CHE654 Design Project #6

Semester 1, 2026

Problem Statement

Project Title

Design, Simulation, and Economic Evaluation of Acetic Acid Production

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Background

Acetic acid is one of the most important commodity chemicals in the petrochemical industry and serves as a key intermediate in the manufacture of vinyl acetate monomer (VAM), purified terephthalic acid (PTA), acetic anhydride, acetate esters, cellulose acetate, pharmaceuticals, food additives, and numerous specialty chemicals. Owing to its widespread applications in the plastics, textiles, adhesives, coatings, packaging, and chemical manufacturing industries, global demand for high-purity acetic acid continues to increase. Consequently, the development of efficient, safe, and economically competitive acetic acid production processes remains an important objective in modern chemical engineering.

Commercially, acetic acid is produced primarily through the catalytic carbonylation of methanol with carbon monoxide in the presence of homogeneous transition-metal catalysts. While the Monsanto process, employing a rhodium catalyst, represented the industry standard for many years, the more recent Cativa® process utilizes an iridium-based catalyst system that offers higher catalyst stability, lower water consumption, improved reaction selectivity, reduced by-product formation, and lower operating costs. As a result, the Cativa® process has become the preferred technology for many newly constructed commercial acetic acid plants.

Despite its high efficiency, the methanol carbonylation process presents several engineering challenges, including catalyst management, efficient carbon monoxide utilization, separation of catalyst-containing reaction mixtures, recovery and recycle of unreacted reactants, corrosion control, energy integration, and purification of glacial acetic acid to commercial specifications. Optimizing reactor operating conditions, minimizing utility consumption, and reducing overall production costs are essential for maintaining commercial competitiveness.

The objective of this project is to design a commercial acetic acid production plant based on the catalytic carbonylation of methanol using Aspen Plus process simulation software. The proposed process will include methanol storage and feed preparation, carbon monoxide compression, catalytic carbonylation reactor, flash separation, catalyst recovery, methanol recycle, purification by multi-stage 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 acetic acid yield while minimizing methanol losses, carbon monoxide 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 methanol price, carbon monoxide cost, catalyst life, acetic acid selling price, utility costs, 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 acetic acid through the catalytic carbonylation of methanol with carbon monoxide.

The specific objectives are to:

1. Develop a complete Process Flow Diagram (PFD) for the commercial production of acetic acid using Aspen Plus.
2. Simulate the complete process, including methanol feed preparation, carbon monoxide compression, carbonylation reactor, flash separation, catalyst recycle, methanol recovery, acetic acid 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, carbonylation reactor, flash drums, recycle systems, distillation columns, condensers, reboilers, and product storage facilities.
6. Optimize key operating variables such as reactor temperature, reactor pressure, methanol-to-carbon monoxide ratio, recycle ratio, and catalyst circulation to maximize acetic acid 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, instrument air, and nitrogen for inerting where applicable.
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 methanol price, carbon monoxide cost, acetic acid selling price, utility costs, catalyst replacement cost, and plant production capacity on project profitability.
12. Assess process safety, corrosion considerations, 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 acetic acid production plant based on the catalytic carbonylation of methanol.

The scope of work includes:

- Review of commercial acetic acid production technologies and selection of the methanol carbonylation 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:
    - Methanol storage and feed preparation
    - Carbon monoxide supply and compression
    - Feed preheating
    - Carbonylation reactor
    - Reactor effluent cooling
    - Flash separation
    - Catalyst-containing liquid recycle
    - Gas recycle and purge
    - Methanol recovery
    - Water removal
    - Acetic acid 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, corrosion control, and overhead.
- Development of discounted cash-flow statements.
- Economic profitability analysis.
- Sensitivity analysis of key technical and economic variables.
- Discussion of process safety, corrosion mitigation, environmental considerations, and recommendations for future process improvements.

The project does not include detailed catalyst chemistry, 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 glacial acetic acid through the catalytic carbonylation of methanol with carbon monoxide.

The principal design assumptions are as follows:

- **Plant Capacity:** 300,000 metric tonnes of glacial acetic acid per year (adjustable according to project requirements).
- **Operating Schedule:** 8,000 operating hours per year.
- **Feedstocks:**
    - Commercial-grade methanol (≥99.9 wt%)
    - Carbon monoxide (≥99.5 mol%)
- **Main Product:** Glacial acetic acid (≥99.8 wt% purity).
- **Reaction:** Methanol carbonylation.
- **Catalyst System:** Literature-based representation of an iridium- or rhodium-catalyzed homogeneous process for simulation purposes.
- **Reactor Type:** Continuous stirred-tank reactor (CSTR) or equivalent homogeneous reactor model.
- **Typical Reactor Temperature:** 170–220°C.
- **Typical Reactor Pressure:** 30–60 bar.
- **Carbon Monoxide Conversion:** Determined by process simulation and recycle configuration.
- **Methanol Recovery:** Distillation and recycle.
- **Product Purification:** Multi-column distillation system to obtain glacial acetic acid.
- **Process Simulation Software:** Aspen Plus.
- **Thermodynamic Property Method:** NRTL for liquid-phase non-ideal mixtures, with Peng–Robinson or another suitable equation of state for gas-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 acetic acid 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:
    - Methanol feedstock
    - Carbon monoxide consumption
    - Steam
    - Cooling water
    - Electricity
    - Nitrogen and utility gases
    - Catalyst replacement and catalyst inventory
    - Corrosion-resistant materials and maintenance
    - Labor
    - Plant overhead
    - Waste treatment and environmental compliance
- Estimation of annual acetic acid 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:
    - Methanol price
    - Carbon monoxide price
    - Acetic acid selling price

- Utility costs
- 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