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A consistent geochemical modelling approach

for long-term assessment of release from contaminated materials to soil and groundwater

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A consistent geochemical modelling approach

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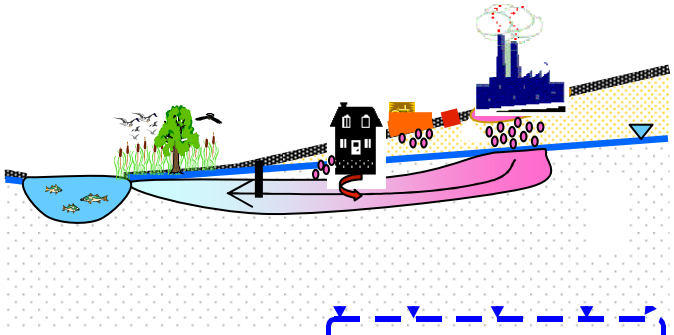
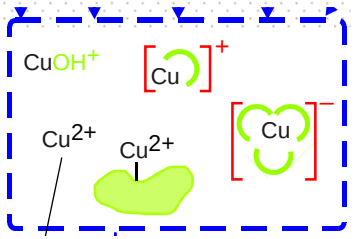
Rob Comans, Joris Dijkstra, Hans van der Sloot, Hans Meeussen & Andre van Zomeren

www.ecn.nl

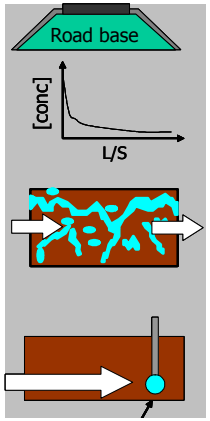
Outline



- ✓ **Introduction**
- ✓ **Generic modelling approach**
  major geochemical processes, models & parameters

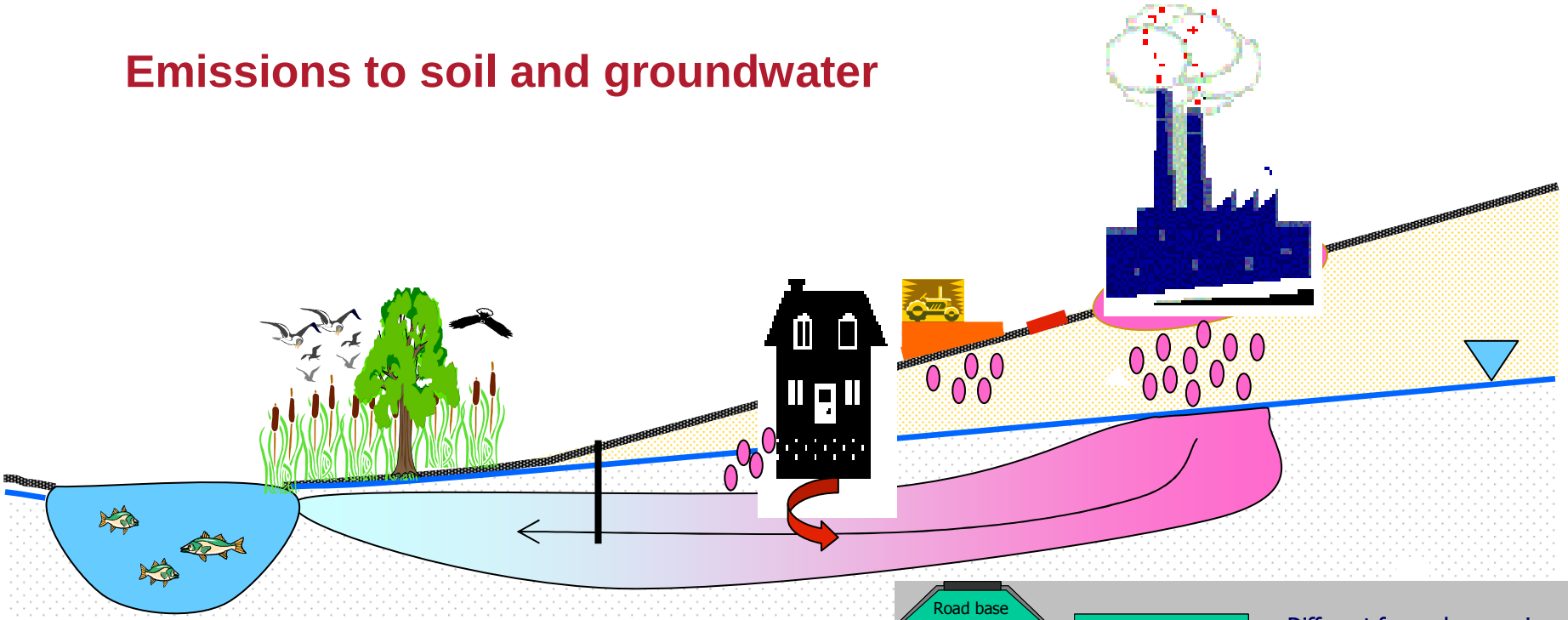


- ✓ **Application to contaminant leaching and speciation in soils**
- ✓ **Application to environmental legislation:**
  emission limits for construction materials



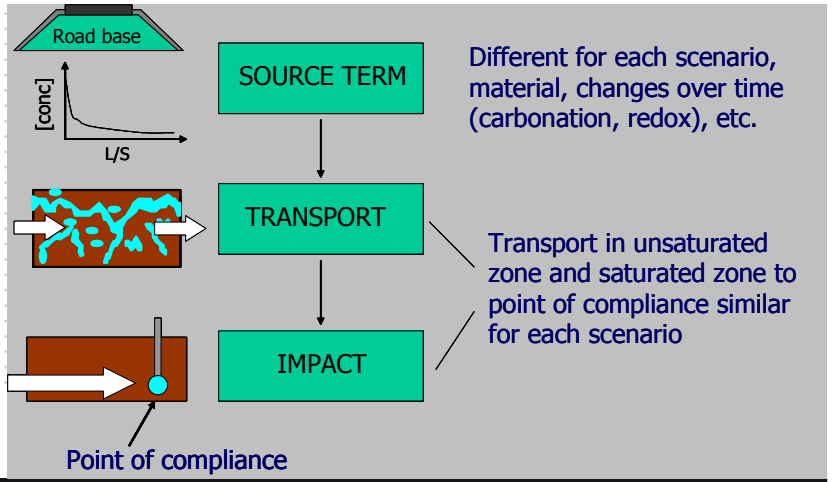
- ✓ **Uncertainties and research questions**
- ✓ **Conclusions**

