
Modeling of Evaporation and Decomposition Processes of H₂SO₄ in SI Cycle

2007. 4. 17

Jong Ho KIM

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**

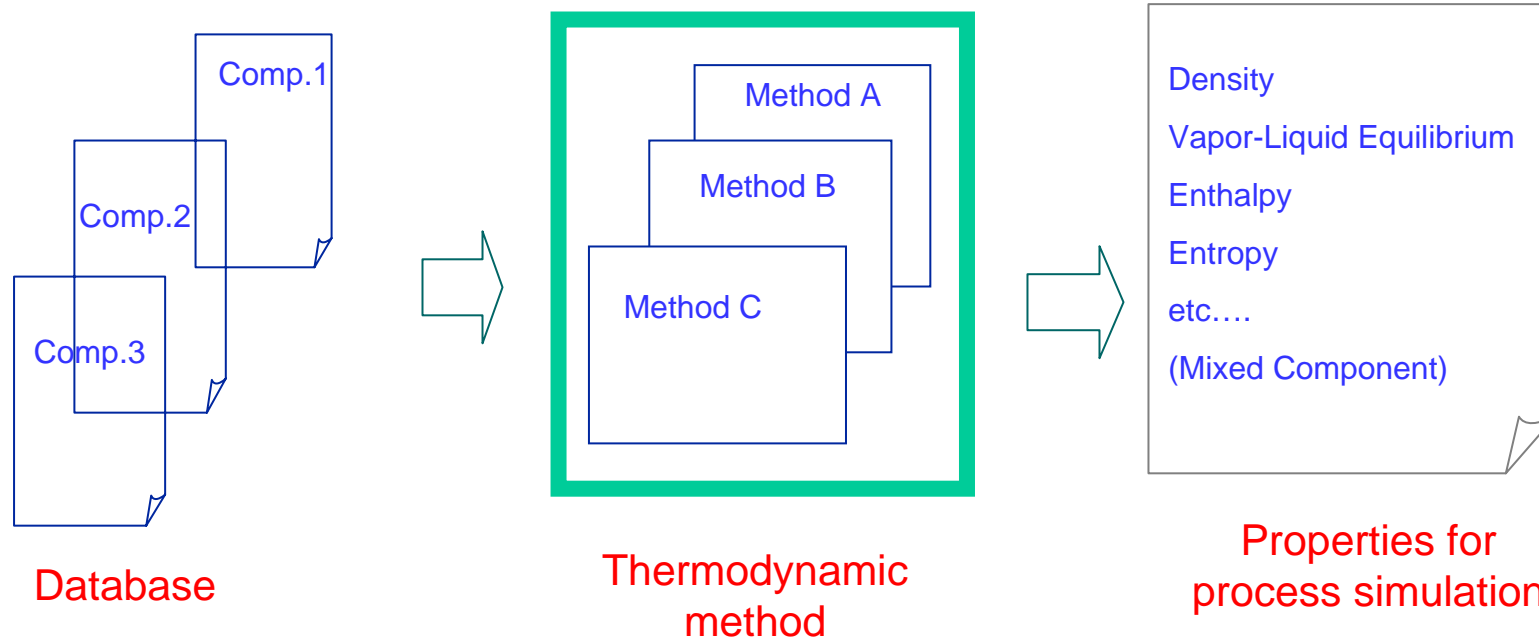
- **Stream flow rates, compositions and physical properties**
- **Equipment sizing, cost evaluation, process optimization**

