

The Simulation Software

PCSiWaPro®



Overview

1. Modelling in the unsaturated soil zone
2. The software PCSiWaPro®
3. The weather generator
4. Applications

Overview

1. Modelling in the unsaturated soil zone

2. The software PCSiWaPro®

3. The weather generator

4. Applications

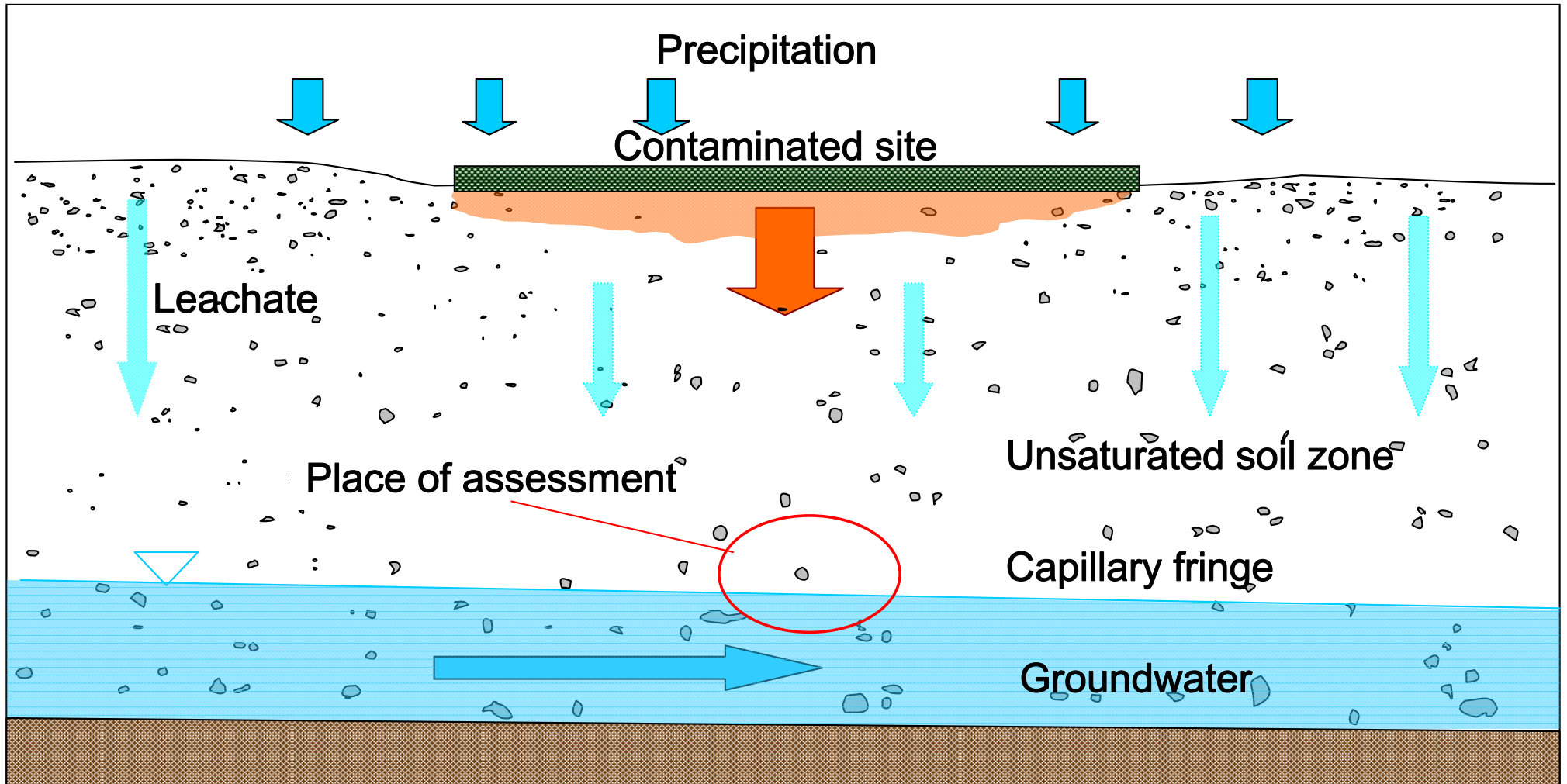
→ **Why** modelling?

- faster, less expensive than field experiments
- risk assessment, prognosis
- scenario analysis (best case/worst case, ...)
- process understanding



→ **But:** The more **processes** included in a model,
the more difficult **parameterization** becomes!

water flow, root water uptake, plant growth, preferential flow,
contaminant transport, sorption, decay, chemical reactions,
soil-surface-interaction, soil-groundwater-interaction, ...



→ Models described by **partial differential equations**:

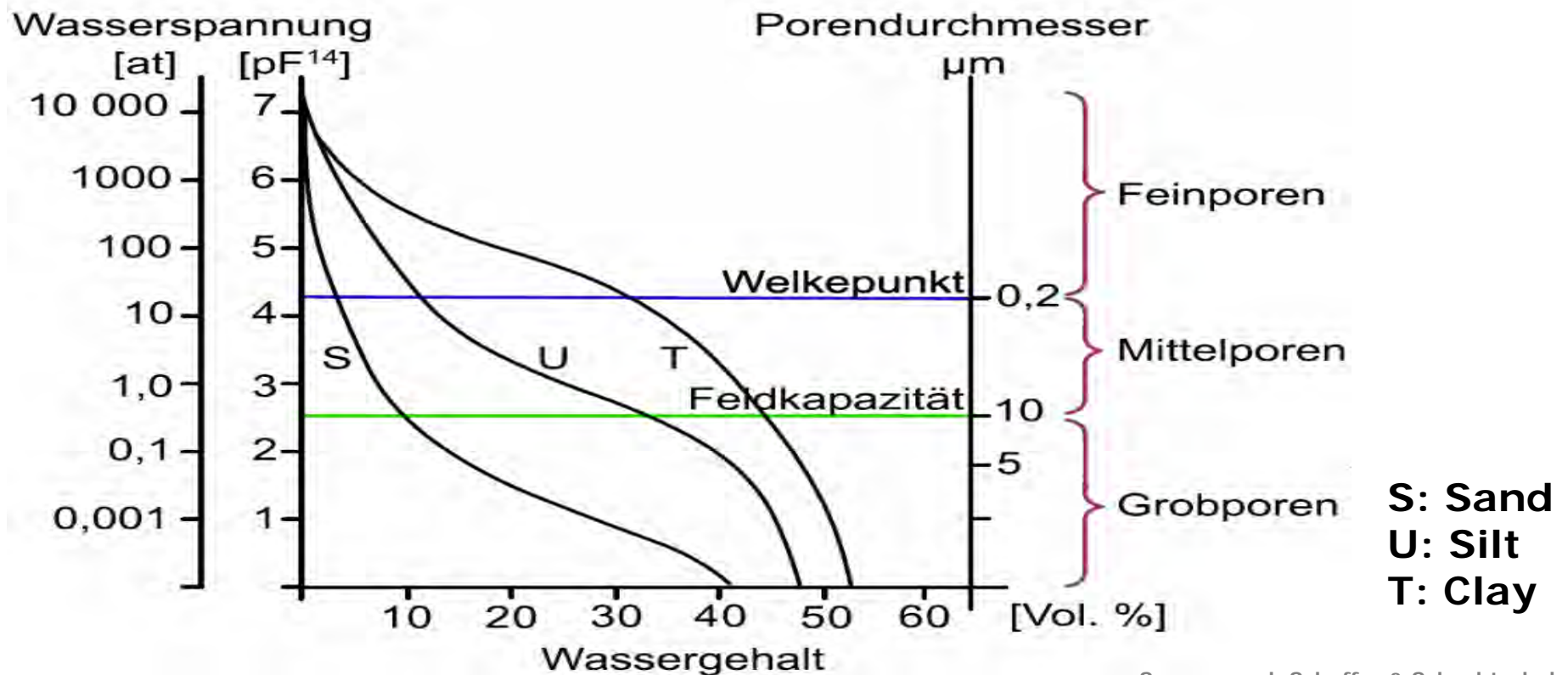
→ **Flow**: RICHARDS-Equation, retention curve parameterization
by VAN GENUCHTEN/LUCKNER

