TECHNISCHE UNIVERSITÄT DRESDEN

Faculty of Environmental Sciences, Institute of Waste Management and Contaminated Site Treatment

The Simulation Software

PCSiWaPro®

DRESDEN concept
Exzellenz aus Wissenschaft und Kultur

Overview

1. Modelling in the unsaturated soil zone

2. The software PCSiWaPro®

3. The weather generator

4. Applications

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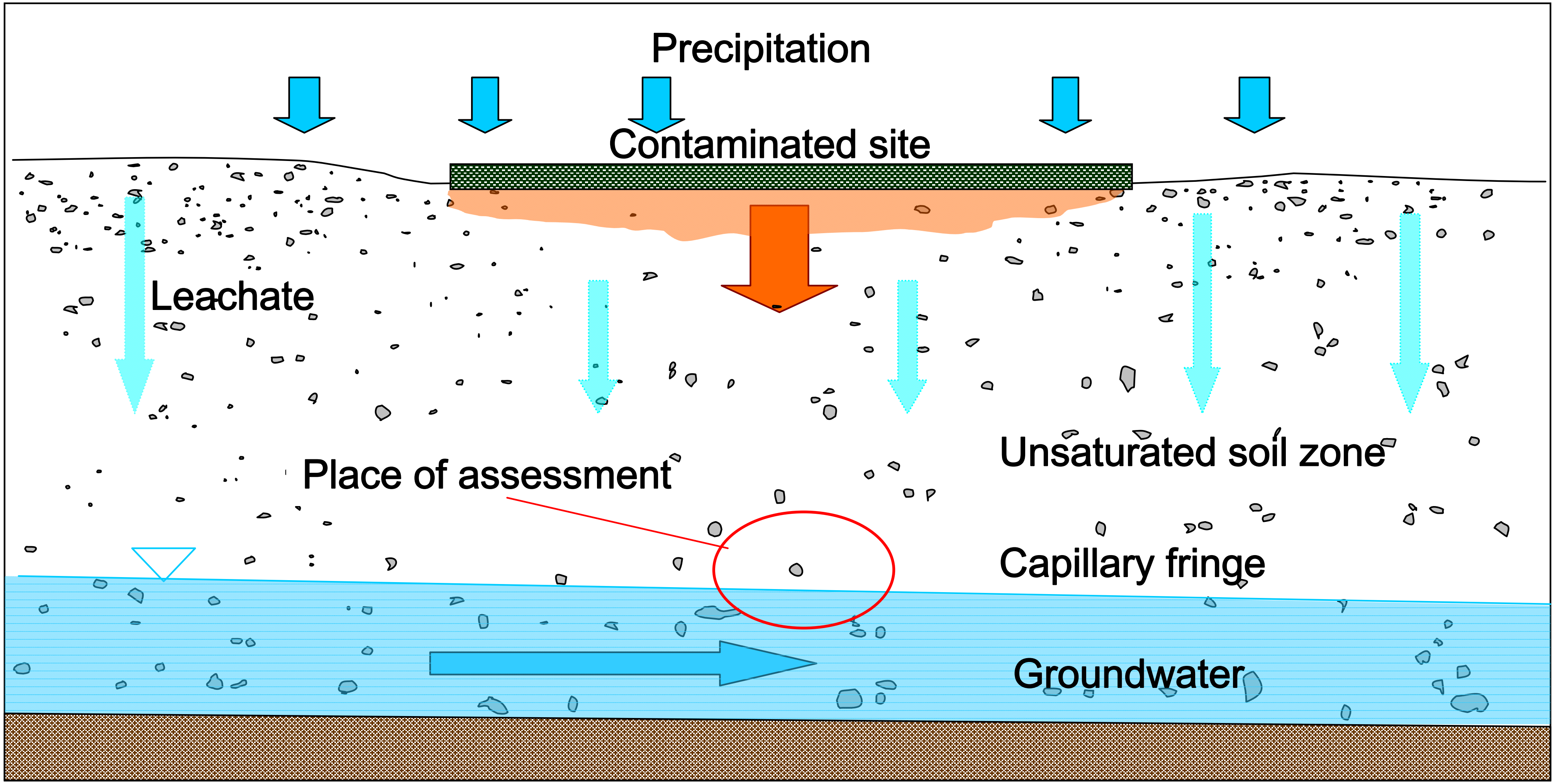
➔ **Why** modelling?

→ 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, ...


Precipitation
Contaminated site
Leachate
Place of assessment
Unsaturated soil zone
Capillary fringe
Groundwater

