CHE654 Design Project #7

Semester 1, 2026

Problem Statement

Project Title

Design, Simulation, and Economic Evaluation of Acrylonitrile Production

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Background

Acrylonitrile is one of the world's most important petrochemical intermediates and is primarily used in the manufacture of acrylic fibers, acrylonitrile-butadiene-styrene (ABS) resins, styrene-acrylonitrile (SAN) copolymers, nitrile rubber (NBR), adiponitrile, carbon fibers, and numerous specialty chemicals. Owing to its excellent chemical stability, mechanical strength, and versatility, acrylonitrile continues to play a vital role in the automotive, electronics, aerospace, construction, and textile industries. Continued growth in these sectors has sustained global demand for acrylonitrile, creating the need for production processes that are technically efficient, economically competitive, energy efficient, and environmentally responsible.

Commercially, more than 90% of the world's acrylonitrile is produced by the catalytic ammoxidation of propylene using ammonia and air in a fluidized-bed reactor, commonly known as the SOHIO process. The highly exothermic reaction is carried out over mixed metal oxide catalysts and simultaneously produces valuable by-products such as acetonitrile and hydrogen cyanide. Efficient heat removal, catalyst performance, reactant conversion, product selectivity, and downstream recovery are critical to achieving high production efficiency while maintaining safe plant operation. The process also presents significant engineering challenges due to the handling of flammable gases, toxic intermediates, highly exothermic reactions, complex gas absorption systems, multiple separation operations, and stringent environmental emission requirements.

The objective of this project is to design a continuous industrial process for the production of high-purity acrylonitrile from propylene, ammonia, and air using the commercial SOHIO ammoxidation process. The proposed process shall be developed using Aspen Plus® to perform rigorous material and energy balances, simulate reaction and separation systems, optimize operating conditions, and minimize utility consumption while satisfying industrial product specifications. Appropriate thermodynamic models shall be selected to accurately represent the gas-phase reaction system and the downstream absorption and distillation processes.

The completed design shall include feed preparation, catalytic reactor, waste heat recovery, quenching, absorber, stripping columns, product purification, by-product recovery, utility systems, and recycle streams. A complete Process Flow Diagram (PFD), equipment sizing methodology, stream summary, utility requirements, process control strategy, and process safety considerations shall be developed to demonstrate the technical feasibility of the proposed plant.

A comprehensive economic evaluation shall also be conducted to determine the commercial viability of the proposed facility. Capital investment and annual operating costs shall be estimated using accepted chemical engineering methodologies, while profitability shall be assessed using indicators such as Total Capital Investment (TCI), Annual Operating Cost (AOC), Net Present Value (NPV), Internal Rate of Return (IRR), Return on Investment (ROI), Payback Period (PBP), and Discounted Cash Flow (DCF). Sensitivity analyses shall be performed to evaluate the influence of fluctuations in raw material prices, product selling prices, utility costs, production capacity, and catalyst life on overall plant profitability.

The final design should demonstrate that the proposed acrylonitrile production plant is technically feasible, economically attractive, operationally safe, and capable of producing polymer-grade acrylonitrile suitable for commercial applications.

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 acrylonitrile.

The objectives of this project are to:

1. Design a continuous industrial process for producing polymer-grade acrylonitrile via the catalytic ammoxidation of propylene.
2. Develop a rigorous Aspen Plus® simulation for the complete process.
3. Perform complete material and energy balance calculations.
4. Select and justify appropriate thermodynamic property methods for reaction and separation systems.
5. Design and optimize the fluidized-bed catalytic reactor to maximize acrylonitrile yield and selectivity.
6. Design downstream gas cooling, absorption, stripping, purification, and by-product recovery systems.
7. Recover valuable by-products such as acetonitrile and hydrogen cyanide whenever economically justified.
8. Minimize energy consumption through heat recovery and process integration.
9. Estimate equipment sizes and utility requirements for all major process units.
10. Conduct comprehensive process safety and environmental assessments.
11. Perform a complete techno-economic evaluation and profitability analysis of the proposed process.

Scope of Work

This project covers the conceptual process design and simulation of a commercial acrylonitrile production plant.