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i} \left[K \left(K_{ij}^A \frac{\partial h}{\partial x_j} + K_{iz}^A \right) \right] - S \quad \theta = \theta_r + \frac{\phi - \theta_{r,w} - \theta_{r,l}}{\left[1 + (\alpha \cdot h_c)^n \right]^{-\frac{1}{n}}}$$

θ	volumetric water content
t	time
x_i	$(x_1=x, x_2=z)$, spatial coordinates
K	hydraulic conductivity
h	pressure head
S	sink/source term

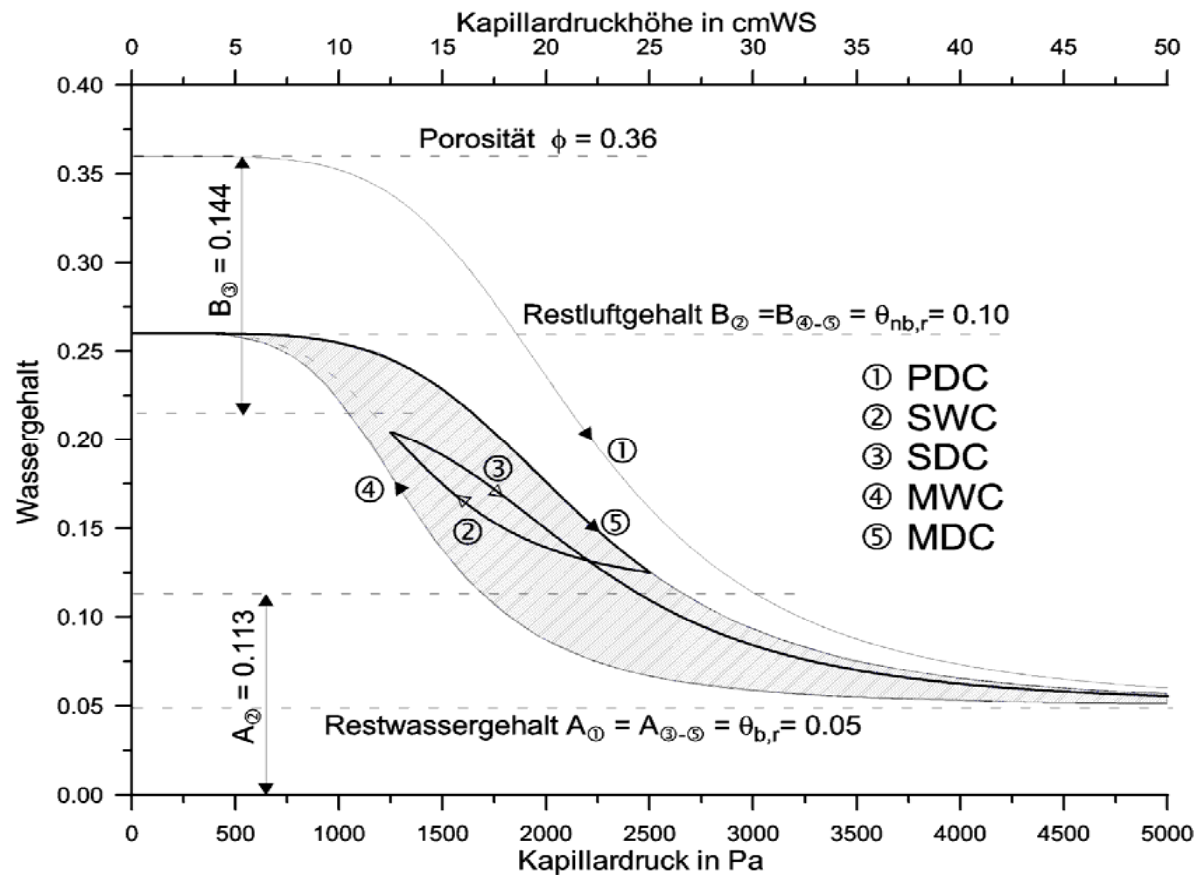
ϕ	porosity
$\theta_{r,w}$	residual water content
$\theta_{r,l}$	residual air content
α	scaling factor (van Genuchten)
n	slope factor (van Genuchten)
h_c	capillary pressure head

→ Retention curve



Source: nach Scheffer & Schachtschabel (2002):
Lehrbuch der Bodenkunde. Heidelberg.

➔ Retention curve: hysteresis



- ① Primary Drainage Curve PDC
- ② Scanning Wetting Curves SWC
- ③ Scanning Drainage Curves SDC
- ④ Main Wetting Curve MWC
- ⑤ Main Drainage Curve MDC

Source: nach Scheffer & Schachtschabel (2002):
Lehrbuch der Bodenkunde. Heidelberg.

