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Evaluation, compilation and comparison of state of the art PHREEQC thermodynamic database files to generate a new one

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Geochemical modelling what for?

- ❑ Water-rock-gas-interactions
- ❑ Mineral precipitation
- ❑ CCS and geothermal exploration
- ❑ Nuclear waste repository
- ❑ Raw material extraction

What's the catch with geochemical modelling?

- Geochemical modelling software needs a thermodynamic database file (TDF) containing thermodynamic quantities like Gibbs Free Energy or solubility constant K of every aqueous, mineral and gaseous species involved
- Individual TDFs are based on varying sources for thermodynamic quantities
- Resulting in deviating model outcomes due to different TDFs used

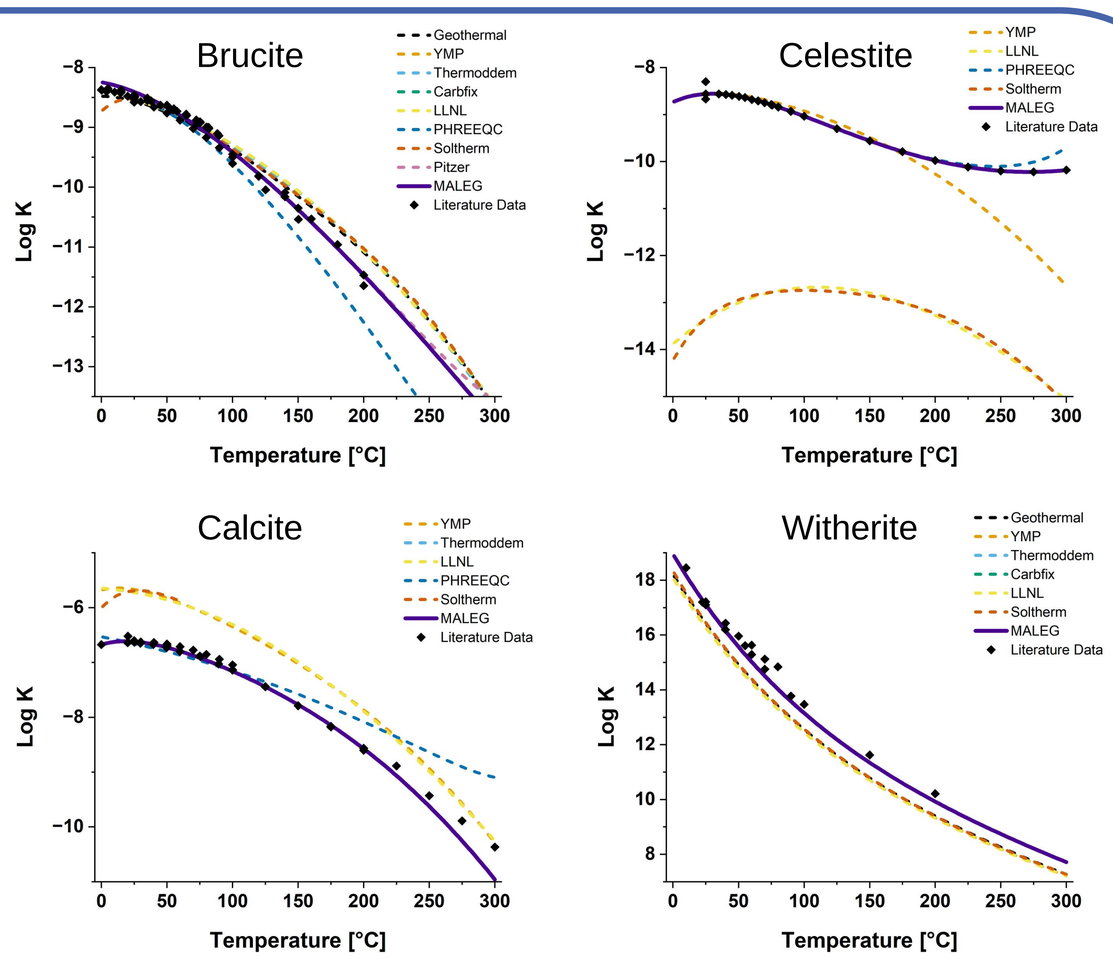
Thermodynamic data constraints

- Thermodynamic quantities are derived from experiments with certain uncertainty and different approaches
- The usable T-P conditions are extrapolated from the valid experimental ranges
- The further away from known values, the higher the deviation

TDF differences

- Contain different species or different reaction paths
- Use different equations of states
- Valid T-P conditions differ for each development concept
- Source of thermodynamic quantities may not be traceable
- Thermodynamic quantities for a species need to be consistent with each other

➡ Compare modelled solubility constant *K* of different TDFs with evaluated literature data to determine best fit to investigate geothermal power plant processes. Snapshots can be seen to the right, full comparison has been done for over 20 mineral phases. MALEG TDF can be downloaded by following the left QR code at the bottom of the poster.



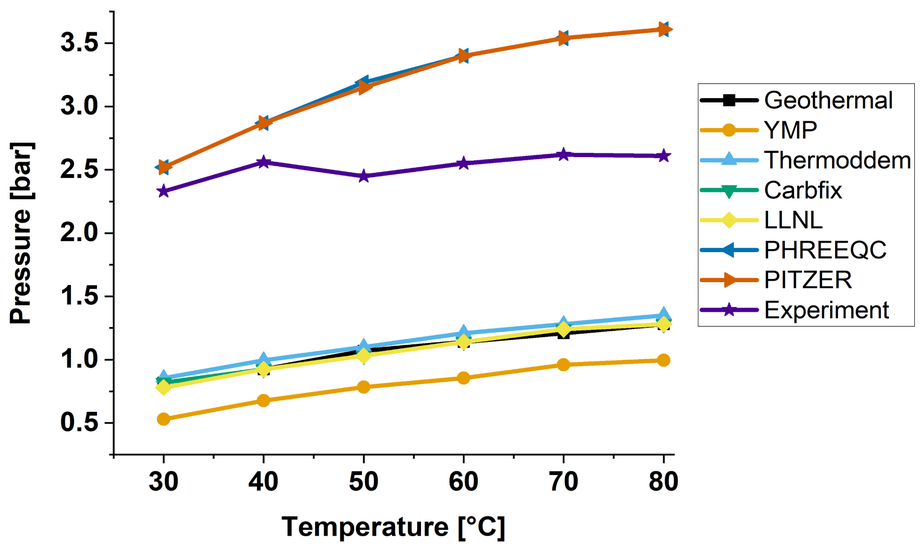
Comparison between modelled vs. measured bubble point in dependance of temperature at a geothermal power plant in the Bavarian molasse basin

- Experiments were conducted in a bypass string under in-situ conditions of the power plant
- The gas bubbles were captured in a specially constructed container
- Each measurement ran for 12 hours
- Only a small portion of the dissolved gas species ventured into the gaseous phase

➡ Only 2 TDFs are kind of close to the experimental data. The TDFs cant reproduce the processes well and either more data is needed or a refinement of the underlying methodology.

Concentration of the completely dissolved gas phase constituents

Gas phase	Nitrogen	Carbon dioxide	Methane	Hydrogen sulfide
Concentration [mmol/l]	0.92	6.88	1.43	0.19



Conclusions and Outlook

- Experimental data are the basis for reliable thermodynamic parameters and accurate modelling results
- Selecting a TDF specialized for the specific problem is key
- Additional efforts are required to generate high-quality experimental data at elevated temperatures, pressures, and varying pH values
- Addressing the data gap for minerals that cannot be investigated with currently available laboratory equipment

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