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

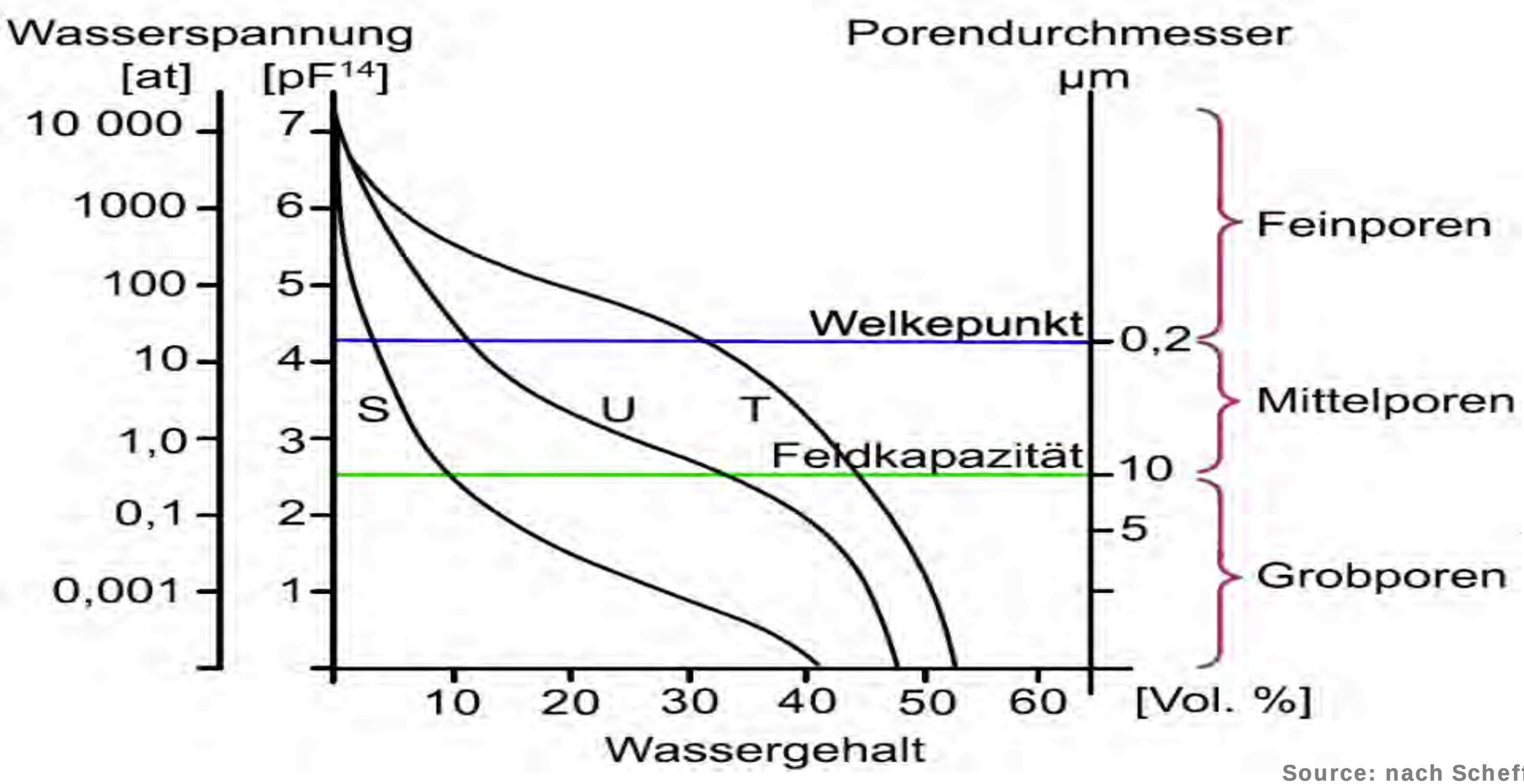
→ **Flow**: RICHARDS-Equation, retention curve parameterization by VAN GENUCHTEN/LUCKNER

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

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

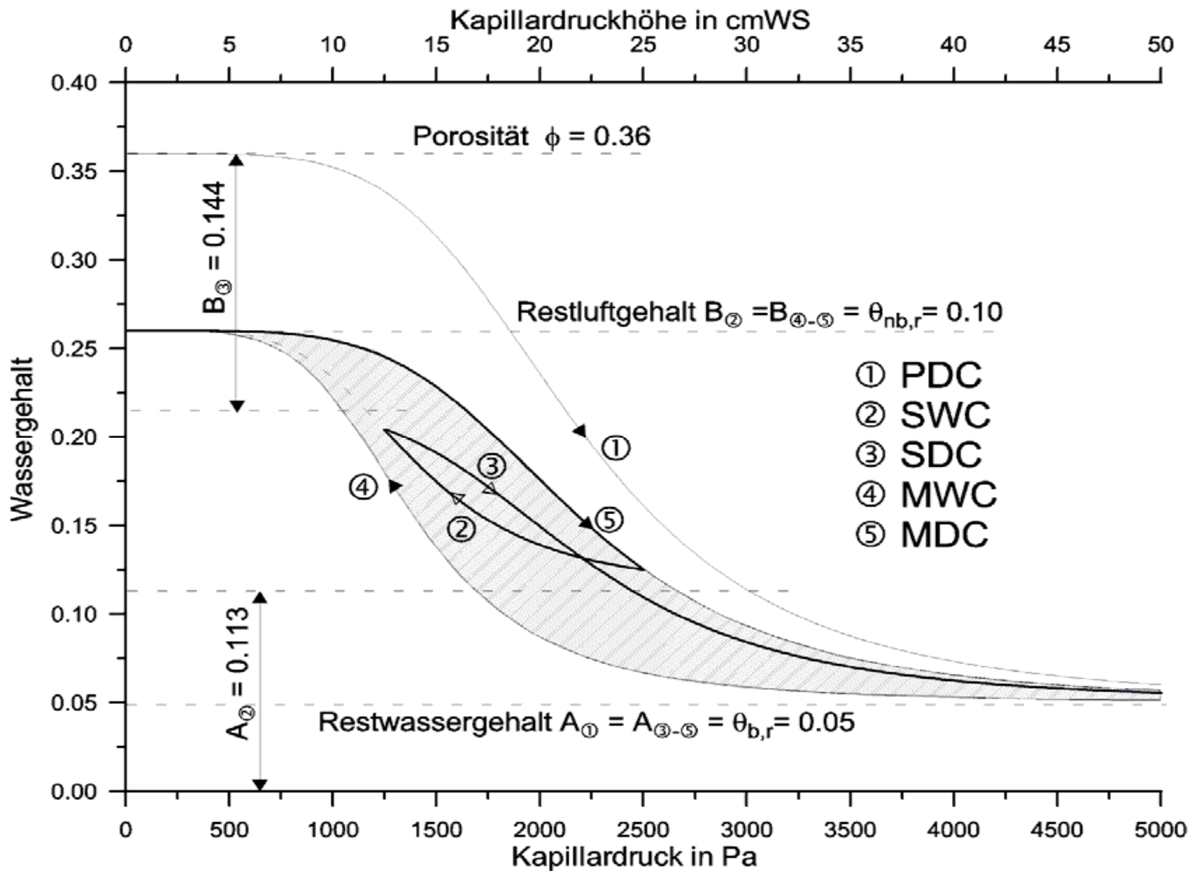
➔ Retention curve



S: Sand
U: Silt
T: Clay

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	γ_w, γ_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

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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

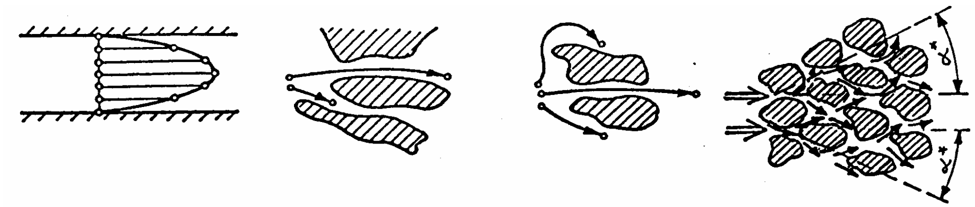
$s_{s,max}$ – max. adsorbed mass on the solid phase, K_L – LANGMUIR-coefficient