→ Models described by **partial differential equations**:

→ **Transport**: Convection-Dispersion-Equation

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial t} = \frac{\partial}{\partial x_i} \left(\theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - S c_s$$

c	concentration	D_{ij}	tensor of dispersion coefficients
s	sorbed concentration	S	sink/source term
P	bulk density	C_s	concentration of sink/source term
t	time	Y_w, Y_s	parameters for 0 st order processes
q_i	i-th component of flux	μ_w, μ_s	parameters for 1 th order processes

→ Models described by **partial differential equations**:

→ **Transport**: Convection-Dispersion-Equation

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial t} = \frac{\partial}{\partial x_i} \left(\theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - S c_s$$

sorption

→ attachment and detachment of contaminants to **soil body**

→ described by **isotherms**

→ Sorption **isotherms**

→ **HENRY**: linear, for low concentrations

$$s_m = \theta \cdot \rho_{fl,m} + \rho_b \cdot K_d \cdot \rho_{fl,m} = (\theta + \rho_b K_d) \rho_{fl,m}$$

→ **FREUNDLICH**: exponential, for fixed number of sorption spots

$$s_m = \theta \cdot \rho_{fl,m} + K_F \cdot \rho_{fl,m}^q$$

→ **LANGMUIR**: non-linear, for high-concentrations

$$s_m = \theta \cdot \rho_{fl,m} + \frac{K_L \cdot \rho_{fl,m}}{1 + K_L \cdot \rho_{fl,m}} \cdot s_{s,max}$$

s_m – adsorbed mass on the solid phase

θ – water content, ρ_b – soil bulk density, $\rho_{fl,m}$ – partial mass density in the fluid phase

K_d – partitioning-(HENRY)-coefficient, q – constant parameter, K_F – FREUNDLICH-coefficient

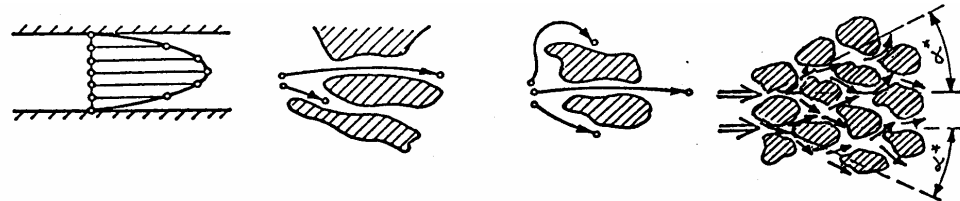
$s_{s,max}$ – max. adsorbed mass on the solid phase, K_L – LANGMUIR-coefficient

→ Models described by **partial differential equations**:

→ **Transport**: Convection-Dispersion-Equation

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial t} = \frac{\partial}{\partial x_i} \left(\theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - S c_s$$

dispersion/
diffusion



→ dispersion coupled to **convection**

→ diffusion due to **BROWNIAN** movement

→ Models described by **partial differential equations**:

→ **Transport**: Convection-Dispersion-Equation

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial t} = \frac{\partial}{\partial x_i} \left(\theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - S c_s$$

convection

→ transport with the **flow of water**

→ Models described by **partial differential equations**:

→ **Transport**: Convection-Dispersion-Equation

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial t} = \frac{\partial}{\partial x_i} \left(\theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - S c_s$$

0th/1st order internal reactions

→ **internal** production or degradation

$$\frac{ds_m}{dt} = -\mu_m \cdot S_m$$

→ example: exponential **decay**

$$S_m = S_{m,0} \cdot e^{-\mu_m \cdot t}$$

→ Models described by **partial differential equations**:

→ **Transport**: Convection-Dispersion-Equation

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial t} = \frac{\partial}{\partial x_i} \left(\theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - S c_s$$

→ contaminant concentration at model **boundary**

sink/
source

→ **source term** functions

- How to use these equations to **simulate** model behaviour
 - **input data**
 - **soil** parameters (conductivities, porosities, ...)
 - **contaminant** parameters (diffusion coefficient, half-life, ...)
 - **initial** conditions
 - steady-state or transient **boundary** conditions
 - mathematical equation **solving technique**
 - additional input data: **discretization** of the model area (space and time)

Overview

1. Modelling in the unsaturated soil zone

2. The software PCSiWaPro®

3. The weather generator

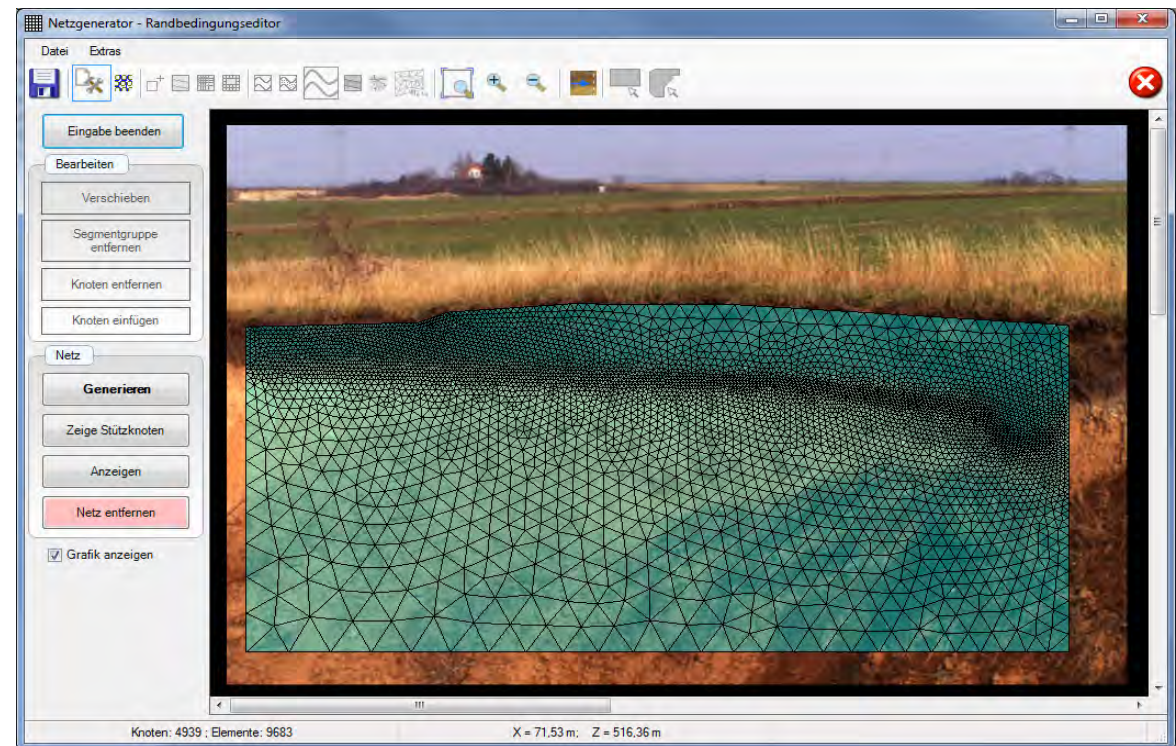
4. Applications

→ **PCSiWaPro®**: a software to **simulate** flow and transport processes in the unsaturated soil zone

