Current Activities which Should Lead to an Article

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Introduction, List of Goals

- Main goal-depth specification of dissertation theme
- Overwiev of mathematical description and algebraic formulation used for reactive transport simulation
- Coupling of two softwares developed at TUL, Flow123d.exe and Semchem.exe under Linux
- Repeat the simulation published in Yeh(2009) with Semchem.exe and compare results obtained by Yeh

Simulation of reactive-transport undergroundwater flow including chemical equilibrium as well as kinetic reactions
Classification of chemical reactions from the Rubin's point of wiev:

- **Sufficiently fast and reversible**
- *Homogeneous*
- *Heterogeneous*
- Surface
- Classical
- **Insufficiently fast and/or irreversible**
- *Homogeneous*
- *Heterogeneous*
- Surface
- Classical

Each of mentioned types is described by another equation.

Overwiev of Mathematical Description and Algebraic Formulation Used for Reactive Transport Simulation

- methods are known for over 20 years
- fabulous article written by Rubin [6].
- software packages minteq [5] $\longrightarrow$ KEMOD [4], Yeh-Pensylvania State University, Northwest Laboratory
- complex software HYDROGEOCHEM [2] based on KEMOD
- application of HYDROGEOCHEM to ilustrative test examples [3]

In present time, Flow123D.exe doesn't include chemistry. Semchem.exe compputes chemistry and transpoort too, but it is too slow.
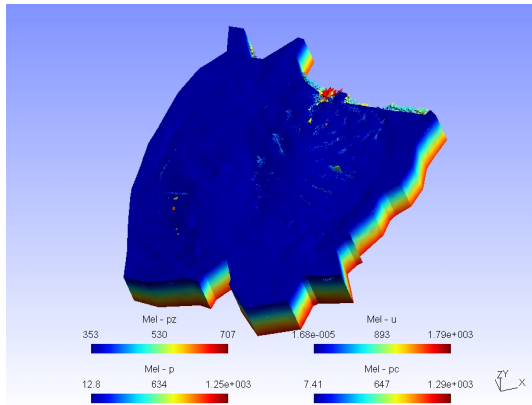
Repeat the Simulation Published in Yeh(2009) with Semchem.exe and Compare Results Obtained by Yeh

In [3] Yeh describes reactive transport whose reactive part consist of 33 reactions involving 42 species. Kinds of reactions are

- Mineral dissolution and surface site formation reactions
- Aqueous complexation reactions
- Adsorption-desorption reactions
- Ion-exchange reactions

Summary
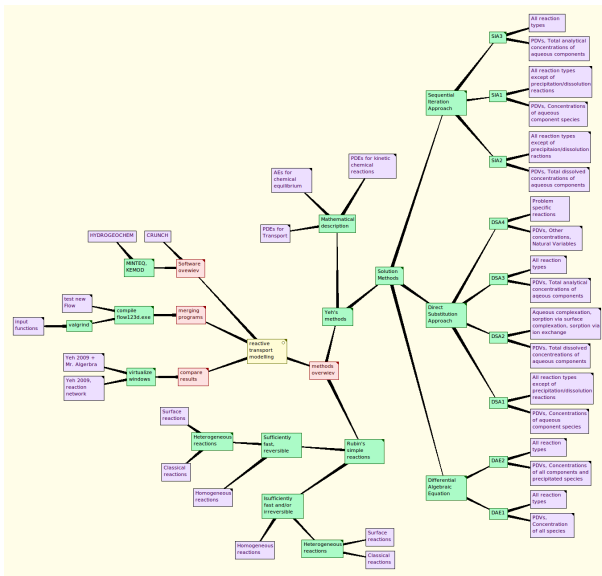
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Karel Hynek Mácha.