➔ 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

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convection

→ transport with the **flow of water**

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

0th/1st order internal reactions

→ **internal** production or degradation

→ example: exponential **decay**

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

$$s_m = s_{m,0} \cdot e^{-\mu_m \cdot t}$$

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

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

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sink/ source

→ contaminant concentration at model **boundary**

→ **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)

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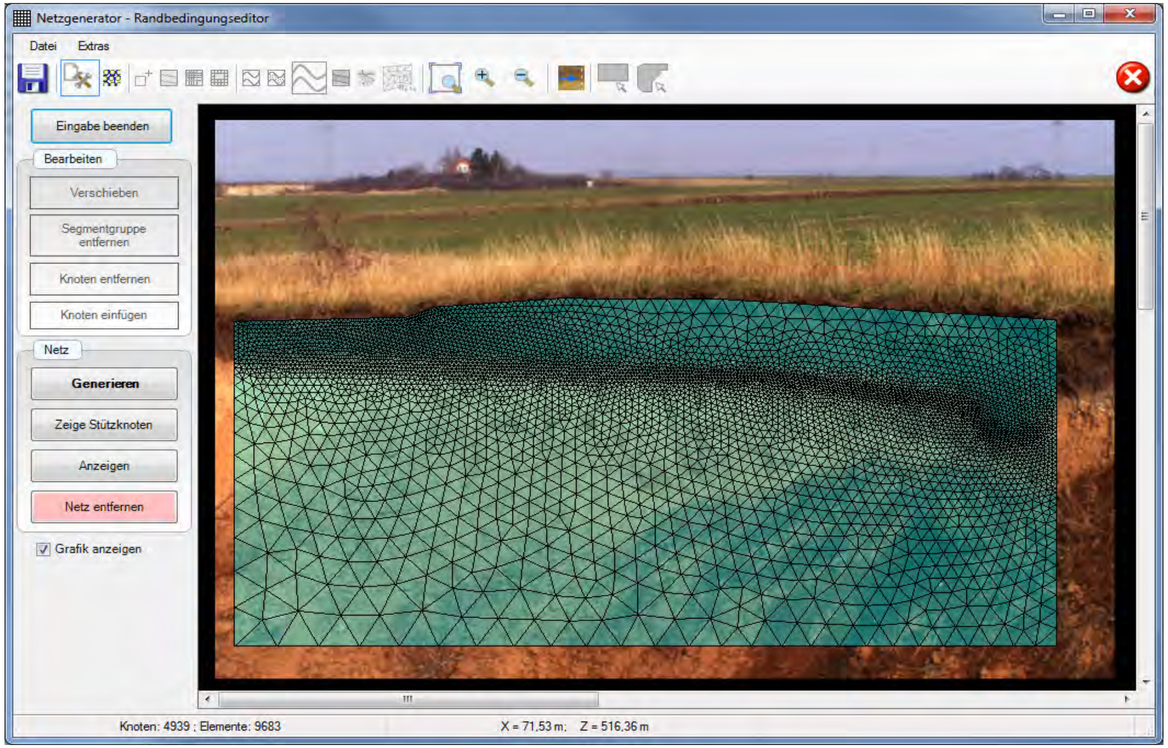
➔ **PCSiWaPro®**: a software to **simulate** flow and transport processes in the unsaturated soil zone

(1) model **generator**

(2) system **solver**

(3) result **viewer**



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

→ **input data**
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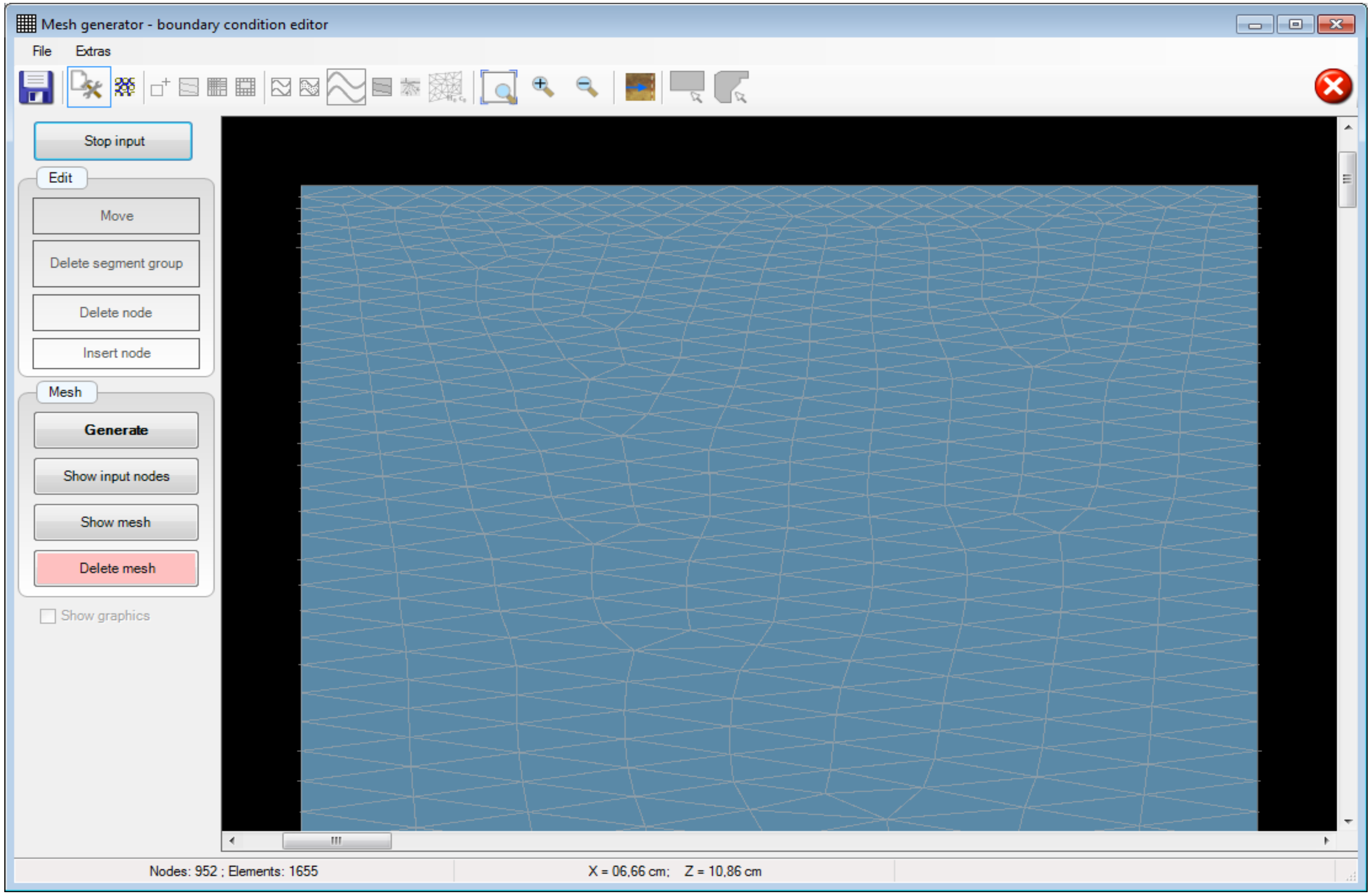
➔ Integrated 1D- or 2D-**mesh generator**