(1) model **generator**

(2) system **solver**

(3) result **viewer**

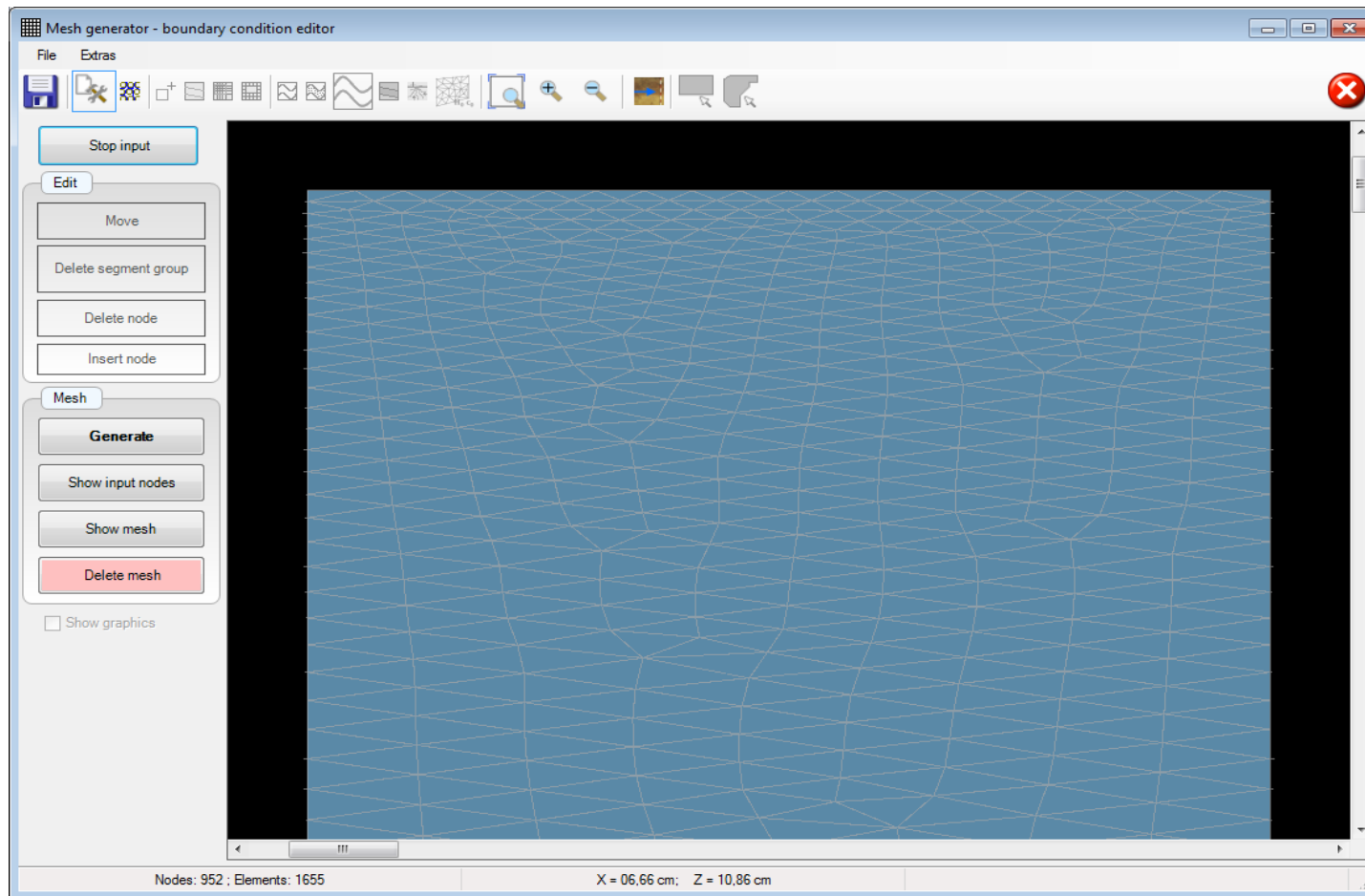


- How to use these equations to simulate model behaviour **with PCSiWaPro®**

- **input data**
 - **soil** parameters (conductivities, porosities, ...)
 - **contaminant** parameters (diffusion coefficient, half-life, ...)
 - **initial** conditions
 - steady-state or transient **boundary** conditions

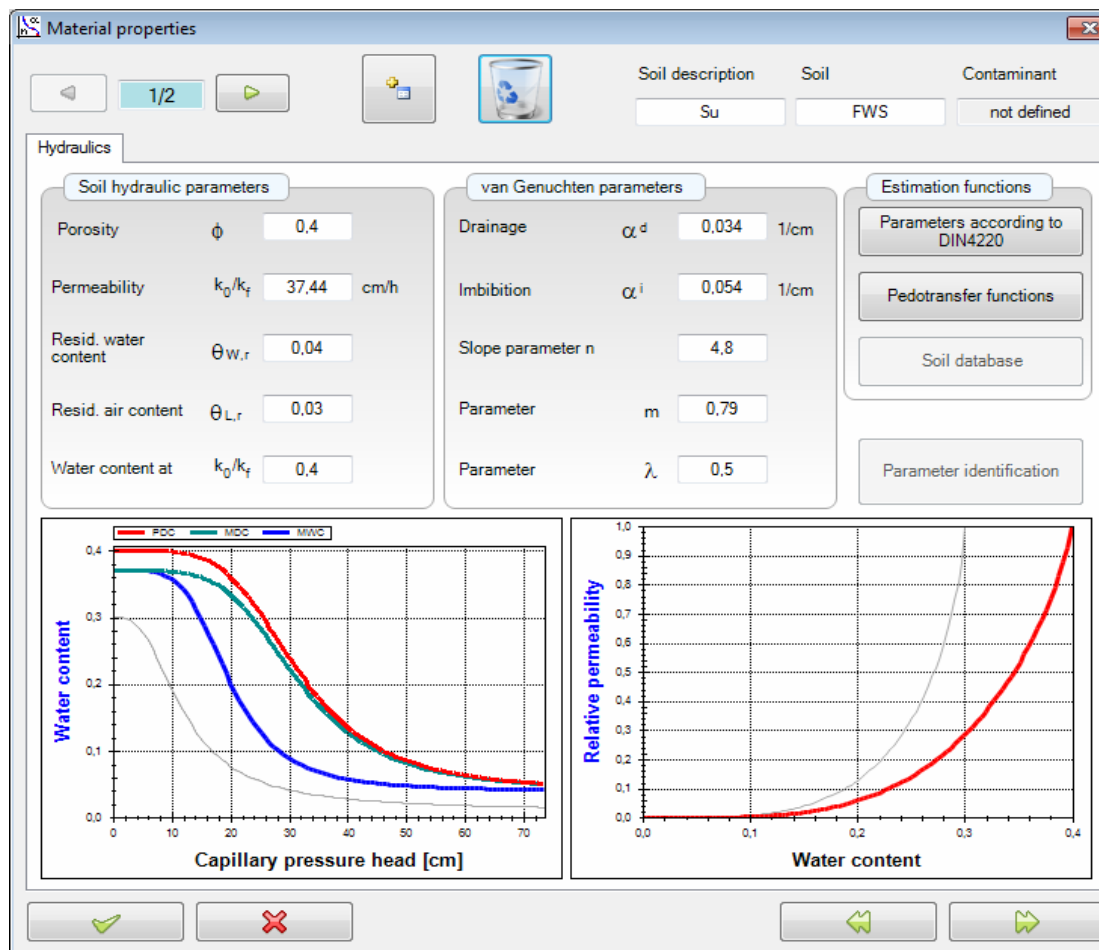
- mathematical equation **solving technique**
 - additional input data: **discretization** of the model area (space and time)

