Bunsen section thermodynamic model for hydrogen production by the sulfur–iodine cycle

Mohamed Kamel Hadj-Kali[a,b], Vincent Gerbaud[a,b,*], Patrick Lovera[c], Olivier Baudouin[d], Pascal Floquet[a,b], Xavier Joulia[a,b], Jean-Marc Borgard[c], Philippe Carles[c]

[a]Université de Toulouse, INP-ENSIACET, UPS, LGC (Laboratoire de Génie Chimique), 4 allée Emile Monso, BP 74233, F-31432 Toulouse
Cedex 4, France
[b]CNRS, LGC (Laboratoire de Génie Chimique), 4 allée Emile Monso, F-31432 Toulouse Cedex 4, France
[c]CEA, DEN, Physical Chemistry Department, F-91191 Gif-sur-Yvette, France
[d]ProSim, Stratège Bâtiment A, BP 27210, F-31672 Labège Cedex, France

article info

abstract

A model for the Bunsen section of the Sulfur–Iodine thermo-chemical cycle is proposed, where sulfur dioxide reacts with excess water and iodine to produce two demixing liquid aqueous phases (H_2SO_4 rich and HI rich) in equilibrium. Considering the mild temperature and pressure conditions, the UNIQUAC activity coefficient model combined with Engels' solvation model is used. The complete model is discussed, with HI solvation by water and by iodine as well as H_2SO_4 solvation by water, leading to a very high complexity with almost hundred parameters to be estimated from experimental data. Taking into account the water excess, a successful reduced model with only 15 parameters is proposed after defining new apparent species. Acids total dissociation and total H_β solvation by water are the main assumptions. Results show a good agreement with published experimental data between 25 _C and 120 _C.