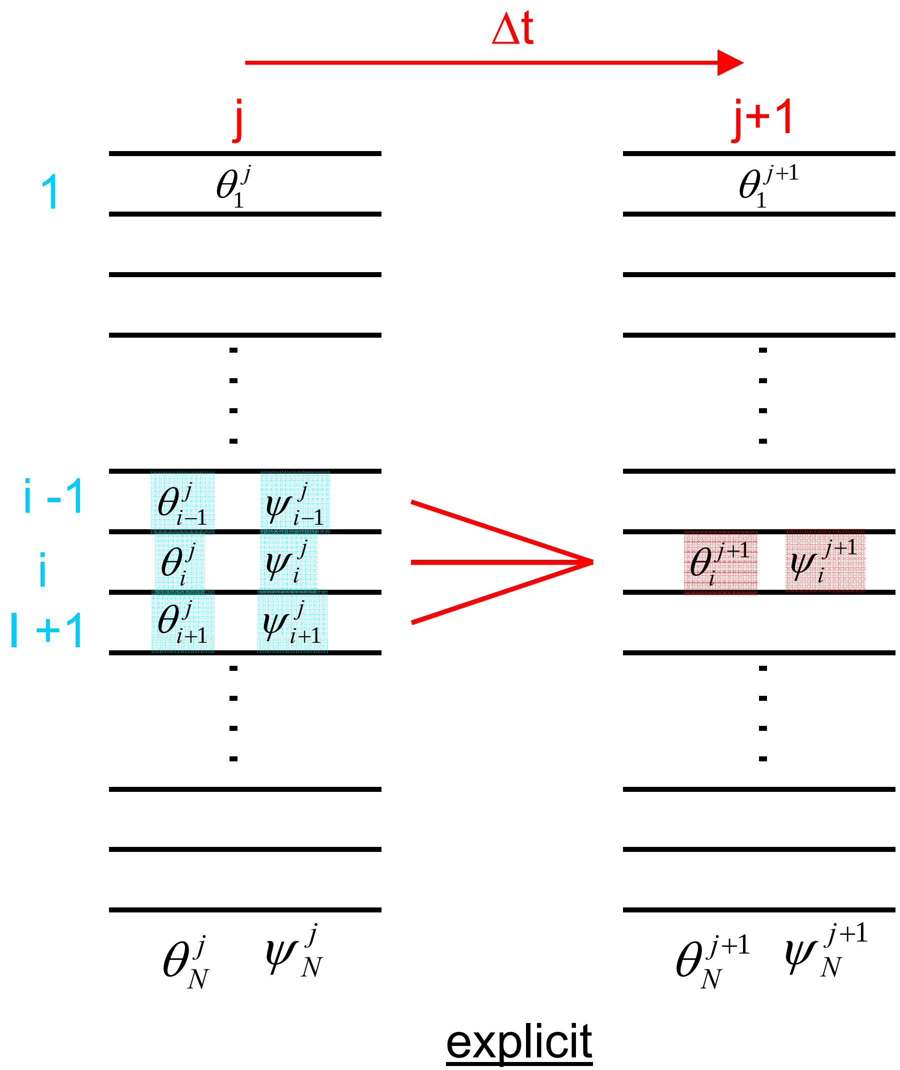
normally: $1 < \Delta z < 10$ cm

in parts of the profile where the changes of θ and ψ are small, Δz can be larger (deeper parts of the profile)

# Numerical Model: explicit scheme




Discretization




Boundary conditions:

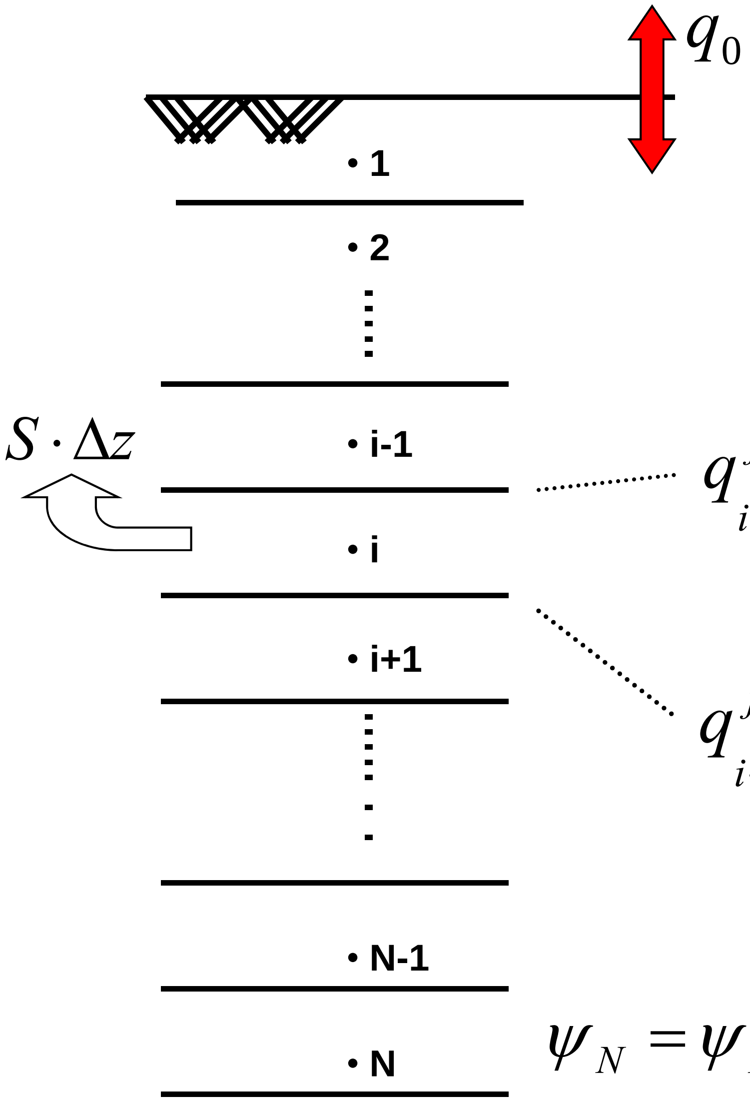
z = 0 and t ≥ 0 : rainfall and evaporation

z>0 and t ≥ 0 : root water uptake S(z,t)

$z_N$(t) and t ≥ 0 : e.g. given water table depth $z_N$(t)