Emissions to soil and groundwater



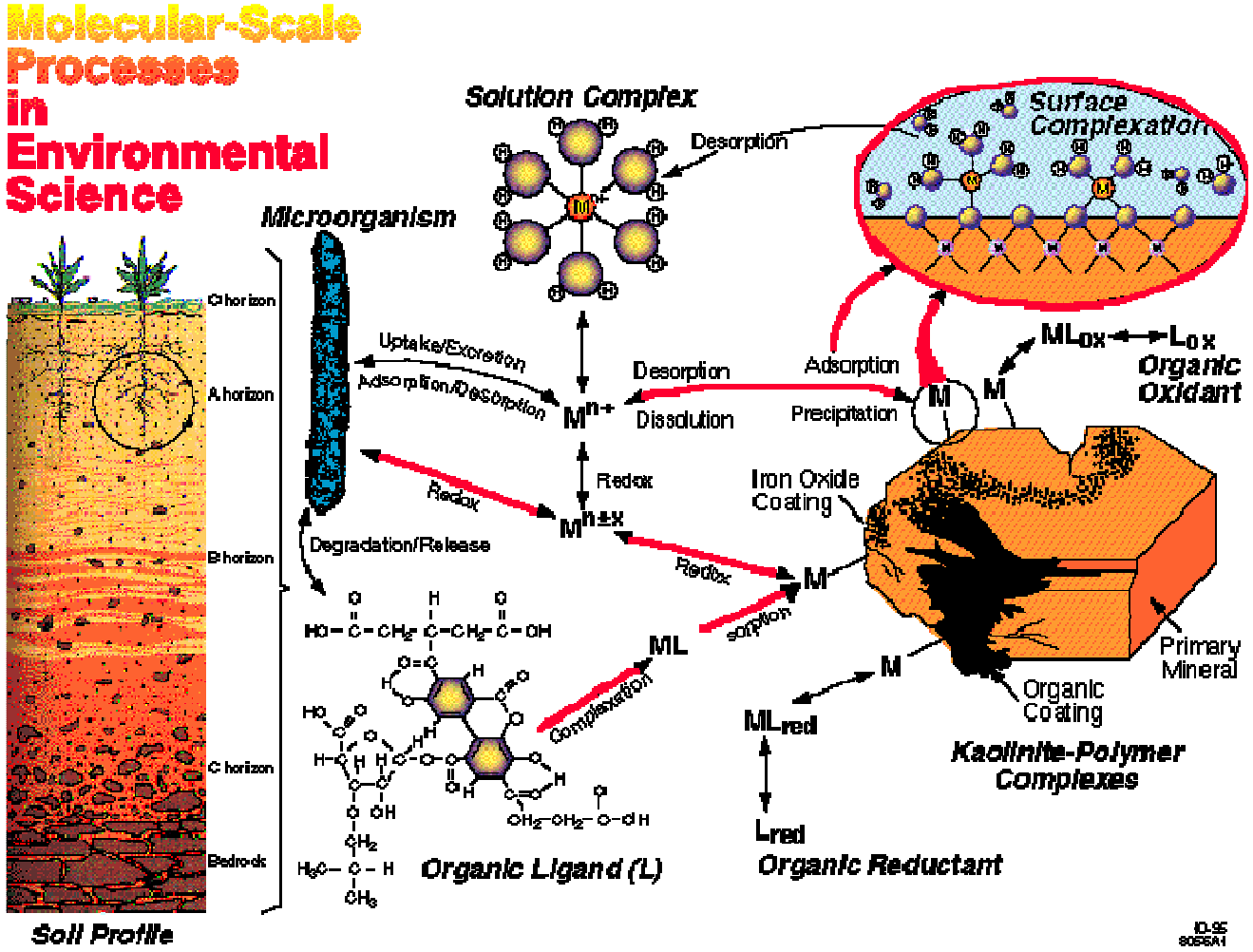
Different scenarios, generic approach:

- Leaching of contaminants (source term)
- Reactive transport
- Impact at a POC



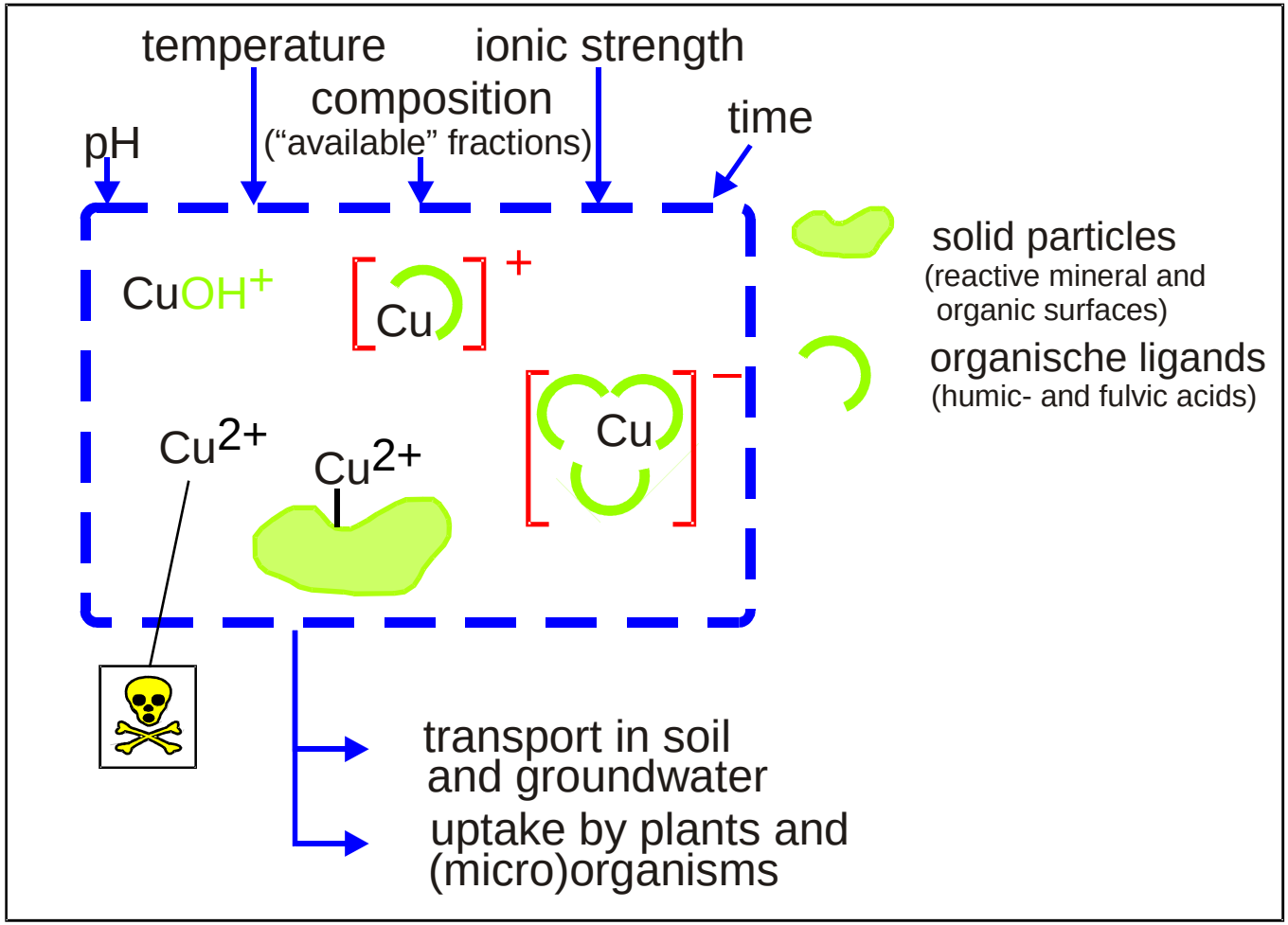
Modified after: Quevauviller (2006)

