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Abstract

Computational methods in chemical equilibrium thermodynamics have found numerous application areas in diverse fields such as metallurgy, petrochemistry, the pulp and paper industry, the study of advanced inorganic materials, environmental science and biochemistry. As many of the cases of interest are not actually in equilibrium, there is a need for methods that extend the application area of multiphase equilibrium solvers to non-equilibrium systems. Likewise there is a need for efficient handling of thermochemical systems that are described by parameters other than those most commonly associated with Gibbs energy, namely temperature, pressure and fixed elemental (and charge) balances.

In the work computational methods and related theory are presented that can be used with a standard Gibbs energy minimiser to solve advanced thermochemical problems. The actual calculations have been performed using the ChemSheet software, but the presentation has aimed to be generic and applicable to other thermochemical codes that allow the user to define thermodynamic data and the stoichiometries of the constituent species in the system.

The examples discussed include electrochemical Donnan equilibrium (particularly applied to aqueous pulp suspensions), surface and interfacial energies of liquid mixtures, systems affected by external magnetic fields and