## Implicit scheme with explicit linearization:

Spatial discretization:




$$\frac{\delta \psi}{\delta t} = \frac{I}{C(\psi)} \cdot \frac{\delta}{\delta z}\left[k(\psi)\left(\frac{\delta \psi}{\delta z} + 1\right)\right] - \frac{S}{C(\psi)}$$

$$\psi = \psi_m$$

$$q_{i-\frac{1}{2}}^{j+1} = -k_{i-\frac{1}{2}}^{j}\left(\frac{\psi_{i-1}^{j+1} - \psi_i^{j+1}}{\Delta z} + 1\right)$$

$$q_{i+\frac{1}{2}}^{j+1} = -k_{i+\frac{1}{2}}^{j}\left(\frac{\psi_{i}^{j+1} - \psi_{i+1}^{j+1}}{\Delta z} + 1\right)$$

$$\psi_N = \psi_I \ !$$

$$\frac{\psi_i^{j+1}-\psi_i^j}{\Delta t}=\frac{1}{C_i^j\Delta z}\left[k^j_{i-\frac{1}{2}}\left(\frac{\psi_{i-1}^{j+1}-\psi_i^{j+1}}{\Delta z}+1\right)-k^j_{i+\frac{1}{2}}\left(\frac{\psi_i^{j+1}-\psi_{i+1}^{j+1}}{\Delta z}+1\right)\right]-\frac{S_i}{C_i^j}$$

<u>rearrange:</u>

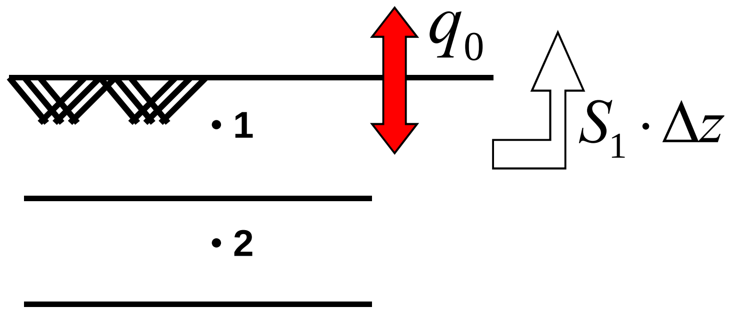
$$-\frac{\Delta t\cdot k^j_{i-\frac{1}{2}}}{C_i^j\Delta z^2}\psi_{i-1}^{j+1}+\left(1+\frac{\Delta t\cdot k^j_{i-\frac{1}{2}}}{C_i^j\Delta z^2}+\frac{\Delta t\cdot k^j_{i+\frac{1}{2}}}{C_i^j\Delta z^2}\right)\psi_i^{j+1}-\frac{\Delta t\cdot k^j_{i+\frac{1}{2}}}{C_i^j\Delta z^2}\psi_{i+1}^{j+1}=$$

$$\psi_i^j+\frac{\Delta t}{C_i^j\Delta z}\left(k^j_{i-\frac{1}{2}}-k^j_{i+\frac{1}{2}}\right)-\frac{S_i\Delta t}{C_i^j}$$

$$\Longrightarrow\quad -A_i\psi_{i-1}^{j+1}+B_i\psi_i^{j+1}-C_i\psi_{i+1}^{j+1}=D_i$$

<u>Upper boundary condition</u>: solution for the 1th node

$$q_{1\frac{1}{2}}^{j+1} = -k_{1\frac{1}{2}}^{j}\left(\frac{\psi_1^{j+1}-\psi_2^{j+1}}{\Delta z}+1\right)$$




$$\frac{\psi_1^{j+1}-\psi_1^{j}}{\Delta t} = \frac{q_0}{C_1^j \Delta z} - \frac{\Delta t}{C_1^j \Delta z}\left[k_{1\frac{1}{2}}^{j}\left(\frac{\psi_1^{j+1}-\psi_2^{j+1}}{\Delta z}+1\right)\right] - \frac{S_1}{C_1^j}$$

rearrange:

$$+\left(1+\frac{\Delta t \cdot k_{1\frac{1}{2}}^{j}}{C_1^j \Delta z^2}\right)\psi_1^{j+1} - \left(\frac{\Delta t \cdot k_{1\frac{1}{2}}^{j}}{C_1^j \Delta z^2}\right)\psi_2^{j+1} = \psi_1^{j} + \frac{\Delta t \cdot q_0}{C_1^j \Delta z} - \frac{\Delta t \cdot k_{i\frac{1}{2}}^{j}}{C_1^j \Delta z} - \frac{S_1 \Delta t}{C_1^j}$$

$$\Rightarrow \quad +B_1\psi_1^{j+1} - C_1\psi_2^{j+1} = D_1$$

Lower boundary condition: solution for the node N-1

• N-2

• N-1

• N $\psi_N^j = \psi_N^{j+1} = \psi_N$

$\Rightarrow$ $\psi_{N-i}^{j+i}$ is the last unknown !

$$\frac{\psi_{N-1}^{j+1} - \psi_{N-1}^{j}}{\Delta t} = \frac{1}{C_{N-1}^{j}\Delta z}\left[k_{N-1\frac{1}{2}}^{j}\left(\frac{\psi_{N-2}^{j+1} - \psi_{N-1}^{j+1}}{\Delta z} + 1\right) - k_{N-1\frac{1}{2}}^{j}\left(\frac{\psi_{N-1}^{j+1} - \psi_{N}}{\Delta z} + 1\right)\right] - \frac{S_{N-1}}{C_{N-1}^{j}}$$

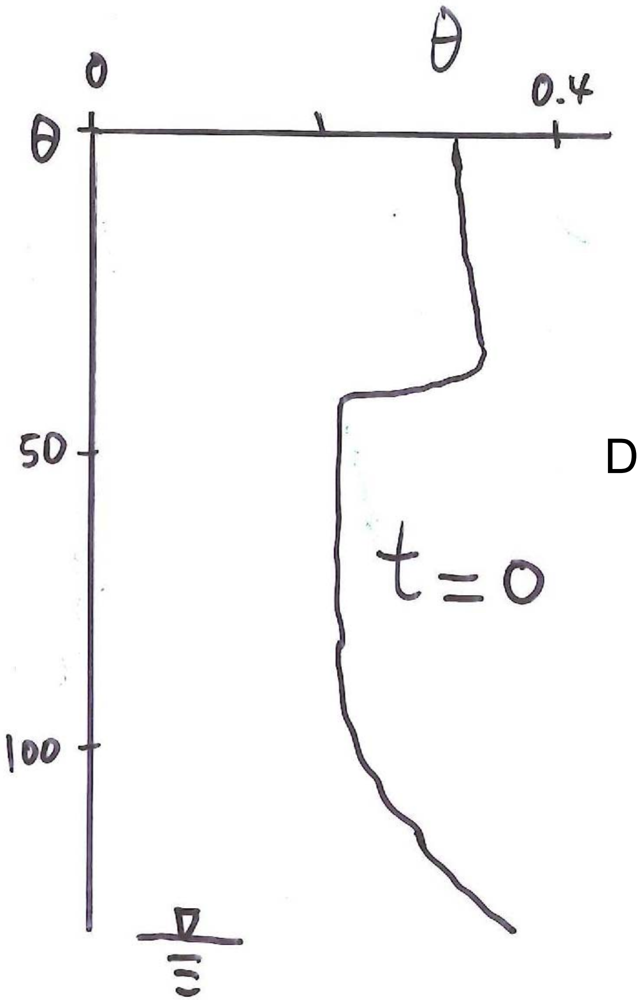
rearrange:

