Karlsruhe Institute of Technology

Institute of Applied Geosciences (AGW)
Geothermal Energy and Reservoir Technology

Validation of thermodynamic databases for hydro-geochemical modeling in geothermal environments

Hydrogeochemical modeling approach to identify the bubbling point in geothermal brines

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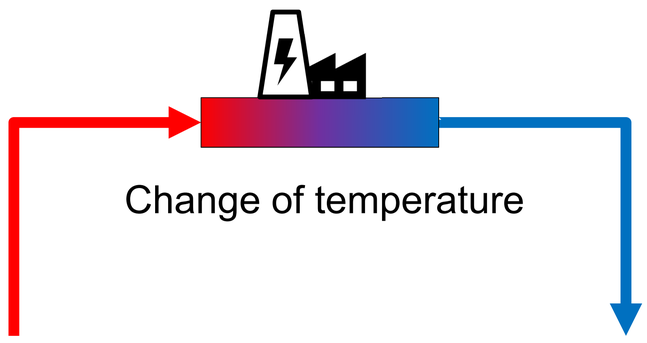
Background

- Brine is in equilibrium with reservoir
- Pressure reduction in the water column
- Potential formation of free gas phase
- pH shift due to H_2S and CO_2 degassing
- Carbonate precipitation
- Corrosion caused by acids



- Reduced solubility for most mineral phases
- Danger due to the occurrence of scaling
- Scaling reduces efficiency & productivity
  → Loss of revenue
- Increase in calcite solubility could lead to reservoir dissolution

Motivation

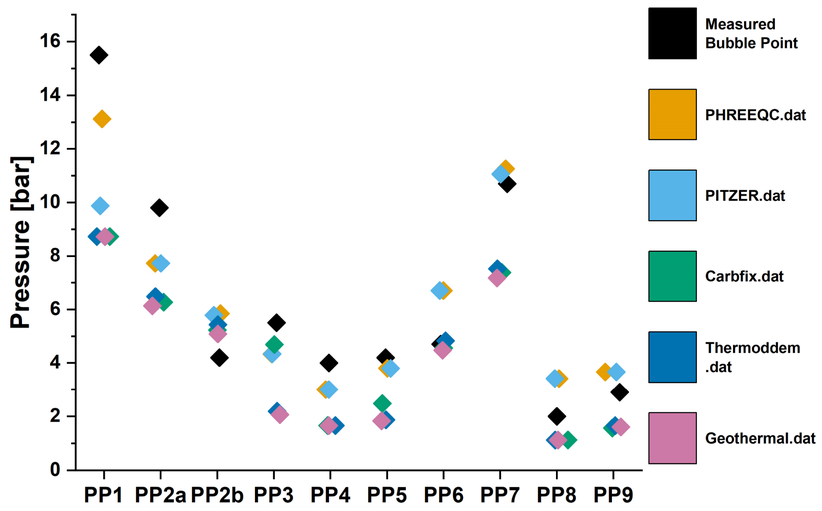
- Prediction of degassing and scaling issues through hydrogeochemical modeling – PHREEQC v3.7
- The program uses thermodynamic databases (TDB) for liquid, solid and gas phases
- Different TDBs use different thermodynamic data, equations of state (EOS) and models
- Not all relevant minerals included in one TDB
- Limitations on the **valid temperature** and **pressure** range apply to each individual TDB and should be extended to the full chemical setting in terms of **pH**, **salinity** and **redox**

Databases

- No published bubble point comparison yet
- Unique set of TDBs

	Origin	Gas EOS	P / T ranges	Unique features
Pitzer.dat Phreeqc.dat	Default TDBs for PHREEQC	Peng-Robinson	Up to 200 °C 1 to 1000 atm	Pitzer-Ion-Activity-Model Redox inactive gas species
LLNL.dat	Converted from Geochemist's Workbench	Ideal gas law	Range varies per mineral between 0 – 300 °C	Large number of species
Carbfix.dat	Result of the Carbfix2 project in Iceland	Peng-Robinson	Range varies per mineral between 0 – 350 °C	An advanced version of LLNL.dat
geothermal .dat	Special TDB for elevated temperatures	Ideal gas law	0 – 300 °C	Specialized for geothermal environments
Thermod dem.dat	From the BRGM for low temperature water-rock interactions	Ideal gas law	Individual for each mineral, mostly up to 300 °C	
YMP.dat soltherm.dat	Converted TDBs from THOUGH-REACT	Ideal gas law	Individual for each mineral, mostly 0 – 300 °C	Does not include methane

Bubble point modeling



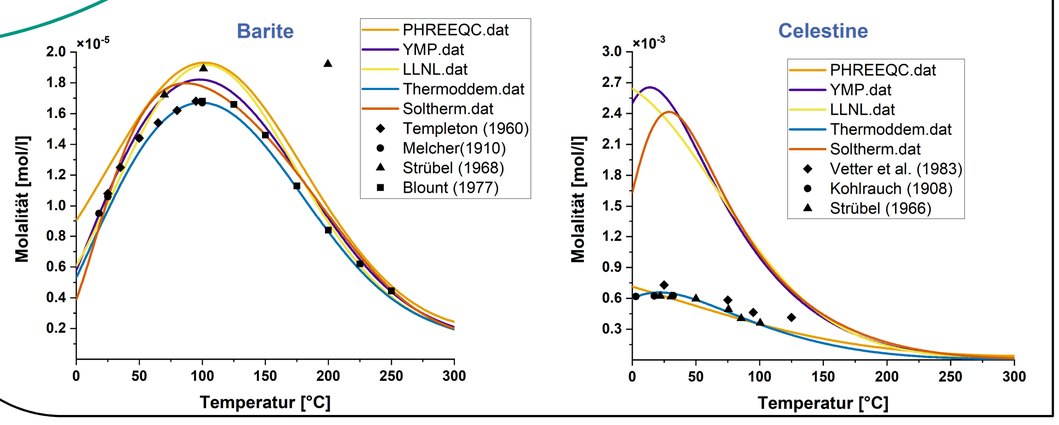
Comparison of the measured bubble point in several power plants (PP) with the predicted bubble point from different PHREEQC TDBs

Modeling approach

- Phreeqc.dat & Pitzer.dat use special approach to exclude N_2, CH_4 and H_2S from redox reactions
- Dissolve the measured gas phase in the brine and gradually reduce the pressure until the bubble point is reached and a free gas phase is formed
- To determine the accuracy of the solubility constants, a low saline brine was in equilibrium with the mineral phase under study
- Experimental data closest to the hydrochemistry of the Bavarian Molasse Basin have been selected
- Solubility validation performed for 22 scaling forming minerals

Solubility modeling

- Experimental data is used as a reference to evaluate the accuracy of the modeling
- The evaluation depends on the quality of the available experimental data



Conclusion

- Active redox reactions of the gas-forming species reduce the bubble point
- Results are highly dependent on location and gas phase composition
- Tendency to underestimate the bubble point in the model
- High uncertainties in the measured data, especially the bubble point
- Merge the best fit to experimental data for each mineral into a new database

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