Reactive Modelling of River Bank Filtration

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Approach to reactive modelling

- **Establish and calibrate a flow model**
- **Verification of conservative transport**
  - **Residence time, particle tracking analyis**
- **Set up a reactive transport model**
  - **Process analysis**
  - **Reaction network**
  - **implementation and simulation**
- **Aim: verify the sampled hydrochemistry**

Modeling Environment (1)

- **PMWIN**
  - **Flow Model (MODFLOW)**
  - **Transport (MT3DMS), multi species**
  - **Reaction (PHT3D)**
    - **Interface to PHREEQC-2 (chemical speciation)**
    - **Use of all skills of PHREEQC-2**
      - **Precipitation/dissolution of solids**
      - **Speciation, redox**
      - **Kinetics (problem adapted formulation)**
      - **Ion exchange**

Modeling Environment (2)

- PHT3D (Prommer, 2001)
  - Definition Reaction Framework Database
  - Definition components
    - as transported species (MT3DMS),
    - or immobile Species
  - PHREEQC-2 processing for each model element
  - assign results to the next transport step (MT3DMS)

Conceptionual chemical model (geochemical response on biodegradation)

- Biodegradation (Kinetics) only by Organic Carbon
- Supply of DOC by mobilisation of matrix OC
- Solid electron acceptors (iron & manganese oxides /oxidhydrates
  - Dissolution precipitation equilibria, redox half reactions
- Dissolved electron acceptors (O_2, NO_3, SO_4)
  - Redox half reactions
- Redox capacity remains constant during kinetic step

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Reaction Network: Components

- **dissolved components (ionar equilibrium)**
  - C(4), Ca, Mg, Na, K, NO_3-N, NO_2-N, N_2-N, NH_4-N, Fe^{2+},Fe^{3+},Mn^{2+},Mn^{3+}, SO_4-S,S^{2-}-S, CH_4, pH, pe
- **dissolved components (Kinetics)**
  - DOC
- **solids (equilibrium)**
  - Calcite, Ferrihydrite ($Fe(OH)_3$), Pyrolusite (MnO_2), Rhodochrosite ($MnCO_3$), FeS_{ppt}, Siderite ($FeCO_3$)
- **solids (Kinetics)**
  - Particular OC

Mathematic Model (Kinetics)

Organic Carbon

Particular Organic Carbon (POC) Supply of DOC

$$r_{POC} = -k_{sol} \cdot \left(c_{DOC} - c_{DOC,limit}\right)$$

Dissolved organic Carbon (DOC) MONOD Kinetics
k_{xx} Decay constants, MONOD constants $K_{xx,}$, Inhibitor constants $K_{inh,xx}$

$$r_{degrad} = r_{O_2} + r_{NO_3} + r_{MnO_2} + r_{FeOOH} + r_{SO_4}$$

$$r_{O_2} = -k_{O_2} \cdot c_{DOC} \cdot \frac{c_{O_2}}{K_{O_2} + c_{O_2}}$$

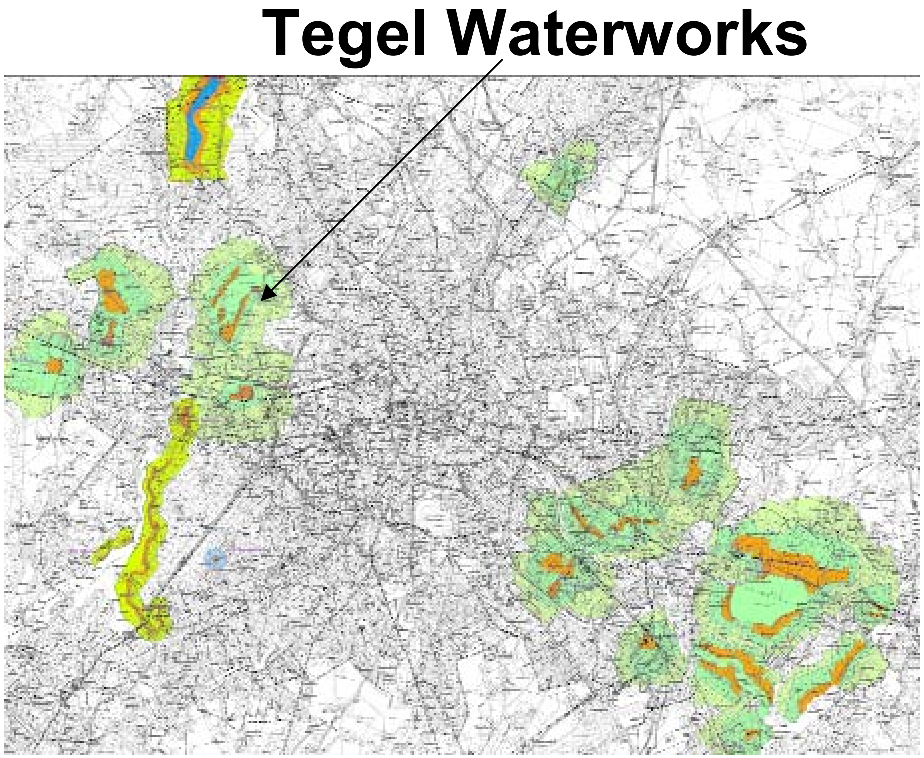
$$r_{NO_3} = -k_{NO_3} \cdot c_{DOC} \cdot \frac{K_{inh,O_2}}{K_{inh,O_2} + c_{O_2}} \cdot \frac{c_{NO_3}}{K_{NO_3} + c_{NO_3}}$$