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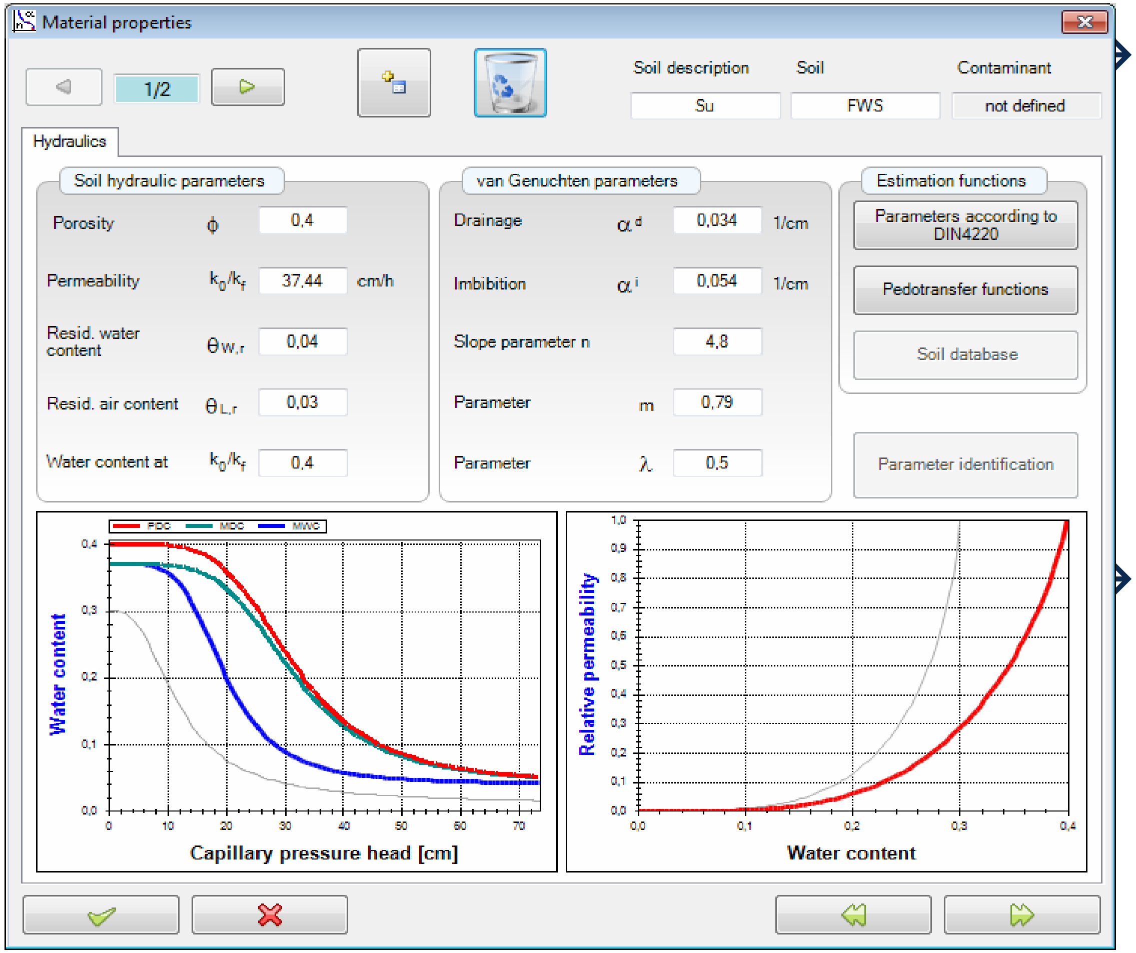
➔ Data input through user-friendly **GUI**



- **input data** from:
  - (1) integrated databases
  - (2) pedotransfer functions
  - (3) measured data

- selection of **model assumptions**
  - → sorption isotherms
  - → source term functions

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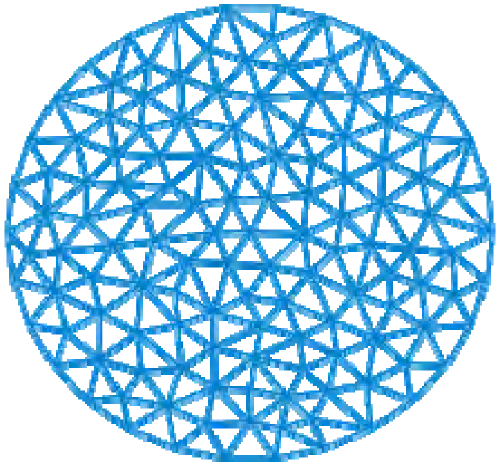
→ Equations solved by:

→ **discretization**
→ space: **finite elements**
→ time: adjusted **finite intervals**
→ explicit, implicit, Crank-Nicholson