■ **Answers “ what if” questions**

- **Effective in SI process design**
-

Basic Concept of Chemical Process Simulator

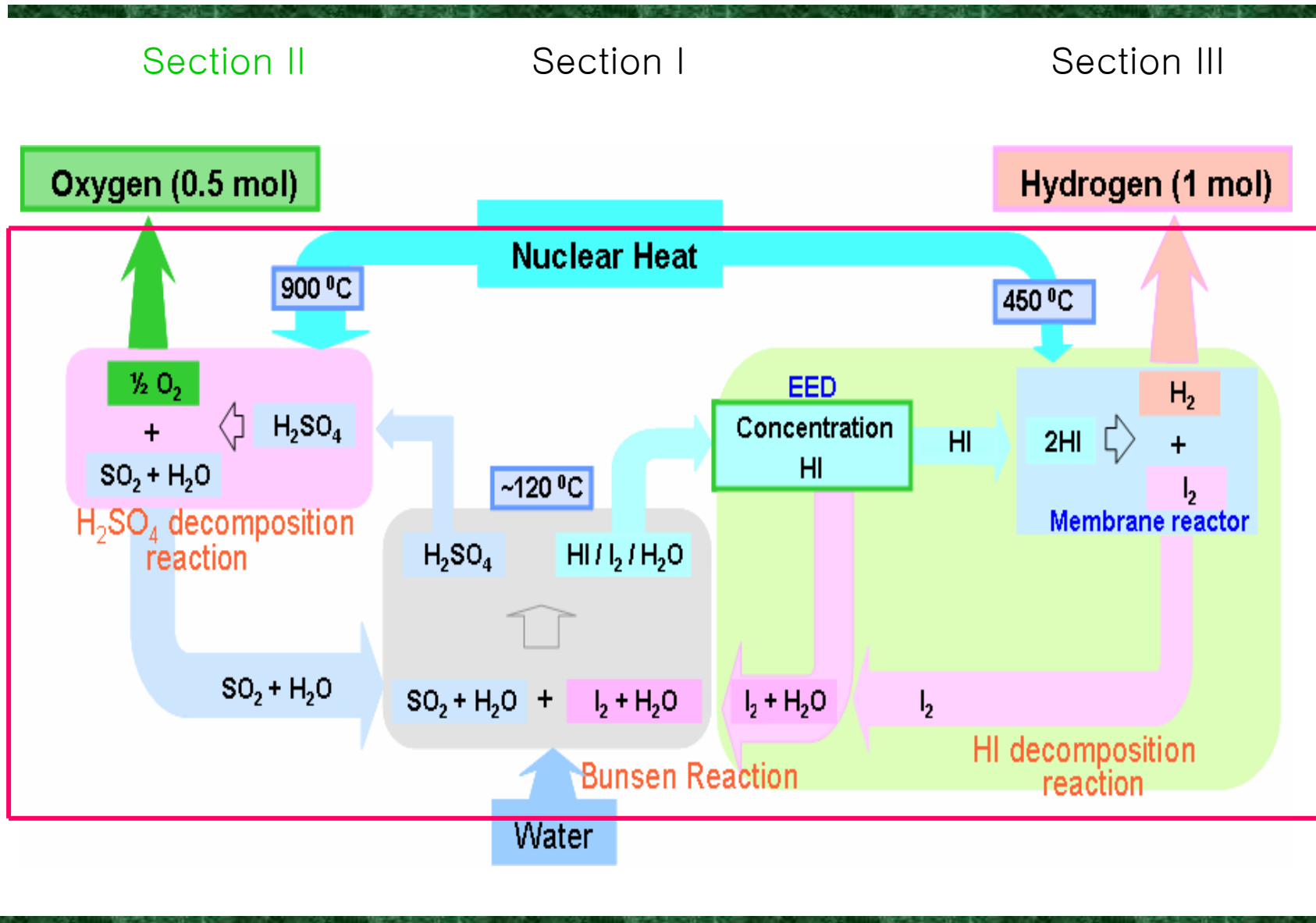
■ Structure



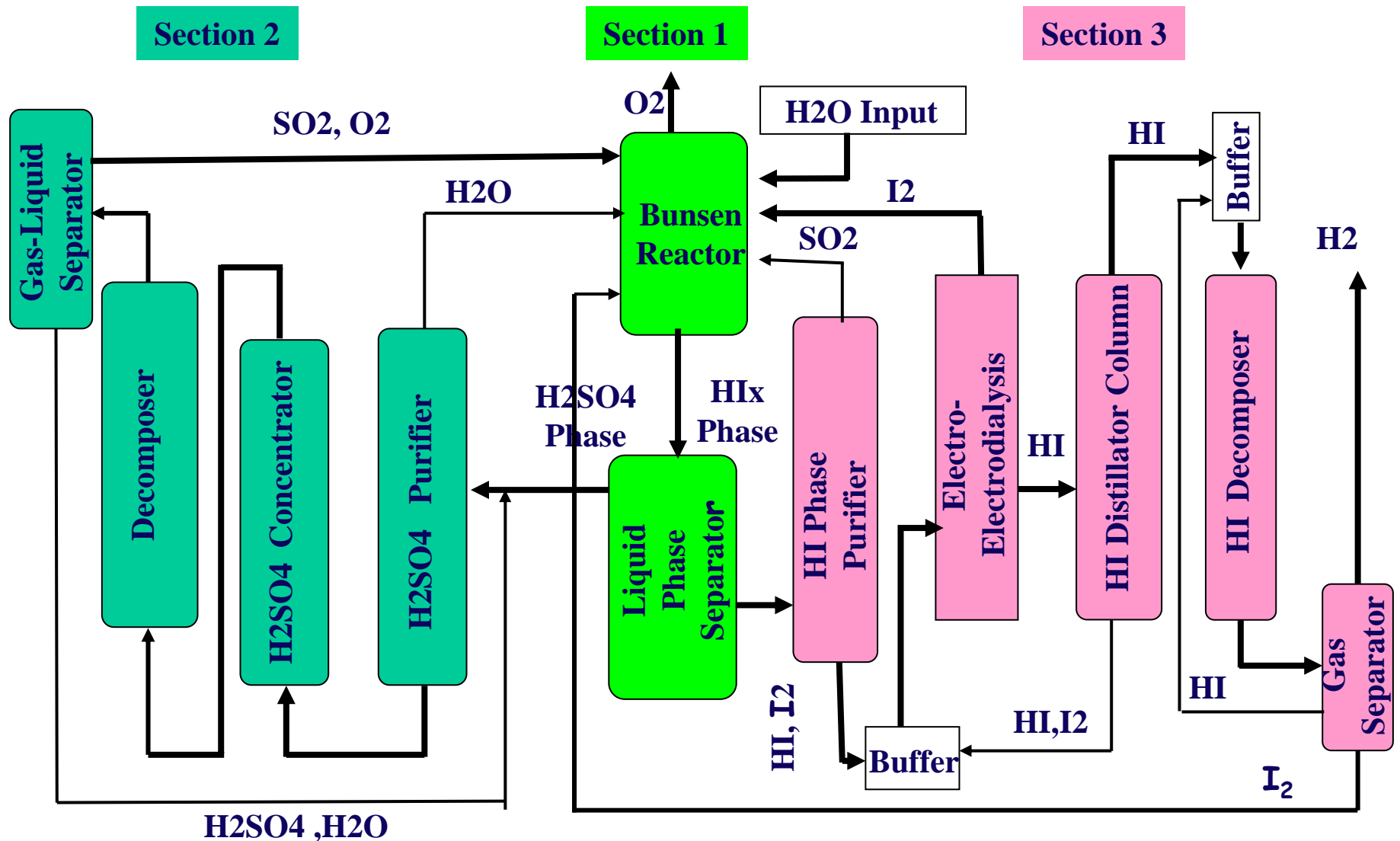
■ Types of the simulator