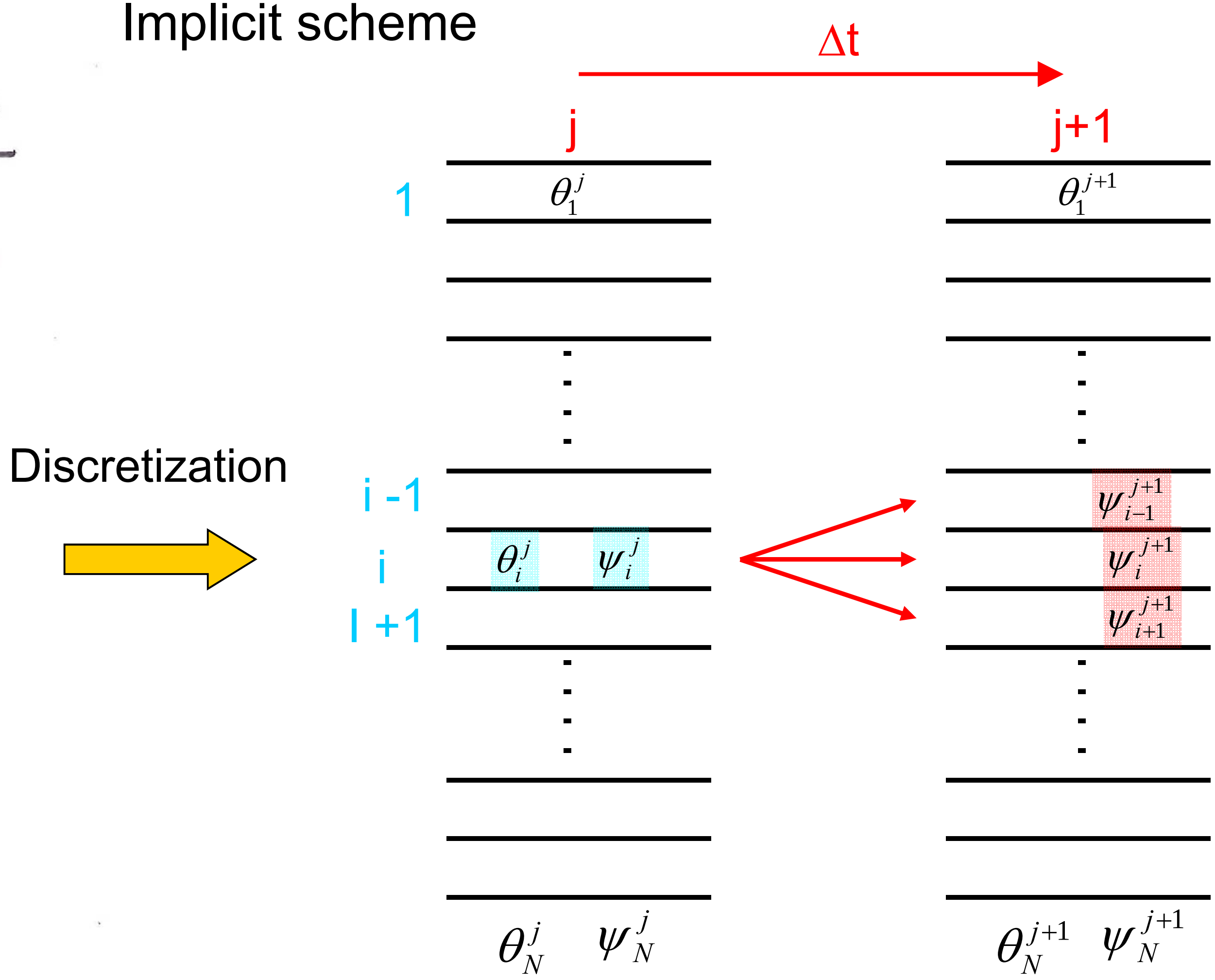
$$-\left(\frac{\Delta t \cdot k_{N-1\frac{1}{2}}^{j}}{C_{N-1}^{j}\Delta z^{2}}\right)\psi_{N-2}^{j+1} + \left(1 + \frac{\Delta t \cdot k_{N-1\frac{1}{2}}^{j}}{C_{N-1}^{j}\Delta z^{2}} + \frac{\Delta t \cdot k_{N-1\frac{1}{2}}^{j}}{C_{N-1}^{j}\Delta z^{2}}\right)\psi_{N-1}^{j+1} = \psi_{N-1}^{j} + \left(\frac{\Delta t \cdot k_{N-\frac{1}{2}}^{j}}{C_{N-1}^{j}\Delta z^{2}}\right)\psi_{N}$$

$$+ \frac{\Delta t}{C_{N-1}^{j}\Delta z}\left(k_{N-1\frac{1}{2}}^{j} - k_{N-1\frac{1}{2}}^{j}\right) - \frac{S_{N-1}\Delta t}{C_{N-1}^{j}}$$

$$\Rightarrow -A_{N-1}\psi_{N-2}^{j+1} + B_{N-1}\psi_{N-1}^{j+1} = D_{N-1}$$

# Numerical Model:
# Implicit scheme




Initial conditions:
- θ(z,t=0)
- ψ(z,t=0)

Boundary conditions:

$z = 0$ and $t \geq 0$ : Rainfall N and Evaporation $E_a$

$z > 0$ and $t \geq 0$ : root water uptake S(z,t)

$z_N(t)$ and $t \geq 0$ : e.g. given water table depth $z_N(t)$

## Solving systems of linear equations:

$$\frac{\psi_i^{j+1}-\psi_i^j}{\Delta t}=\frac{1}{C_i^j\Delta t}\left\{k_{i-\frac{1}{2}}^j\left(\frac{\psi_{i-1}^{j+1}-\psi_i^{j+1}}{\Delta z}+1\right)-k_{i+\frac{1}{2}}^j\left(\frac{\psi_i^{j+1}-\psi_{i+1}^{j+1}}{\Delta z}+1\right)\right\}$$

1. Iterative Methods:
   e.g. Gauss-Seidel iteration scheme

$$-A_i\psi_{i-1}^{j+1}+B_i\psi_i^{j+1}-C_i\psi_{i+1}^{j+1}=D_i$$

General iteration eq. :

$$\left[\psi_i^{j+1}\right]^{m+1}=\frac{A_i}{B_i}\left[\psi_{i-1}^{j+1}\right]^{m+1}+\frac{C_i}{B_i}\left[\psi_{i+1}^{j+1}\right]^{m}+\frac{D_i}{B_i}$$

m, m+1 = m$^{th}$ and (m+1)$^{th}$ approximation of $\psi_i^{j+1}$

if $\left|\left[\psi_i^{j+1}\right]^{m+1}-\left[\psi_i^{j+1}\right]^{m}\right|<\varepsilon$ is satisfied for all i = 1, 2, …, n