Geochemical processes controlling fate of (leached) contaminants



Source: Surface and Aqueous Geochemistry Group, Stanford, USA

Key to generic modelling approach: contaminant speciation



Naar: M. Gfeller & R. Schulin, ETH, Zürich

Multi-surface geochemical modelling of leaching processes

"Available" concentrations:
→ Leaching/extraction at low pH (≈0.5)

Major ion chemistry:
pH, major (competing) ions, inorganic ligands
(NIST-thermodynamic database)[1]

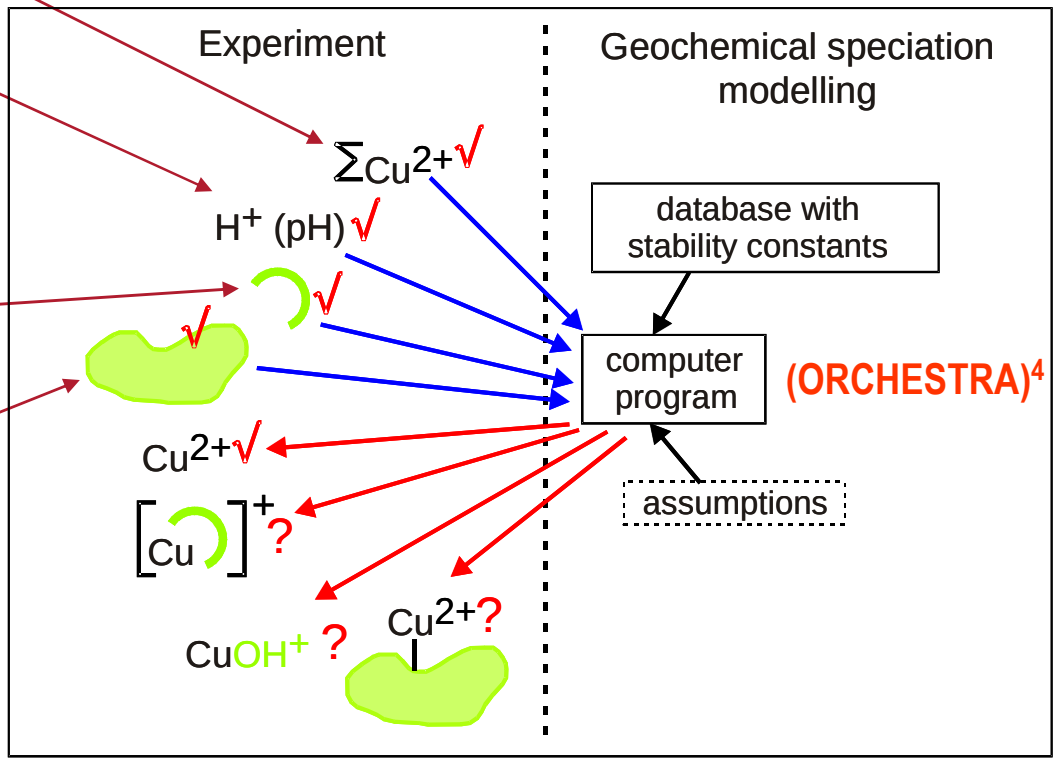
Dissolved organic matter:
Humic and fulvic acids
(NICA model)[2]

Reactive surfaces in the solid phase:
- OM (humic/fulvic acids)

(NICA model)[2]
- Fe/Al (hydr)oxides

(Two layer SCM)[3]
- Clay particles

(Donnan model)

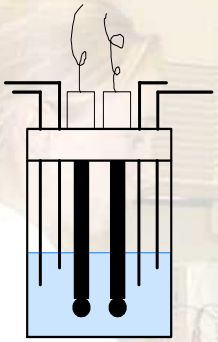


Modified after M. Gfeller & R. Schulin, ETH, Zürich

[1] MINTEQ 4.0/NIST; [2] Milne et al. (2003); [3] Dzombak & Morel (1990); [4] Meeussen (2003)

Approach to identification of geochemical processes:

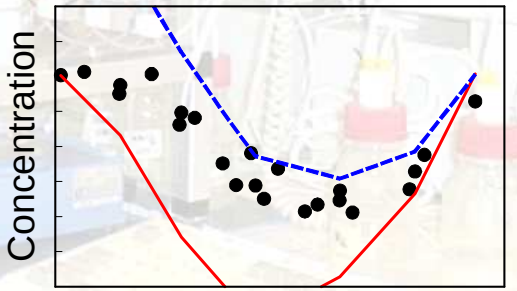
"Geochemical fingerprints"



pH-dependent solubility

Model

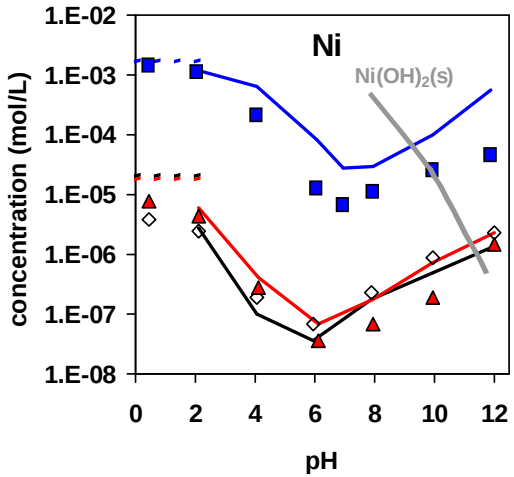
?

