CHE654 Design Project #7

Semester 1, 2025

Project Title:

Design and Economic Evaluation of Sulfolane Production via Reaction of 1,3-Butadiene and Sulfur Dioxide

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Problem Statement:

Sulfolane (tetrahydrothiophene-1,1-dioxide) is a widely used industrial solvent, especially in gas sweetening and extractive distillation processes due to its high polarity and thermal stability. The conventional synthesis involves the reaction of **1,3-butadiene** with **sulfur dioxide (SO_2)** to form **3-sulfolene**, which is subsequently hydrogenated to yield sulfolane.

This project aims to **simulate the full production process of sulfolane** in **Aspen Plus**, from raw materials to final purification, using **chemical reaction engineering principles and economic analysis**. The simulation will include:

- Detailed process modeling,
- Reactor and separation unit design,
- Thermodynamic and kinetic evaluation,
- Mass and energy balances,
- Utility consumption,
- Economic metrics such as Net Present Value (NPV), Internal Rate of Return (IRR), and Payback Period.

Project Objectives:

1. **Model the synthesis of sulfolane** from 1,3-butadiene and SO_2 using Aspen Plus.
2. Include a reaction pathway:
    - **Step 1:** [1,3-butadiene + SO_2 → 3-sulfolene] (cycloaddition)
    - **Step 2:** [3-sulfolene + H_2 → sulfolane] (hydrogenation)
3. Design and simulate appropriate **reactors**, **separators**, and **purification units**.
4. Validate the process using provided **kinetic and thermodynamic data**.
5. Conduct **material and energy balance** across the process.
6. Evaluate the **economic feasibility** using Aspen Process Economic Analyzer (APEA) or other tools.

Input Data:

Feed Conditions:

- **1,3-Butadiene:**
  - Purity: ≥ 99%
  - Feed rate: 100 kmol/h
  - State: Gas
- **SO_2:**
  - Purity: ≥ 99.5%
  - Feed rate: 100 kmol/h
  - State: Gas

Reaction Kinetics:

Step 1: Cycloaddition Reaction

- **Reaction:**
  $C_4H_6 + SO_2 \rightarrow C_4H_6SO_2$ (3-sulfolene)

  Rate law:

  $r_1 = k_1 \cdot C_{C_4H_6} \cdot C_{SO_2}$

  Rate constant:

  $k_1 = 0.15\,\mathrm{L/mol \cdot min} \cdot \exp\left(-\frac{5500}{T}\right)$, with T in K
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Step 2: Hydrogenation

- **Reaction:**
  $C_4H_6SO_2 + H_2 \rightarrow C_4H_8SO_2$ (sulfolane)

  Rate law:

  $r_2 = k_2 \cdot C_{\text{3-sulfolene}} \cdot C_{H_2}$

  Rate constant:

  $k_2 = 0.09\,\mathrm{L/mol \cdot min} \cdot \exp\left(-\frac{4800}{T}\right)$, with T in K

Thermodynamic Data:

Use **NRTL** or **SRK** property method for vapor-liquid equilibrium.
Reactor temperatures:

- Cycloaddition: 90–150 °C

- Hydrogenation: 100–150 °C
  Operating pressure:
- 5–10 atm

Proposed Process Flow Diagram (PFD):

Units:

1. **Feed conditioning**
2. **Reactor R-1:** Cycloaddition reactor (PFR or CSTR)
3. **Separator S-1:** Removal of unreacted SO_2 and 1,3-butadiene
4. **Reactor R-2:** Hydrogenation reactor (fixed-bed or CSTR)
5. **Distillation column:** Separation of sulfolane from other species
6. **Recycle stream:** Unreacted SO_2 and butadiene
7. **Pumps, heat exchangers**, and **cooling utilities**

A simplified schematic or Aspen-generated PFD can be included separately.

Deliverables:

1. Aspen Plus simulation file (.bkp)
2. Mass and energy balances for the entire process
3. Equipment sizing and utility requirements
4. Economic analysis including:
   - Capital cost estimation
   - Operating cost breakdown
   - Cash flow analysis
   - IRR, NPV, and Payback Period
5. Sensitivity analysis (e.g., raw material cost, energy consumption)
6. Final report with process discussion and recommendations
