CHE654 Design Project #7

Semester 1, 2026

Problem Statement

Project Title

Design, Simulation, and Economic Evaluation of Isopropyl Alcohol Production

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Background

Isopropyl Alcohol (IPA), also known as isopropanol or 2-propanol, is one of the most important oxygenated solvents produced by the petrochemical industry. It is widely used in pharmaceuticals, personal care products, electronics manufacturing, coatings, printing inks, disinfectants, cleaning formulations, and chemical synthesis. In addition to its role as an industrial solvent, IPA serves as a valuable intermediate in the production of acetone, isopropyl esters, and numerous specialty chemicals. The sustained growth of the healthcare, electronics, automotive, and consumer goods industries has resulted in a continuous global demand for high-purity isopropyl alcohol.

Commercially, isopropyl alcohol is produced primarily through the direct catalytic hydration of propylene with water. Compared with the older indirect sulfuric acid hydration process, direct hydration offers higher selectivity, reduced corrosion, lower environmental impact, simplified process operation, and lower operating costs. The process typically employs a fixed-bed catalytic reactor operating at elevated temperature and pressure, followed by separation, recycle of unreacted propylene, and purification through multi-stage distillation. Despite its commercial maturity, the process presents several engineering challenges, including equilibrium limitations, optimization of the water-to-propylene ratio, efficient propylene recycle, energy-intensive distillation, and minimization of utility consumption.

The objective of this project is to design a commercial isopropyl alcohol production plant based on the catalytic direct hydration of propylene using Aspen Plus process simulation software. The proposed process will include propylene storage and feed preparation, water supply and feed conditioning, catalytic hydration reactor, reactor effluent cooling, gas-liquid separation, propylene recycle, purification by distillation, dehydration to obtain high-purity isopropyl alcohol, 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 isopropyl alcohol yield while minimizing propylene losses, energy consumption, and operating costs. 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 propylene price, utility costs, catalyst life, isopropyl alcohol selling price, 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, 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 Isopropyl Alcohol (IPA) through the direct catalytic hydration of propylene.

The specific objectives are to:

1. Develop a complete Process Flow Diagram (PFD) for the commercial production of isopropyl alcohol using Aspen Plus.
2. Simulate the complete process, including propylene feed preparation, water feed conditioning, catalytic hydration, gas-liquid separation, propylene recycle, IPA purification, dehydration, 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, feed heaters, catalytic reactors, flash separators, recycle compressors, distillation columns, condensers, reboilers, decanters (if required), and product storage facilities.
6. Optimize key operating variables such as reactor temperature, reactor pressure, water-to-propylene molar ratio, recycle ratio, and conversion to maximize IPA yield while minimizing by-product formation and utility consumption.
7. Investigate heat recovery and process integration opportunities to improve thermal efficiency and reduce energy requirements.
8. Estimate utility requirements, including steam, cooling water, electricity, instrument air, and nitrogen for inerting where appropriate.
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 propylene price, utility costs, catalyst life, IPA selling price, 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 isopropyl alcohol production plant based on the direct catalytic hydration of propylene.

The scope of work includes:

- Review of commercial IPA production technologies and selection of the direct hydration 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:
    - Propylene storage and feed preparation
    - Feed compression
    - Water feed preparation
    - Feed preheating
    - Direct hydration reactor
    - Reactor effluent cooling
    - High-pressure gas-liquid separation
    - Propylene recycle and purge
    - Crude IPA recovery
    - IPA purification and dehydration 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 catalyst development, 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 isopropyl alcohol through the direct catalytic hydration of propylene.

The principal design assumptions are as follows:

- **Plant Capacity:** 100,000 metric tonnes of isopropyl alcohol per year (adjustable according to project requirements).
- **Operating Schedule:** 8,000 operating hours per year.
- **Feedstocks:**
  - Polymer-grade propylene (≥99.5 wt%)
  - Process water (demineralized)
- **Main Product:** Isopropyl alcohol (≥99.9 wt% purity).
- **By-products:** Small quantities of diisopropyl ether (DIPE) and other minor oxygenated compounds, depending on operating conditions.
- **Reaction:** Direct catalytic hydration of propylene.
- **Catalyst:** Commercial solid acid catalyst (represented by literature-based kinetics or equilibrium data for simulation).
- **Reactor Type:** Fixed-bed catalytic reactor.
- **Typical Reactor Temperature:** 180–260°C.
- **Typical Reactor Pressure:** 30–80 bar.
- **Water-to-Propylene Molar Ratio:** Typically 0.6–1.2.
- **Propylene Recovery:** Gas-liquid separation followed by recycle compression.
- **Product Purification:** Multi-column distillation system to obtain high-purity IPA.
- **Process Simulation Software:** Aspen Plus.
- **Thermodynamic Property Method:** NRTL or UNIQUAC for the non-ideal liquid-phase IPA–water system, with Peng–Robinson or another suitable equation of state for vapor-phase calculations where required.
- **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 isopropyl alcohol 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:
    - Propylene feedstock
    - Process water
    - Steam
    - Cooling water
    - Electricity
    - Nitrogen and utility gases
    - Catalyst replacement
    - Labor
    - Maintenance
    - Plant overhead
    - Waste treatment and environmental compliance
- Estimation of annual isopropyl alcohol production and product sales revenue, with consideration of any recoverable by-products such as diisopropyl ether.
- 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:
    - Propylene price
    - Utility costs
    - IPA selling price
    - Catalyst 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 parameters and 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