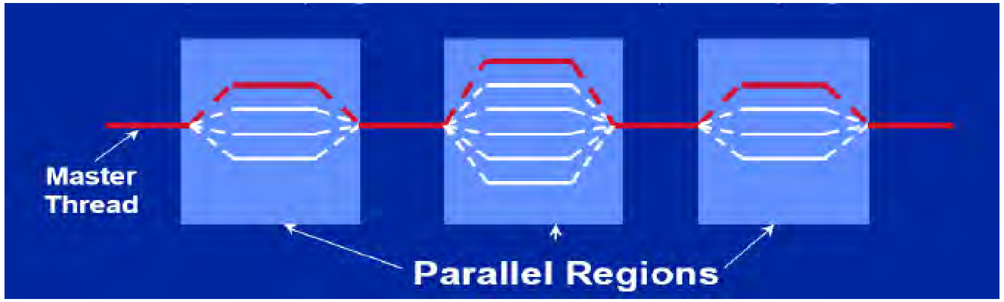
→ repeated solution of **linear equation system** for each timestep
→ **direct**: GAUSSian elimination
→ **iterative**: preconditioned conjugate gradient method

→ **Problem**: long simulation runtimes

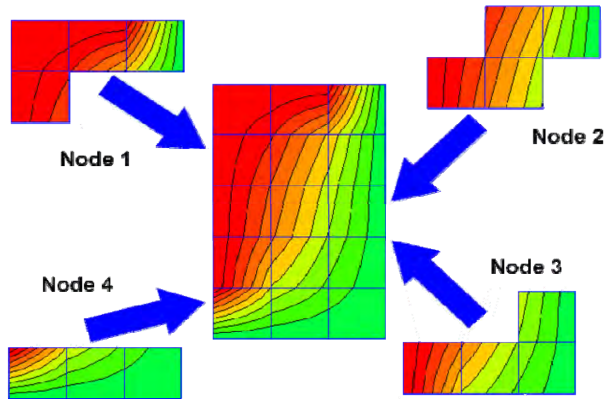
➔ Current research topic: source code **parallelization**

→ dividing work into **mutually independent** parts

Incremental parallelism (OpenMP)



domain decomposition (MPI)

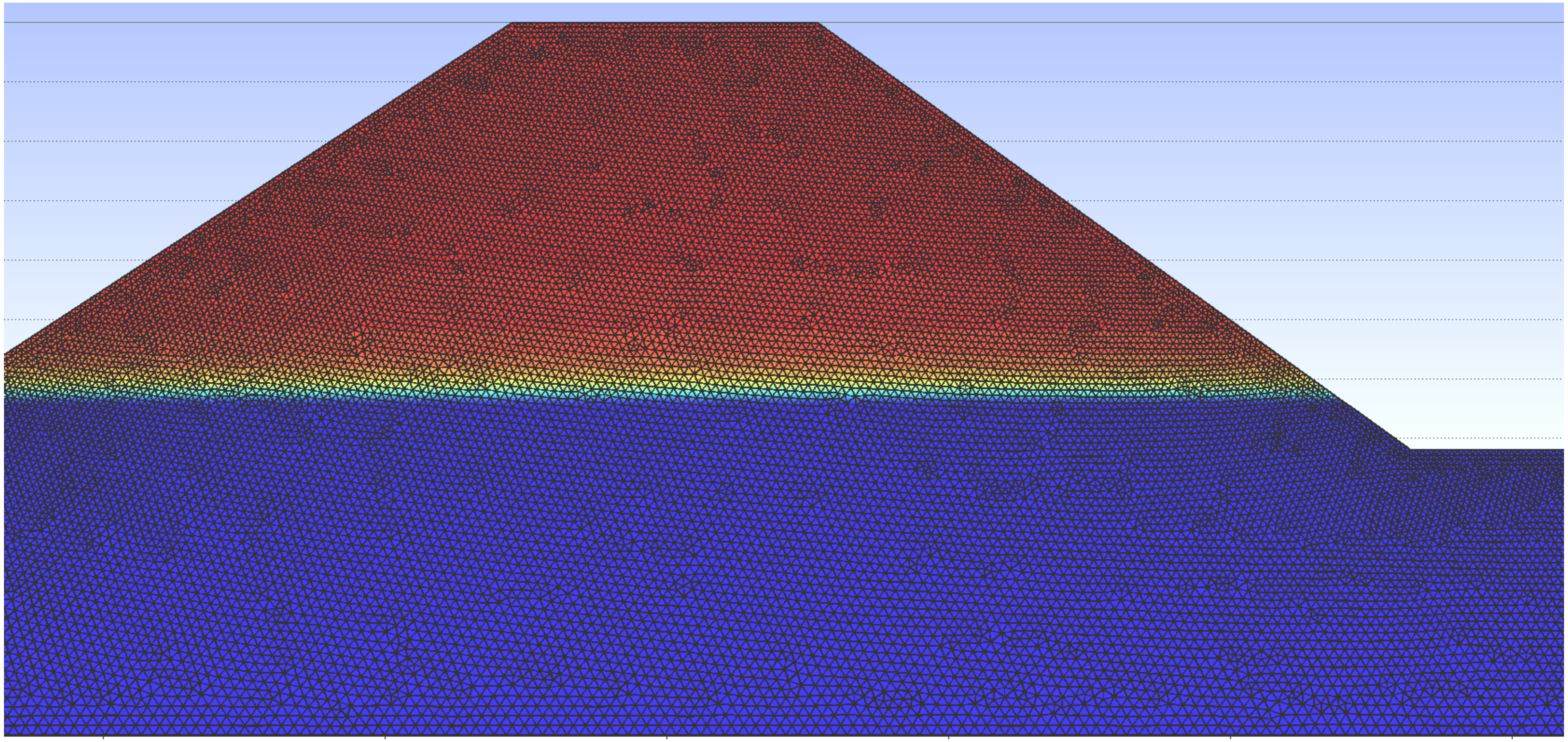


→ computationally most **expensive** tasks:

