

## Content

1	Introduction .....	5
2	Flow modeling.....	7
2.1	Basic terms.....	7
2.2	Steps in preparation of a flow model .....	8
3	Transport modeling.....	11
3.1	Basic terms.....	11
3.2	Example of transport modeling.....	14
3.2.1	Introduction.....	14
3.2.2	Used numerical tools.....	15
3.2.3	Input data and description of the model.....	15
3.2.4	Boundary conditions .....	16
3.2.5	Flow model.....	20
3.2.6	Calibration of the flow model .....	21
3.2.7	Calculation of different hydraulic variants.....	27
3.3	Transport model .....	29
4	Principles of hydrogeochemistry .....	35
4.1	Sampling of water and solids.....	35
4.2	Introduction to thermodynamics .....	40
4.3	Redox reactions.....	46
4.4	Geochemical kinetics.....	48
4.5	Adsorption and cation exchange.....	51
5	Geochemical modeling.....	59
5.1	Types and strategy of geochemical modeling.....	59
5.2	Types of geochemical programs .....	60
5.3	Examples of geochemical modeling .....	63
5.3.1	Speciation modeling.....	63
5.3.1.1	Principles and modeling strategy.....	63
5.3.1.2	Case study: speciation in arsenic affected aquifers in Bangladesh.....	65
5.3.2	Inverse geochemical modeling.....	73
5.3.2.1	Principles and modeling strategy.....	73
5.3.2.2	Case study: inverse geochemical modeling of the Guarani Aquifer system in Brazil .....	74

5.3.2.3	Case study: inverse geochemical modeling at site contaminated by petroleum hydrocarbons at Hnevice, Czech Republic.....	76
5.3.3	Forward geochemical modeling.....	79
5.3.3.1	Principles and modeling strategy.....	79
5.3.3.2	Case study: neutralization of acid mine drainage in a batch.....	82
5.3.3.3	Case study: titration of acid mine drainage water .....	83
6	Reactive transport modeling.....	85
6.1	Principles and modeling strategy.....	85
6.2	Case study: modeling of acid mine drainage neutralization .....	86
6.3	Case study: modeling of Cd adsorption in a column .....	89
6.4	Case study: modeling diffusion of tritium with decay in landfill liner.....	92
6.5	Case study: modeling of natural attenuation and iron cycling at Hnevice site, Czech Republic .....	94
6.6	Case study: reactive transport modeling of acid plume in sandstones .....	98
6.6.1	Site geology and hydrogeology.....	98
6.6.2	Hydrogeology.....	98
6.6.3	Reactive transport modeling .....	100
6.6.4	Simulation results.....	104
6.6.5	Conclusions.....	114
	Literature.....	115