CHE654 Design Project #1

Semester 1, 2026

Problem Statement

Project Title

Design, Simulation, and Economic Evaluation of KA Oil Production from Cyclohexane

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Background

Cyclohexanol and cyclohexanone, collectively known as **KA (Ketone-Alcohol) Oil**, are important intermediate chemicals used primarily in the manufacture of adipic acid and caprolactam, the key raw materials for producing nylon-6,6 and nylon-6, respectively. The increasing global demand for engineering plastics, synthetic fibers, automotive components, and consumer products has resulted in a continuous need for efficient and economically viable KA oil production processes.

The conventional industrial process for KA oil production involves the partial oxidation of cyclohexane using air or oxygen in the presence of suitable catalysts. Because the desired oxidation products are more reactive than cyclohexane itself, maintaining high selectivity while achieving an acceptable conversion remains a major engineering challenge. Excessive oxidation can lead to undesirable by-products, reduced product yield, and increased separation and purification costs.

The objective of this project is to design a chemical process for the commercial production of KA oil from cyclohexane using Aspen Plus. The proposed process should include feed preparation, catalytic oxidation, product separation, recycle streams, and product purification to obtain cyclohexanol and cyclohexanone at the desired specifications. Appropriate thermodynamic models, reaction kinetics or conversion assumptions, and process operating conditions should be selected based on industrial practice and published literature.

In addition to process simulation, the project will include equipment sizing, utility requirements, heat integration opportunities, and plant-wide material and energy balances. A comprehensive economic evaluation will be performed to estimate the total capital investment, annual operating costs, product revenue, and overall profitability. Economic indicators such as Net Present Value (NPV), Internal Rate of Return (IRR), Payback Period, and Return on Investment (ROI) will be calculated to assess the commercial feasibility of the proposed plant. Sensitivity analyses will also be conducted to evaluate the effects of fluctuations in raw material prices, product selling prices, plant capacity, and utility costs on the project's profitability.

The final process design should demonstrate technical feasibility, economic viability, energy efficiency, and safe operation while identifying opportunities for process optimization and improved sustainability.

Objective

The primary objective of this project is to develop a technically feasible and economically viable process for the commercial production of KA (Ketone-Alcohol) Oil, consisting of cyclohexanol and cyclohexanone, from the catalytic oxidation of cyclohexane.

The specific objectives are to:

1. Develop a complete process flow diagram (PFD) for the production of KA oil using Aspen Plus.
2. Perform material and energy balance calculations for all major process units.
3. Select suitable thermodynamic models and reaction parameters to accurately simulate the oxidation process.
4. Design and size the major process equipment, including reactors, separators, distillation columns, heat exchangers, pumps, compressors, and storage vessels.
5. Optimize operating conditions to maximize cyclohexane conversion while maintaining high selectivity toward cyclohexanol and cyclohexanone.
6. Minimize utility consumption through process integration and heat recovery where appropriate.
7. Estimate the capital investment and annual operating costs for the proposed plant.
8. Evaluate the economic performance using profitability indicators such as Net Present Value (NPV), Internal Rate of Return (IRR), Payback Period (PBP), and Return on Investment (ROI).
9. Conduct sensitivity analyses to determine the effects of variations in feedstock prices, product prices, utility costs, and production capacity on project profitability.
10. Assess the technical feasibility, economic sustainability, and overall commercial attractiveness of the proposed process.

Scope of Work

This project covers the conceptual design and simulation of an industrial plant for producing KA oil from cyclohexane using catalytic liquid-phase oxidation.

The scope of the project includes:

- Review of industrial KA oil production technologies and selection of a suitable commercial process.
- Development of the process flow diagram (PFD).
- Selection of thermodynamic models and physical property methods.

- Simulation of all major process units using Aspen Plus.
- Material and energy balance calculations.
- Design and sizing of major process equipment.
- Utility system estimation, including steam, cooling water, electricity, and compressed air requirements.
- Heat integration and energy optimization where applicable.
- Equipment cost estimation using standard chemical engineering cost correlations.
- Estimation of total capital investment (TCI) and annual operating costs (AOC).
- Profitability analysis based on product sales, raw material costs, and operating expenses.
- Cash-flow analysis over the project lifetime.
- Sensitivity analysis of key economic variables.
- Discussion of process safety, environmental considerations, and recommendations for future process improvements.

Detailed mechanical design, piping design, instrumentation, structural engineering, and plant construction scheduling are outside the scope of this project.

Design Basis

The process is designed to produce commercial-grade KA oil through the catalytic oxidation of cyclohexane using air as the oxidizing agent.

The principal design assumptions include:

- **Plant Capacity:** 100,000 metric tonnes of KA oil per year (adjustable based on project requirements).
- **Operating Time:** 8,000 operating hours per year.
- **Feedstock:** Commercial-grade cyclohexane and atmospheric air.
- **Main Products:** Cyclohexanol and cyclohexanone.
- **Reaction Type:** Liquid-phase catalytic oxidation.
- **Reactor Configuration:** Continuous stirred-tank reactor (CSTR) or industrial equivalent.
- **Process Simulation Software:** Aspen Plus.
- **Thermodynamic Method:** NRTL, UNIQUAC, or Peng–Robinson, selected based on phase behavior and literature recommendations.
- **Economic Base Year:** Clearly stated and used consistently throughout the analysis.
- **Plant Lifetime:** 20 years.
- **Construction Period:** 2 years.
- **Corporate Income Tax:** Assumed according to the selected country or region.
- **Discount Rate:** Typically 10–12% unless otherwise specified.
- **Product Specifications:** Commercial-grade KA oil meeting downstream adipic acid or caprolactam production requirements.

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

Economic Evaluation Methodology

The economic feasibility of the proposed KA oil 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 manufacturing costs, including raw materials, utilities, labor, maintenance, depreciation, waste treatment, and overhead.
- Estimation of annual revenue based on plant production capacity and market prices for cyclohexanol and cyclohexanone.
- Development of annual 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 investigate the impact of variations in cyclohexane price, KA oil selling price, utility costs, catalyst costs, and production rate on the project's economic performance.

The project will be considered economically attractive if the calculated NPV is positive at the selected discount rate, the IRR exceeds the minimum acceptable rate of return, and the payback period falls within an acceptable industrial investment horizon.

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