- Aspen Plus
- ChemCAD
- Prosim

Overview of the SI cycle



Overview of the SI Cycle



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.
-

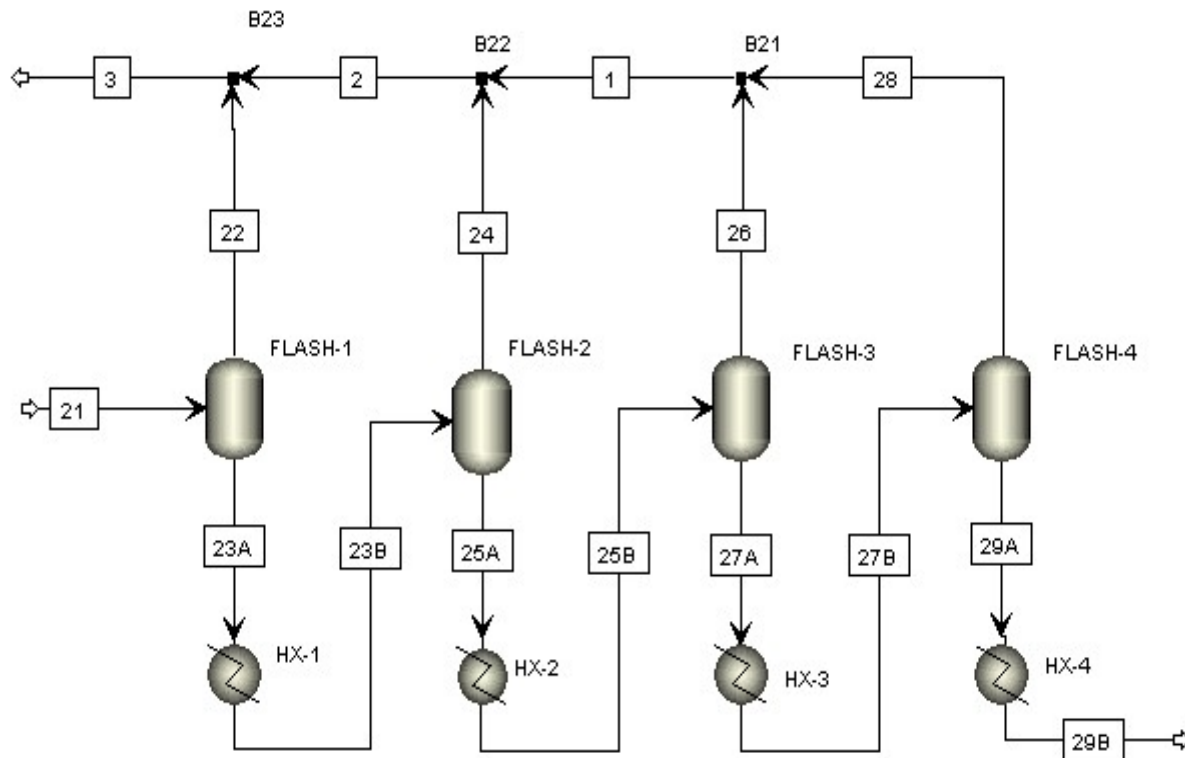
Modeling of Sulfuric Acid Evaporation Process