→ Integrated 1D- or 2D-mesh generator



- How to use these equations to simulate model behaviour **with PCSiWaPro®**
- **input data**
 - **soil** parameters (conductivities, porosities, ...)
 - **contaminant** parameters (diffusion coefficient, half-life, ...)
 - **initial** conditions
 - steady-state or transient **boundary** conditions
- mathematical equation **solving technique**
 - additional input data: **discretization** of the model area (space and time)

→ Data input through user-friendly **GUI**



→ **input data** from:

- (1) integrated databases
- (2) pedotransfer functions
- (3) measured data

→ selection of **model assumptions**

- sorption isotherms
- source term functions

- How to use these equations to simulate model behaviour **with PCSiWaPro®**

- **input data**
 - **soil** parameters (conductivities, porosities, ...)
 - **contaminant** parameters (diffusion coefficient, half-life, ...)
 - **initial** conditions
 - steady-state or transient **boundary** conditions

- **mathematical equation solving technique**
 - additional input data: **discretization** of the model area (space and time)

→ Equations solved by:

→ **discretization**

→ space: **finite elements**

→ time: adjusted **finite intervals**

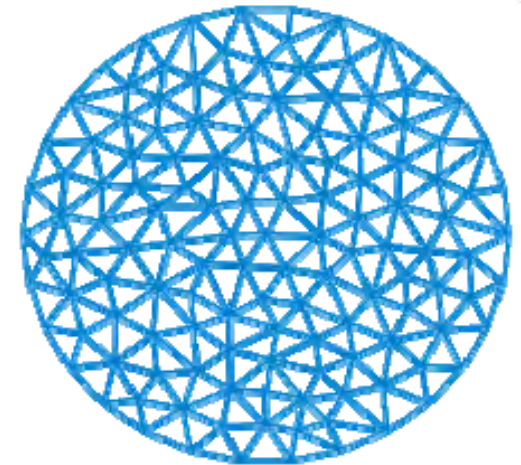
→ explicit, implicit, Crank-Nicholson

→ repeated solution of **linear equation system**
for each timestep

→ **direct**: GAUSSian elimination

→ **iterative**: preconditioned conjugate gradient method

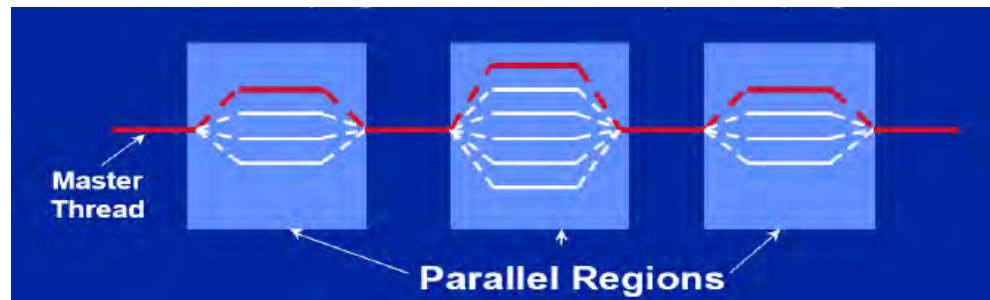
→ **Problem**: long simulation runtimes



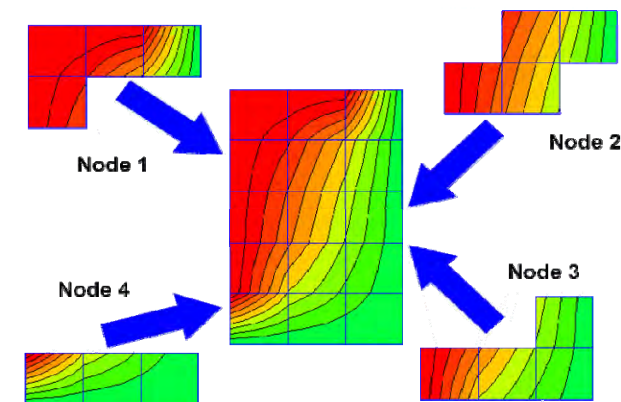
→ Current research topic: source code **parallelization**

→ dividing work into **mutually independent** parts

Incremental parallelism (OpenMP)



domain decomposition (MPI)

