CHE654 Design Project #5

Semester 1, 2026

Problem Statement

Project Title

Design, Simulation, and Economic Evaluation of Methyl Isobutyl Ketone (MIBK) Production

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Background

Methyl Isobutyl Ketone (MIBK) is an important oxygenated solvent widely used in the coatings, paints, adhesives, printing inks, pharmaceuticals, agrochemicals, lubricants, and specialty chemical industries. Owing to its excellent solvency, moderate evaporation rate, and favorable compatibility with numerous organic compounds, MIBK has become one of the most commercially significant ketone solvents. In addition to its role as an industrial solvent, MIBK is also used as an intermediate in the manufacture of extraction agents, antioxidants, and various fine chemicals. The continued growth of the coatings, automotive, construction, and electronics industries has sustained a strong global demand for high-purity MIBK.

Commercially, MIBK is primarily produced from acetone through a sequence of catalytic reactions involving aldol condensation to form diacetone alcohol (DAA), dehydration of DAA to mesityl oxide (MO), and catalytic hydrogenation of MO to MIBK. Modern industrial processes may integrate these reactions using multifunctional catalysts; however, the conventional multi-step process remains widely practiced due to its operational flexibility, high selectivity, and ease of product purification. The process presents several engineering challenges, including reaction selectivity, catalyst performance, hydrogen utilization, separation of multiple oxygenated compounds, recycle stream management, and optimization of energy consumption and operating costs.

The objective of this project is to design a commercial MIBK production plant based on the catalytic conversion of acetone using Aspen Plus process simulation software. The proposed process will include acetone storage and feed preparation, catalytic aldol condensation, dehydration, hydrogenation, gas-liquid separation, recycle systems, product purification by distillation, and associated utility systems. Appropriate thermodynamic property methods, reactor models, and operating conditions will be selected based on published industrial data and accepted engineering practice.

The project will include complete material and energy balance calculations, equipment sizing, utility requirement estimation, and process optimization to maximize MIBK yield while minimizing acetone losses, hydrogen consumption, and energy requirements. Heat integration opportunities will be investigated to recover process heat and improve overall thermal efficiency.

A comprehensive techno-economic evaluation will be performed to assess the commercial feasibility of the proposed process. Capital investment, annual operating costs, raw material costs, utility consumption, catalyst replacement, maintenance expenses, and product revenues will be estimated. Project profitability will be evaluated using Net Present Value (NPV), Internal Rate of Return (IRR), Payback Period (PBP), Return on Investment (ROI), Profitability Index (PI), and Break-even Analysis. Sensitivity analyses will also be conducted to investigate the effects of fluctuations in acetone price, hydrogen cost, MIBK selling price, utility costs, catalyst life, and plant production capacity on the overall economic performance of the project.

The final process design should demonstrate technical feasibility, operational safety, energy efficiency, environmental responsibility, and economic viability while identifying opportunities for process optimization, improved heat integration, catalyst utilization, and sustainable operation in accordance with established industrial practice.

Objective

The primary objective of this project is to develop a technically feasible, safe, energy-efficient, and economically viable process for the commercial production of high-purity Methyl Isobutyl Ketone (MIBK) through the catalytic conversion of acetone using the conventional aldol condensation–dehydration–hydrogenation process.

The specific objectives are to:

1. Develop a complete Process Flow Diagram (PFD) for the commercial production of MIBK using Aspen Plus.
2. Simulate the entire process, including acetone feed preparation, catalytic aldol condensation, dehydration, hydrogenation, gas-liquid separation, hydrogen recycle, product purification, and utility systems.
3. Perform complete material and energy balance calculations for all major process units.
4. Select appropriate thermodynamic property methods and reactor models based on industrial practice and published literature.
5. Design and size the major process equipment, including storage tanks, pumps, heat exchangers, reactors, compressors, flash separators, recycle compressors, distillation columns, condensers, reboilers, and product storage facilities.
6. Optimize key operating variables such as reactor temperature, pressure, acetone conversion, hydrogen-to-feed ratio, and recycle ratio to maximize MIBK yield and selectivity while minimizing by-product formation.
7. Investigate heat recovery and process integration opportunities to improve thermal efficiency and reduce utility consumption.
8. Estimate utility requirements, including steam, cooling water, electricity, fuel gas (if applicable), and instrument air.
9. Estimate capital investment and annual operating costs using accepted chemical engineering economic methods.

10. Evaluate project profitability using Net Present Value (NPV), Internal Rate of Return (IRR), Payback Period (PBP), Return on Investment (ROI), Profitability Index (PI), and Break-even Analysis.
11. Conduct sensitivity analyses to determine the effects of fluctuations in acetone price, hydrogen price, MIBK selling price, utility costs, catalyst life, and plant production capacity on project profitability.
12. Assess process safety, environmental performance, and sustainability in accordance with accepted industrial engineering practice.

Scope of Work

This project covers the conceptual process design and simulation of a commercial Methyl Isobutyl Ketone (MIBK) production plant based on the catalytic conversion of acetone.

The scope of work includes:

- Review of commercial MIBK production technologies and selection of the conventional acetone condensation process.
- Development of the overall Process Flow Diagram (PFD).
- Selection of appropriate thermodynamic property methods.
- Simulation of the complete process using Aspen Plus.
- Modeling of the major process sections, including:
    - Acetone storage and feed preparation
    - Feed pumping and preheating
    - Aldol condensation reactor
    - Dehydration reactor
    - Hydrogen compression
    - Hydrogenation reactor
    - Reactor effluent cooling
    - Gas-liquid separation
    - Hydrogen recycle and purge
    - Distillation system for acetone recovery, intermediate separation, and MIBK purification
    - Product storage
- Material and energy balance calculations.
- Design and sizing of major process equipment.
- Utility consumption estimation.
- Heat integration and energy recovery analysis.
- Equipment cost estimation using published cost correlations.
- Estimation of Fixed Capital Investment (FCI), Working Capital Investment (WCI), and Total Capital Investment (TCI).
- Estimation of annual operating costs, including raw materials, utilities, catalyst replacement, labor, maintenance, and overhead.
- Development of discounted cash-flow statements.
- Economic profitability analysis.

