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Thermolab: a thermodynamics laboratory for non-linear transport processes in open systems

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We developed a numerical thermodynamics laboratory called "Thermolab" to study the effects of the thermodynamic behavior of non-ideal solution models on reactive transport processes in open systems. The equations of state of internally consistent thermodynamic datasets are implemented in MATLAB functions and form the basis for calculating Gibbs energy. A linear algebraic approach is used in Thermolab to compute Gibbs energy of mixing for multi-component phases to study the impact of the non-ideality of solution models on transport processes. The Gibbs energies are benchmarked with experimental data, phase diagrams and other thermodynamic software. Constrained Gibbs minimization is exemplified with MATLAB codes and iterative refinement of composition of mixtures may be used to increase precision and accuracy. All needed transport variables such as densities, phase compositions, and chemical potentials are obtained from Gibbs energy of the stable phases after the minimization in Thermolab. We demonstrate the use of precomputed local equilibrium data obtained with Thermolab in reactive transport models. In reactive fluid flow the shape and the velocity of the reaction front vary depending on the non-linearity of the partitioning of a component in fluid and solid. We argue that non-ideality of solution models has to be taken into account and further explored in reactive transport models. Thermolab Gibbs energies can be used in Cahn-Hilliard models for non-linear diffusion and phase growth. This presents a transient process towards equilibrium and avoids computational problems arising during precomputing of equilibrium data.