■ 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.
-

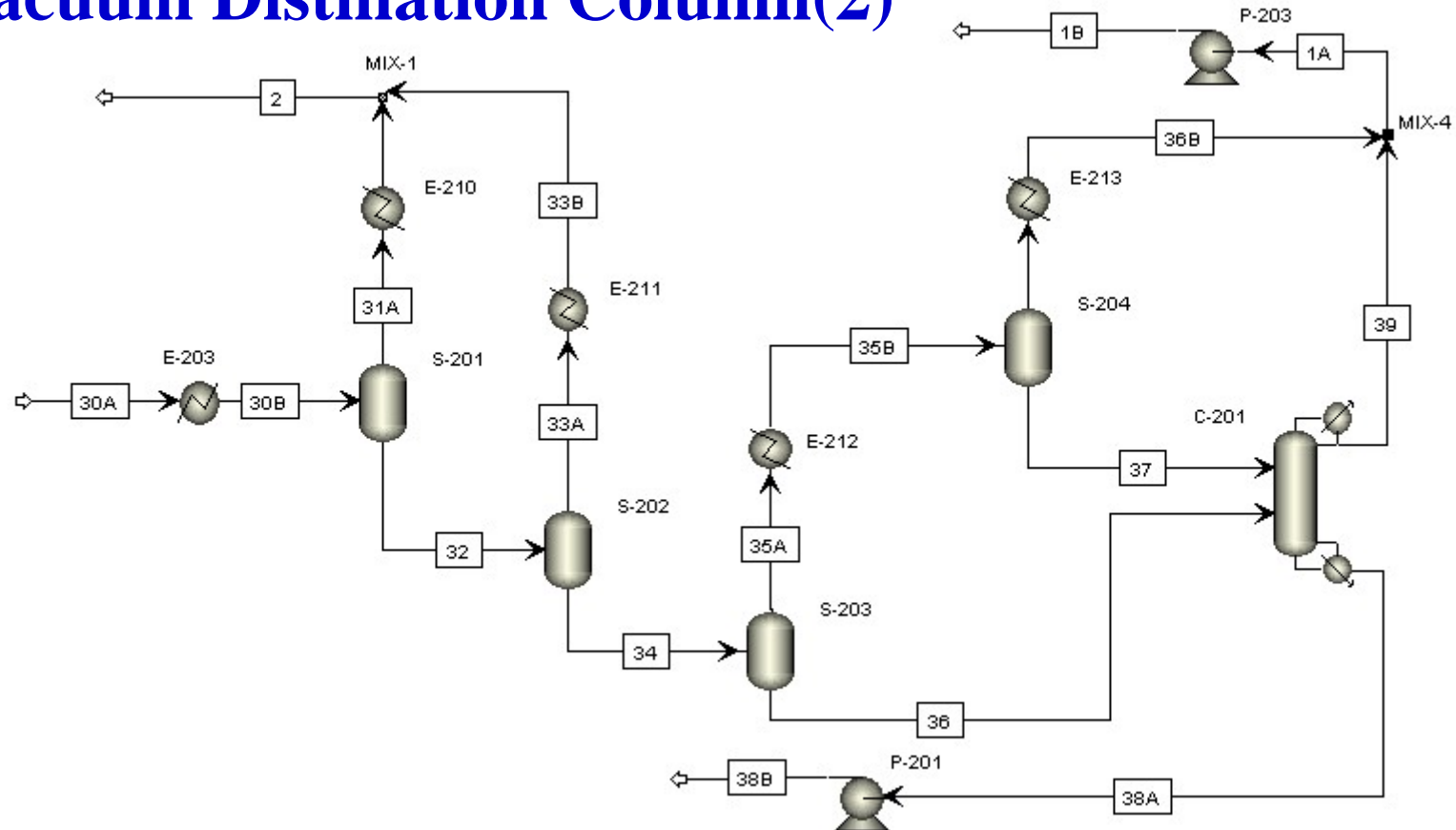
Modeling of Sulfuric Acid Evaporation Process

■ Isobaric Concentrator(1)



Modeling of Sulfuric Acid Evaporation Process

■ Vacuum Distillation Column(2)