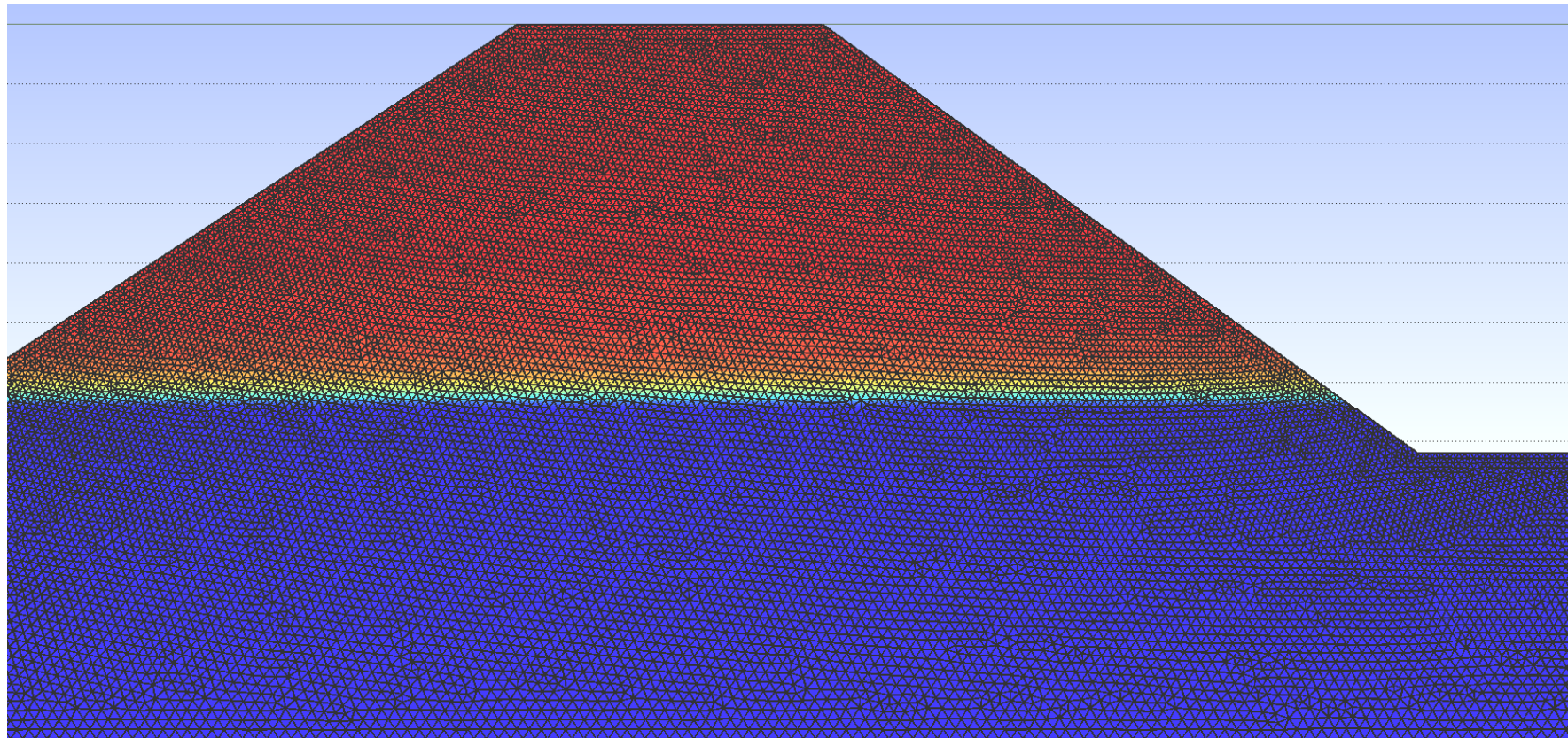


→ computationally most **expensive** tasks:

→ matrix assembly, system solver

→ integrating and testing of **parallel solver libraries**

→ **Simulation** (dam seepage example)



Overview

1. Modelling in the unsaturated soil zone

2. The software PCSiWaPro®

3. The weather generator

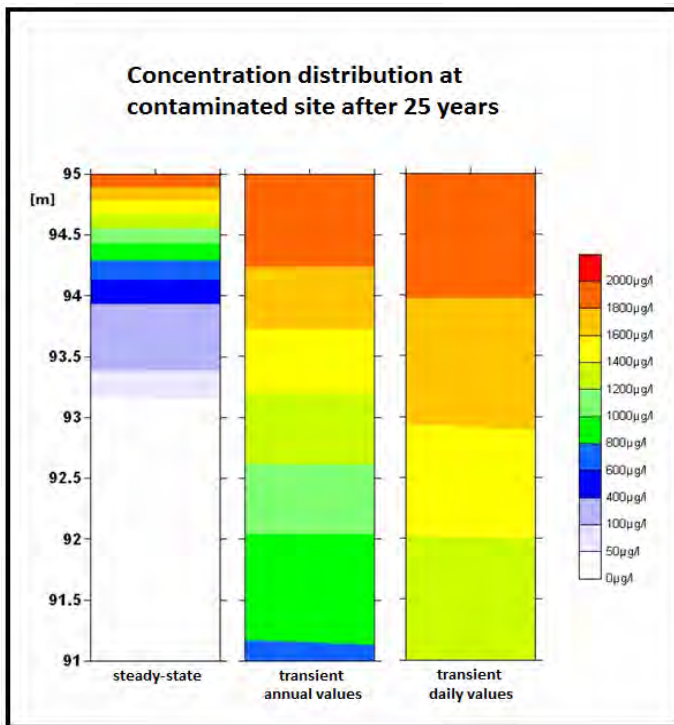
4. Applications

- How to use these equations to simulate model behaviour
with PCSiWaPro®

- **input data**
 - **soil** parameters (conductivities, porosities, ...)
 - **contaminant** parameters (diffusion coefficient, half-life, ...)
 - **initial** conditions
 - steady-state or **transient boundary conditions**

- mathematical equation **solving technique**
 - additional input data: **discretization** of the model area
(space and time)

→ Computation of upper boundary condition with the integrated **weather generator**



→ **input data**

→ precipitation

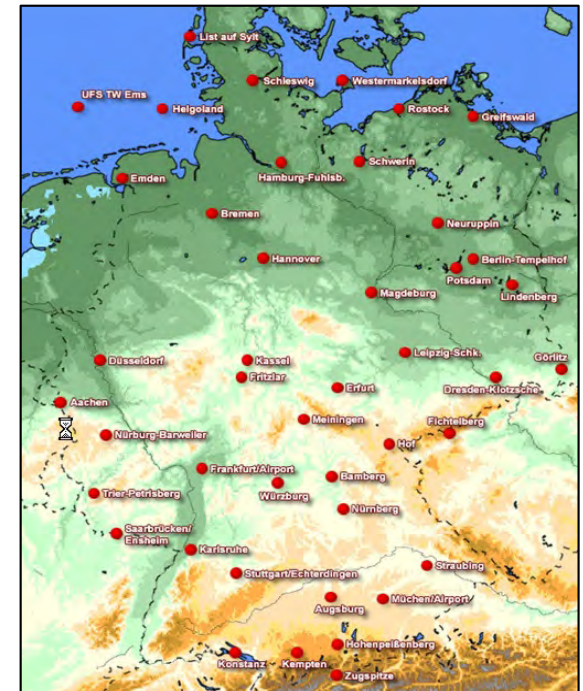
→ evapotranspiration

→ vegetation cover

→ slope

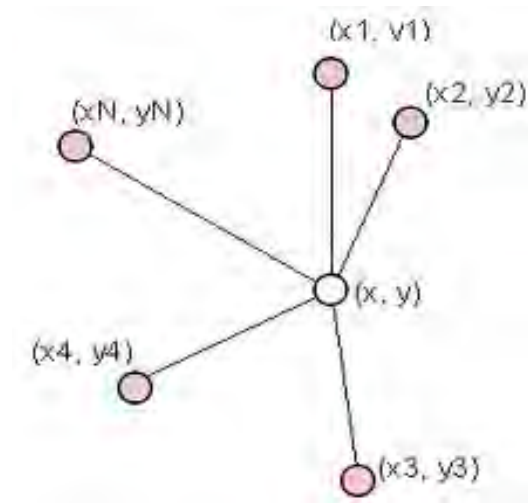
→ ...