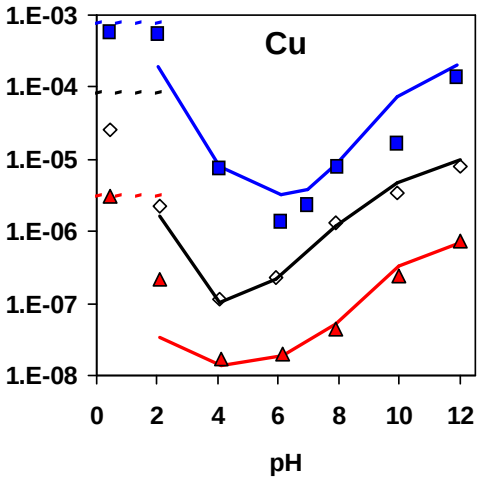


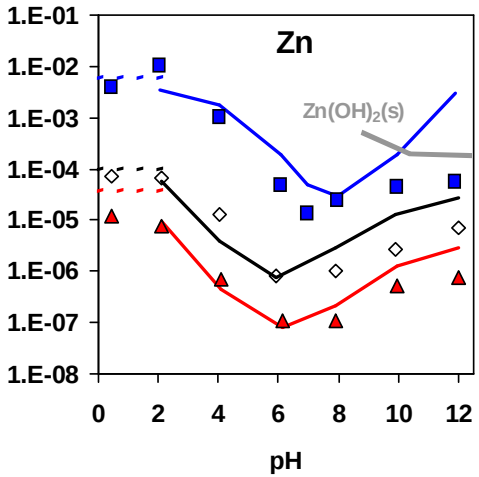
!

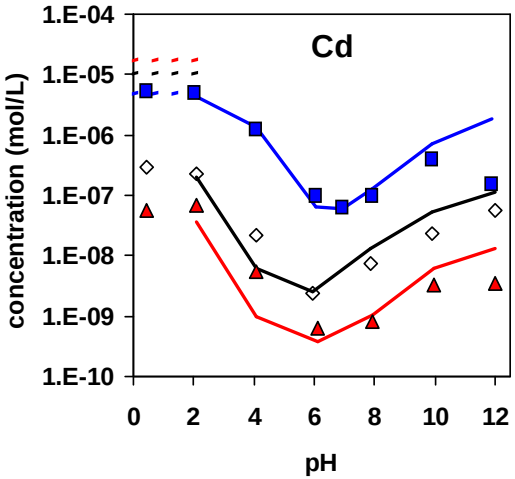
See also: Dijkstra et al. (2004) Environ. Sci. Technol. 38, 4390-4395.

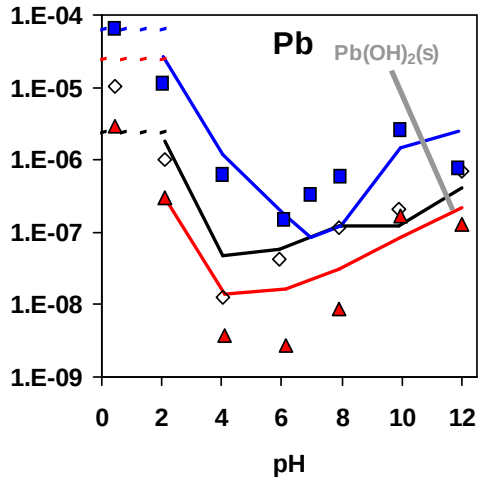
Leaching of heavy metals from contaminated soils