⇓

sufficient approximation

1. node:

$$+B_1\psi_1^{j+1} - C_1\psi_2^{j+1} = D_1$$

$$(\psi_1^{j+1})^{m+1} = (\frac{C_1}{\mathrm{B}_1}(\psi_2^{j+1})^m + \frac{D_1}{\mathrm{B}_1})$$

1. Iteration m=1:

$$[\psi_1^{j+1}]^2 = (\frac{C_1}{\mathrm{B}_1}[\psi_2^{j+1}]^1 + \frac{D_1}{\mathrm{B}_1})$$

2 – (N-1) nodes

$$-A_i\psi_{i-1}^{j+1} + B_i\psi_i^{j+1} - C_i\psi_{i+1}^{j+1} = D_i$$

$$\left[\psi_i^{j+1}\right]^{m+1} = \frac{A_i}{B_i}\left[\psi_{i-1}^{j+1}\right]^{m+1} + \frac{C_i}{B_i}\left[\psi_{i+1}^{j+1}\right]^m + \frac{D_i}{B_i}$$

1. Iteration m=1:

$$\left[\psi_i^{j+1}\right]^2 = \frac{A_i}{B_i}\left[\psi_{i-1}^{j+1}\right]^2 + \frac{C_i}{B_i}\left[\psi_{i+1}^{j+1}\right]^1 + \frac{D_i}{B_i}$$

2 – (N-1) nodes

$$-A_i\psi_{i-1}^{j+1} + B_i\psi_i^{j+1} - C_i\psi_{i+1}^{j+1} = D_i$$

$$\left[\psi_i^{j+1}\right]^{m+1} = \frac{A_i}{B_i}\left[\psi_{i-1}^{j+1}\right]^{m+1} + \frac{C_i}{B_i}\left[\psi_{i+1}^{j+1}\right]^{m} + \frac{D_i}{B_i}$$

1. Iteration m= 4:

$$\left[\psi_i^{j+1}\right]^{5} = \frac{A_i}{B_i}\left[\psi_{i-1}^{j+1}\right]^{5} + \frac{C_i}{B_i}\left[\psi_{i+1}^{j+1}\right]^{4} + \frac{D_i}{B_i}$$



$$\left|\left[\psi_i^{j+1}\right]^{m+1} - \left[\psi_i^{j+1}\right]^{m}\right| < \varepsilon$$ is satisfied for all i = 1, 2, …, n

↓

sufficient approximation

2. Direct methods: e.g. Gauss elimination

If we have N-1 internal mesh points, we have the following system of linear equations:

$$+b_1u_1 - c_1u_2 = d_1 \qquad \textbf{(1)} \qquad \mathrm{u}_1 = \psi_1^{j+1}$$

$$-a_2u_1 + b_2u_2 - c_2u_3 = d_2 \qquad \textbf{(2)}$$

$$-a_iu_{i-2} + b_iu_i - c_iu_{i+1} = d_i \qquad \textbf{(i)}$$

$$-a_{N-1}u_{N-2} + b_{N-1}u_{N-1} = d_{N-1} \qquad \textbf{(N-1)}$$

- a‘s, b‘s, c‘s and d‘s are known
- elimination: u1 from eq.2
  u2 from eq.3
  etc.

Assume the following stage of elimination:

$$a_{i-1}u_{i-1} - c_{i-1}u_i = S_{i-1}$$

$$-a_i u_{i-1} + b_i u_i - c_i u_{i+1} = d_i$$

Eliminating $u_{i-1}$ leads to:

$$\left(b_i - \frac{a_i c_{i-1}}{a_{i-1}}\right)u_i - c_i u_{i+1} = d_i + \frac{a_i S_{i-1}}{a_{i-1}}$$

or $\alpha_i u_i - c_i u_{i+1} = S_i$

with $\alpha_i = b_i - \frac{a_i C_{i-1}}{\alpha_{i-1}}$

and $S_i = d_i + \frac{a_i S_{i-1}}{\alpha_{i-1}}$

$$\alpha_1 = b_1$$

$$S_1 = d_1$$

The last pair of simultaneous equations are:

$$\alpha_{N-2} u_{N-2} - c_{N-2} u_{N-1} = S_{N-2}$$

and

$$-a_{N-1} u_{N-2} - b_{N-1} u_{N-1} = d_{N-1}$$

Elimination of $u_{N-2}$ leads to:

$$[b_{N-1} - \frac{a_{N-1} c_{N-2}}{\alpha_{N-2}}] u_{N-1} = d_{N-1} + \frac{a_{N-1} S_{N-2}}{\alpha_{N-2}}$$

or:

$$\alpha_{N-1} u_{N-1} = S_{N-1}$$

By backward substitution we will find the unknown $u_i$:

$$u_{N-1} = \frac{S_{N-1}}{a_{N-1}}$$

$$u_i = \frac{1}{\alpha_i}\left(S_i + c_i u_{i+1}\right) \quad \text{i=N-2, N-3,….,1}$$