→ output: daily values of precipitation

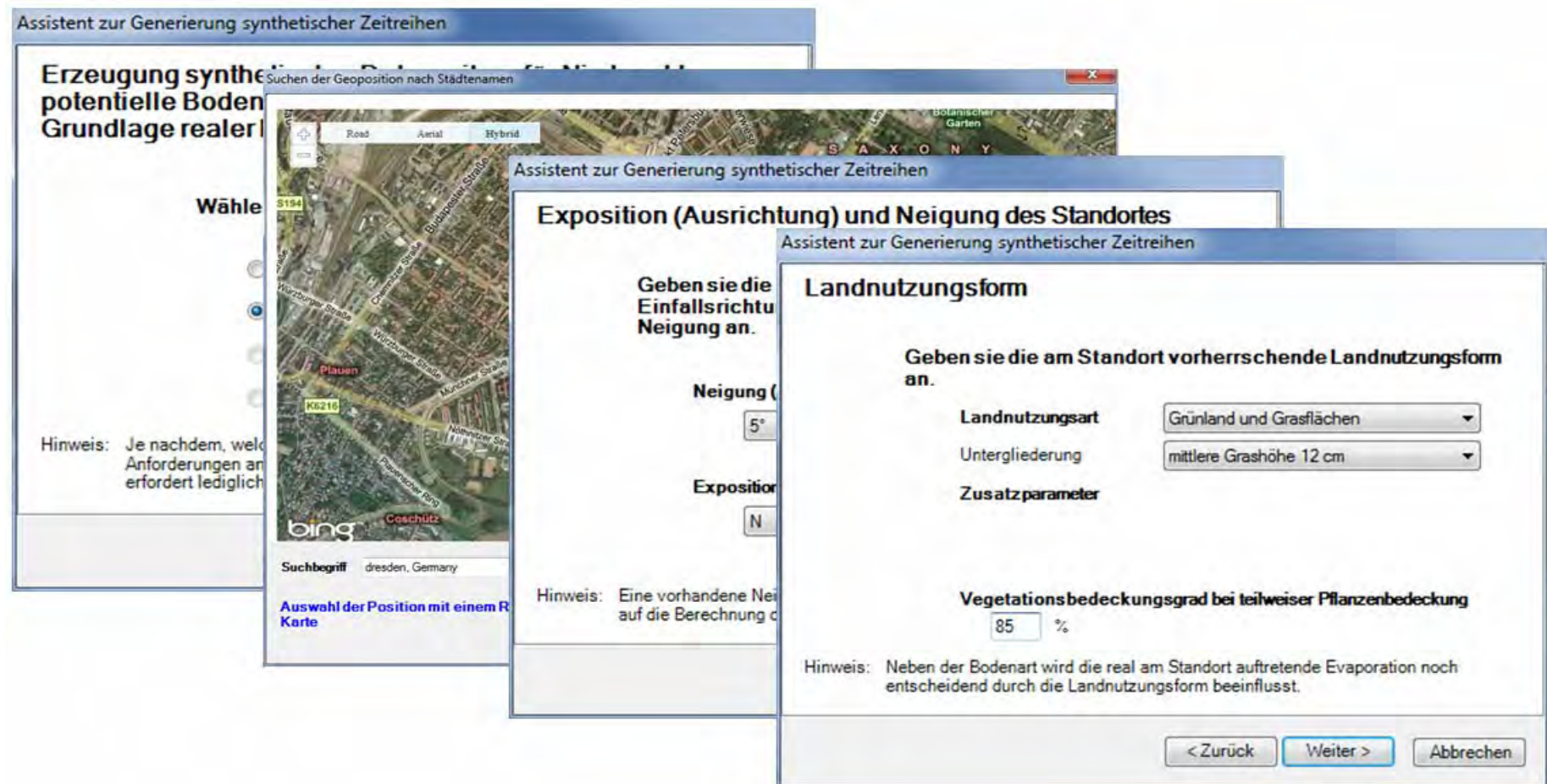


→ Time series generation by:

- (1) statistical **characterization** of input time series
- (2) spatial **interpolation** of statistical parameters
- (3) **sampling** of synthetical time series
→ past, present and **future**



➔ Data input through **assistant**

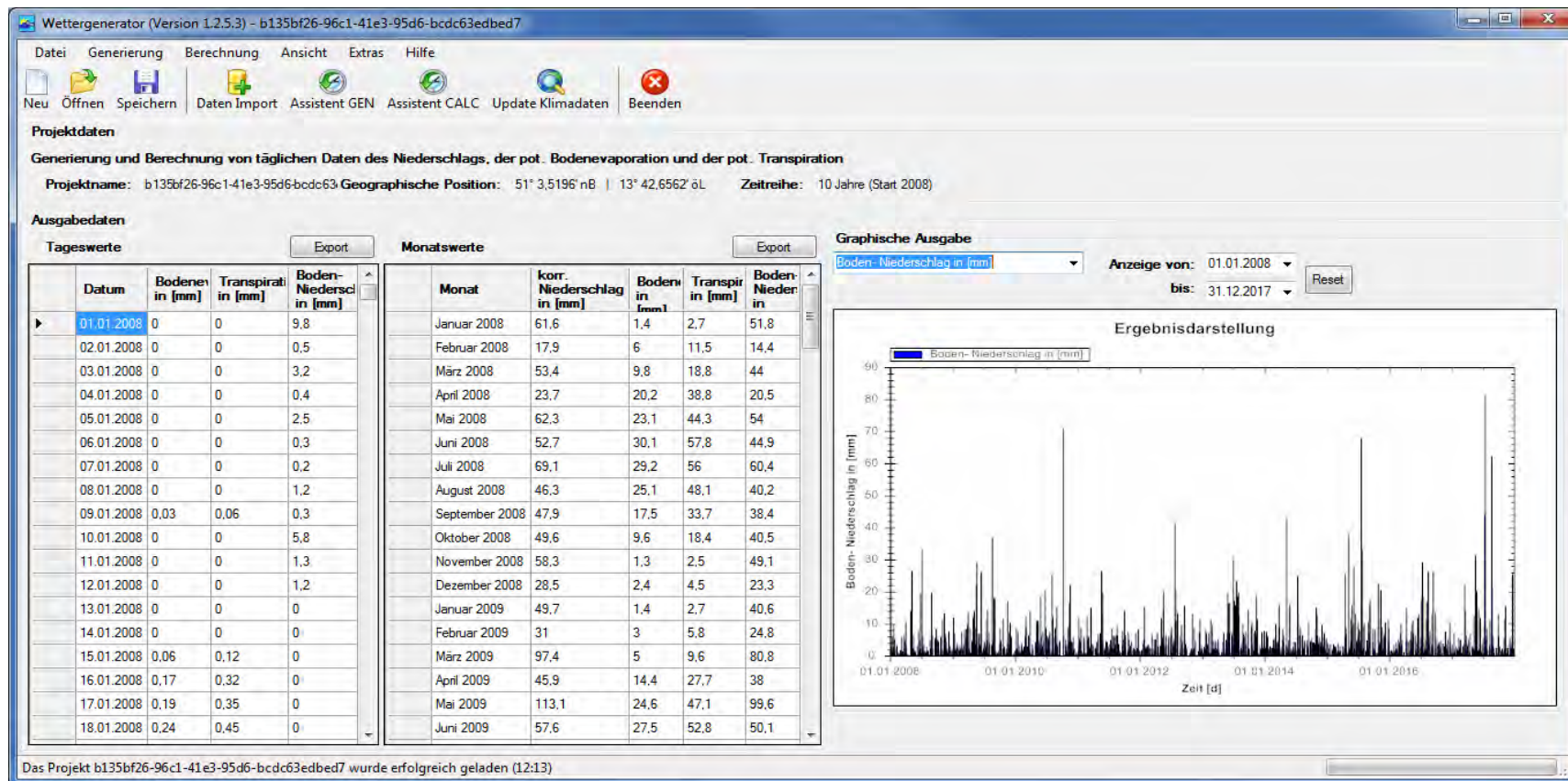


The screenshot displays the 'Assistant zur Generierung synthetischer Zeitreihen' (Assistant for the generation of synthetic time series) software interface. It consists of several overlapping windows:

- Main Window:** Titled 'Erzeugung synthetischer Zeitreihen', it includes a search bar for geolocation by city name, a 'Wähle' (Choose) button, and a hint: 'Hinweis: Je nachdem, welche Anforderungen an die synthetische Zeitreihe gestellt werden, sind unterschiedliche Eingangsparameter erforderlich lediglich'. A search term 'dresden, Germany' is visible.
- Map Window:** Shows a Bing map of Dresden, Saxony, Germany, with a search bar and map controls.
- Exposition (Ausrichtung) und Neigung des Standortes:** A window for inputting orientation and slope. It asks for 'Geben sie die Einfallrichtung an.' (Specify the orientation) and 'Neigung (Neigungswinkel) an.' (Specify the slope angle). The slope is set to 5° and the orientation to N. A hint states: 'Hinweis: Eine vorhandene Neigungswinkel auf die Berechnung der synthetischen Zeitreihe einfließen.' (Note: An existing slope angle will influence the calculation of the synthetic time series).
- Landnutzungsform (Land use type):** A window for selecting the dominant land use type at the location. It asks for 'Geben sie die am Standort vorherrschende Landnutzungsform an.' (Specify the dominant land use type at the location). The selected type is 'Grünland und Grasflächen' (Grassland and grass areas). Other options include 'Untergliederung' (Subclassification) set to 'mittlere Grashöhe 12 cm' (average grass height 12 cm) and 'Zusatzparameter' (Additional parameters). It also includes a 'Vegetationsbedeckungsgrad bei teilweiser Pflanzenbedeckung' (Vegetation cover degree at partial plant cover) set to 85%. A hint notes: 'Hinweis: Neben der Bodenart wird die real am Standort auftretende Evaporation noch entscheidend durch die Landnutzungsform beeinflusst.' (Note: In addition to soil type, the real evaporation occurring at the location is also decisively influenced by the land use type).

Navigation buttons at the bottom of the 'Landnutzungsform' window include '< Zurück' (Back), 'Weiter >' (Next), and 'Abbrechen' (Cancel).

- ➔ Graphical visualization of result **time series**
- ➔ **automatic transfer** to PCSiWaPro® model



Overview

1. Modelling in the unsaturated soil zone

2. The software PCSiWaPro®

3. The weather generator

4. Applications

→ Applications of **PCSiWaPro**® in the following fields:

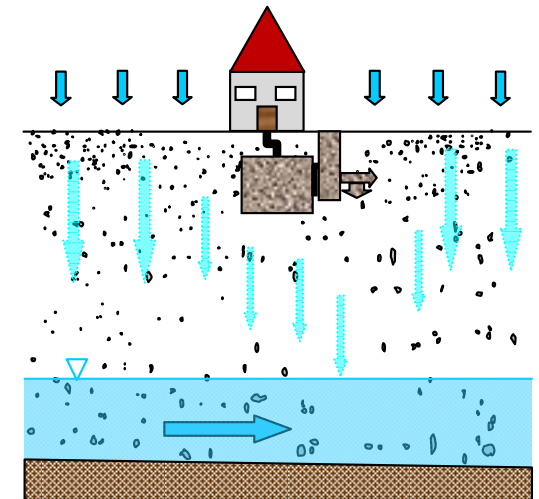
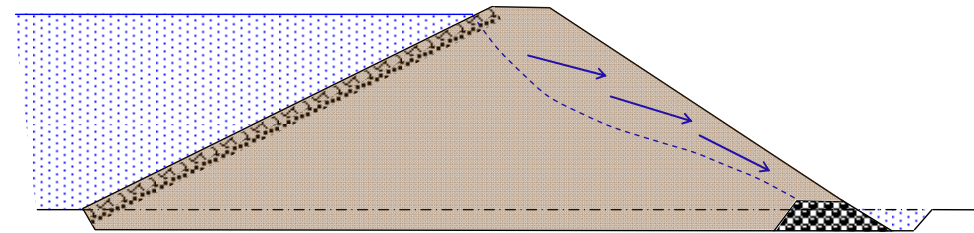
→ leachate forecast

→ earth dams

→ capillary barriers

→ landfill coverage

→ small-scale sewage treatment plants

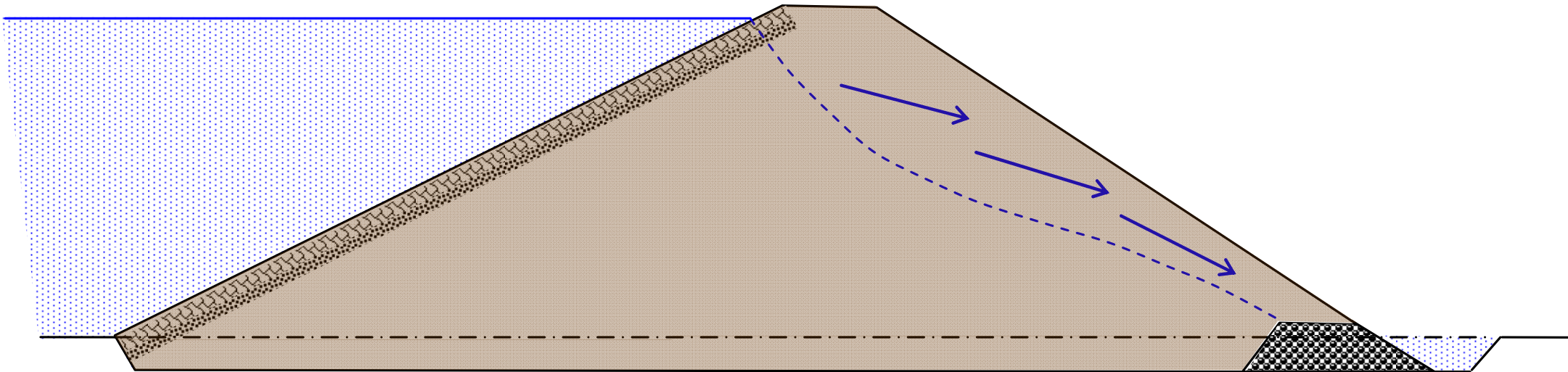


→ Completed applications with **PCSiWaPro**[®]:

→ Seepage in an **earth dam**

How long / how far will the unsaturated zone be wetted
until instabilities occur?

Influence of structural measures (drainage, blocking walls, ...)



→ Completed applications with **PCSiWaPro®**:

→ Simulation of a capillary barrier in a **tipping trough**