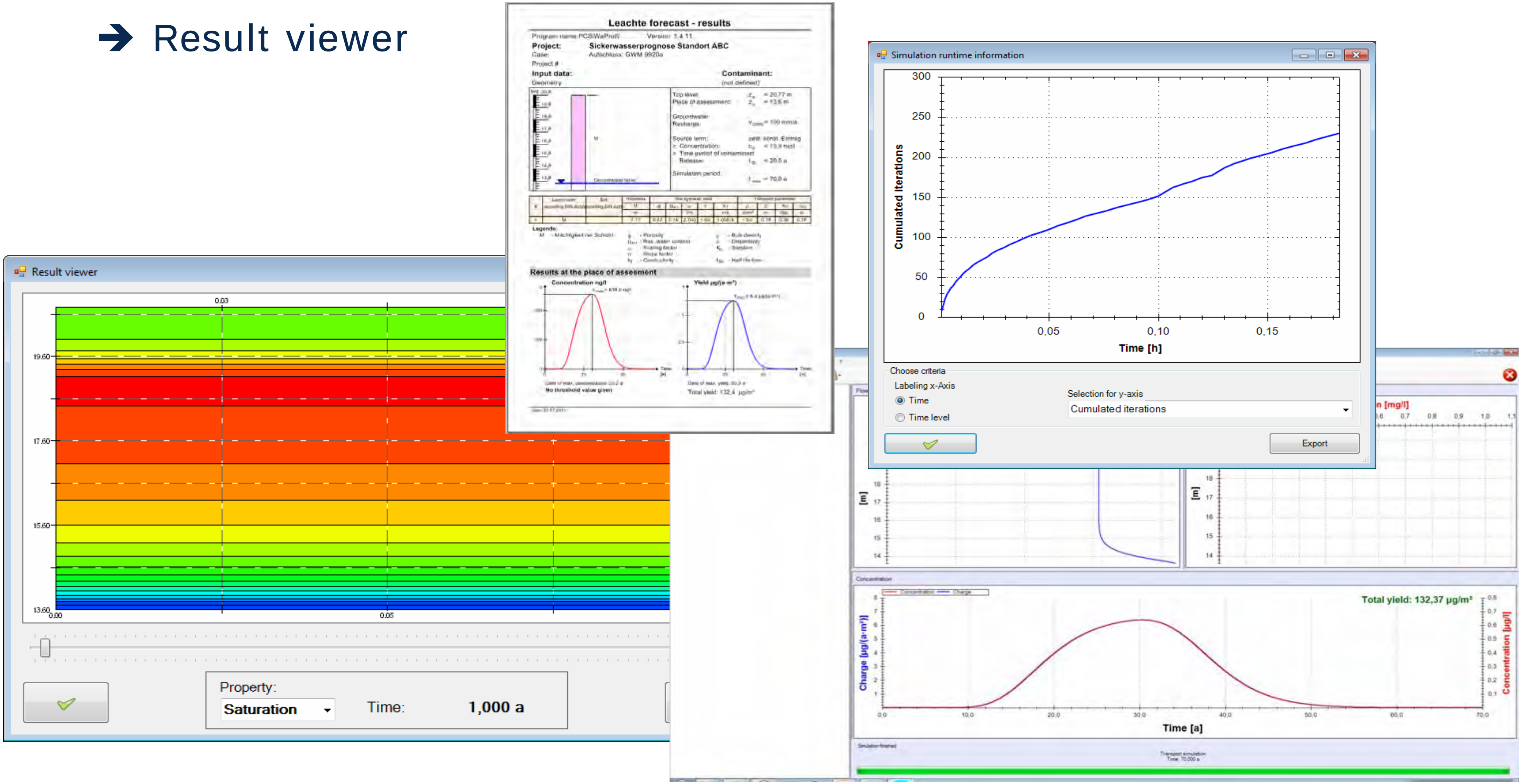
→ matrix assembly, system solver

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

➔ **Simulation** (dam seepage example)



➔ Result viewer



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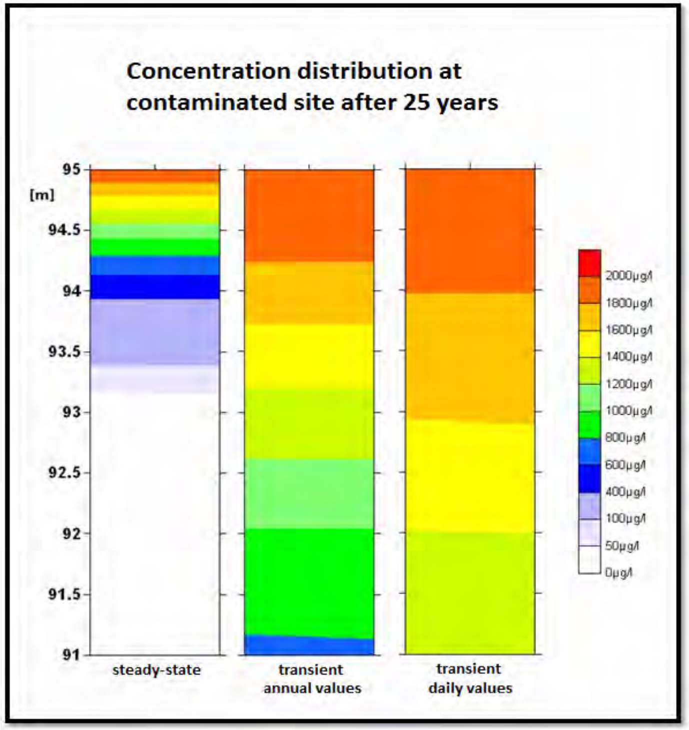
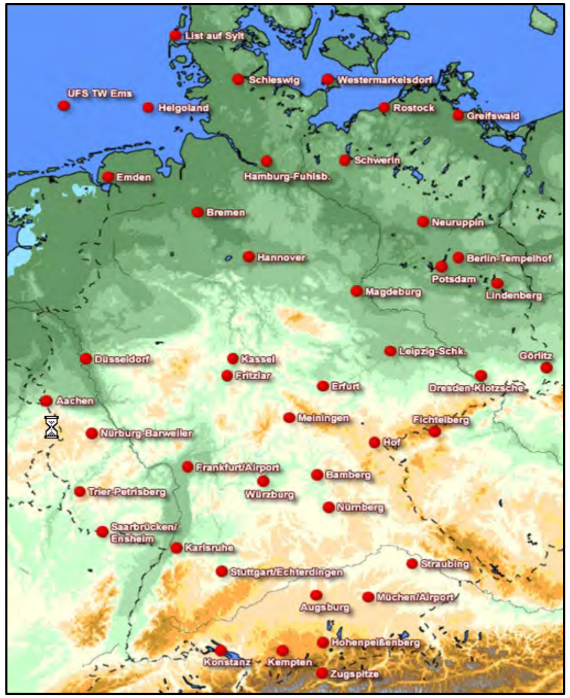
➔ Computation of upper boundary condition with the integrated **weather generator**



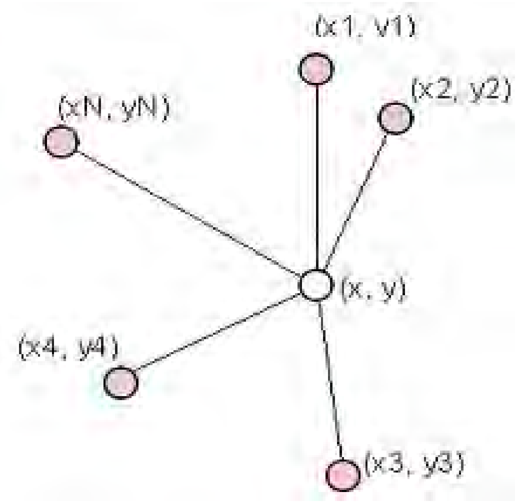
→ **input** data
- → precipitation
- → evapotranspiration
- → vegetation cover
- → slope
- → ...

