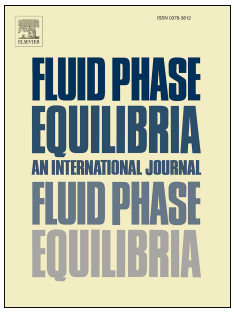
Accepted Manuscript



Thermodynamic modeling of the hybrid sulfur (HyS) cycle for hydrogen production

Harnoor Kaur, Meng Wang, Maximilian B. Gorensek, Chau-Chyun Chen

PII: S0378-3812(17)30509-5

DOI: 10.1016/j.fluid.2017.12.025

Reference: FLUID 11698

To appear in: *Fluid Phase Equilibria*

Received Date: 27 July 2017

Revised Date: 19 December 2017

Accepted Date: 20 December 2017

Please cite this article as: H. Kaur, M. Wang, M.B. Gorensek, C.-C. Chen, Thermodynamic modeling of the hybrid sulfur (HyS) cycle for hydrogen production, *Fluid Phase Equilibria* (2018), doi: 10.1016/j.fluid.2017.12.025.

Thermodynamic Modeling of the Hybrid Sulfur (HyS) Cycle for Hydrogen Production

Harnoor Kaur[1], Meng Wang[1], Maximilian B. Gorensek[2], Chau-Chyun Chen[1,*]

[1]Department of Chemical Engineering, Texas Tech University, Lubbock, TX 79409-3121, USA

[2]Savannah River National Laboratory, Aiken, SC 29808, USA

* Corresponding author. Tel.: +1 806.834.3098. Email address: chauchyun.chen@ttu.edu

Abstract

We have developed a comprehensive thermodynamic model for the ternary system sulfur dioxide + sulfuric acid + water based on a previously published thermodynamic model of the aqueous sulfuric acid system using the symmetric electrolyte NRTL (eNRTL) activity coefficient model. The eNRTL binary interaction parameters and the chemical equilibrium constants are regressed from experimental SO_2 solubility data in aqueous sulfuric acid solutions. The model accurately represents all thermodynamic properties including vapor-liquid equilibrium, liquid-liquid equilibrium, calorimetric properties, and speciation over a wide acid concentration range, from pure water to pure sulfuric acid and pure sulfur dioxide, and temperatures from 273.15 to 393.15 K. The model should be very useful in supporting process research, development, and design of advanced water-splitting processes based on the hybrid sulfur (HyS) cycle.

Keywords:

sulfur dioxide, sulfuric acid, electrolyte NRTL model, water-splitting, hybrid sulfur cycle