Modeling of Sulfuric Acid Decomposition Process

■ Recuperator

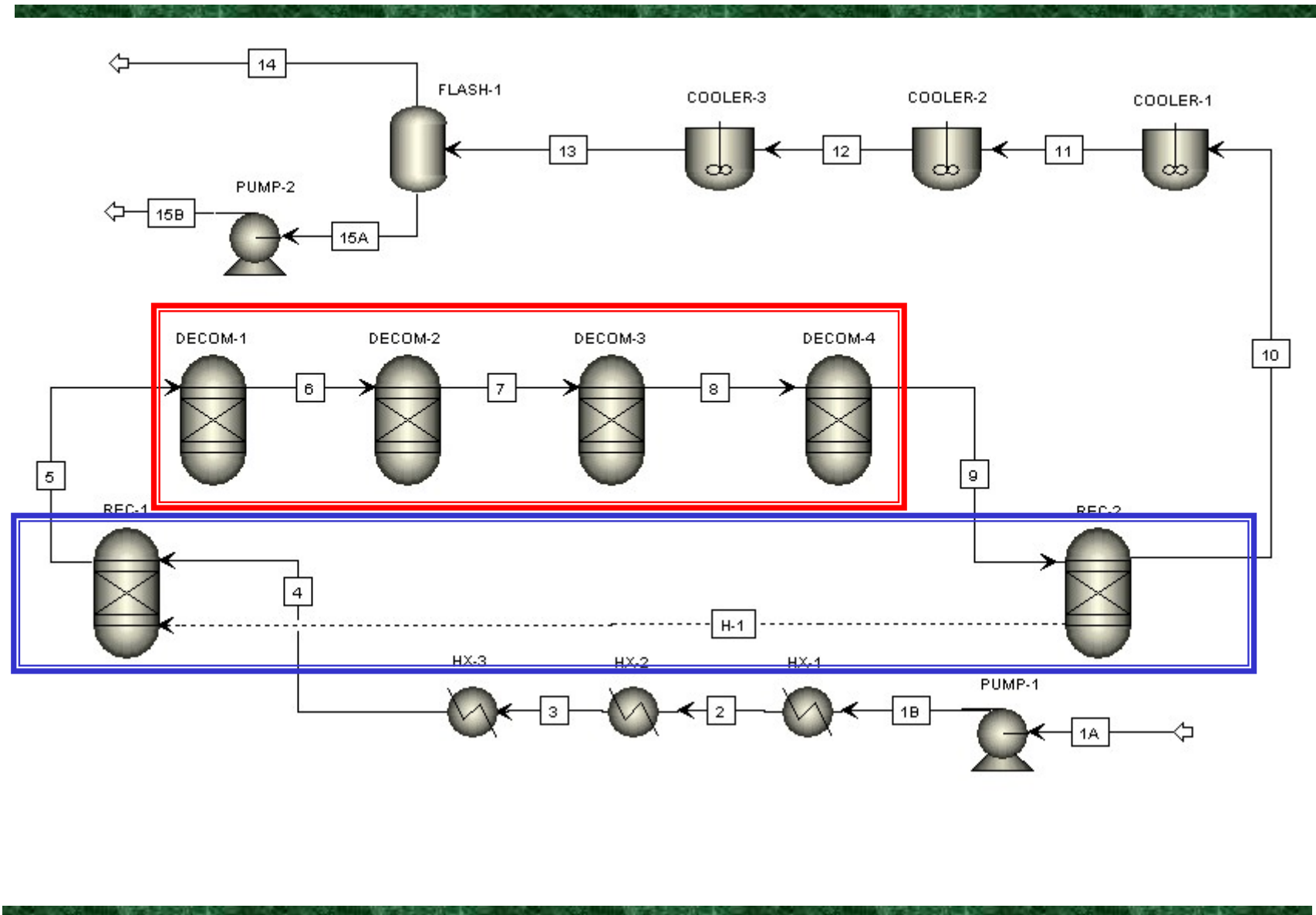
- Description :
 - The sulfuric acid is heated to the vaporization temperature in the recuperator.
 - Some of the sulfuric acid decomposes into SO_3 and H_2O .
 - The recuperator retrieves much of the heat remaining after sulfuric acid decomposition.
 - Modeling :
 - The recuperator is modeled as two Gibbs reactors coupled by a heat stream.
-