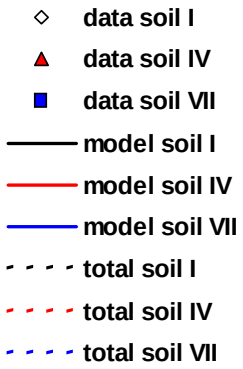






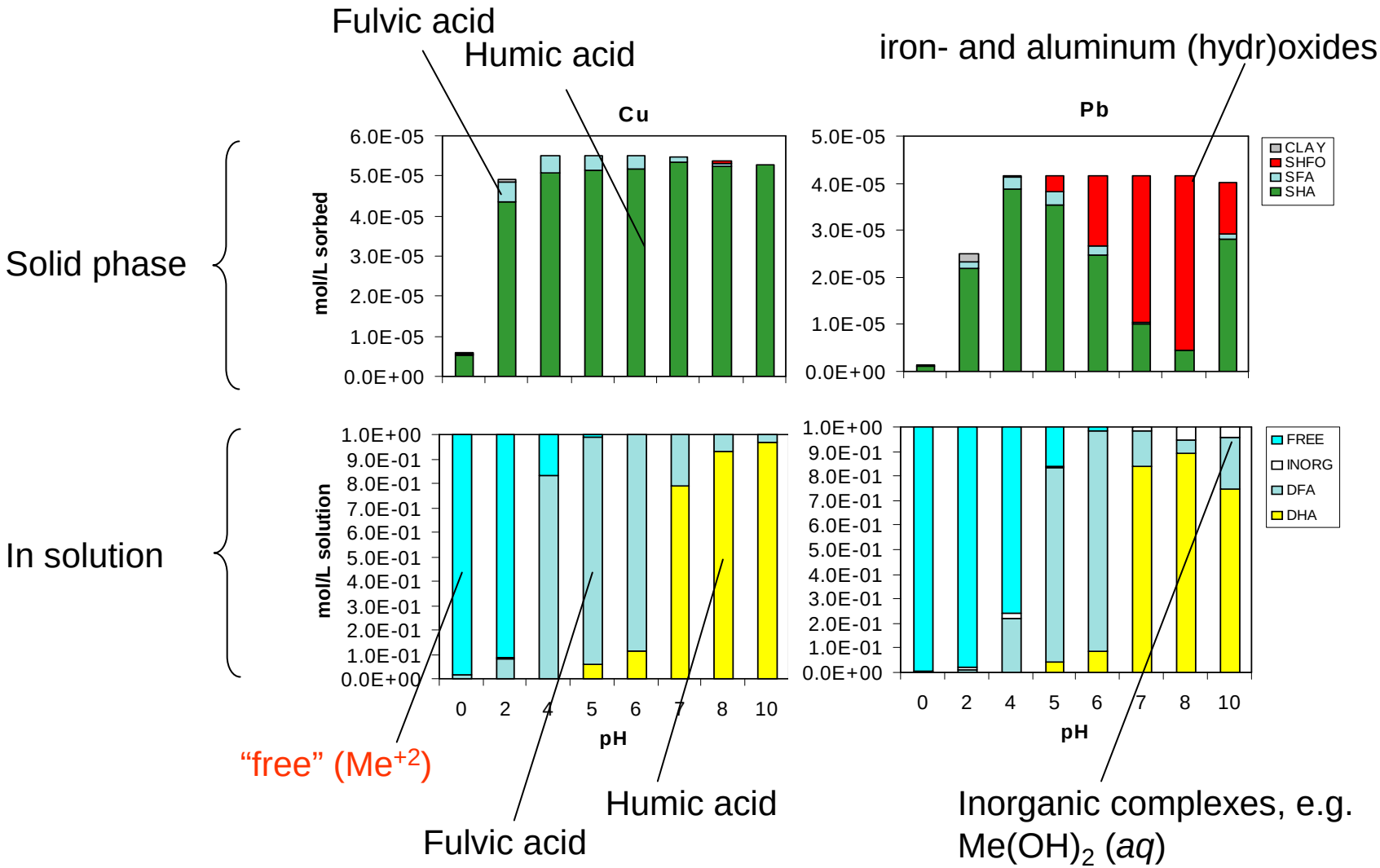




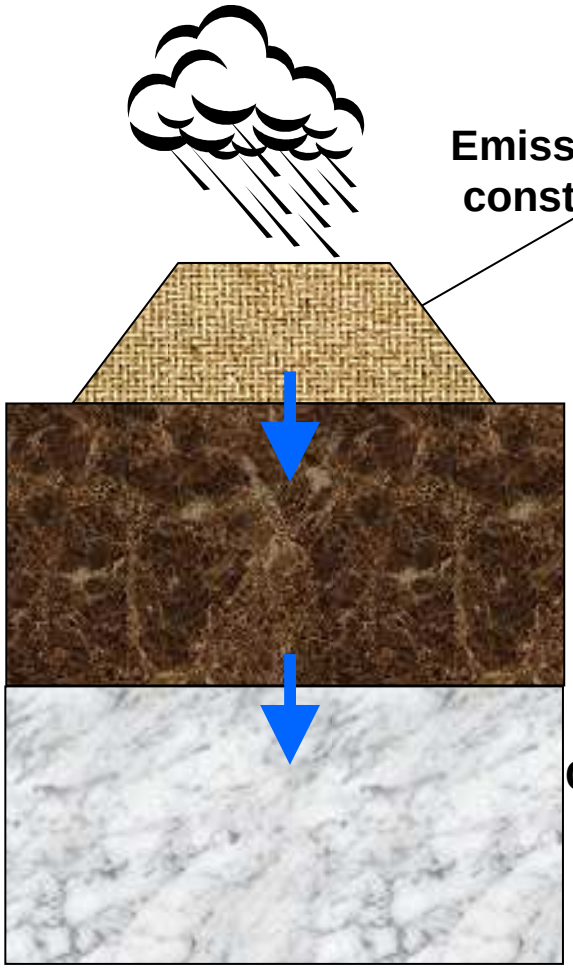


Dijkstra et al., *Environmental Science and Technology* (2004), 38, 4390-4395

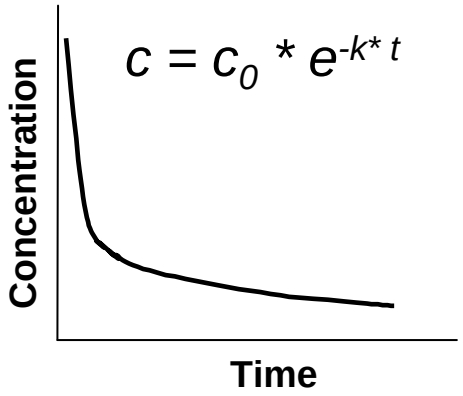
Speciation of heavy metals in contaminated soils



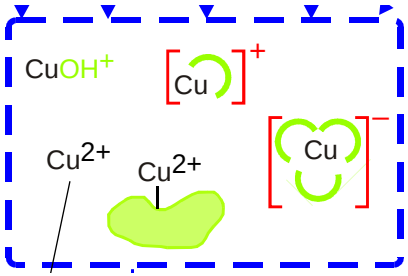
Development maximum emission values Dutch Soil Quality Act



Emission from construction:

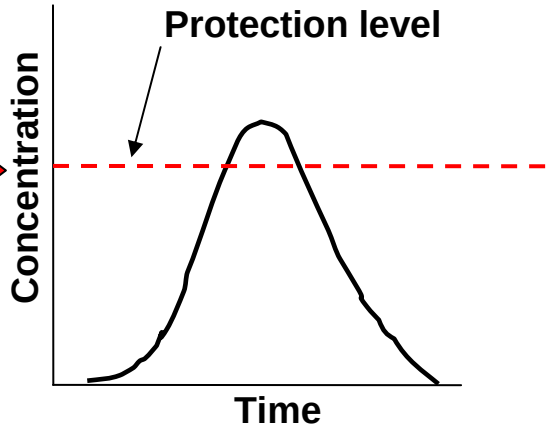


Transport through soil:

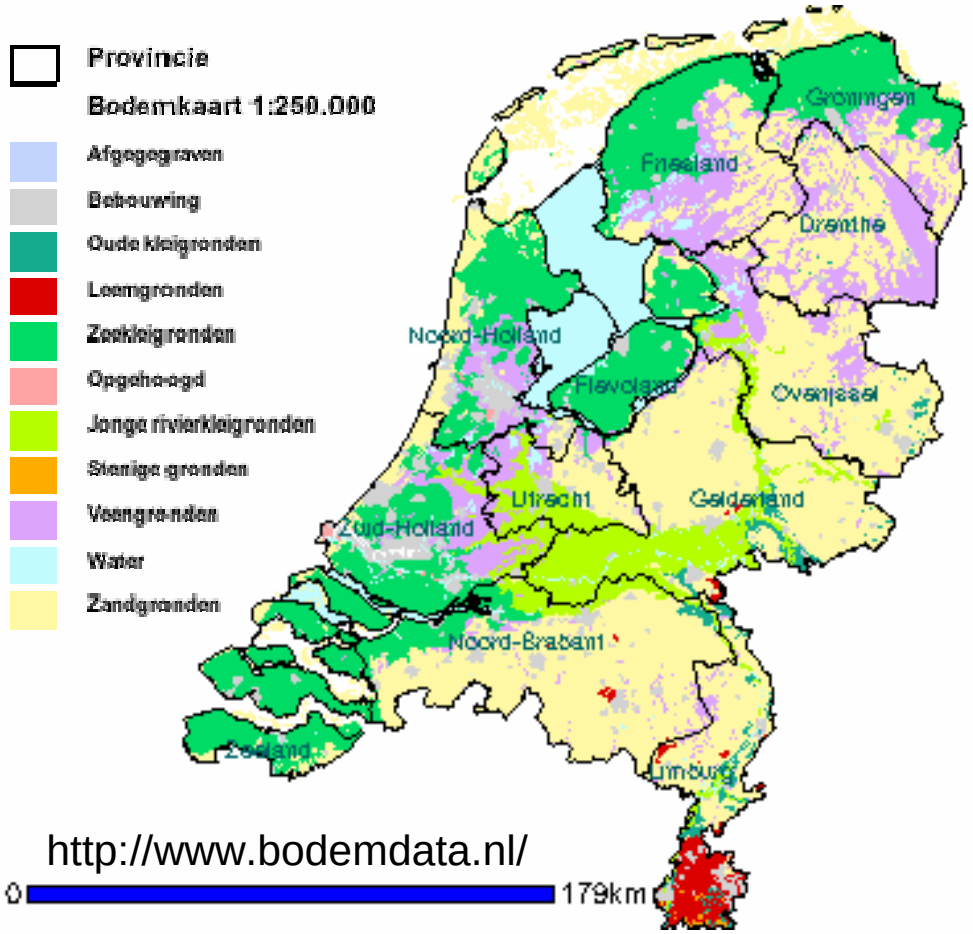


Concentration in groundwater

(t=100 y / t=1000 y)



