

## CHE654 Design Project #10

Semester 1, 2025

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### 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.

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#### Process Description:

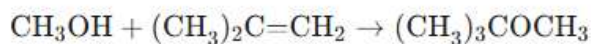
##### 1. Feed Preparation:

- **Methanol (MeOH)** and **isobutylene (IB)**, often present in **C<sub>4</sub> hydrocarbon streams** from a refinery or steam cracker, are purified and preheated before entering the reactor.
- Optional: If a mixed C<sub>4</sub> 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:



- 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.
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#### **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.
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#### **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
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### **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.
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