$$r_{MnO_2} = -k_{MnO_2} \cdot c_{DOC} \cdot \frac{K_{inh,O_2}}{K_{inh,O_2} + c_{O_2}} \cdot \frac{K_{inh,NO_3}}{K_{inh,NO_3} + c_{NO_3}} \cdot \frac{c_{MnO_2}}{K_{MnO_2} + c_{MnO_2}}$$

$$r_{FeOOH} = -k_{FeOOH} \cdot c_{DOC} \cdot \frac{K_{inh,O_2}}{K_{inh,O_2} + c_{O_2}} \cdot \frac{K_{inh,NO_3}}{K_{inh,NO_3} + c_{NO_3}} \cdot \frac{K_{inh,MnO_2}}{K_{inh,MnO_2} + c_{MnO_2}} \cdot \frac{c_{FeOOH}}{K_{FeOOH} + c_{FeOOH}}$$

$$r_{SO_4} = -k_{SO_4} \cdot c_{DOC} \cdot \frac{K_{inh,O_2}}{K_{inh,O_2} + c_{O_2}} \cdot \frac{K_{inh,NO_3}}{K_{inh,NO_3} + c_{NO_3}} \cdot \frac{K_{inh,MnO_2}}{K_{inh,MnO_2} + c_{MnO_2}} \cdot \frac{K_{inh,Feooh}}{K_{inh,FeOOH} + c_{FeOOH}} \cdot \frac{c_{SO_4}}{K_{SO_4} + c_{SO_4}}$$

Waterworks protection areas Berlin

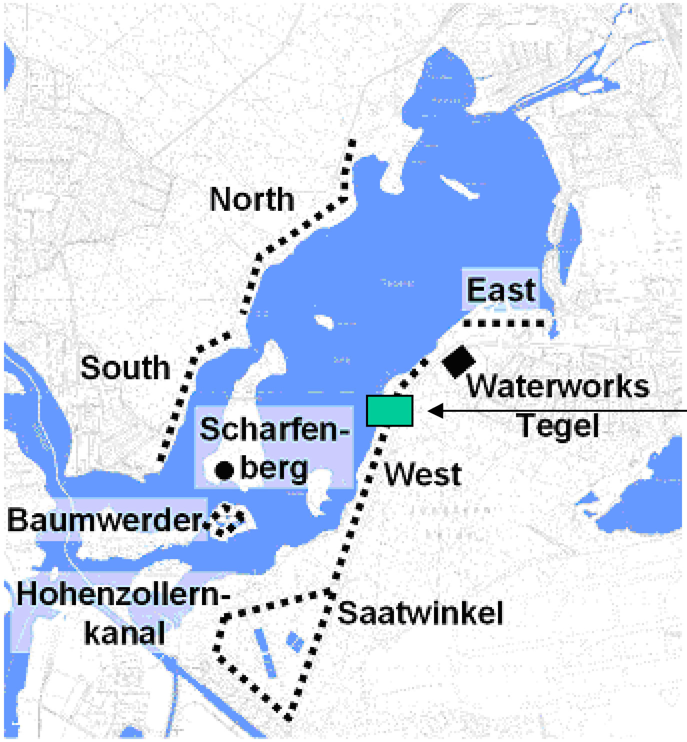


Schutzzonen

- Zone I (Fassungsbereich mit Brunnengalerien)
- Zone II (engere Schutzzone)
- Zone III (nach Festsetzung durch Rechtsverordnung)
- Zone III A (nach Festsetzung durch Rechtsverordnung)
- Zone III B (nach Festsetzung durch Rechtsverordnung)
- Zone III (nach 46er Anordnung)
- Schutzgebietsgrenze in Brandenburg
- Betriebsgelände Wasserwerk
- Schutzzone auf Gewässerfläche
- Blattschnitt entsprechend der Anlage zur Wasserschutzgebietsverordnung

