CHE654 Design Project #3

Semester 1, 2026

Problem Statement

Project Title

Design, Simulation, and Economic Evaluation of Cyclohexane Production via Benzene Hydrogenation

---

Background

Cyclohexane is an important petrochemical intermediate that serves as the primary feedstock for the manufacture of cyclohexanol and cyclohexanone (KA oil), which are subsequently converted into adipic acid and caprolactam for the production of nylon-6,6 and nylon-6. In addition to its role as a chemical intermediate, cyclohexane is widely used as an industrial solvent and as a feedstock in numerous petrochemical processes. The continued growth of the automotive, textile, engineering plastics, and consumer goods industries has sustained a strong global demand for cyclohexane and its derivatives.

Commercially, cyclohexane is produced primarily by the catalytic hydrogenation of benzene using hydrogen over nickel- or noble metal-based catalysts under elevated temperature and pressure. This process offers nearly complete benzene conversion, high selectivity toward cyclohexane, and reliable operation at industrial scale. Nevertheless, the process involves significant challenges related to reactor temperature control due to the highly exothermic nature of the hydrogenation reaction, efficient hydrogen utilization, heat recovery, product purification, and optimization of operating costs. Increasing energy prices and stricter environmental regulations further emphasize the importance of designing energy-efficient and economically competitive cyclohexane production facilities.

The objective of this project is to design a commercial cyclohexane production plant based on the catalytic hydrogenation of benzene using Aspen Plus process simulation software. The proposed process will include benzene storage and feed preparation, hydrogen compression, feed preheating, catalytic hydrogenation reactor, product cooling, gas-liquid separation, hydrogen recycle, cyclohexane 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 established engineering practice.

The project will include complete material and energy balance calculations, equipment sizing, utility requirement estimation, and process optimization to maximize cyclohexane yield while minimizing energy consumption and hydrogen losses. Heat integration opportunities will be evaluated to recover reaction heat and improve overall process 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 influence of benzene price, hydrogen cost, cyclohexane selling price, plant capacity, and utility costs on the overall economic performance of the plant.

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, and sustainable operation in accordance with current 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 cyclohexane through the catalytic hydrogenation of benzene using hydrogen.

The specific objectives are to:

1. Develop a complete Process Flow Diagram (PFD) for the production of cyclohexane using Aspen Plus.
2. Simulate the entire process, including feed preparation, hydrogen compression, catalytic hydrogenation, product cooling, gas-liquid separation, hydrogen recycle, cyclohexane 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, compressors, heat exchangers, hydrogenation reactor, separators, recycle compressors, distillation columns, and product storage facilities.
6. Optimize key operating variables such as reactor temperature, pressure, hydrogen-to-benzene molar ratio, and recycle ratio to maximize cyclohexane yield and selectivity.
7. Investigate heat recovery and process integration opportunities to improve overall thermal efficiency and reduce utility consumption.
8. Estimate utility requirements, including cooling water, steam, electricity, fuel gas, 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 benzene price, hydrogen price, cyclohexane selling price, utility costs, and plant production capacity on project profitability.
12. Evaluate 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 cyclohexane production plant based on the catalytic hydrogenation of benzene using hydrogen.

The scope of work includes:

- Review of commercial cyclohexane production technologies and selection of the catalytic hydrogenation process.
- Development of the 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:
  - Benzene storage and feed preparation
  - Hydrogen supply and compression
  - Feed preheating
  - Catalytic hydrogenation reactor
  - Product cooling
  - Gas-liquid separation
  - Hydrogen recycle and purge
  - Cyclohexane purification by distillation
  - 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 cyclohexane by catalytic hydrogenation of benzene.

The principal design assumptions are as follows:

- **Plant Capacity:** 150,000 metric tonnes of cyclohexane per year (adjustable according to project requirements).
- **Operating Schedule:** 8,000 operating hours per year.
- **Feedstocks:**
    - Commercial-grade benzene (≥99.9 wt%)
    - High-purity hydrogen (≥99.9 mol%)
- **Main Product:** Cyclohexane (≥99.9 wt% purity).
- **Reaction:** Catalytic hydrogenation of benzene.
- **Catalyst:** Nickel-based catalyst (or platinum/palladium catalyst, depending on process selection).
- **Reactor Type:** Fixed-bed catalytic reactor.
- **Typical Reactor Temperature:** 150–250°C.
- **Typical Reactor Pressure:** 20–40 bar.
- **Hydrogen-to-Benzene Molar Ratio:** 3–6.
- **Hydrogen Recovery:** Achieved through gas-liquid separation and recycle.
- **Cyclohexane Purification:** Distillation to commercial product specifications.
- **Process Simulation Software:** Aspen Plus.
- **Thermodynamic Property Method:** Peng–Robinson Equation of State or another appropriate hydrocarbon property package.
- **Plant Lifetime:** 20 years.
- **Construction Period:** 2 years.
- **Discount Rate:** 10–12%.
- **Corporate Income Tax:** Based on the selected country or regional regulations.
- **Economic Base Year:** Clearly stated and applied consistently throughout the economic analysis.

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

Economic Evaluation Methodology

The economic feasibility of the proposed cyclohexane 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:
  - Benzene feedstock
  - Hydrogen consumption
  - Cooling water
  - Steam
  - Electricity
  - Fuel gas (if required)
  - Catalyst replacement
  - Labor
  - Maintenance
  - Plant overhead
  - Waste treatment and environmental compliance
- Estimation of annual cyclohexane production and product sales revenue.
- 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:
  - Benzene price
  - Hydrogen price
  - Cyclohexane selling price
  - Utility costs
  - 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 economic parameters and evaluate the robustness of the project under different 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