

Constrained and Generalized Free Energy Models Using ChemSheet

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ABSTRACT

Theory and computational methods to solve equilibrium and non-equilibrium problems that are defined by conditions such as external magnetic field, fixed surface area or sub-volume, external magnetic field or constrained reaction or mass transfer extents using ChemSheet/ChemApp are presented.

New virtual components are defined to the system stoichiometry to either correspond to the added constraint such as surface area or extent of reaction, or to facilitate the adjustment of the molar free energy based on the added work term (such as magnetic work) or equivalent free energy contribution (biochemical systems with fixed pH or ionic strength). If necessary, the standard state chemical potential, corresponding to pure substance in the new conditions may also be redefined.

Application areas include systems para-equilibrium systems, paramagnetic systems, surface energies of mixtures, adjusted standard states in biochemical systems, nanoparticles and time development of reactive systems.