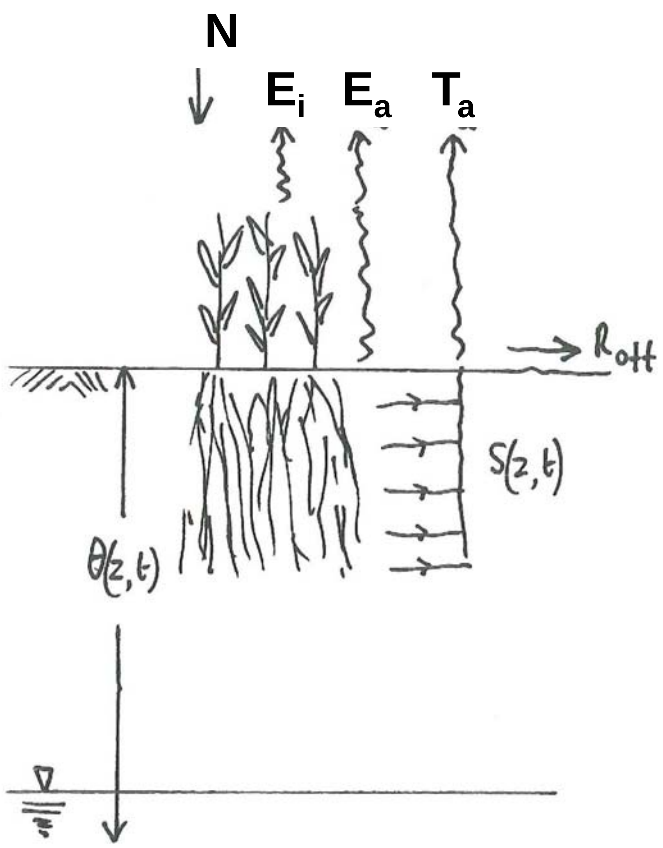
**Time-depth-curves:**

a method to visualize the vertical movement of water in the soil

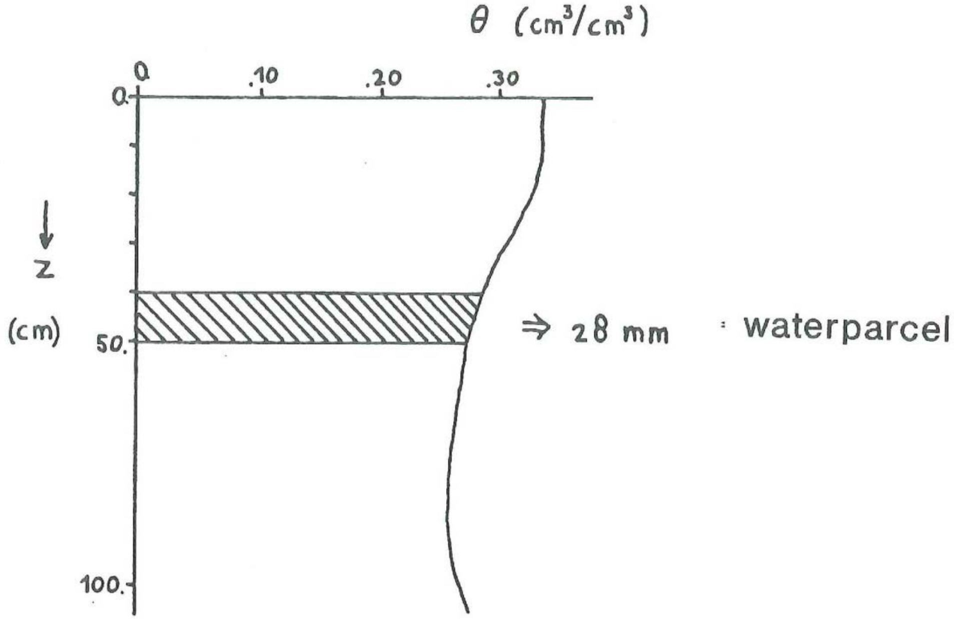
Data needed to : - generate time-depth-curves
- calculate the water balance of water-parcels between time-depth-curves

are:

- Precipitation N (cm(d)
- Interception $E_i$ (cm/d)
- actual Evaporation $E_a$(cm/d)
- root water uptake as a function of time and depth S(z,t) (cm³/cm³.d)
- volumetric water content as a function of time and depth θ(z,t) (cm³/cm³.d)
- surface runoff $R_{off}$ (cm/d)



