

CHE654 Design Project #6

Semester 1, 2025

Problem Statement

Project Title

Simulation and Economic Analysis of n-Butanol Production via the Oxo Process from Propylene Using Aspen Plus

Background

n-Butanol (C_4H_9OH) is an important industrial alcohol used as a **solvent**, **chemical intermediate**, and in **plasticizers** and **coatings**. A common industrial route for its production is the **Oxo process** (hydroformylation), where **propylene** reacts with **synthesis gas** ($CO + H_2$) to form **butyraldehyde**, which is then **hydrogenated** to **n-butanol**.

This project focuses on designing and simulating the production of n-butanol from **propylene** using the **oxo process** in **Aspen Plus**, followed by an **economic evaluation** of the process using major financial indicators to determine its viability.

Objectives

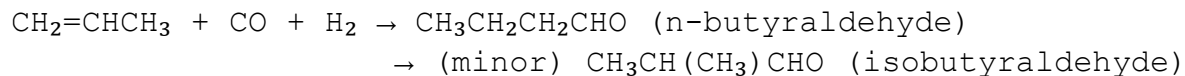
1. **Simulate** the production of n-butanol from propylene using the **Oxo process** in Aspen Plus.
 2. Develop a comprehensive **process flow diagram (PFD)** with key unit operations.
 3. Conduct **mass and energy balances** for each unit operation.
 4. Estimate **raw material and utility requirements**.
 5. Perform a detailed **economic analysis**, including:
 - Internal Rate of Return (IRR)
 - Net Present Value (NPV)
 - Payback Period
 - Annual Cash Flow
 6. Evaluate the **technical and financial feasibility** of the proposed process.
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Process Chemistry

1. Hydroformylation (Oxo Reaction)

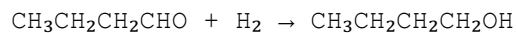
Propylene + CO + H₂ → Butyraldehydes (n- and iso-)



- **Catalyst:** Rhodium- or cobalt-based homogeneous catalyst
 - **Conditions:** Moderate temperature (100–150°C), high pressure (20–40 bar)
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2. Hydrogenation of Aldehydes

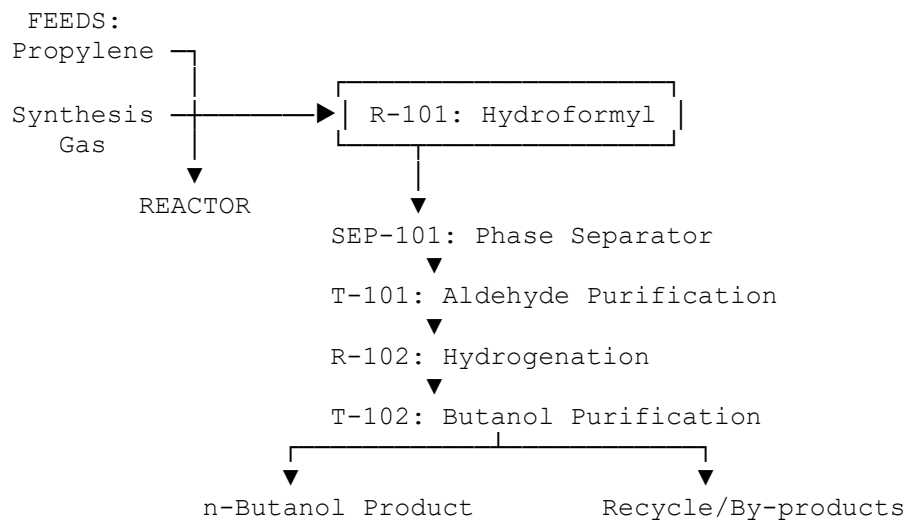
Butyraldehyde + H₂ → *n*-Butanol



- **Catalyst:** Nickel or copper-based
 - **Conditions:** 120–200°C, 10–20 bar
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Conceptual Process Flow Diagram (PFD)



Aspen Plus Simulation Setup

1. Thermodynamic Model

- **NRTL** or **UNIQUAC** for liquid–liquid and vapor–liquid equilibrium
 - **Peng-Robinson** or **SRK** for high-pressure vapor-phase components
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2. Component List

Component	Formula	Role
Propylene	C ₃ H ₆	Feed
Carbon Monoxide	CO	Feed (syngas)
Hydrogen	H ₂	Feed (syngas)
<i>n</i> -Butyraldehyde	C ₄ H ₈ O	Intermediate
Isobutyraldehyde	C ₄ H ₈ O	By-product
<i>n</i> -Butanol	C ₄ H ₉ OH	Final product
Water	H ₂ O	By-product
Inerts (CH ₄ , N ₂)	Various	Purge

3. Typical Operating Conditions

Unit	Temp (°C)	Pressure (bar)	Notes
Hydroformylation	100–150	20–40	Rh or Co catalyst
Phase Separator	40–80	~10–20	Remove unreacted gases
Hydrogenation	120–200	10–20	Ni or Cu catalyst
Distillation	Varies	~1–2	Product purification

4. Feed Data (Example Basis)

Component	Flowrate (kmol/h)	Purity (%)
Propylene	100	99.9
CO	100	99.5
H ₂	200	99.5

Target Production: ~**50,000 tonnes/year** of *n*-butanol
Operating Days: **330 days/year**

Economic Evaluation Framework

A. Capital Costs (CapEx)

- Reactors (high-pressure)
 - Gas separators
 - Distillation towers
 - Heat exchangers, compressors
 - Catalyst recovery (optional)
 - Instrumentation & control
 - Safety systems
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B. Operating Costs (OpEx)

Category	Description
Raw Materials	Propylene, CO, H ₂
Catalyst	Rh or Co complex, Ni, Cu
Utilities	Steam, electricity, cooling water
Maintenance & Labor	Plant operation
Waste Treatment	Off-gas, aqueous purge

C. Financial Indicators

Indicator	Purpose
IRR	Return on investment over time
NPV	Net value of all future cash flows
Payback Period	Time to recover initial investment
Annual Cash Flow	Profit after expenses each year

D. Economic Assumptions (Typical Values)

Parameter	Value
Project Life	15 years
Discount Rate	10%
Depreciation	10 years, straight-line
Operating Days/Year	330
Tax Rate	30%

Parameter	Value
Startup Year Loss	100% CapEx recovery over life

Final Deliverables

1. **Aspen Plus Simulation File:** Flowsheet with all major units
 2. **Process Flow Diagram (PFD):** Detailed and labeled
 3. **Material and Energy Balances**
 4. **Utility Requirements and Consumption**
 5. **Cost Estimates:** CapEx and OpEx
 6. **Economic Evaluation Spreadsheet:**
 - IRR
 - NPV
 - Payback period
 - Annual cash flows
 7. **Technical Report** summarizing:
 - Process design
 - Simulation results
 - Economic conclusions
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