Nubyira Process Designers

Executive Summary

This project presents the design, simulation, and economic evaluation of a continuous stirred-tank reactor (CSTR) based plant for the production of chlorobenzenes. It includes a dual-column distillation system for efficient separation of unreacted benzene, monochlorobenzenes, and dichlorobenzenes. Advanced process modeling, control, and dynamic simulations were conducted using Aspen HYSYS, supported by comprehensive material and energy balances, equipment design, and cost estimation.

Introduction

The chemical industry increasingly demands efficient, sustainable methods for producing high-demand chemicals like chlorobenzenes. This project explores an integrated design approach combining core chemical engineering concepts with modern simulation tools to develop a scalable, operable plant model for chlorobenzene production.

Process Overview

The plant uses benzene and chlorine as feedstock, with a CSTR reactor producing mono- and dichlorobenzenes. A two-column distillation system separates the products: Column 1 recovers unreacted benzene; Column 2 separates monochlorobenzene (MCB) and dichlorobenzene (DCB).

Reaction and Kinetics

Primary Reaction:
$C_6H_6 + Cl_2 \rightarrow C_6H_5Cl + HCl$
Kinetic Model:
- 1st-order with respect to benzene
- Temperature: 60-100C
- Catalyst: FeCl

Rate laws were implemented in Aspen HYSYS.

Process Design and Simulation

Aspen HYSYS was used for steady-state and dynamic simulations. The CSTR was modeled as isothermal. Distillation columns were simulated with rigorous thermodynamic methods. Energy integration was achieved using heat exchanger networks.

Equipment Sizing and Selection

Key equipment includes:
- CSTR (jacketed, volume based on residence time)
- Heat Exchangers (shell-and-tube)

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- Distillation Columns (20-25 stages)
- Pumps sized using hydraulic design principles.

PFDs and P&IDs

Process Flow Diagrams (PFDs) and Piping & Instrumentation Diagrams (P&IDs) were developed to capture process control logic, safety instrumentation, and flow paths using standard ISA symbols.

Plant Layout and 3D Visualization

The plant was spatially modeled using Autodesk Inventor. Equipment was placed with considerations for maintenance, operability, and safety zones. 3D visualizations supported design reviews.

Dynamic Simulation and Control Strategy

Dynamic simulations assessed plant stability. PID controllers managed reactor temperature and column reflux. Control loops were tuned and tested for robustness under disturbances.

Economic Analysis

Capital costs included equipment, installation, and infrastructure. Operating costs covered utilities, raw materials, and labor. Financial metrics like NPV and ROI confirmed economic feasibility.

Conclusions

This project shows the integrated application of chemical engineering principles in designing a complete chlorobenzene production plant. It validates both technical and economic viability and contributes to the early foundation of Nubyira Process Designers.

Sample Process Diagram

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