SENSUT Berlin (2006)

Well production areas Lake Tegel



Modelling Area

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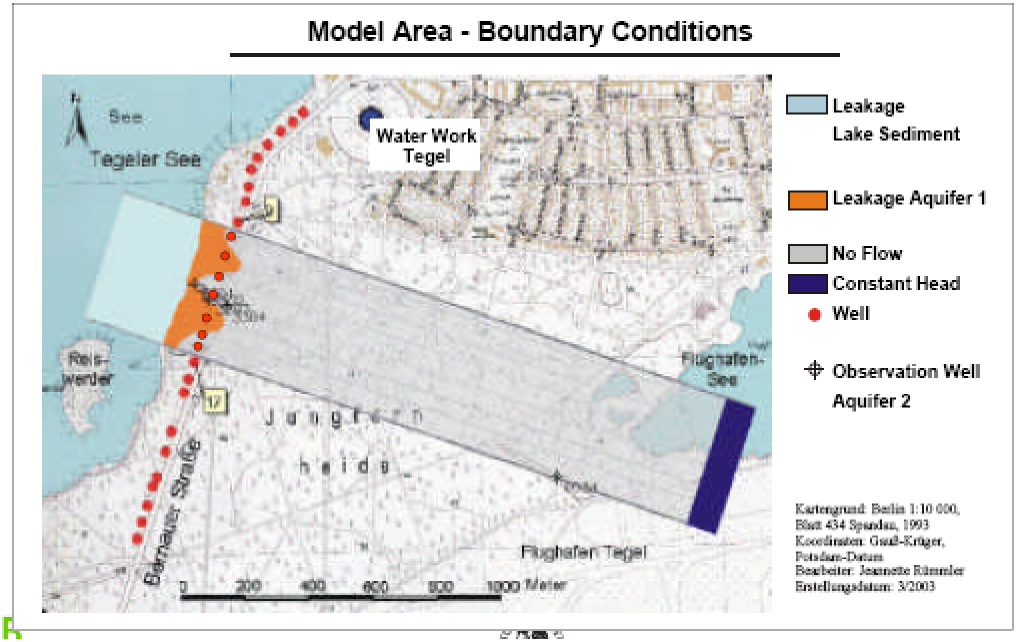
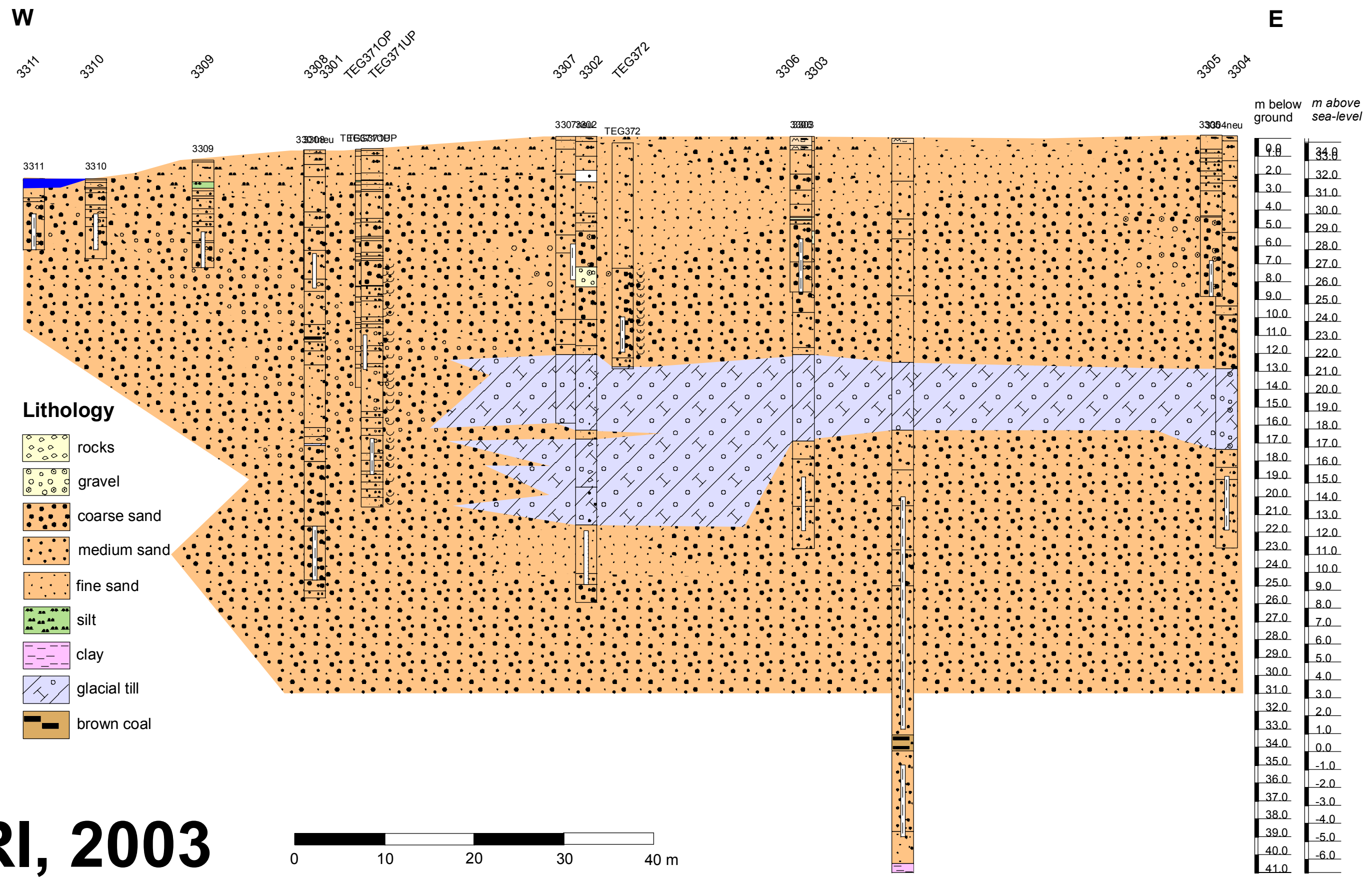