Modeling of Sulfuric Acid Decomposition Process

■ Decomposer

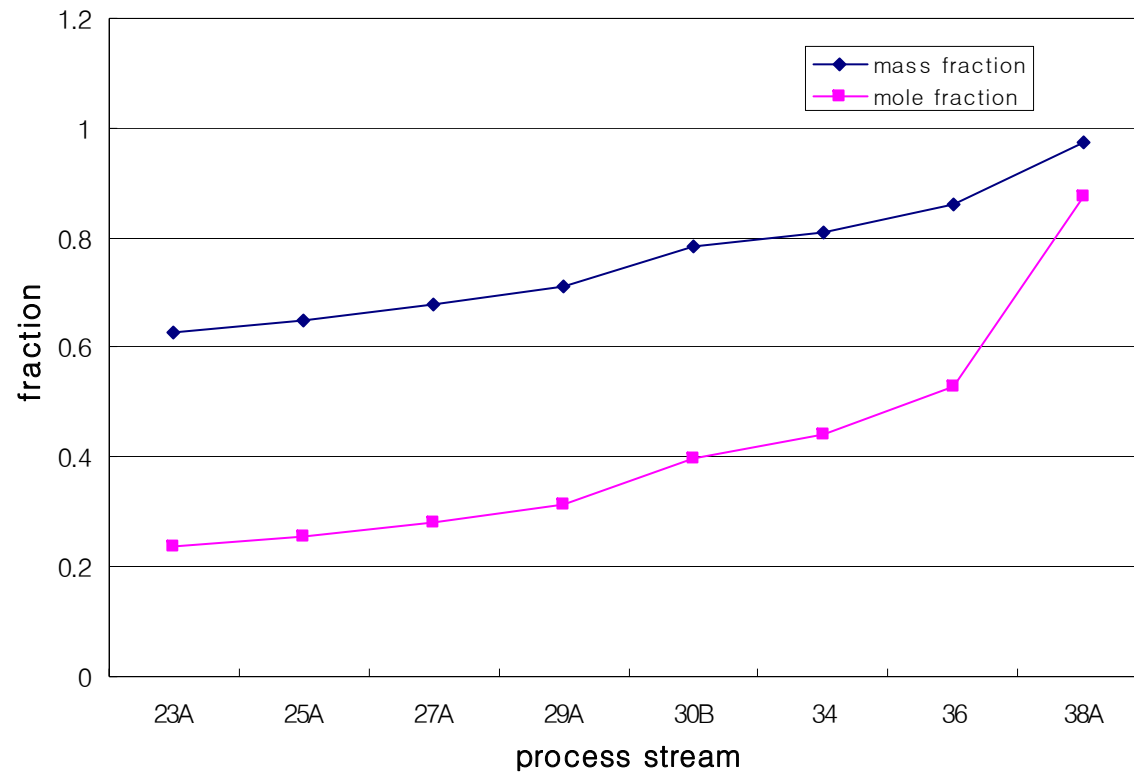
- Description :
 - SO_3 decomposes into SO_2 and O_2 .
 - Small amount of undecomposed H_2SO_4 is decomposing into SO_3 and H_2O .
 - The outlet stream from decomposer is cooled, transferring heat to the decomposer feed.
 - Modeling :
 - The decomposer is modeled as a series of four Gibbs reactors.
-

Modeling of Sulfuric Acid Decomposition Process



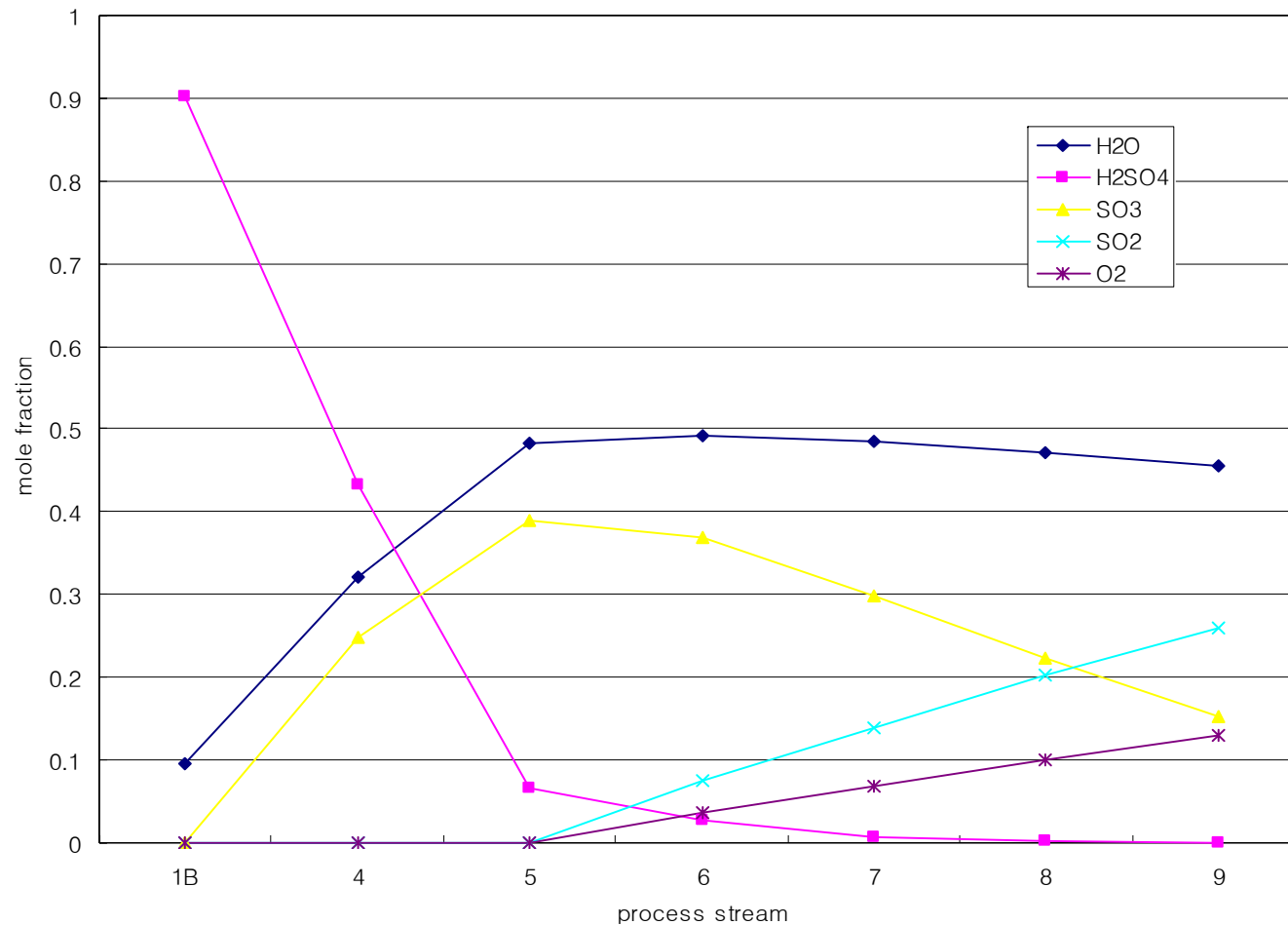
Modeling of Sulfuric Acid Evaporation Process

