CHE654 Design Project #10

Semester 1, 2025

Problem Statement: Aspen Plus Simulation of MTBE Production via Catalytic Etherification of Methanol and Isobutylene

Objective:

To simulate and analyze the **production of methyl tert-butyl ether (MTBE)** through the **catalytic etherification** of **methanol** and **isobutylene** using **Aspen Plus**. The project involves developing a complete process flowsheet, generating **mass and energy balances**, and performing an **economic evaluation** to determine the **financial feasibility** of the process.

Process Description:

1. **Feed Preparation:**
    - **Methanol (MeOH)** and **isobutylene (IB)**, often present in **C_4 hydrocarbon streams** from a refinery or steam cracker, are purified and preheated before entering the reactor.
    - Optional: If a mixed C_4 stream is used, a separation unit is required to isolate **isobutylene**.
2. **Reaction – Etherification Reactor:**
    - The etherification occurs in a **fixed-bed catalytic reactor** or **reactive distillation column**, often using an **acidic ion-exchange resin catalyst**.

      The primary reaction is:

      $$CH_3OH + (CH_3)_2C{=}CH_2 \rightarrow (CH_3)_3COCH_3$$

    - Side reactions are minimal under optimal conditions, but excess methanol is typically used to drive the reaction to completion.
    - Operating conditions: ~30–100°C and ~1–2 MPa.
3. **Separation and Product Purification:**
    - The reactor effluent is sent to a **separator/distillation unit** to:
        - Recover unreacted methanol and isobutylene for recycle.
        - Purify **MTBE** as the main product.

        - Remove any heavy or light by-products.

4. **Recycle:**
    - Unconverted methanol and isobutylene are recycled to improve raw material utilization and reduce waste.

Simulation Tasks in Aspen Plus:

- Model the **reactor** using either **RPlug** (if kinetic data is available) or **RCSTR** with stoichiometric conversion.
- Alternatively, simulate the **reactive distillation** approach if applicable using **RadFrac** with reaction stages.
- Include **separation trains**: distillation columns, flash drums, or absorption systems.
- Design **recycle streams** for unreacted reactants.
- Perform complete **mass and energy balances** across all units.
- Integrate heat exchangers for energy recovery and utility savings.

Economic Evaluation:

- Estimate:
    - **Capital costs** for reactors, distillation columns, compressors, heat exchangers, and other equipment.
    - **Operating costs**, including raw materials (methanol, isobutylene), utilities, and labor.
    - **Revenue** based on MTBE market price and production rate.
- Financial analysis includes:
    - **Net Present Value (NPV)**
    - **Internal Rate of Return (IRR)**
    - **Payback Period**
    - **Break-even analysis**
- Perform **sensitivity analysis** on:
    - Feedstock cost
    - Product price

- Reactor conversion
- Utility consumption

Expected Outcomes:

- A complete Aspen Plus simulation of MTBE production with all major process units and recycle loops.
- Detailed **mass and energy balances** for each stream and unit operation.
- Evaluation of **reactor efficiency**, conversion, and selectivity.
- A clear **economic feasibility report**, including profitability metrics and break-even analysis.
- Recommendations for process optimization or scale-up potential.
