CHE654 Design Project #8

Semester 1, 2025

Problem Statement: Aspen Plus Simulation of Acetic Anhydride Production from Acetone

Objective:

To simulate and evaluate the production of acetic anhydride using acetone as the feedstock, via the thermal cracking of acetone to form ketene and methane, followed by the reaction of ketene with acetic acid. The study will utilize Aspen Plus to develop a rigorous process model and perform an economic evaluation to determine the financial viability of the process.

Process Description:

1. Feed Preparation:
    - Acetone is fed into a cracking furnace operating at high temperatures (~700–750°C) where it undergoes pyrolysis:

      $$CH_3COCH_3 \rightarrow CH_2CO + CH_4$$

        - Products: ketene (CH_2CO) and methane (CH_4).
2. Separation:
    - The gaseous product stream from the furnace is cooled and sent to a separator where methane is removed as a by-product.
    - Ketene is purified for use in the next step.
3. Synthesis of Acetic Anhydride:
    - Ketene is reacted with acetic acid in a reactor to produce acetic anhydride:

      $$CH_2CO + CH_3COOH \rightarrow (CH_3CO)_2$$

    - Product Recovery:
    - The reactor output is cooled, and acetic anhydride is separated and purified.
    - Any unreacted acetic acid is recycled back to the reactor.

Simulation Tasks in Aspen Plus:

- Model the thermal cracking reactor using an RGIBBS or RYIELD reactor.
- Simulate the ketene purification and methane separation steps.

- Model the ketene-acetic acid reaction using an RPLUG or RCSTR reactor.
- Design heat exchangers, separators, and recycle loops.
- Include a sensitivity analysis for reactor temperature, conversion rates, and separation efficiency.

Economic Evaluation:

- Perform a cost estimation using Aspen Economic Analyzer or Aspen Process Economic Analyzer (APEA).
- Estimate:
    - Total Capital Investment (TCI)
    - Operating Costs (OPEX)
    - Raw material costs (acetone, acetic acid)
    - Product revenue from acetic anhydride and by-product methane (if utilized).
- Conduct financial analysis including:
    - Net Present Value (NPV)
    - Internal Rate of Return (IRR)
    - Payback Period
    - Break-even analysis
- Consider market prices of acetic anhydride and assess project viability under different production scales.

Expected Outcomes:

- A fully developed Aspen Plus flowsheet simulating all process units.
- Optimal operating conditions for maximum product yield and energy efficiency.
- Economic indicators to assess the profitability of the process.
- Recommendations for process improvements or scale-up potential.