Modeling of Evaporation and Decomposition Processes of $\text{H}_2\text{SO}_4$ in SI Cycle

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Outline

- Basic Concepts of Chemical Process Simulator
- Overview of the SI Cycle - Section 2 Process
- Modeling of Sulfuric Acid Evaporation Process
- Modeling of Sulfuric Acid Decomposition Process
- Summary
Basic Concept of Chemical Process Simulator

- **Models**
  - Characteristic equations of a chemical process with a computer program

- **Uses underlying physical relationships**
  - Mass balance, enthalpy balance
  - Equilibrium relationships
  - Rate correlations (reaction and mass/heat transfer)

- **Predicts**
  - Stream flow rates, compositions and physical properties
  - Equipment sizing, cost evaluation, process optimization

- **Answers “what if” questions**
  - Effective in SI process design
Basic Concept of Chemical Process Simulator

**Structure**

- Comp.1
- Comp.2
- Comp.3

**Thermodynamic method**

- Method A
- Method B
- Method C

**Database**

- Density
- Vapor-Liquid Equilibrium
- Enthalpy
- Entropy
- etc., (Mixed Component)

**Properties for process simulation**

**Types of the simulator**

- Aspen Plus
- ChemCAD
- Prosim
Overview of the SI Cycle

Section 1

Bunsen Reactor

H2SO4, H2O

HI, I2

HI Phase Purifier

Electro-Electrodialysis

HI Distillator Column

HI Decomposer

H2

Gas Separator

HI

HI, I2

Buffer

HI, I2

SO2, O2

H2O

HI, I2

HI Phase Purifier

Liquid Phase Separator

H2SO4 Phase

H2SO4 Concentrator

H2SO4 Purifier

Decomposer

Gas-Liquid Separator

H2O Input

HI

O2

Section 2

Section 3
Overview of the SI Cycle

- The function of Section 2

  - Concentration of Sulfuric Acid
    - less material heat to high temperature means less sensible heat must be supplied.
    - smaller heat exchanger
    - less cost

  - Decomposition of Concentrated Sulfuric Acid
Modeling of Sulfuric Acid Evaporation Process

- **Isobaric Concentrator (1)**

  - **Description:**
    - The sulfuric acid is pumped to the operating pressure of isobaric concentrator.
    - The concentration increases at the exit of isobaric concentrator.

  - **Modeling:**
    - Isobaric concentrator is modeled as the heater followed by an adiabatic flash tank.
### Vacuum Distillation Column(2)

- **Description**:
  - The liquid product of isobaric concentrator is further concentrated in a series of three reduced pressure flashes before entering the vacuum distillation column.
  - The bottom product of the vacuum distillation column is almost concentrated to the azeotropic concentration.

- **Modeling**:
  - Vacuum distillation column is modeled with the combination of flash tanks and RADFRAC.
Modeling of Sulfuric Acid Evaporation Process

- Isobaric Concentrator(1)
Modeling of Sulfuric Acid Evaporation Process

- Vacuum Distillation Column(2)
Modeling of Sulfuric Acid Decomposition Process

- **Recuperator**

  - **Description**:
    - The sulfuric acid is heated to the vaporization temperature in the recuperator.
    - Some of the sulfuric acid decomposes into SO$_3$ and H$_2$O.
    - The recuperator retrieves much of the heat remaining after sulfuric acid decomposition.

  - **Modeling**:
    - The recuperator is modeled as two Gibbs reactors coupled by a heat stream.
Modeling of Sulfuric Acid Decomposition Process

- **Decomposer**

  • Description:
    - SO$_3$ decomposes into SO$_2$ and O$_2$.
    - Small amount of undecomposed H$_2$SO$_4$ is decomposing into SO$_3$ and H$_2$O.
    - The outlet stream from decomposer is cooled, transferring heat to the decomposer feed.

  • Modeling:
    - The decomposer is modeled as a series of four Gibbs reactors.
Modeling of Sulfuric Acid Decomposition Process
Modeling of Sulfuric Acid Evaporation Process

- Sulfuric Acid Fraction Change in Process Stream
Modeling of Sulfuric Acid Decomposition Process

- Mole Fraction Change in Process Stream
Modeling of Sulfuric Acid Decomposition Process

- Mole Fraction Change vs. Temp.
Complete Simulation Flowsheet for Section 2

1. Feed to section 1
2. 3-cooker
   \[SO_3 + H_2O = H_2SO_4\]
3. 4-stage isobaric concentrator
4. Recuperator 1
5. 4-stage decomposer: decomposition of \(SO_3, H_2SO_4\)
6. Recuperator 2
7. Vacuum distillation column
8. Water to section 1
9. Concentrated sulfuric acid
10. Preheater
Summary

- The flow-sheet for the sulfuric acid evaporation and decomposition processes has been developed based on the S-I cycle.

- Some sensitivity analyses indicate that:
  - Concentration is more effective in vacuum distillation column than in isobaric concentrator.
  - Most of the sulfuric acid has decomposed into SO$_3$ and H$_2$O at the exit of recuperator.
  - In the decomposer, most of SO$_3$ has decomposed into SO$_2$ and O$_2$ with small amount of H$_2$SO$_4$ decomposition.
THANK YOU!