

## Thermodynamic modeling of HIX part of the Iodine – Sulfur thermocycle

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The thermochemical water splitting cycle is an environmentally attractive way to produce hydrogen without using fossil fuels. Among a hundreds possible cycles, the sulfur – iodine (IS) is a promising one, expected to become a major source of hydrogen production from nuclear or solar energy.

The IS process cycle is divided into three sections; namely: (1) the Bunsen section whose purpose is to produce the two immiscible liquid acid phases: one containing mainly sulfuric acid and the other hydrogen iodide and iodine (2) sulfuric acid concentration and decomposition section and (3) Hydrogen iodide concentration and decomposition section, known by HIX section.

The thermodynamics of aqueous sulfuric acid system has already been described by chemical engineers and the challenge actually remains in describing the thermodynamics of the HIX system ( $\text{H}_2\text{O} - \text{HI} - \text{I}_2$ ) which is a strong electrolyte system, extremely complex because of various phase behavior that occurs (vapor – liquid – liquid – solid) over the large range of pressure and temperature spanned in the process.

A review of existing models shows that two approaches can be adopted to deal with phases equilibrium ; (1) homogeneous one in which the same equation of state is applied to different phases in equilibrium and (2) combined approach where the vapor phase is described by an equation of state and the liquid one by a coefficient activity model.

The homogeneous approach would be effective for the high pressure HIX system but cannot capture alone the strong non ideality of the liquid phase. That may explain why the current HIX model written by Neumann<sup>i</sup> has been done based on an activity coefficient model coupled with a solvation formalism proposed by Engels<sup>ii</sup>. Unfortunately, activity coefficient models fail for critical compounds in mixtures as is the case for HI under temperature conditions expected in the process.

Based on this analysis, we propose a novel modeling of the HIX system that matches all the constraints enounced.

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<sup>i</sup> Neumann D., 1987, Diplomaufgabe, RWTH Aachen.

<sup>ii</sup> Engels H., 1990, “Phase equilibria and phase diagrams of electrolytes”. Chemistry data Series, Volume XI, Part I. Published by DECHEMA.