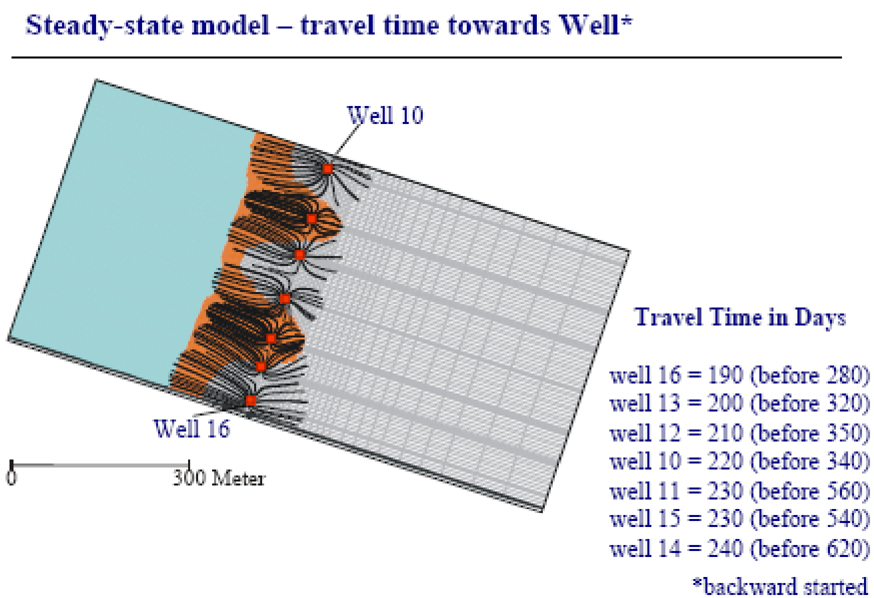
Funded by NASRI (Natural and Artificial Systems for Recharge and Infiltration) set up by VEOLIA Water