Major Dutch soil types: sand, clay, peat

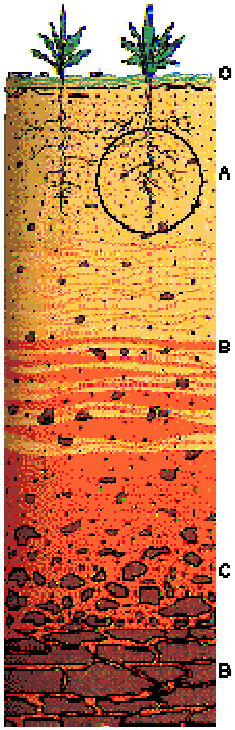


http://www.bodemdata.nl/

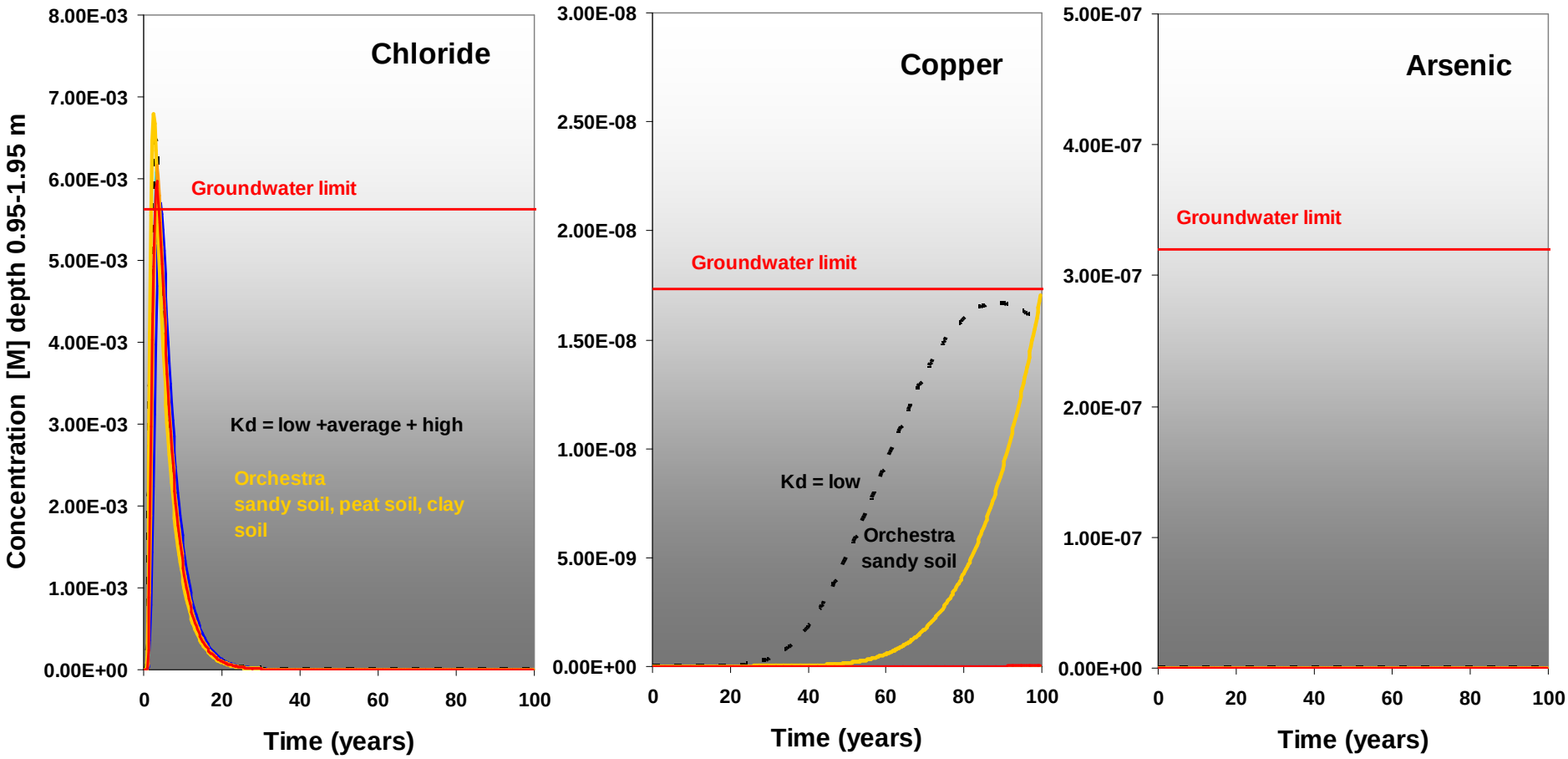
Stone database (Alterra)

Specific depth profiles:

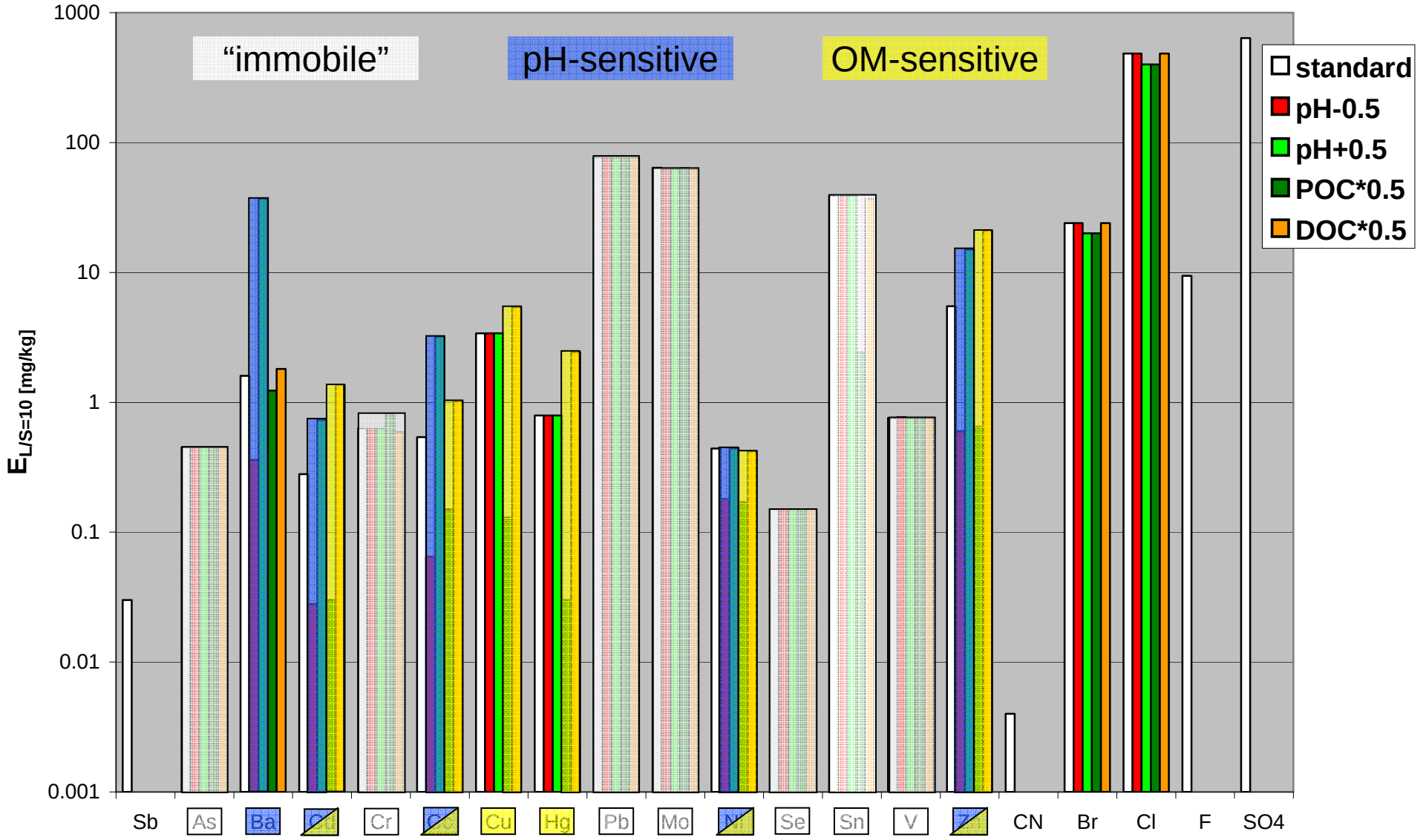
- *pH*
- *Reactive mineral/ -organic surfaces*
- *Hydrological properties*



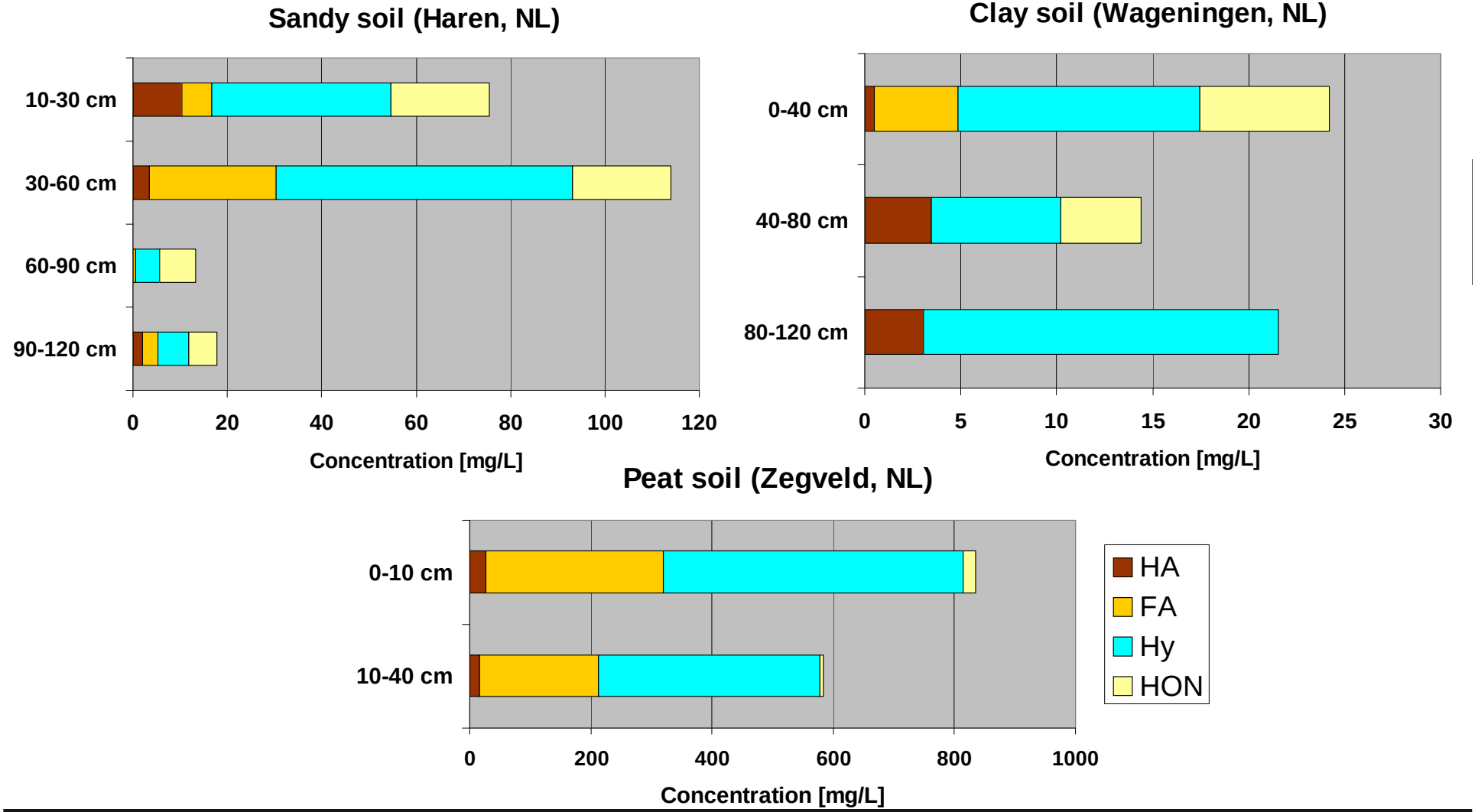
Soil Profile


Chloride
Concentration [M] depth 0.95-1.95 m
8.00E-03
7.00E-03
6.00E-03
5.00E-03
4.00E-03
3.00E-03
2.00E-03
1.00E-03
0.00E+00
Groundwater limit
Kd = low +average + high
Orchestra
sandy soil, peat soil, clay soil
0
20
40
60
80
100
Time (years)
Copper
3.00E-08
2.50E-08
2.00E-08
1.50E-08
1.00E-08
5.00E-09
0.00E+00
Groundwater limit
Kd = low
Orchestra
sandy soil
0
20
40
60
80
100
Time (years)
Arsenic
5.00E-07
4.00E-07
3.00E-07
2.00E-07
1.00E-07
0.00E+00
Groundwater limit
0
20
40
60
80
100
Time (years)

