Process Analysis and Optimization

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Application of Optimization Techniques in Chemical Engineering

Problem 1: Optimization of Plug Flow Reactor (PFR) Design

Objective: To maximize the conversion of a first-order irreversible reaction ($A \rightarrow B$) in a PFR, for a given feed rate and reactor volume using optimization techniques.

Given Parameters (Assumed):

- Reaction: $A \rightarrow B$
- Rate law: $-r_A = kC_A$
- First-order reaction: $k = 0.1\ s^{-1}$ (assumed)
- Feed flow rate: $F_{A0} = 10$ mol/s
- Reactor volume: $V = 100$ L

Model Equations:

PFR Design Equation:

$$V = \int (F_{A0} / -r_A)\, dX$$

Since $-r_A = kC_A = kC_{A0}(1 - X)$, then:

$$V = (F_{A0} / kC_{A0}) * \int (1 / (1 - X))\, dX$$

$$V = (F_{A0} / kC_{A0}) [-\ln(1 - X)]$$

Solving for X:

$$X = 1 - \exp(-kC_{A0}V / F_{A0})$$

Optimization Approach:

Objective Function: Maximize X

Constraints:

- Fixed reactor volume V
- Fixed feed rate F_{A0}

As per the equation, conversion X increases with initial concentration C_{A0}.

Therefore, maximize C_{A0} within limits to maximize X.

Result and Conclusion:

Assuming C_{A0} = 1 mol/L:

$X = 1 - \exp(-0.1 * 1 * 100 / 10) = 1 - \exp(-1) \approx 0.632$

Conclusion: Operating at higher C_{A0} increases conversion. Optimization suggests maximizing C_{A0} within design limits.

Problem 2: Optimization of Distillation Column

Objective: To minimize total cost by optimizing the number of theoretical stages (N) and reflux ratio (R).

Cost Components:

1. Capital Cost (CC): Increases with number of stages (N)
2. Operating Cost (OC): Increases with reflux ratio (R)

Optimization Strategy:

Use Underwood-Gilliland Shortcut Method:

- Estimate minimum reflux ratio R_{min}
- Estimate minimum number of stages N_{min}
- Apply Gilliland correlation:

  $Y = (N - N_{min}) / (N + 1)$

  $X = (R - R_{min}) / (R + 1)$

Objective Function:

Total Cost (TC) = $\alpha N + \beta R$

Where:

α = cost per stage

β = cost per unit reflux

Optimization Procedure:

1. Calculate R_{min} using Underwood equations
2. Vary R from R_{min} to $2R_{min}$ and calculate N using Gilliland correlation
3. Calculate TC for each pair (N, R)
4. Choose the combination that minimizes TC

Illustrative Example:

Assume:
- $R_{min} = 1.5$
- $N_{min} = 12$
- $\alpha = 1000$, $\beta = 5000$

Try R = 1.5, 2.0, 2.5, 3.0
Calculate corresponding N and TC for each R
Determine the optimal combination (N, R) with minimum TC

Conclusion:

- Higher R decreases N but increases OC
- Higher N reduces R but increases CC
- Optimal point is a balance between capital and operating cost

Usually found near R = 1.4 to 1.6 * R_{min}

This assignment demonstrates how optimization techniques can be used effectively in chemical reactor and separation process design. Mathematical modeling and trade-off analysis are essential tools in achieving cost-effective engineering solutions.