Hydrogeological section along the transect Lake Tegel



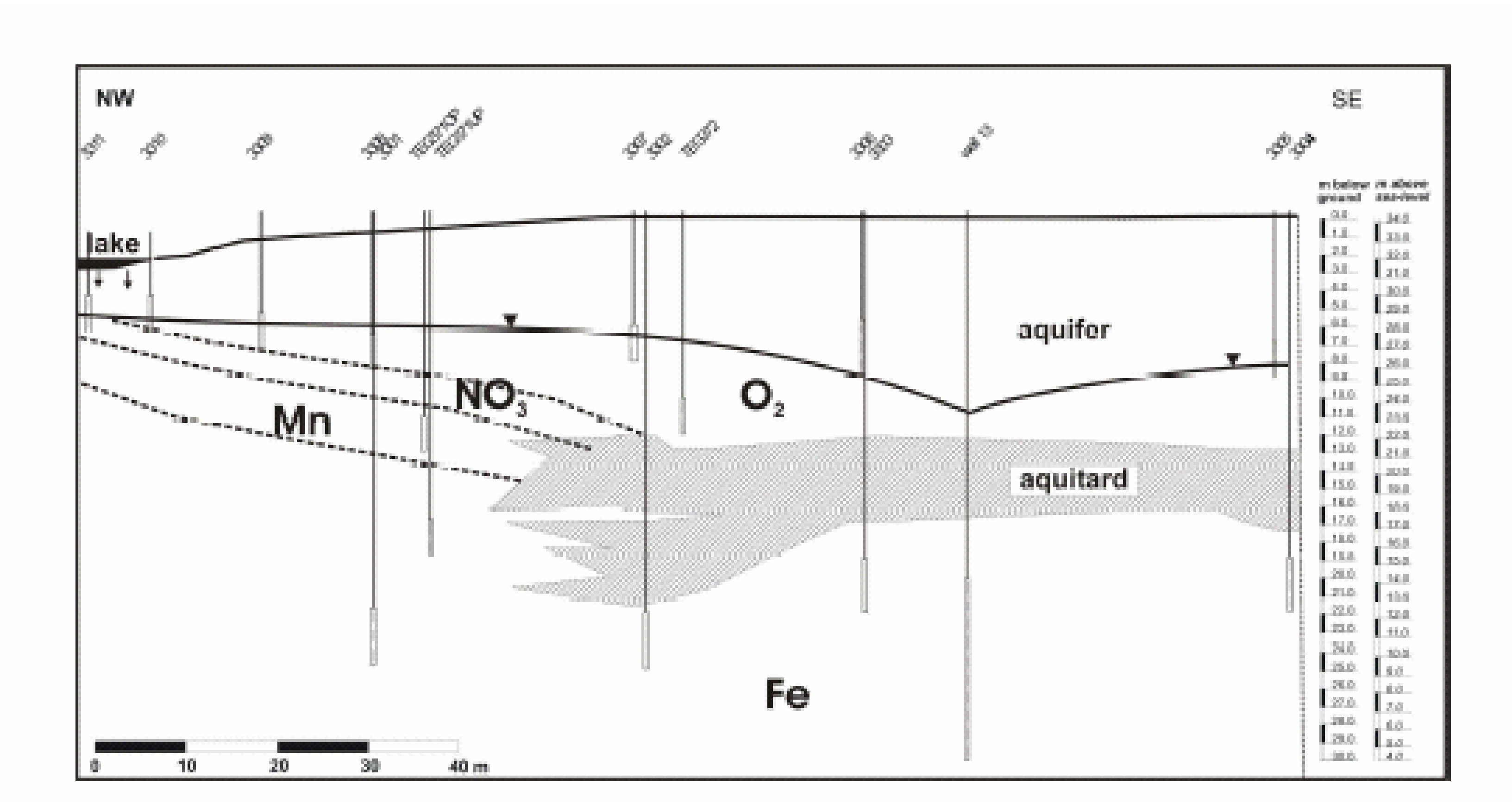
NASRI, 2003

Bank filtration flow modelling



NASRI, 2003 (Diplomarbeit Rümler)

