CHE654 Design Project #5

Semester 1, 2025

Problem Statement

Project Title

Simulation and Economic Assessment of Ethylene Dichloride (EDC) Production via Direct Chlorination of Ethylene Using Aspen Plus

Background

Ethylene dichloride (EDC, C₂H₄Cl₂) is a key intermediate in the chemical industry, primarily used in the production of vinyl chloride monomer (VCM), which is the main precursor to polyvinyl chloride (PVC). The most common method of EDC production is the direct chlorination of ethylene with chlorine gas, typically in the presence of a catalyst like ferric chloride (FeCl₃).

This project aims to simulate the EDC production process using **Aspen Plus**, analyze material and energy balances, and evaluate the **economic feasibility** based on key financial indicators, including **Internal Rate of Return (IRR)**, **Net Present Value (NPV)**, **payback period**, and **cash flow analysis**.

© Objectives

- 1. **Design and simulate** the EDC production process via **direct chlorination** in Aspen Plus.
- 2. Develop a detailed **process flow diagram (PFD)** including all major unit operations.
- 3. Perform material and energy balances across the process.
- 4. Estimate utilities and raw material requirements.
- 5. Conduct an **economic evaluation**, including:
 - o Internal Rate of Return (IRR)
 - Net Present Value (NPV)
 - Payback Period
 - Annual Cash Flow Analysis
- 6. Assess the **technical and financial feasibility** of the proposed process.

Process Chemistry

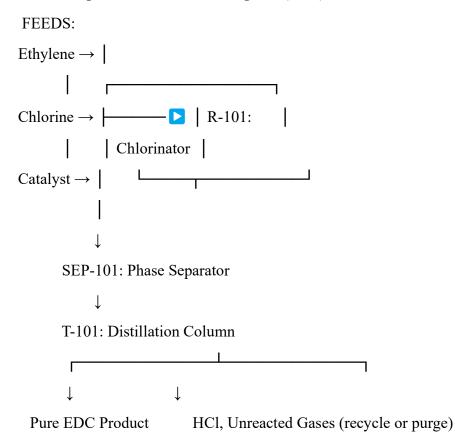
Main Reaction (Direct Chlorination):

 C_2H_4 (Ethylene) + Cl_2 (Chlorine) $\rightarrow C_2H_4Cl_2$ (Ethylene Dichloride)

 $\Delta H = -218 \text{ kJ/mol}$ (Exothermic)

- Catalyst: Ferric chloride (FeCl₃) or other Lewis acid catalysts
- Reaction typically occurs in liquid phase under moderate conditions

E Conceptual Process Flow Diagram (PFD)



Aspen Plus Simulation Setup

1. Thermodynamic Property Method

- Use NRTL or UNIQUAC for liquid-phase separations
- Use Peng-Robinson (PR) for vapor-liquid equilibrium if gas-phase is involved

2. Component List

Component Formula Role

Ethylene C₂H₄ Feed

Chlorine Cl₂ Feed

EDC C₂H₄Cl₂ Product

Hydrogen Chloride HCl By-product

Nitrogen N₂ Purge/blanketing (optional)

Catalyst (FeCl₃) – Not modeled explicitly in basic simulation

3. Typical Operating Conditions

Unit Temperature (°C) Pressure (bar) Description

Reactor 45–70 2–5 Liquid phase, stirred or fixed bed

Separator 50–100 ~1–2 Vapor-liquid separation

Distillation 100–150 (reboiler) ~1 Purify EDC

🚺 Input Data for Aspen Plus Simulation

A. Feed Data (Example Basis)

Stream Flowrate (kmol/h) Purity (%) Notes

Ethylene 100 99.9 Feed gas

Chlorine 100 99.5 Feed gas/liquid

Catalyst Fixed Batch input Not included in balance

Basis: 50,000 tonnes/year EDC production

Plant availability: 330 days/year

🐞 Economic Evaluation Framework

A. Capital Expenditure (CapEx)

- Chlorination reactor
- Phase separator
- Distillation system
- Heat exchangers and pumps
- Storage tanks (EDC is hazardous—requires special materials)
- Safety systems (HCl handling, ventilation)
- Catalyst and recycle infrastructure

B. Operating Expenditure (OpEx)

Category Description

Raw materials Ethylene and chlorine

Catalyst Ferric chloride replacement (if any)

Utilities Steam, electricity, cooling water

Maintenance & labor Plant operation

Waste handling Vent gas treatment, HCl neutralization

C. Financial Indicators

Indicator Purpose

IRR Expected return on capital investment

NPV Present value of future cash flows

Payback Period Time required to recover investment

Cash Flow Yearly profitability after expenses

D. Economic Assumptions (Sample)

Parameter Value

Project Life 15 years

Parameter Value

Discount Rate 10%

Depreciation 10-year straight line

Operating Days/Year 330

Startup Duration 1 year

Tax Rate 30%

✓ Final Deliverables

- 1. Aspen Plus Simulation File (.bkp): Full flowsheet, unit operations, stream tables
- 2. Process Flow Diagram (PFD): Visual process layout
- 3. Material & Energy Balance Report
- 4. Utility Consumption Summary
- 5. Capital and Operating Cost Estimates
- 6. Economic Analysis Spreadsheet: IRR, NPV, Payback Period
- 7. Final Technical & Financial Report