- Sulfuric Acid Fraction Change in Process Stream



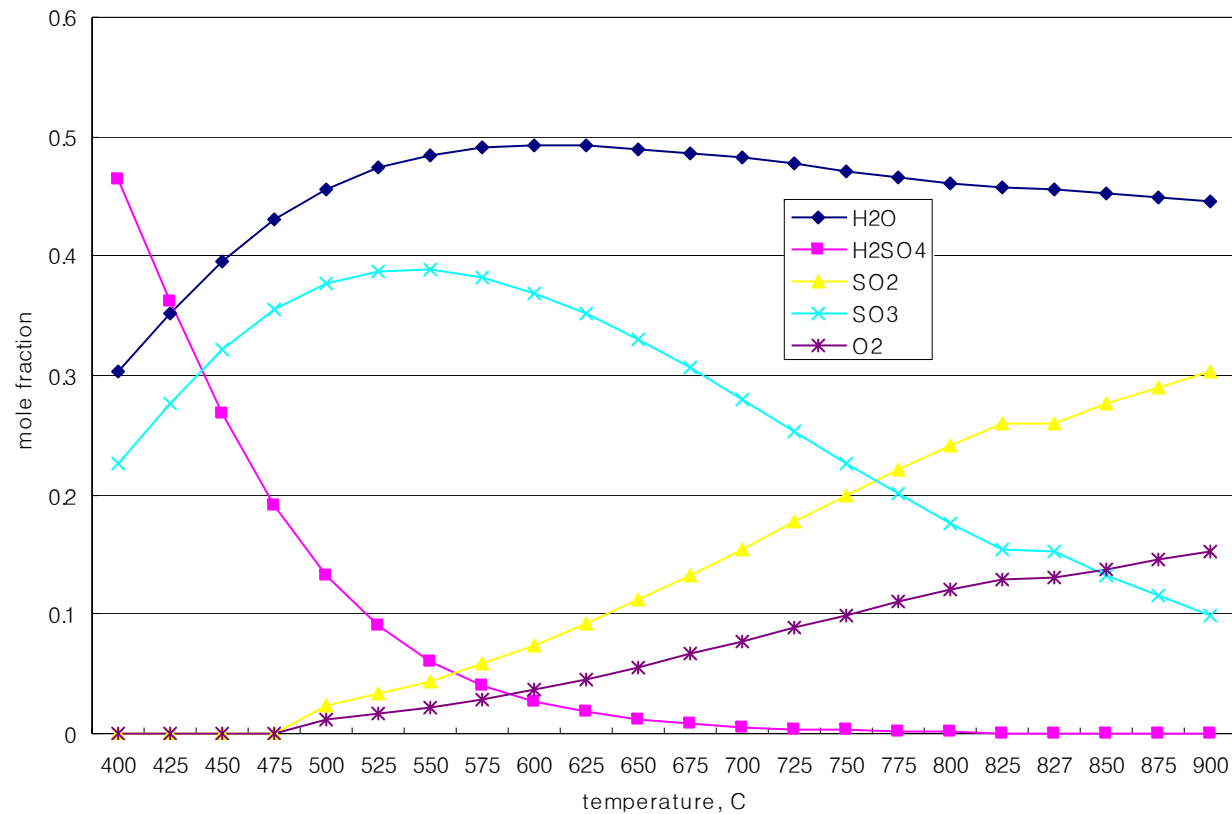
Modeling of Sulfuric Acid Decomposition Process