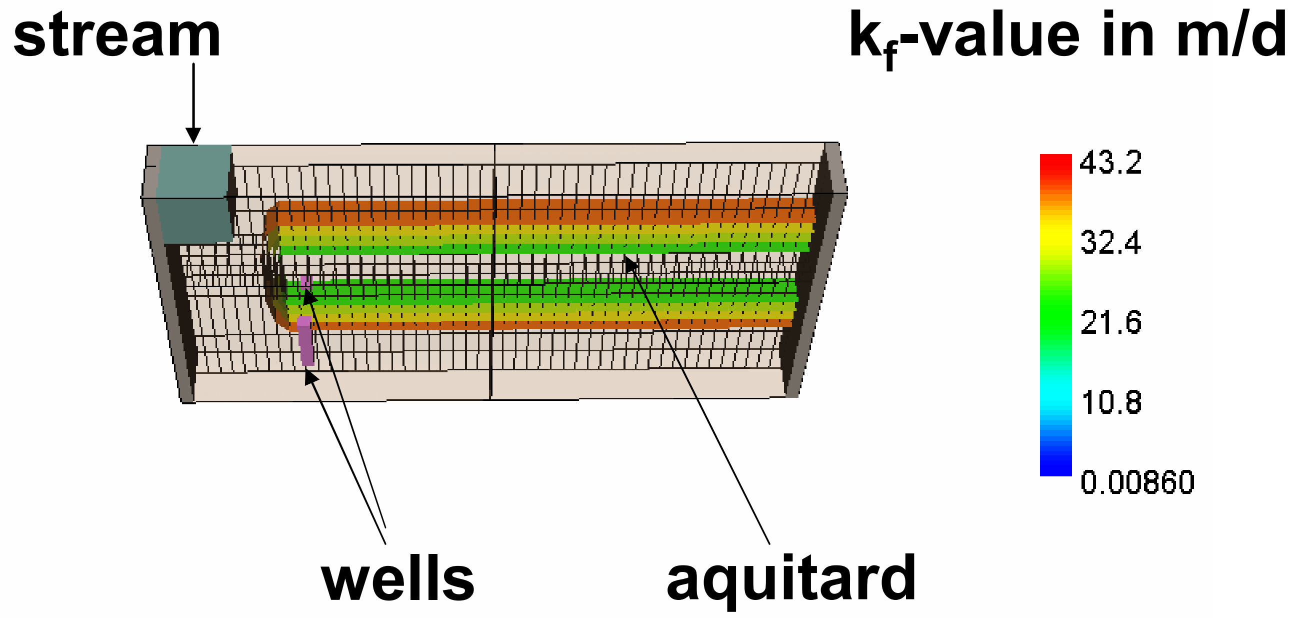
Hydrochemistry: observed redox zonation



Conceptual reactive Transport model

- 3D Model
  - lateral extension 1000 m x 50 m,
  - thickness of 50 m
  - Constant potential on the landside boundary
  - leakage with semipermeable colmation at the left boundary („Lake Tegel“)
  - Oscillating pumping regime
  - local geological setting conceptionally incorporated

3D Model configuration

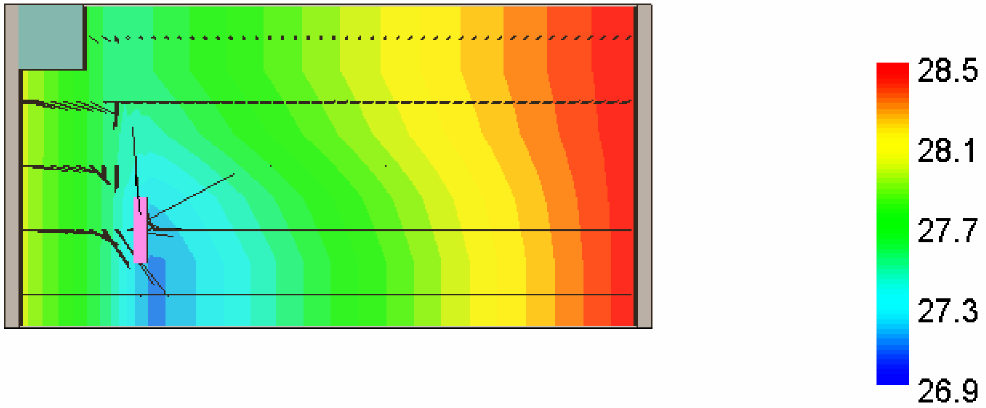


Pumping regime

- The pumping regime at Wellfield West Tegel is strongly instastionary.
- 3 modelled alternating pumping wells
  - 2 wells Q max. 450 m^3/d at the model margin
  - 1 well Q max 900 m^3/d
  - Simulation: after 1 year start of pumping, total simulation duration 3 years
  - Alternating pumping 10 days interval
  - If the central well is pumping the other wells are switched off (and the reverse)

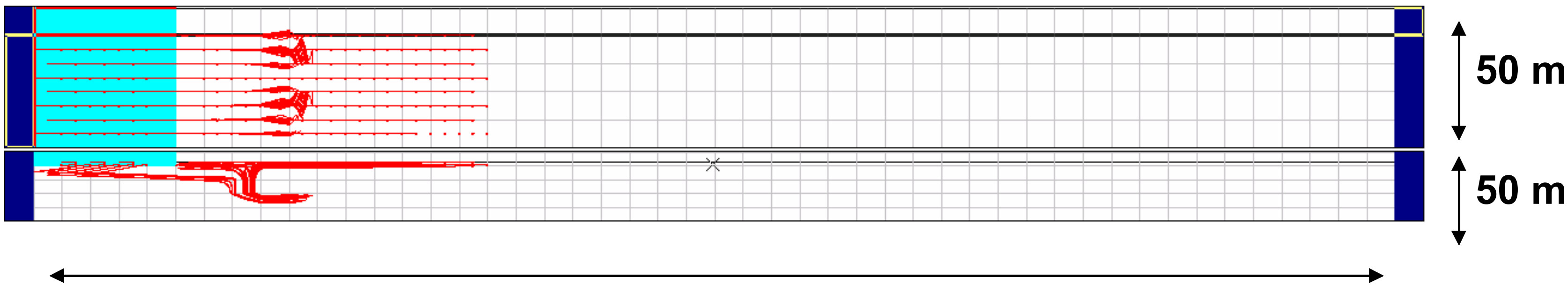
Simulated piezometer heads during pumping

Piezometer head (m a. s. l.)