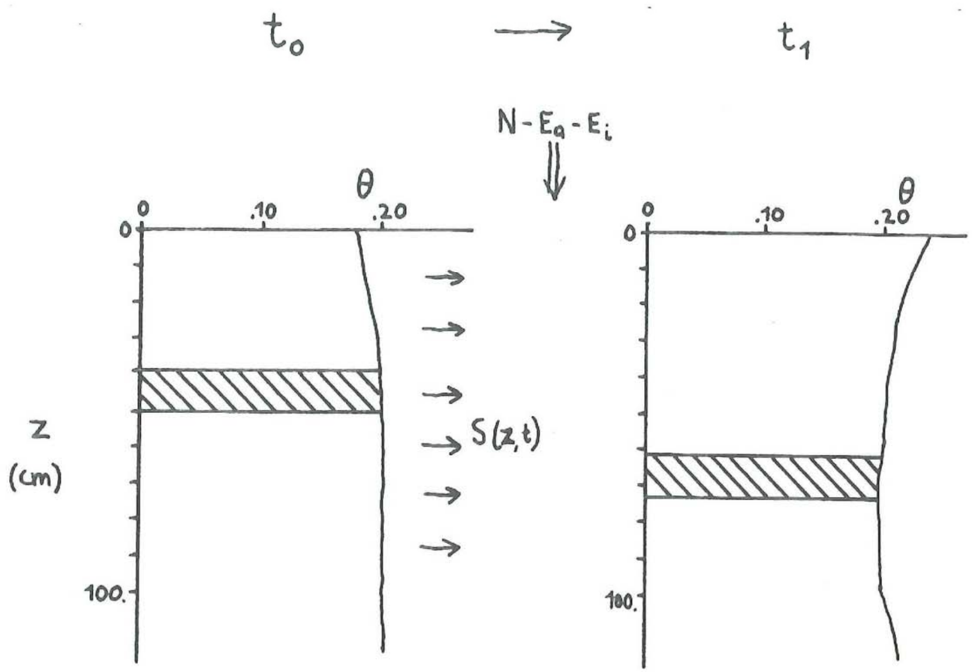
initialize waterparcels at t=0

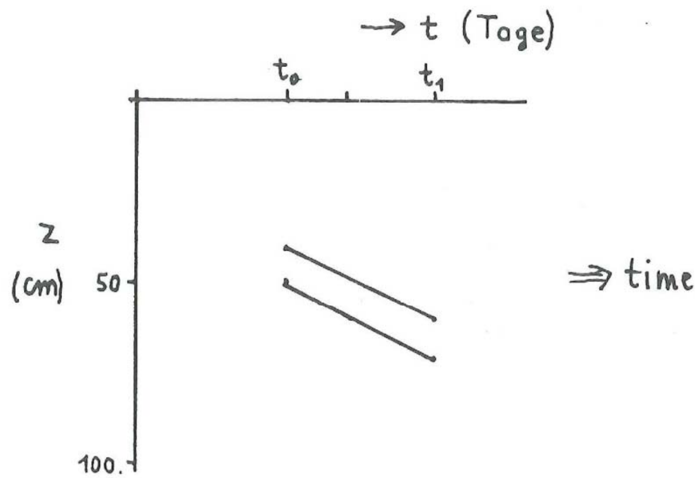



assumptions: only piston flow
no diffusion-dispersion

$$W = \int_{z1=40}^{z2=50} \theta(z,0)\, dz = 28\,\text{mm}$$

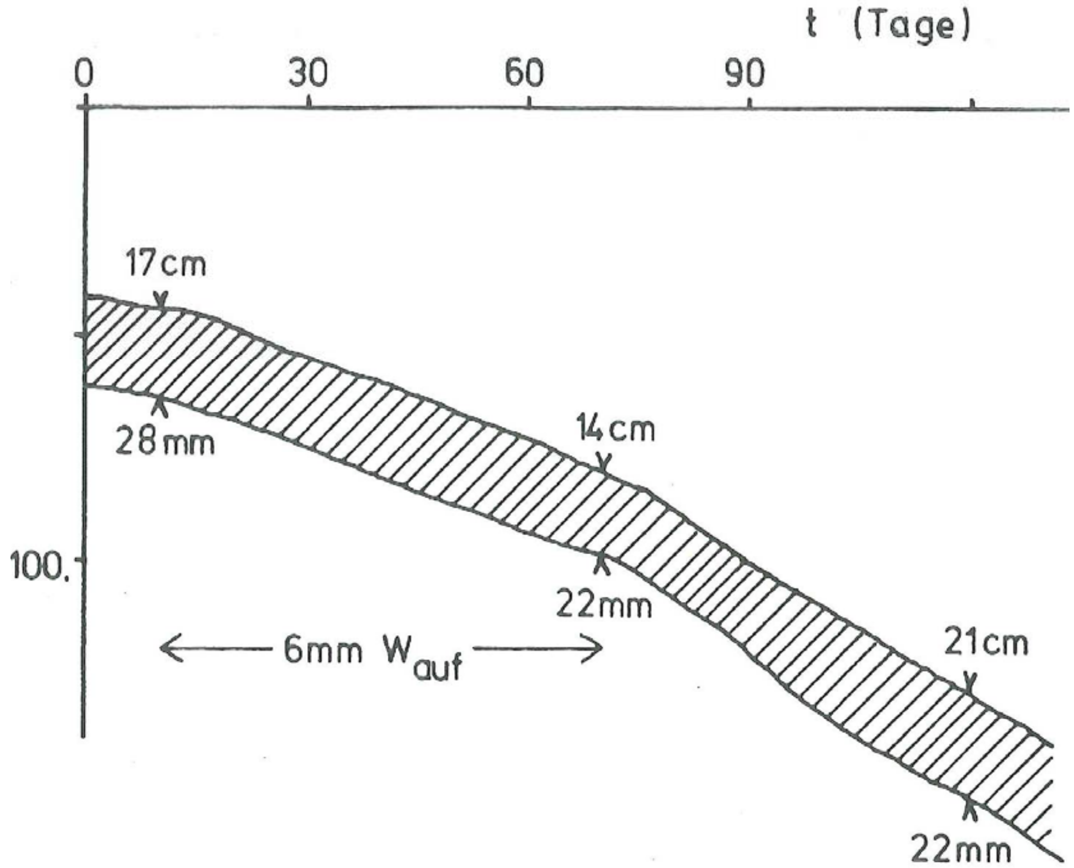
## movement of a waterparcel



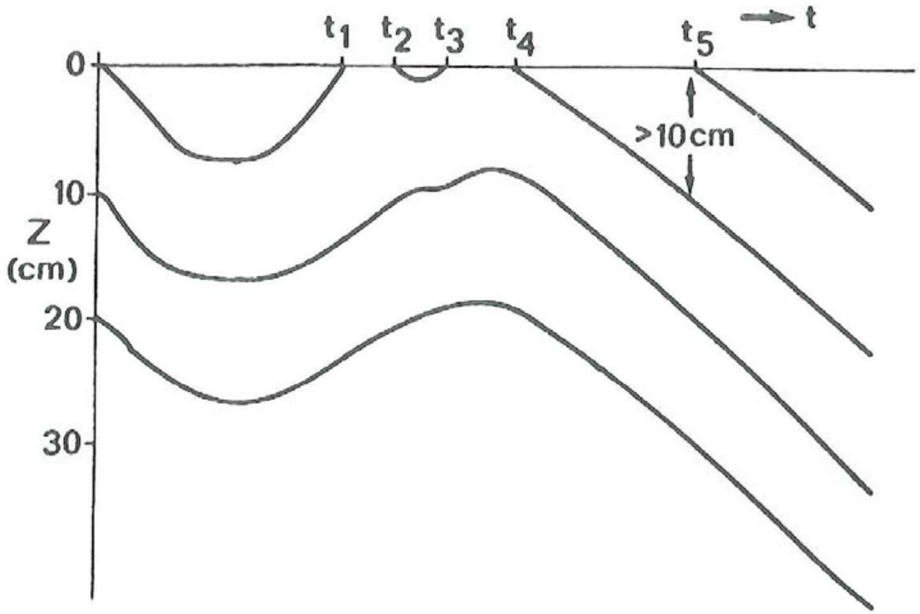




$$\int_0^{z_{t1}} \theta(z,t_1)dz = \int_0^{z_{t0}} \theta(z,t_0)\,dz + \int_{t_0}^{t_1} (N - E_a - E_i)\,dt - \int_{t_0}^{t_1} \int_0^{z_t} S(z,t)\,dz dt$$

## time-depth-curves of a waterparcel



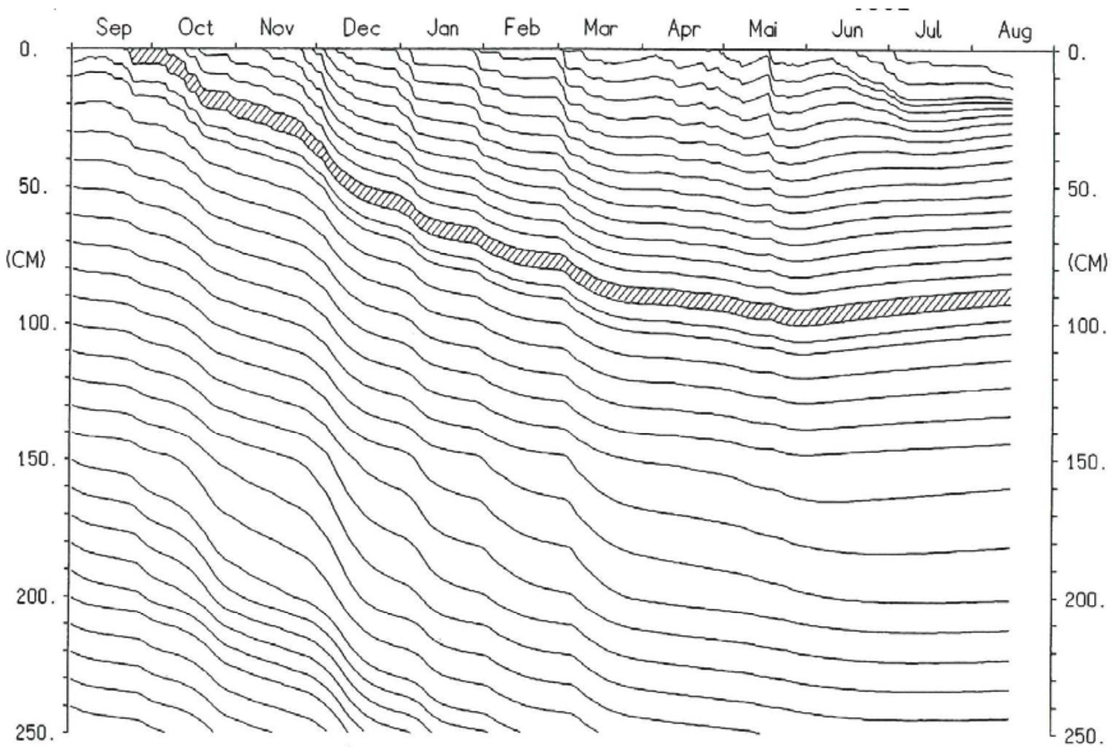
## creation of new waterparcels:




criteria: - certain dates
- amount of water in waterparcel
- thickness of the waterparcel