■ Mole Fraction Change in Process Stream



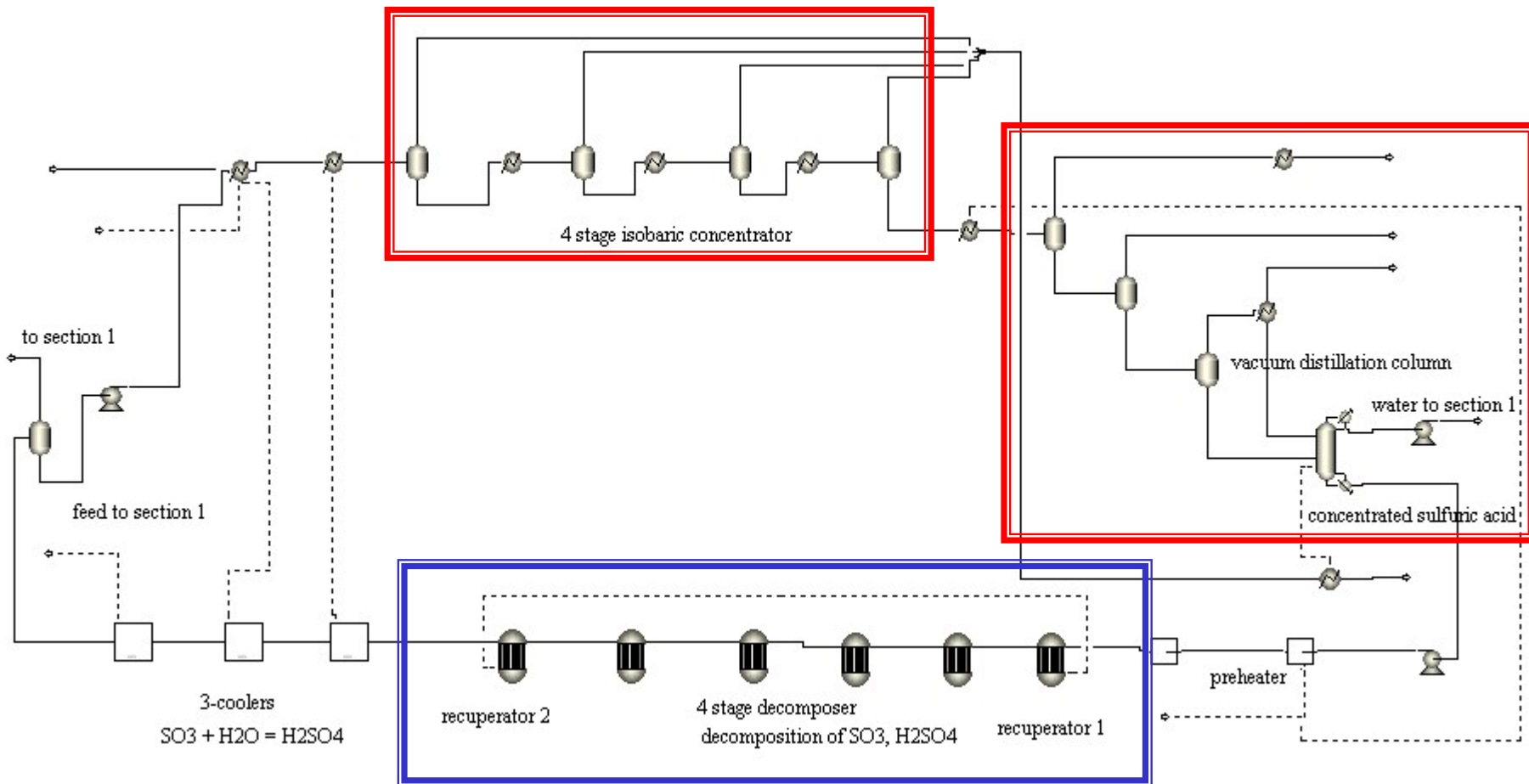
Modeling of Sulfuric Acid Decomposition Process

■ Mole Fraction Change vs. Temp.



Flow-sheet of SI process –Section 2

- Complete Simulation Flowsheet for Section 2



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_2O 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_2SO_4 decomposition.
-

THANK YOU !