Flow pathes during oscillating pumping

Plan view



Vertical view

instationary flow field, variable pumping

Assigning initial and boundary reactive transport conditions

- **Initials**
  - **Based on groundwater analyses**
  - **Problem: matrix composition**
- **Boundary conditions**
  - **Based on surface water analyses (Lake Tegel)**
  - **Inflow land side: groundwater analyses**

Presentation of reactive transport calculation results

- prognostic simulation of hydrochemistry instationary pumping conditions
- Simulation time 3 a
- Chemical initials and boundary conditions from NASRI data base

Chemical initials and boundary conditions (1)

Component	Initials+constant head cells Oxic	Initials+constant head cells Anoxic	Inflow concentration stream
pH	6.918	7.212	8.20
pe	13.791	1.458	4.34
C(+4)	5.668e-003	3.296e-003	2.837e-3
C(-4)	1e-20	1e-20	1e-20
Ca	4.174e-003	2.938e-003	2.239e-3
Na	1.302e-003	1.428e-003	2.185e-3
Mg	7.741e-004	3.169e-004	4.568e-4
Cl	1.242e-003	1.609e-003	1.97e-3
K	5.146e-005	4.018e-005	3.019e-4
N(+5)	1.258e-004	1e-20	1.429e-4
N(+3)	1.786e-017	1e-20	1.08e-16
N(0)	1e-20	1.572e-005	3.696e-23
N(-3)	1e-20	1e-20	1e-20

Chemical initials and boundary conditions (2)

Component	Initials+constant head cells Oxic	Initials+constant head cells Anoxic	Inflow concentration stream
Fe(2)	3.020e-017	1.320e-005	1e-20
Fe(3)	4.437e-008	3.311e-008	1e-20
Mn(2)	9.895e-015	7.882e-006	1e-20
Mn(3)	1e-20	1e-20	1e-20
S(-2)	1e-20	1e-20	1e-20
S(6)	2.636e-003	1.729e-003	1.448e-3
O(0)	1.134e-003	1e-20	1.113e-3
DOC	1e-7	1e-4	1e-5
POC	1e-4	0.02	0.00
Calcite	0.014775	0.01479	0.00
Ferrihydrite $Fe(OH)_3$	0.0283	0.0283	0.00
Pyrolusite MnO_2	0.00095	0	0.00
Rhodochrosite $MnCO_3$	0	0.00095	0.00
Siderite $FeCO_3$	0	8.32e-6	0.00

Chemical boundary conditions recharge (1)

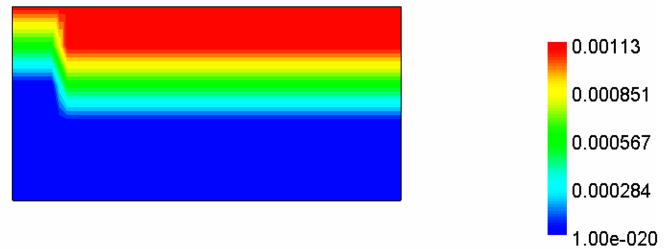
Komponente	Recharge (GWN)
pH	4.056
pe	16.566
C(+4)	1.082e-5
C(-4)	0.00
Ca	2.233e-5
Na	6.189e-5
Mg	2.334e-5
Cl	8.295e-5
K	6.366e-5
N(+5)	1.934e-4
N(+3)	4.089e-17
N(0)	0.00
N(-3)	0.00

Groundwater recharge: 100 mm/a

Chemical boundary conditions recharge (2)

Component	Groundwater Recharge
Fe(2)	1e-20
Fe(3)	1e-20
Mn(2)	1e-20
Mn(3)	1e-20
S(-2)	0.00
S(6)	5.462e-5
O(0)	5.012e-4
DOC	0.00
POC	0.00
Calcite	0.00
Ferrihydrite $Fe(OH)_3$	0.00
Pyrolusite MnO_2	0.00
Rhodochrosite $MnCO_3$	0.00
Siderite $MnCO_3$	0.00