ORCHESTRA emission values



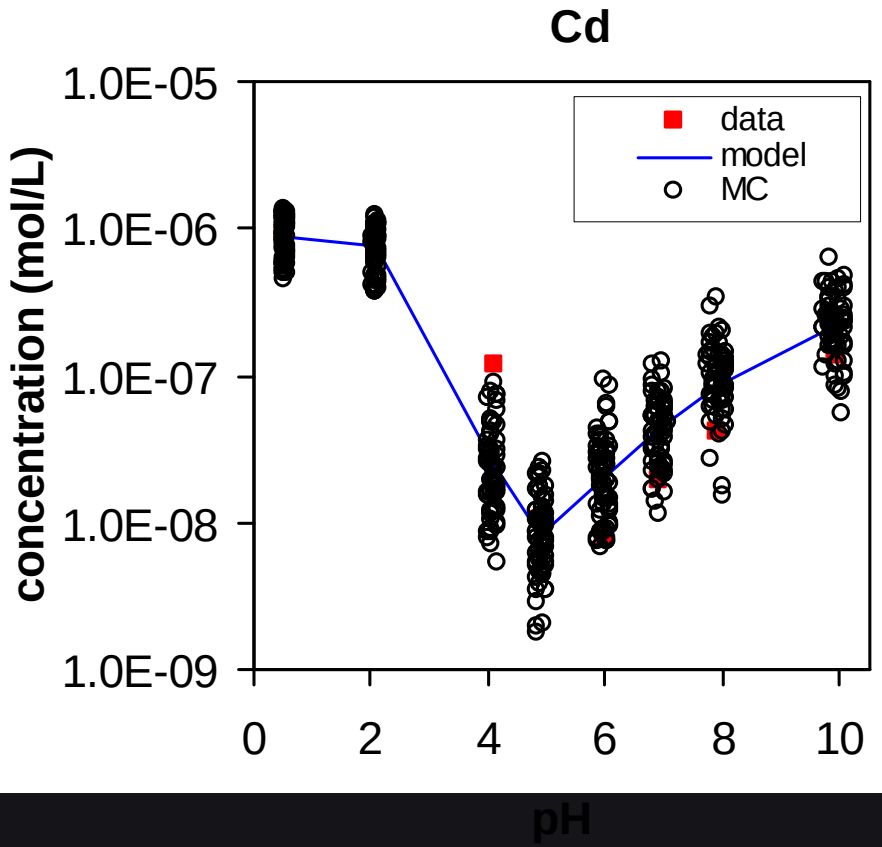
Application of new rapid method for (dissolved) organic matter reactivity*

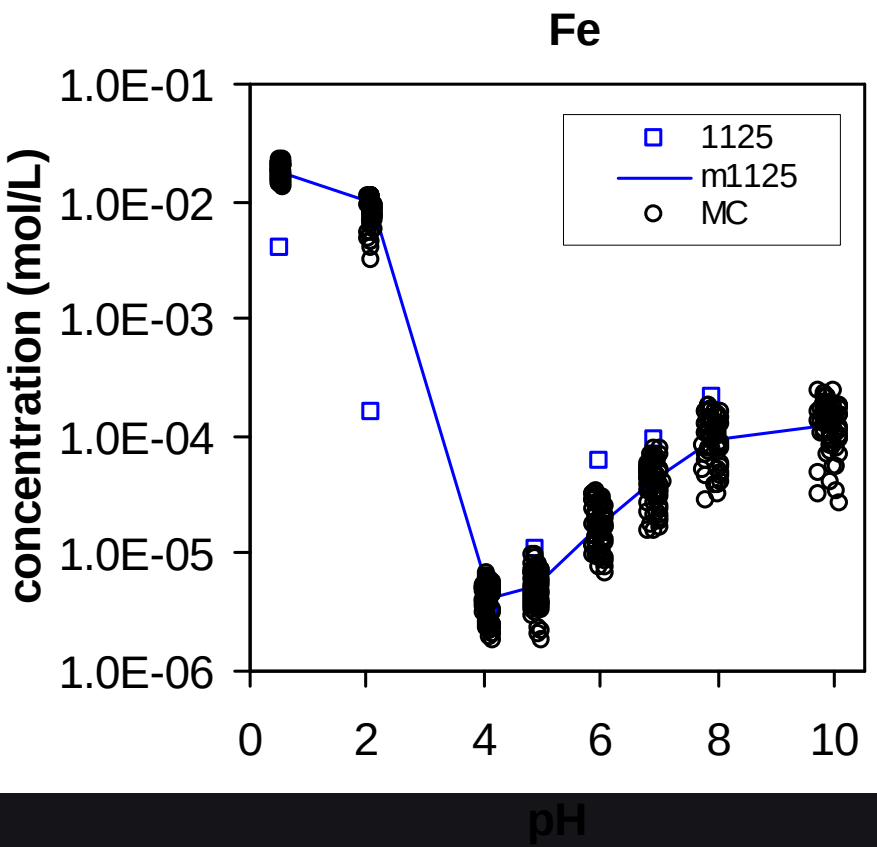


*) van Zomeren & Comans (2007) Environ. Sci. Technol. 41, 6755-6761.

Uncertainty in model predictions – Monte Carlo analysis

- **Key parameters:** e.g. contaminant availability, reactive surfaces, reactive fraction of DOC, competing ions
- **Thermodynamic constants:** e.g. solubility, complexation, sorption





Conclusions

- ✓ **Multi-surface geochemical modelling** based on fundamental thermodynamic parameters (no fitting!) → generic approach (variety of contaminated materials), e.g. for:
  - ➢ process identification
  - ➢ environmental risk assessment
- ✓ pH-dependent leaching/solubility → **"geochemical fingerprints"** of underlying processes that can be used to predict reactive transport of contaminants
- ✓ **New direction** in development of environmental (emission) limits in The Netherlands: mechanistic geochemical modelling
- ✓ Dominant role of **(dissolved) organic carbon** (humic and fulvic acids) in contaminant speciation and leaching from soils and other contaminated materials
- ✓ **Quantitative accounting of uncertainties** in model predictions required