Time-depth-curves of:

- Loess soil
- Summer wheat crop
- GW-table at 2.5 m
- Period: Sept - Aug



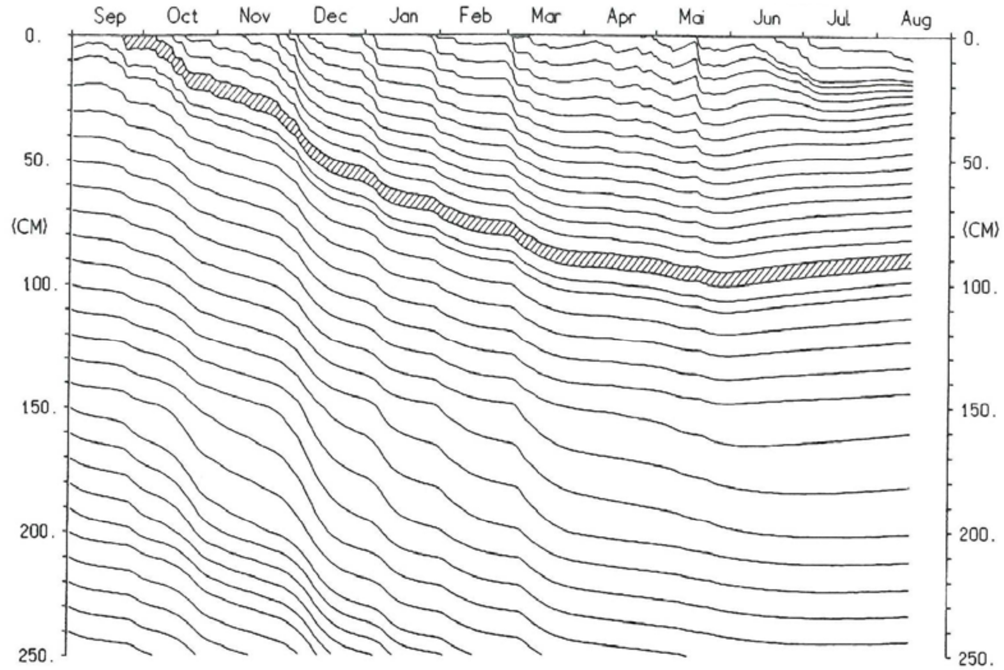

Water balance of :

B : WATER PARCELS PRESCRIBED AT THE BEGINNING OF THE SIMULATION PERIOD :

| DEPTH-RANGE(T=0) CM | W(T=0) CM | W-UPT CM | W(T=T) CM | DEPTH-RANGE(T=T) CM |
|---|---|---|---|---|
| 0.0 - 5.0 | 1.52 | 0.19 | 1.81 | 92.6 - 98.5 |
| 5.0 - 10.0 | 1.52 | 0.01 | 1.51 | 98.5 - 103.4 |
| 10.0 - 20.0 | 3.04 | 0.00 | 3.04 | 103.4 - 113.2 |
| 20.0 - 30.0 | 3.10 | 0.00 | 3.10 | 113.2 - 123.1 |
| 30.0 - 40.0 | 3.29 | 0.00 | 3.29 | 123.1 - 133.5 |
| 40.0 - 50.0 | 3.31 | 0.00 | 3.31 | 133.5 - 143.9 |
| 50.0 - 60.0 | 3.42 | 0.00 | 3.42 | 143.9 - 160.1 |
| 60.0 - 70.0 | 3.42 | 0.00 | 3.42 | 160.1 - 181.6 |

Time-depth-curves of:

- Loess soil
- Summer wheat crop
- GW-table at 2.5 m
- Period: Sept - Aug




Water balance of :

A : WATER PARCELS CREATED DURING THE SIMULATION PERIOD

| DATUM | * RAIN * CM | EI CM | EA CM | W-UPT CM | W(T=T) CM | DEPTH-RRAGE CM |
|---|---|---|---|---|---|---|
| 3. 7 205.1 - 15. 8 249.0 | 4.11 | 1.10 | 0.16 | 1.12 | 1.74 | 0.0 - 9.5 |
| 18. 6 190.8 - 3. 7 205.1 | 3.44 | 0.85 | 0.19 | 1.87 | 0.53 | 9.5 - 13.7 |
| 18. 5 159.5 - 18. 6 190.8 | 5.44 | 0.67 | 1.51 | 2.79 | 0.47 | 13.7 - 17.7 |
| 29. 4 140.3 - 18. 5 159.5 | 4.69 | 0.07 | 2.44 | 2.02 | 0.16 | 17.7 - 19.0 |
| 3. 3 83.9 - 29. 4 140.3 | 6.08 | 0.00 | 4.07 | 1.77 | 0.24 | 19.0 - 21.0 |
| 1. 3 82.0 - 3. 3 83.9 | 2.11 | 0.00 | 0.11 | 1.72 | 0.28 | 21.0 - 23.5 |
| 30. 1 51.7 - 1. 3 82.0 | 2.43 | 0.00 | 0.43 | 1.68 | 0.32 | 23.5 - 26.3 |
| 26. 1 47.2 - 30. 1 51.7 | 2.10 | 0.00 | 0.10 | 1.54 | 0.46 | 26.3 - 30.4 |
| 4. 1 25.4 - 26. 1 47.2 | 2.03 | 0.00 | 0.03 | 1.48 | 0.52 | 30.4 - 34.5 |
| 24.12 14.5 - 4. 1 25.4 | 2.11 | 0.00 | 0.11 | 1.28 | 0.72 | 34.5 - 40.2 |
| 7.12 -2.0 - 24.12 14.5 | 2.08 | 0.00 | 0.08 | 1.08 | 0.92 | 40.2 - 46.4 |
| 3.12 -6.1 - 7.12 -2.0 | 2.06 | 0.00 | 0.06 | 0.91 | 1.09 | 46.4 - 52.6 |
| 29.11 -10.3 - 3.12 -6.1 | 2.04 | 0.00 | 0.04 | 0.81 | 1.19 | 52.6 - 58.3 |
| 25.11 -15.0 - 29.11 -10.3 | 2.07 | 0.00 | 0.07 | 0.75 | 1.25 | 58.3 - 63.8 |
| 11.11 -28.9 - 25.11 -15.0 | 2.31 | 0.00 | 0.31 | 0.62 | 1.38 | 63.8 - 69.6 |
| 18.10 -52.5 - 11.11 -28.9 | 2.62 | 0.00 | 0.62 | 0.41 | 1.59 | 69.6 - 75.6 |
| 13.10 -57.5 - 18.10 -52.5 | 2.17 | 0.00 | 0.17 | 0.37 | 1.63 | 75.6 - 81.5 |
| 6.10 -64.7 - 13.10 -57.5 | 2.51 | 0.00 | 0.51 | 0.33 | 1.67 | 81.5 - 86.9 |
| 20. 9 -80.1 - 6.10 -64.7 | 3.09 | 0.00 | 1.09 | 0.27 | 1.73 | 86.9 - 92.6 |
| 0. 0 0.0 - 20. 9 -80.1 | 2.17 | 0.00 | 1.69 | 0.19 | 1.81 | 92.6 - 98.5 |

## Notation for functions of several variables

Assume $u$ is a function of the independent variables $x$ and $t$. Subdivide the $x$-$t$ plane into sets of equal rectangles of sides $\delta x = h$, $\delta t = k$, as shown in Fig. 1.4, and let the co-ordinates $(x, t)$ of the representative mesh point $P$ be

$$x = ih; \quad t = jk,$$

where $i$ and $j$ are integers.

