CHE654 Design Project #1

Semester 1, 2025

🧩 Problem Statement

Project Title

Design, Simulation, and Economic Evaluation of Methyl Ethyl Ketone (MEK) Production from n-Butane via n-Butene Intermediate

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Background

Methyl Ethyl Ketone (MEK) is a valuable industrial solvent used extensively in coatings, adhesives, and chemical synthesis. Its production from petrochemical feedstocks has drawn attention due to increasing demand and profitability. A viable route involves the **dehydrogenation of n-butane to produce n-butene**, which is subsequently **partially oxidized to MEK**. This pathway allows for high selectivity and integration into existing petrochemical infrastructure.

Objective

To develop and evaluate a full-scale process for MEK production from n-butane via n-butene as an intermediate using **Aspen Plus** for process simulation and **economic analysis** for feasibility assessment.

Scope of Work

1. Process Simulation

- Develop a detailed **process flow diagram (PFD)** for the conversion of **n-butane to MEK via n-butene**.
- Simulate the process using **Aspen Plus**, including:
    - **Feed preparation**
    - **Dehydrogenation of n-butane to n-butene**
    - **Oxidation of n-butene to MEK**
    - **Separation and purification**
    - **Recycle and purge systems** (if applicable)
- Perform **mass and energy balances**.

- Conduct **sensitivity analysis** on temperature, pressure, and conversion rates.

2. Economic Evaluation

- Estimate **capital and operating costs** using Aspen Economic Analyzer or external cost estimation tools.
- Perform **financial analysis**, including:
    - **Net Present Value (NPV)**
    - **Internal Rate of Return (IRR)**
    - **Payback Period**
    - **Cash Flow Analysis** over the project lifetime (e.g., 10–20 years)
- Include assumptions on:
    - Plant capacity (e.g., tons of MEK per year)
    - Equipment cost index
    - Inflation/discount rates
    - Raw material and utility costs
    - Product selling price

🔁 **Process Overview and PFD**

🧪 **Major Process Steps**

1. **Feed Conditioning**
    - n-Butane is compressed and preheated.
2. **Dehydrogenation Reactor (R-101)**
    - n-Butane → n-Butene + H_2
3. **Intermediate Separation (V-101)**
    - Removal of hydrogen and light gases.
4. **Oxidation Reactor (R-102)**
    - n-Butene + O_2 → MEK + Byproducts
5. **Cooling and Quenching**
6. **MEK Separation and Purification**
    - Distillation column(s) to recover pure MEK.

7. **Byproduct Management and Recycle Loops**

🏗️ Process Flow Diagram

(This can be redrawn in Aspen or a PFD editor based on units listed above.)

🔢 Aspen Plus Simulation: Required Input Data

1. Components

- n-Butane (C_4H_{10})
- n-Butene (C_4H_8)
- Oxygen (O_2), Nitrogen (N_2)
- Hydrogen (H_2)
- MEK (C_4H_8O)
- Water (H_2O), CO, CO_2

2. Reactions

a. Dehydrogenation (Endothermic):

C4H10 → C4H8 + H2

- Reactor Type: RPlug
- Kinetics: Power law (literature-based) or assume conversion
- Typical Conditions: 500–600 °C, ~5–10 atm

b. Oxidation (Exothermic):

C4H8 + 1.5O2 → C4H8O (MEK) + H2O

- Side reactions:
    - Combustion to CO/CO_2
- Reactor Type: RStoic or RPlug
- Temperature: 200–350 °C

3. Feed and Operating Conditions

- n-Butane flow: 100–500 kmol/hr

- Air as oxidant: O_2/N_2 (21/79 mol%)
- Heat exchangers for preheating/cooling
- Pressure: 5–20 atm (depending on stage)
- Use **Peng-Robinson EOS** or **SRK** for vapor-phase systems

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📈 Economic Analysis Inputs

Capital Costs

- Equipment sizing and costing using Aspen Plus or external references
- Installation factors
- Contingency and indirect costs

Operating Costs

- Raw materials: n-Butane, air, water
- Utilities: Steam, cooling water, electricity
- Labor, maintenance, overhead

Revenue Assumptions

- Market price of MEK (e.g., $1.5–$2.0/kg)
- Byproduct credit (e.g., hydrogen)

Financial Parameters

- Project life: 10–20 years
- Discount rate: 8–12%
- Tax rate: 25–30%
- Depreciation: Straight-line or MACRS

📊 Expected Deliverables

1. Aspen Plus flowsheet with convergence
2. Stream and utility tables
3. Equipment sizing report
4. Economic indicators:
    - Capital investment summary

- Operating cost breakdown
- NPV, IRR, Payback Period
- Annual cash flow chart

5. Optimization results (if applicable)
6. Sustainability or environmental assessment (optional)

Would you like help building a **starter Aspen Plus file**, **sample cash flow sheet in Excel**, or assistance with **reaction kinetics estimation** from literature?