Problem Statement

Project Title

Design, Simulation, and Economic Evaluation of Benzene Production via Hydrodealkylation of Toluene

---

Background

Benzene is one of the most important basic petrochemicals and serves as a key raw material for the manufacture of styrene, cumene, cyclohexane, phenol, aniline, detergents, synthetic fibers, engineering plastics, pharmaceuticals, and numerous specialty chemicals. The continuing growth of the petrochemical, automotive, construction, and consumer products industries has sustained a strong global demand for high-purity benzene. Consequently, the development of efficient, reliable, and economically competitive benzene production processes remains an important objective of the chemical and petrochemical industries.

Although benzene is recovered from catalytic reformate and pyrolysis gasoline in petroleum refineries, a significant proportion of commercial benzene is produced by the catalytic hydrodealkylation (HDA) of toluene. In this process, toluene reacts with hydrogen at elevated temperature and pressure to produce benzene and methane with high selectivity. The HDA process offers operational flexibility by converting surplus toluene into higher-value benzene while maintaining high product purity and excellent commercial reliability. However, the process presents several engineering challenges, including high-temperature reactor operation, efficient hydrogen utilization, recycle gas management, heat recovery, product purification, and optimization of energy consumption and operating costs.

The objective of this project is to design a commercial benzene production plant based on the catalytic hydrodealkylation of toluene using Aspen Plus process simulation software. The proposed process will include toluene storage and feed preparation, hydrogen compression, feed preheating, hydrodealkylation reactor, effluent cooling, gas-liquid separation, hydrogen recycle, methane purge, benzene purification by distillation, toluene recovery and recycle, 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 benzene yield while minimizing hydrogen consumption and energy requirements. Heat integration opportunities will be investigated to recover waste heat from the reactor effluent 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 effects of fluctuations in toluene price, hydrogen cost, benzene selling price, utility costs, and plant 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 benzene through the catalytic hydrodealkylation (HDA) of toluene using hydrogen.

The specific objectives are to:

1. Develop a complete Process Flow Diagram (PFD) for the commercial production of benzene using Aspen Plus.
2. Simulate the entire process, including feed preparation, hydrogen compression, feed preheating, hydrodealkylation reactor, gas-liquid separation, hydrogen recycle, benzene purification, toluene recovery, 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, fired heaters, catalytic reactors, heat exchangers, flash separators, recycle compressors, distillation columns, condensers, reboilers, and product storage facilities.
6. Optimize key operating variables such as reactor temperature, reactor pressure, hydrogen-to-toluene molar ratio, and recycle ratio to maximize benzene yield while minimizing hydrogen consumption and energy usage.
7. Investigate heat recovery and process integration opportunities to improve thermal efficiency and reduce utility consumption.
8. Estimate utility requirements, including fuel gas, steam, cooling water, electricity, 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 toluene price, hydrogen price, benzene selling price, utility costs, 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 benzene production plant based on the catalytic hydrodealkylation (HDA) of toluene using hydrogen.

The scope of work includes:

- Review of commercial benzene production technologies and selection of the hydrodealkylation 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:
    - Toluene storage and feed preparation
    - Hydrogen supply and compression
    - Feed preheating
    - Hydrodealkylation reactor
    - Reactor effluent cooling
    - High-pressure gas-liquid separation
    - Hydrogen recycle and purge
    - Benzene purification by distillation
    - Toluene recovery and recycle
    - 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 benzene by catalytic hydrodealkylation of toluene.

The principal design assumptions are as follows:

- **Plant Capacity:** 200,000 metric tonnes of benzene per year (adjustable according to project requirements).
- **Operating Schedule:** 8,000 operating hours per year.
- **Feedstocks:**
    - Commercial-grade toluene (≥99.5 wt%)
    - High-purity hydrogen (≥99.9 mol%)
- **Main Product:** Benzene (≥99.9 wt% purity).
- **Main By-product:** Methane (fuel gas or export gas).
- **Reaction:** Catalytic hydrodealkylation of toluene.
- **Catalyst:** Chromium oxide, molybdenum-based catalyst, or other commercial HDA catalyst depending on process selection.
- **Reactor Type:** Fixed-bed catalytic reactor.
- **Typical Reactor Temperature:** 550–700°C.
- **Typical Reactor Pressure:** 30–60 bar.
- **Hydrogen-to-Toluene Molar Ratio:** 4–8.
- **Hydrogen Recovery:** Gas-liquid separation followed by recycle compression.
- **Product Purification:** Distillation for benzene purification and toluene recovery.
- **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:** According to the selected country or regional regulations.
- **Economic Base Year:** Clearly specified and used consistently throughout the 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 benzene 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:
    - Toluene feedstock
    - Hydrogen consumption
    - Fuel gas
    - Steam
    - Cooling water
    - Electricity
    - Catalyst replacement
    - Labor
    - Maintenance
    - Plant overhead
    - Waste treatment and environmental compliance
- Estimation of annual benzene production and product sales revenue, with consideration of methane by-product utilization where applicable.
- 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:
    - Toluene price
    - Hydrogen price
    - Benzene 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 key economic drivers 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