CHE654 Design Project #2

Semester 1, 2025

🧩 Problem Statement

Project Title

Simulation and Economic Evaluation of Aniline Production from Benzene via Nitrobenzene Using Aspen Plus

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Background

Aniline ($C_6H_5NH_2$) is a key industrial chemical widely used in the manufacture of dyes, rubber processing chemicals, pharmaceuticals, agrochemicals, and polyurethane precursors (such as MDI). The most common industrial route to aniline involves **nitration of benzene** to produce **nitrobenzene**, followed by **catalytic hydrogenation** to produce aniline.

This process is well-established and efficient, but plant design, energy integration, and cost evaluation remain crucial to determine the **technical and financial feasibility** of scaling or optimizing the production. This project will simulate the production process in **Aspen Plus**, design all key process units, and evaluate its **economic viability** using standard financial indicators such as **IRR**, **NPV**, and **payback period**.

Objectives

1. **Simulate the production of aniline** from benzene via nitrobenzene using Aspen Plus.
2. Define all necessary **reaction pathways, unit operations, and process conditions**.
3. Perform **material and energy balances** and simulate separation, reaction, and heat integration units.
4. Design a **process flow diagram (PFD)** suitable for scale-up or pilot plant design.
5. Carry out a **comprehensive economic evaluation**, including:
    - Capital and operating costs
    - Cash flow analysis
    - Net Present Value (NPV)
    - Internal Rate of Return (IRR)
    - Payback period

6. Recommend process improvements and assess the project's financial feasibility.

🔁 Process Description

The production of aniline from benzene typically occurs in two main steps:

1. **Nitration of Benzene:**
   - Benzene reacts with nitric acid (and sulfuric acid as a catalyst) to form **nitrobenzene**.
   - This is an exothermic liquid-phase reaction.
2. **Hydrogenation of Nitrobenzene:**
   - Nitrobenzene is catalytically hydrogenated using H_2 gas to form **aniline** and water.
   - This step requires high pressure and temperature and is typically gas-phase or trickle-bed.

🏗️ Conceptual Process Flow Diagram (PFD)

FEED 1: Benzene ─┐

├─> R-101: Nitration Reactor ─> V-101: Phase Separator

FEED 2: HNO_3 ─────┘ ↓

Nitrobenzene + H_2 ─> R-102: Hydrogenation Reactor

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T-101: Distillation Column

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Products: Aniline (main), Water (byproduct)

Optional recycle or vent systems may be added.

🧪 Aspen Plus Simulation Setup

1. Thermodynamic Model

- Use **NRTL** or **UNIQUAC** for liquid-phase nitration.
- Use **Peng-Robinson** for vapor-phase hydrogenation if gas-phase model is used.

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2. Components

Component	Formula	Role
Benzene	C_6H_6	Raw material
Nitric Acid	HNO_3	Nitrating agent
Nitrobenzene	$C_6H_5NO_2$	Intermediate
Hydrogen	H_2	Reducing agent
Aniline	$C_6H_5NH_2$	Final product
Water	H_2O	Byproduct
Sulfuric Acid	H_2SO_4	Catalyst (not consumed)

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3. Reaction Equations

a. Nitration:

C6H6 + HNO3 → C6H5NO2 + H2O

- Reactor Type: **RStoic** or **RCSTR**
- Conditions: ~50–80°C, 1–2 atm
- Conversion: ~90–95% of benzene

b. Hydrogenation:

C6H5NO2 + 3H2 → C6H5NH2 + 2H2O

- Reactor Type: **RPlug** or **RGibbs**
- Catalyst: Pd/C or Ni
- Conditions: 150–250°C, 10–30 atm
- Conversion: > 98% of nitrobenzene

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4. Process Units (Aspen Blocks)

Unit ID	Type	Description
R-101	RStoic	Nitration of benzene
V-101	Flash2	Phase separation (removal of acids)
R-102	RPlug	Hydrogenation of nitrobenzene
T-101	RadFrac	Separation and purification of aniline
E-101	HeatX	Utility heat exchangers

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5. Operating Conditions (Typical)

Unit	Temperature	Pressure	Notes
R-101	60–80°C	1–2 atm	Nitration
V-101	50°C	1 atm	Separation of acids/water
R-102	180–220°C	20–30 atm	Hydrogenation with Ni or Pd/C
T-101	100–140°C	~1 atm	Aniline separation/distillation

📈 **Economic Evaluation Scope**

A. Capital Cost Estimates

- Based on equipment sizing and Aspen Economic Evaluator or CAPCOST
- Includes installation, contingency, and indirect costs

B. Operating Cost Estimates

- Feedstock prices (e.g., benzene, nitric acid, hydrogen)
- Utilities (steam, cooling water, electricity)
- Catalyst cost (Pd, Ni), waste treatment, labor

C. Revenue Assumptions

- Aniline market price: ~$1.5–2.5/kg
- Annual production target: e.g., **10,000 TPA**

D. Financial Indicators

Metric	Description
NPV	Net Present Value over project life
IRR	Internal Rate of Return
Payback Period	Time to recover total investment
Cash Flow Analysis	Year-by-year operating margin and profit

E. Assumptions

- Project life: 15–20 years
- Discount rate: 10–12%
- Construction time: 2 years
- Depreciation: Straight-line (or MACRS)
- 330 operating days/year

✅ Deliverables

- Aspen Plus simulation file (.bkp or .apw)
- Complete PFD and stream tables
- Equipment list and utility consumption summary
- Excel spreadsheet for:
  - Capital and operating cost estimation
  - Cash flow and profitability analysis
  - NPV, IRR, and payback calculation
- Recommendations for optimization