Denote the value of $u$ at $P$ by

$$u_P = u(ih, jk) = u_{i,j}.$$

Then by equation (1.4),

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_P = \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \simeq \frac{u\{(i+1)h, jk\} - 2u\{ih, jk\} + u\{(i-1)h, jk\}}{h^2}.$$

i.e.

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \simeq \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}, \qquad (1.8)$$

with a leading error of order $h^2$. Similarly,

$$\left(\frac{\partial^2 u}{\partial t^2}\right)_{i,j} \simeq \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2}, \qquad (1.9)$$

with a leading error or order $k^2$.

With this notation the forward-difference approximation for $\partial u/\partial t$ at $P$ is

$$\frac{\partial u}{\partial t} \simeq \frac{u_{i,j+1} - u_{i,j}}{k}, \qquad (1.10)$$

with a leading error of $O(k)$.

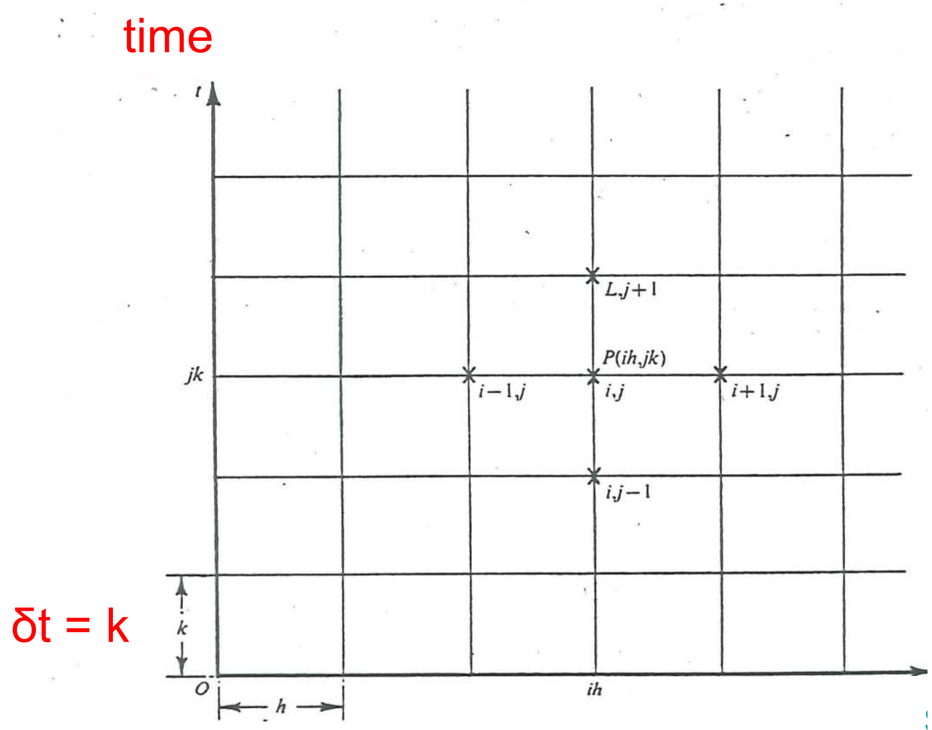



Fig. 1.4

δx = h

(Smith, 19

## Finite-difference approximations to derivatives

When a function $u$ and its derivatives are single-valued, finite and continuous functions of $x$, then by Taylor's theorem,

$$u(x+h)=u(x)+hu'(x)+\tfrac{1}{2}h^2u''(x)+\tfrac{1}{6}h^3u'''(x)+\dots \qquad (1.1)$$

and

$$u(x-h)=u(x)-hu'(x)+\tfrac{1}{2}h^2u''(x)-\tfrac{1}{6}h^3u'''(x)\dots \qquad (1.2)$$

Addition of these expansions gives

$$u(x+h)+u(x-h)=2u(x)+h^2u''(x)+O(h^4), \qquad (1.3)$$

where $O(h^4)$ denotes terms containing fourth and higher powers of $h$. Assuming these are negligible in comparison with lower powers of $h$ it follows that,

$$u''(x)=\left(\frac{d^2u}{dx^2}\right)_{x=x}\simeq\frac{1}{h^2}\{u(x+h)-2u(x)+u(x-h)\}, \qquad (1.4)$$

with a leading error on the right-hand side of order $h^2$.

Subtraction of equation (1.2) from equation (1.1) and neglect of terms of order $h^3$ leads to

$$u'(x)=\left(\frac{du}{dx}\right)_{x=x}\simeq\frac{1}{2h}\{u(x+h)-u(x-h)\}, \qquad (1.5)$$

with an error of order $h^2$.

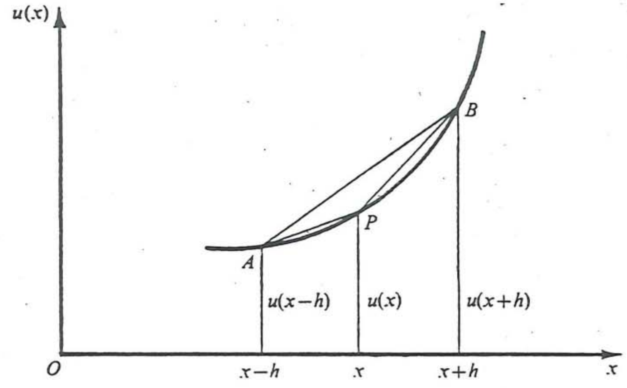



**Fig. 1.3**

Equation (1.5) clearly approximates the slope of the tange by the slope of the chord $AB$, and is called a *central-di* approximation. We can also approximate the slope of the tan $P$ by either the slope of the chord $PB$, giving the *forward-di* formula,

$$u'(x)\simeq\frac{1}{h}\{u(x+h)-u(x)\},$$

or the slope of the chord $AP$ giving the *backward-differen* mula

$$u'(x)\simeq\frac{1}{h}\{u(x)-u(x-h)\}.$$

Both (1.6) and (1.7) can be written down immediately from tions (1.1) and (1.2) respectively, assuming second and powers of $h$ are negligible. This shows that the leading er these forward and backward-difference formulae are both $O$