Transactions of the Korean Nuclear Society Spring Meeting
Jeju, Korea, May 10-11, 2007

Modeling of a Stoichiometric Bunsen Reaction

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1. Introduction

IS (Iodine-Sulfur) process consists of three coupled reactions described in equations (1)~(3). The net reaction is that one mole of water dissociates into one mole of hydrogen and a half mole of oxygen as in equation (4).

$SO_2 + I_2 + 2H_2O \rightarrow H_2SO_4 + 2HI$ ------(1)
$H_2SO_4 \rightarrow SO_2 + H_2O + 1/2\ O_2$ ---------(2)
$2\ HI \rightarrow I_2 + H_2$ -------------------------- -(3)
$H_2O \rightarrow H_2 + 1/2\ O_2$ --------------------- (4)

The equation (1) is known as a Bunsen reaction. Stoichimetrically speaking, one mole of iodine, one mole of sulfur dioxide and 2 moles of water react to produce 1 mole of sulfuric acid and 2 moles of hydrogen iodide in Bunsen reaction. The reactants, SO_2 and I_2, are recycled from equation (2) and equation (3), respectively.

The purpose of this study is to establish the simulation model of a stoichiometric Bunsen reaction in the IS process using unit and flow-sheet models that is provided by chemical process simulator.

2. Modeling of a Stoichiometric Bunsen Reaction

2.1 Process Description

In Bunsen reaction, I_2 and SO_2, the products of sulfuric acid decomposition and HI decomposition reaction respectively, are recycled to a Bunsen reactor. These components are mixed and reacted with water and forms liquid mixture which are later separated into heavy phase solution(HI_x), light phase solution(H_2SO_4), and gas phases(SO_2, H_2O).

In the booster reactor, SO_2 and I_2 are combined with H_2O to produce H_2SO_4 and HI_x by the reverse Bunsen reaction. The concentration of sulfuric acid with light phase solution increases.

O_2 is purified in the scrubbing column before it is discharged into the atmosphere. In the upper part of scrubbing column, O_2 is purified by contacting with pure water. In the lower part of the column, large amount of I_2 in the scrubbing water reacts with SO_2 to produce H_2SO_4 and HI.

2.2 Simulation Models

1) Bunsen reactor

Most of Bunsen reaction takes place in the Bunsen reactor. Small amount of Bunsen reaction takes place in sulfuric acid booster, SO_2 absorption tower and O_2 scrubber.

The Bunsen reactor is simulated as a RSTOIC that can properly describe the stoichiometric equation.

2) Three-phase Separator

Three-phase Separator, one of the most important units in Bunsen reaction, splits the Bunsen reaction products into (1)heavy HIx phase, (2) light H_2SO_4 phase, and (3) gas phase. This is simulated as a 3 phase separator model.

3) Sulfuric acid boost reactor

In the sulfuric acid boost reactor, the concentration of the sulfuric acid is concentrated from 15 mole% to 20 mole %. At the top of the booster reactor, the sulfuric acid proceeds to section II and O_2 proceeds to O_2 scrubber. At the bottom, the mixture of $HI/I_2/H_2O$ is recycled to Bunsen reactor. The Sulfuric acid boost reactor is simulated as a combination of RSTOIC model and Flash tank.

4) SO_2 Absorption Tower

The liquid product from the bottom of O2 scrubber is mixed with $HI/I_2/H_2O$ recycled from reaction(3), and proceeds to SO_2 absorption tower. In SO_2 absorption tower, this mixture reacts with SO_2 from HIx/SO_2 stripper and further proceed to reaction(2). This is simulated as a RADFRAC model.

5) O_2 scrubber

In O_2 scrubber, Bunsen reaction takes place. O_2 gas is purified as the small amount of SO_2 that was contained in the O_2 is removed by Bunsen reaction. . Most of purified O_2 is vented to the atmosphere and a part of O_2 is recycled to H_2SO_4 stripping tower to strip SO_2. O_2 scrubber is simulated as a combination of RSTOIC and Flash tank model.

6) Pumps, Compressors, etc.

The other units such as pump, compressor, and valve are simulated with the standard model in the chemical process simulator for this unit. The unit models and streams are connected each other with mixers and splitters.

3. Results

Unit models and corresponding flow streams have been developed for the stoichiometric Bunsen reaction with chemical process simulator. These unit models and flow streams have been integrated to develop overall simulated flow-sheet for Bunsen reaction. It is shown in Fig. 1. The overall flow-sheet for Bunsen reaction can be modified when more accurate and reliable thermodynamic data are produced in the future.

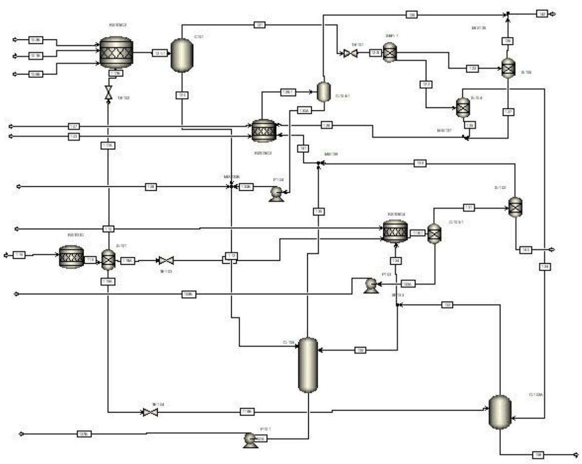

Fig. 1. Overall simulated flow-sheet for Bunsen Reaction

ACKNOWLEDGEMENTS

This study has been carried out under the Nuclear R & D Program supported by the Ministry of Science and Technology (MOST) of Korea.

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