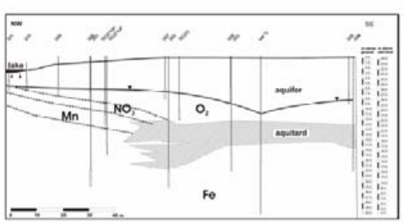
Results (1):O_2

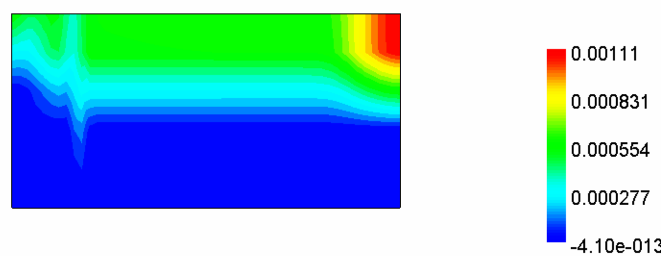


Start

Observation **Simulation**

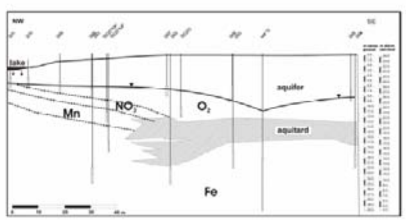
after 3 a

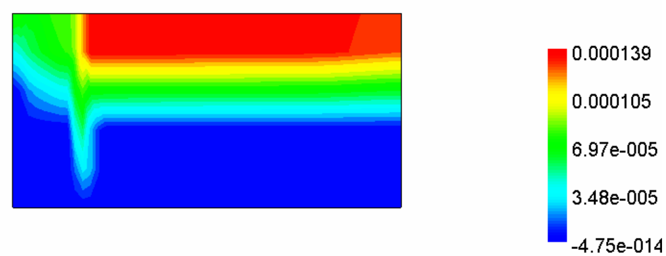




Results (2): NO_3-N

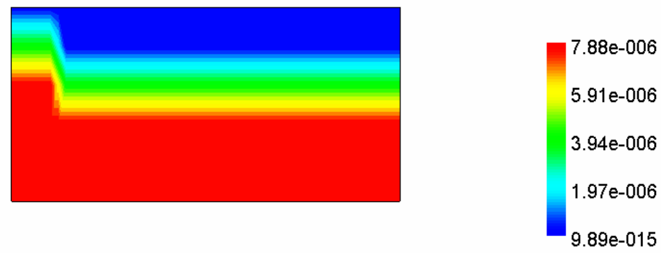
Start





nach 3 a

Results (4):Mn



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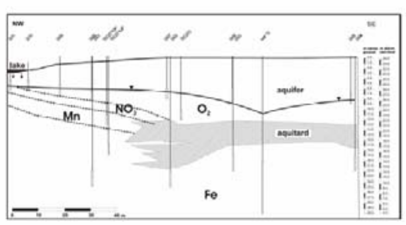
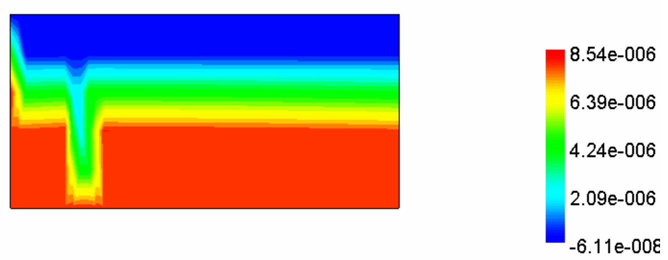
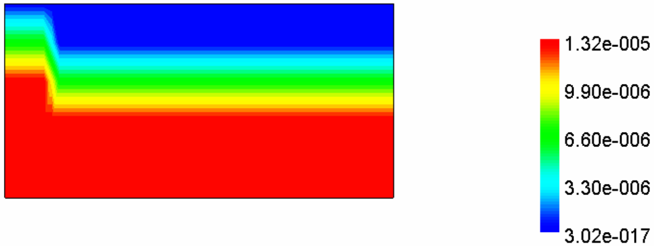




nach 3 a

Results (5): Fe



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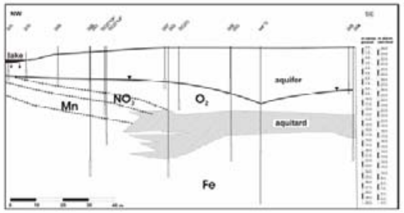

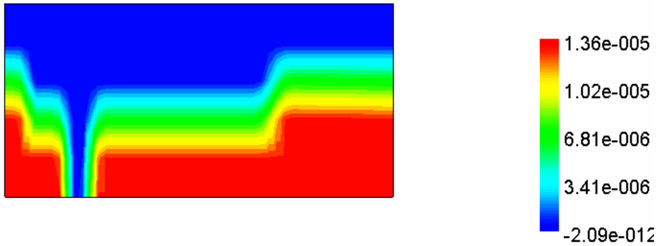

after 3 years

Conclusions

- **Reactive transport modelling is a usefull tool**
  - **For all problems and test sites involving changes in hydrochemical groundwater compositions**
  - **To define redox conditions for the stability /instability of pharmaceutical trace compounds during river bank filtration**

Thank you very much for your attention!