The scope of work includes:

Literature Review

- Commercial acrylonitrile manufacturing technologies
- SOHIO process chemistry
- Catalyst systems
- Industrial operating conditions
- Product specifications
- Environmental regulations

Process Development

- Process selection
- Reaction stoichiometry
- Reactor operating conditions
- Process flow development
- Process Flow Diagram (PFD)

Aspen Plus® Simulation

- Property method selection
- Material balance
- Energy balance
- Reactor simulation
- Absorption simulation
- Distillation simulation
- Recycle convergence
- Process optimization

Equipment Design

Preliminary design of:

- Feed compressors
- Air compressor
- Ammonia vaporizer
- Fluidized-bed reactor
- Waste heat boiler
- Quench tower
- Absorber

- Stripper
- Distillation columns
- Heat exchangers
- Pumps
- Compressors
- Storage tanks
- Utility systems

Utility System Design

Estimate requirements for:

- High-pressure steam
- Cooling water
- Electricity
- Instrument air
- Nitrogen
- Refrigeration (if required)

Economic Evaluation

Estimate:

- Capital investment
- Operating costs
- Manufacturing costs
- Product revenue
- Plant profitability

Design Basis

The process is designed for the continuous commercial production of high-purity acrylonitrile.

The principal design assumptions are as follows:

Plant Capacity

200,000 metric tonnes per year of acrylonitrile

Plant Operation

- Continuous operation
- 330 operating days/year
- 24 hours/day
- 7,920 operating hours/year

Product Specification

Acrylonitrile purity: ≥99.5 wt%
Water: ≤0.2 wt%
Organic impurities: Within polymer-grade specifications

Feedstocks

- Propylene
- Anhydrous ammonia
- Air

Process Route

Catalytic vapor-phase ammoxidation of propylene using the commercial SOHIO process with a fluidized-bed mixed-metal oxide catalyst.

Reactor Performance (Typical Industrial Targets)

Propylene conversion: 95–99%
Acrylonitrile selectivity: 75–83%
Acetonitrile: 2–5%
Hydrogen cyanide: 3–7%
Carbon oxides and other by-products: Minimized through process optimization.

Process Simulation

Software: Aspen Plus®

Suggested property methods:

- Peng–Robinson
- RK-SOAVE
- NRTL (liquid purification where appropriate)

Final property method selection shall be justified using published thermodynamic data.

Product Recovery

Overall acrylonitrile recovery: Greater than 98%

Economic Evaluation Methodology

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

The economic assessment includes:

The proposed process shall be evaluated using accepted chemical engineering economic analysis procedures.

Capital Investment

Estimate:

- Purchased equipment cost
- Installation
- Instrumentation
- Piping
- Electrical systems
- Buildings
- Yard improvements
- Engineering
- Construction
- Contingency

Determine:

- Fixed Capital Investment (FCI)
- Working Capital (WC)
- Total Capital Investment (TCI)

Annual Operating Cost

Estimate: Variable Costs

- Propylene
- Ammonia
- Air compression
- Steam
- Cooling water
- Electricity
- Catalyst replacement
- Waste treatment

Fixed Costs

- Labor
- Maintenance
- Insurance
- Property taxes
- Plant overhead

- Administrative expenses

Determine: Annual Operating Cost (AOC)

Revenue Analysis

Estimate annual revenue from:

- Acrylonitrile
- Acetonitrile
- Hydrogen cyanide (if recovered and marketed)

Profitability Analysis

Determine:

- Gross Annual Revenue
- Gross Profit
- Net Profit
- Manufacturing Cost
- Unit Production Cost
- Return on Investment (ROI)
- Payback Period (PBP)
- Discounted Payback Period (DPBP)
- Net Present Value (NPV)
- Internal Rate of Return (IRR)
- Profitability Index (PI)
- Discounted Cash Flow (DCF)

The economic analysis shall assume:

- Plant life: 20 years
- Construction period: 2 years
- Discount rate: 8–12%
- Corporate income tax and depreciation based on the selected regional economic assumptions

Sensitivity Analysis

Evaluate the effects of variations in:

- Propylene price
- Ammonia price
- Acrylonitrile selling price
- Utility costs
- Plant capacity

- Catalyst lifetime
- Product selectivity
- Plant operating factor

The analysis shall identify the most influential economic variables and assess the robustness of the proposed investment under changing 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