From Pyro to Bio:
Applications of the Constrained Gibbs Energy Method

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ABSTRACT

During the last decade, ChemSheet software and its sister products have been adapted by both industrial users and active scientists worldwide. Due to the generic modelling principles of the ChemApp programming library and its flexible connection through ChemSheet with various computational tools, the applications range from high temperature systems to biochemical analysis, including materials chemistry, industrial reactor scale-up and process simulation. Industrial models and expert systems have been developed e.g. for chemical industry, pulp and paper, cement and lime manufacturing, metallurgy, steelmaking, power production and environmental technologies.

Within ChemSheet, the new Constrained Free Energy method has been developed, allowing for the use of immaterial constraints in the conservation matrix of the minimization problem. The new method enables the association of the conservation matrix with structural, physical, chemical and energetic attributes. Thus the scope of free energy calculations can be extended beyond the conventional studies of global chemical equilibria and equilibrium phase diagrams. The presentation will cover the application of the Constrained Free Energy method for reactive phase diagrams, giving some examples on industrial process simulation and including biochemical research.