- Sensitivity analysis of key technical and economic variables.
- Discussion of process safety, environmental considerations, and recommendations for future process improvements.

The project does not include detailed mechanical design, piping and instrumentation design (P&ID), structural engineering, civil engineering, detailed control system design, or plant construction scheduling.

Design Basis

The process is designed for the continuous commercial production of high-purity Methyl Isobutyl Ketone (MIBK) through the catalytic conversion of acetone.

The principal design assumptions are as follows:

- **Plant Capacity:** 50,000 metric tonnes of MIBK per year (adjustable according to project requirements).
- **Operating Schedule:** 8,000 operating hours per year.
- **Feedstocks:**
    - Commercial-grade acetone (≥99.5 wt%)
    - High-purity hydrogen (≥99.9 mol%)
- **Main Product:** Methyl Isobutyl Ketone (≥99.5 wt% purity).
- **Reaction Pathway:**
    - Aldol condensation of acetone to diacetone alcohol (DAA)
    - Dehydration of DAA to mesityl oxide (MO)
    - Hydrogenation of MO to MIBK
- **Catalysts:** Commercial catalysts appropriate for each reaction step (or a multifunctional catalyst if an integrated reactor configuration is selected).
- **Reactor Configuration:** Continuous stirred-tank reactors (CSTRs), fixed-bed reactors, or an equivalent industrial arrangement, depending on the selected process.
- **Typical Aldol Condensation Temperature:** 20–80°C.
- **Typical Dehydration Temperature:** 100–180°C.
- **Typical Hydrogenation Temperature:** 100–180°C.
- **Typical Hydrogenation Pressure:** 10–30 bar.
- **Hydrogen Recovery:** Gas-liquid separation followed by recycle compression.
- **Product Purification:** Multi-column distillation system to recover unreacted acetone and purify MIBK.
- **Process Simulation Software:** Aspen Plus.
- **Thermodynamic Property Method:** NRTL for the liquid-phase oxygenated system, with Peng–Robinson or another appropriate equation of state where vapor-phase behavior requires it.
- **Plant Lifetime:** 20 years.
- **Construction Period:** 2 years.
- **Discount Rate:** 10–12%.
- **Corporate Income Tax:** According to the selected country or regional regulations.

- **Economic Base Year:** Clearly specified and used consistently throughout the economic analysis.

Where industrial operating data are unavailable, engineering assumptions supported by published literature and accepted industrial practice will be adopted.

Economic Evaluation Methodology

The economic feasibility of the proposed MIBK production plant will be evaluated using standard chemical engineering economic analysis methods.

The economic assessment includes:

- Estimation of purchased equipment costs based on equipment sizing and published cost correlations.
- Determination of installed equipment costs using appropriate installation factors.
- Estimation of Fixed Capital Investment (FCI), Working Capital Investment (WCI), and Total Capital Investment (TCI).
- Calculation of annual operating costs, including:
    - Acetone feedstock
    - Hydrogen consumption
    - Steam
    - Cooling water
    - Electricity
    - Fuel gas (where applicable)
    - Catalyst replacement
    - Labor
    - Maintenance
    - Plant overhead
    - Waste treatment and environmental compliance
- Estimation of annual MIBK production and product sales revenue, with consideration of any valuable by-products or recovered intermediates.
- Development of discounted cash-flow statements over the plant operating life.
- Evaluation of project profitability using:
    - Gross Profit
    - Net Profit
    - Return on Investment (ROI)
    - Payback Period (PBP)
    - Net Present Value (NPV)
    - Internal Rate of Return (IRR)
    - Profitability Index (PI)
    - Break-even Analysis
- Sensitivity analyses to evaluate the impact of changes in:
    - Acetone price
    - Hydrogen price

- MIBK selling price
- Utility costs
- Catalyst life and replacement cost
- Plant production capacity
- Discount rate

The project will be considered economically feasible if the Net Present Value is positive at the selected discount rate, the Internal Rate of Return exceeds the company's minimum acceptable rate of return, and the Payback Period falls within an acceptable industrial investment horizon. Sensitivity analyses will be used to identify the most influential technical and economic variables and to evaluate the robustness of the proposed process under different operating and market conditions.

Detailed Design of a Heat Exchanger

You are to pick one heat exchanger in your process to carry out its detailed design. You should use ASPEN Exchanger Design & Rating (EDR) in the ASPEN Plus simulator to carry out the detailed design. For this heat exchanger design, the following information should be provided:

- Diameter of shell
- Number of tube and shell passes
- Number of tubes per pass
- Tube pitch and arrangement (triangular/square/..)
- Number of shell-side baffles, if any, and their arrangement (spacing, pitch, type)
- Diameter, tube-wall thickness, shell-wall thickness, and length of tubes
- Calculation of both shell- and tube-side film heat transfer coefficients
- Calculation of overall heat transfer coefficient (you may assume that there is no fouling on either side of the exchanger)
- Heat transfer area of the exchanger
- Shell-side and tube-side pressure drops (calculated, not estimated)
- Materials of construction
- Approximate cost of the exchanger

A detailed sketch of the exchanger should be included along with a set of comprehensive calculations in an appendix for the design of the chosen heat exchanger.

Process Flow Diagram