→ output: <u>daily</u> values of precipitation

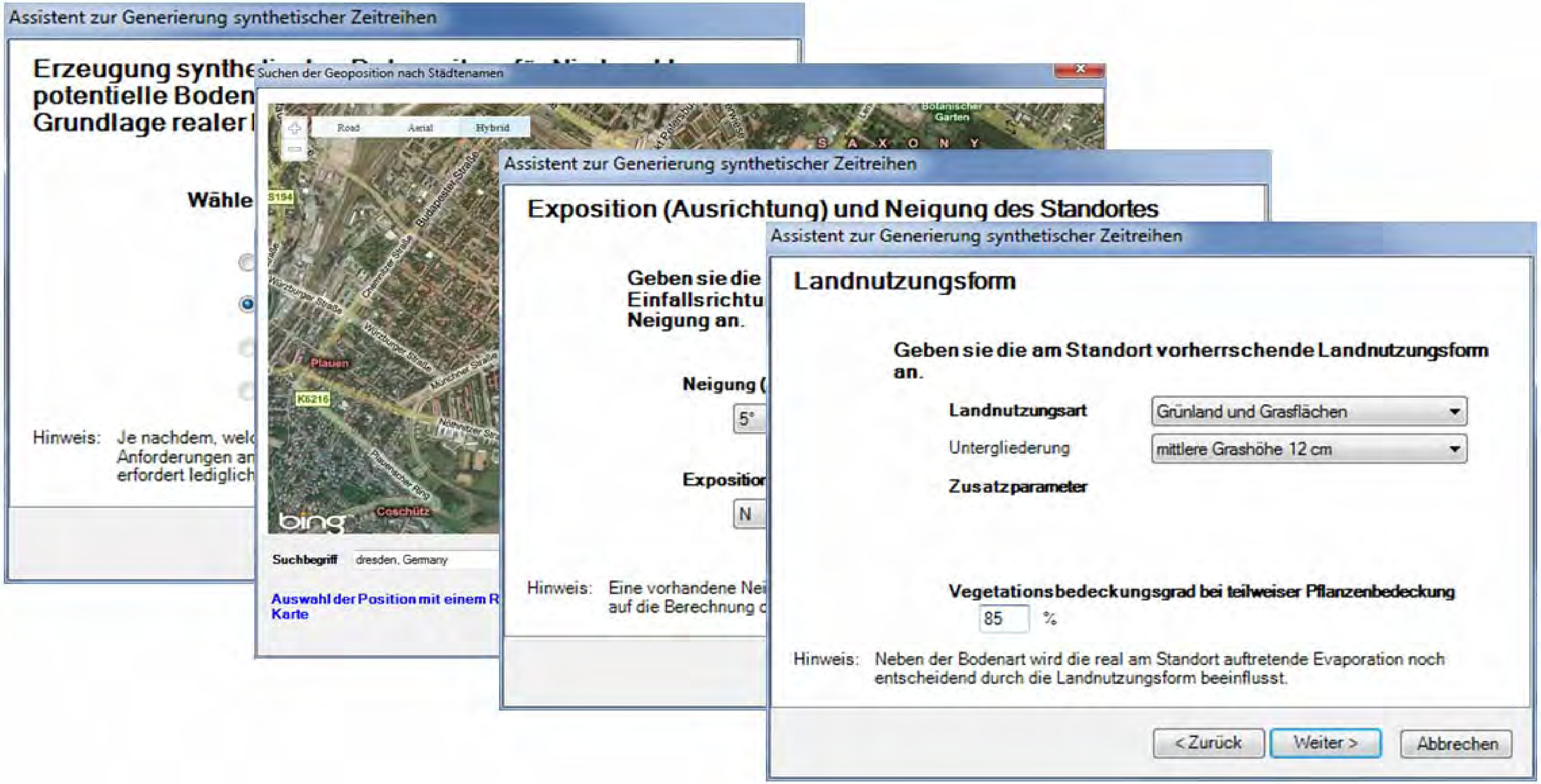


➔ **Time series generation** by:

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

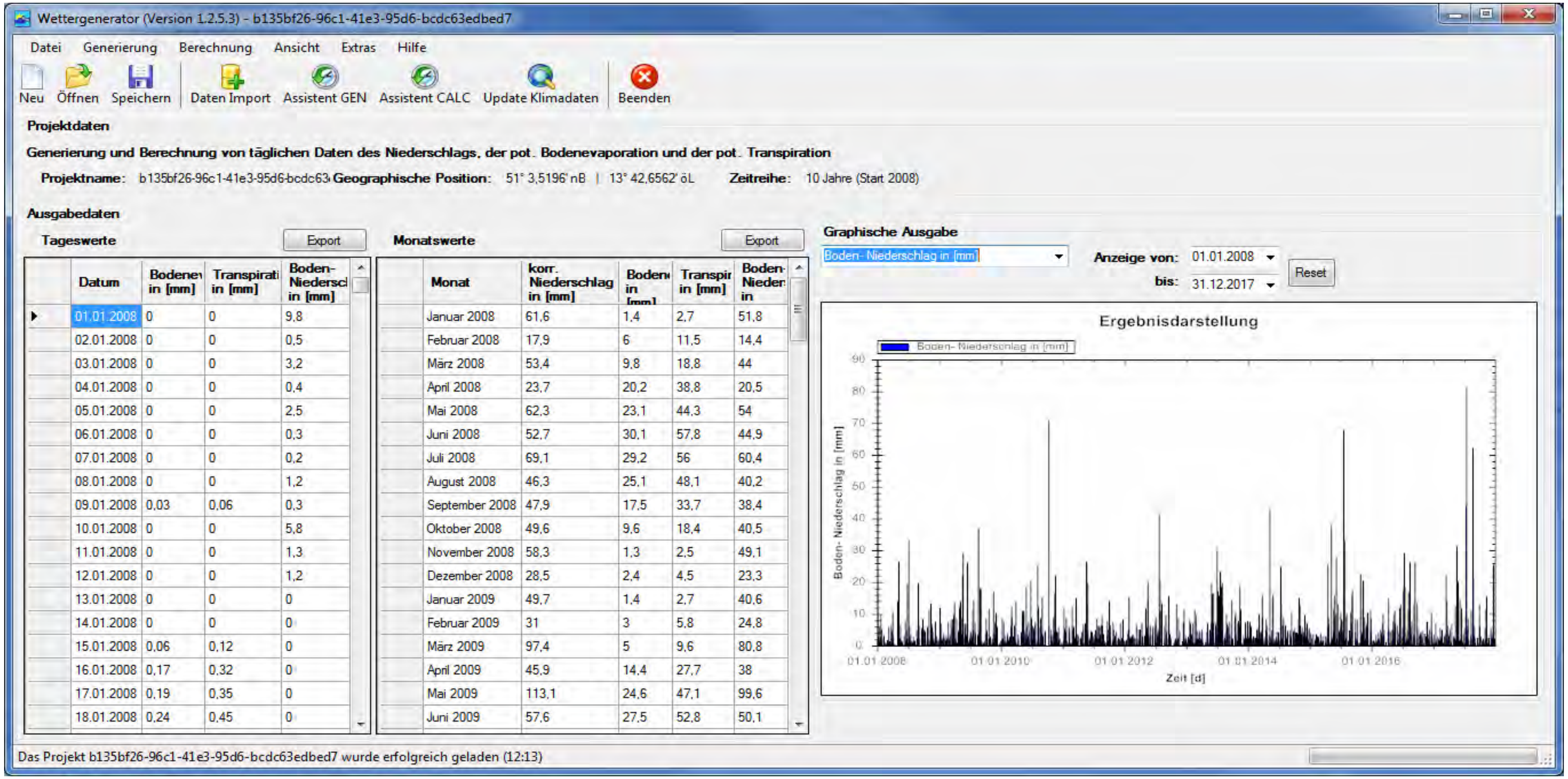


➔ Data input through **assistant**



➔ Graphical visualization of result **time series**

→ **automatic transfer** to PCSiWaPro® model



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

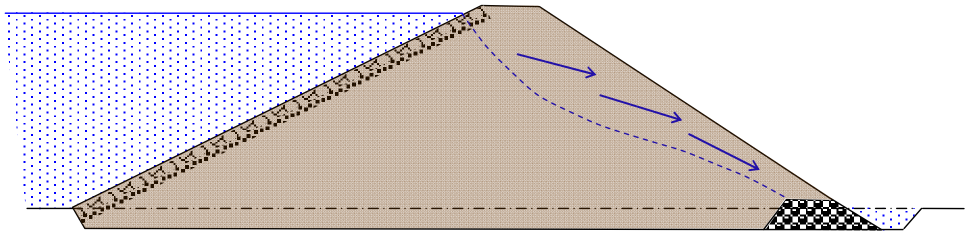
→ leachate forecast

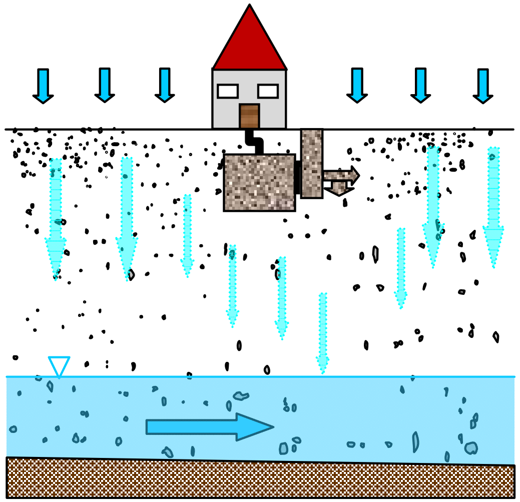
→ earth dams

→ capillary barriers

→ landfill coverage

→ small-scale sewage treatment plants



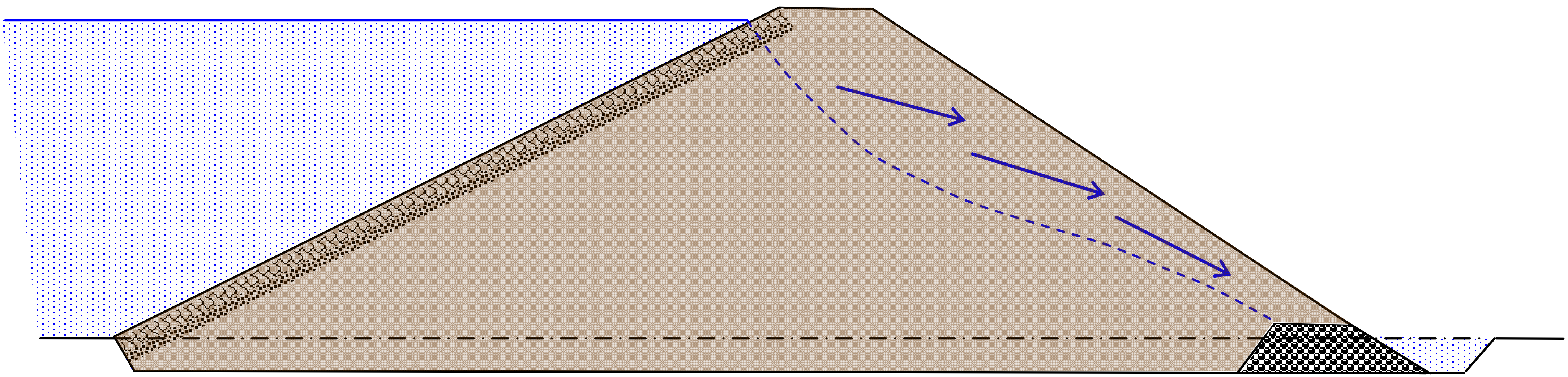


➔ Completed applications with **PCSiWaPro®**:

→ 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**

Which materials should be used?

What are requirements for the dimensioning of the tipping trough?