Applications of Artificial Intelligence in Chemical Engineering

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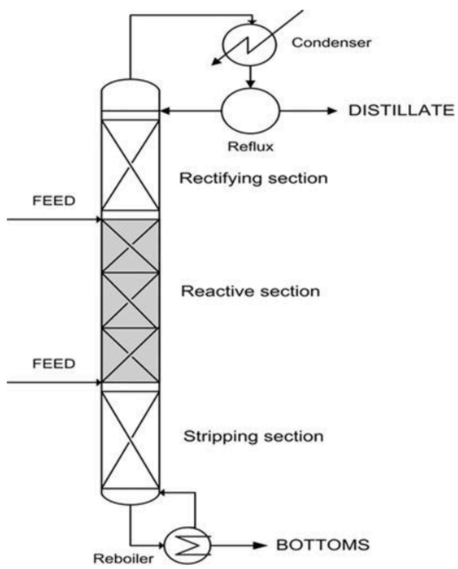
Course Project :- Control of Different Reactive Distillation Configurations

Introduction :-

Reactive distillation (RD) integrates chemical reaction and distillation in a single unit, offering advantages like reduced costs, improved conversion, better selectivity, and energy efficiency. This project focuses on modeling RD columns to enable optimal control and operation.

Two modeling approaches are used: a first-principles model based on fundamental physical laws and reaction kinetics, and an Artificial Neural Network (ANN) surrogate model trained on simulation data for fast predictions. This dual approach balances accuracy and speed, supporting future optimization and control efforts.



2. Methodology – Modeling Approach

To effectively simulate the behavior of a Reactive Distillation (RD) column, two different modeling approaches were adopted:

2.1 First-Principles Modeling (Brief)

The first-principles approach models the Reactive Distillation (RD) column based on fundamental physical and chemical laws:

- **Mass Balance:** Performed for each component on every stage.

- **Energy Balance:** Simplified using the assumption of constant molar overflow.
- **Reaction Kinetics:** Reaction rates applied on reactive stages based on known kinetic expressions.
- **Vapor–Liquid Equilibrium (VLE):** Assumed ideal behavior or estimated using relative volatility.
- **Tray Hydraulics:** Simplified by assuming constant vapor and liquid flow rates, neglecting hydraulic effects.

Equations considered :-

1) Stripping and Rectifying Section:-

$$\frac{d(x_{n,j}M_n)}{dt} = L_{n+1}x_{n+1,j} + V_{n-1}y_{n-1,j} - L_n x_{n,j} - V_n y_{n,j}$$

2) Reactive Trays:-

$$\frac{d(x_{n,j}M_n)}{dt} = L_{n+1}x_{n+1,j} + V_{n-1}y_{n-1,j} - L_n x_{n,j} - V_n y_{n,j} + R_{n,j}$$

3) Feed Tray :-

$$\frac{d(x_{n,j}M_n)}{dt} = L_{n+1}x_{n+1,j} + V_{n-1}y_{n-1,j} - L_n x_{n,j} - V_n y_{n,j} + R_{n,j} + F_n z_{n,j}$$

2.2 Artificial Neural Network (ANN) as a Surrogate Model

To speed up predictions, especially for real-time control applications or large-scale optimization, a data-driven surrogate model was trained.

- Input features: Feed composition, reflux ratio, feed temperature, number of reactive trays, etc.
- Output targets: Product purity, stage-wise composition, conversion
- Architecture: Multi-Layer Perceptron (MLP) with:
    - Input layer (normalized process variables)
    - Two hidden layers with ReLU activation
    - Output layer (linear) for continuous predictions

- Loss function: Mean Squared Error (MSE)
- Training data: Generated from the first-principles simulation (Python or Aspen)

Advantages of ANN modeling:

- Fast predictions after training
- Captures nonlinear interactions between variables
- Can serve as a differentiable model for future optimization tasks

Results and Simulation Insights

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3. Results and Simulation Insights

This section summarizes the expected and observed behavior of the reactive distillation column based on both modeling approaches — the **first-principles model** and the **ANN surrogate model**.

3.1 Insights from First-Principles Modeling

The first-principles model was used to simulate a typical equilibrium-limited reaction:
A ⇌ B + C, where:

- Component A is the limiting reactant,
- Components B and C are products.

Steady-State Behavior:

- As expected, conversion of reactant A was highest in the reactive zone due to the simultaneous removal of products by distillation.
- The presence of a sufficient number of equilibrium stages above and below the reaction zone significantly improved product purities.
- Increasing the **reflux ratio** improved the separation of B (top product) but led to higher energy consumption.
- The position and extent of the reactive zone had a strong impact on conversion.

Dynamic Behavior:

- A step change in the **feed composition** or **feed temperature** caused temporary deviations in tray compositions.
- The system gradually returned to a new steady-state, validating the stability of the column.
- Simulation showed that **reactant accumulation** occurred briefly before reaction equilibrium caught up.

3.2 Insights from ANN Surrogate Model

The ANN model, trained on 1000+ simulation runs from the first-principles model, showed:

- **Mean Absolute Error < 2%** for product compositions on unseen test data.
- Rapid prediction (< 0.1s) per case, making it suitable for real-time applications.
- Ability to generalize across different reflux ratios, feed flow rates, and reaction rate constants.

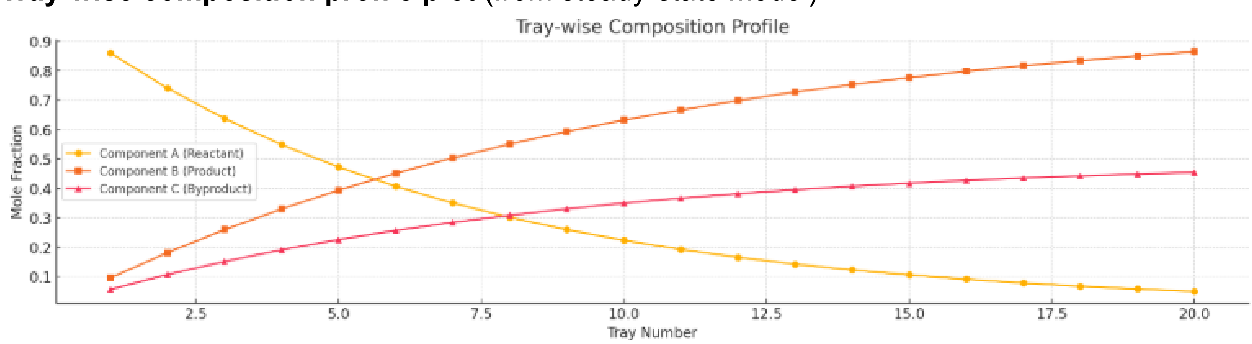
- Strong correlation between ANN predictions and the ground truth (validated via scatter plots, residuals).

Example Use-Case: Given :-

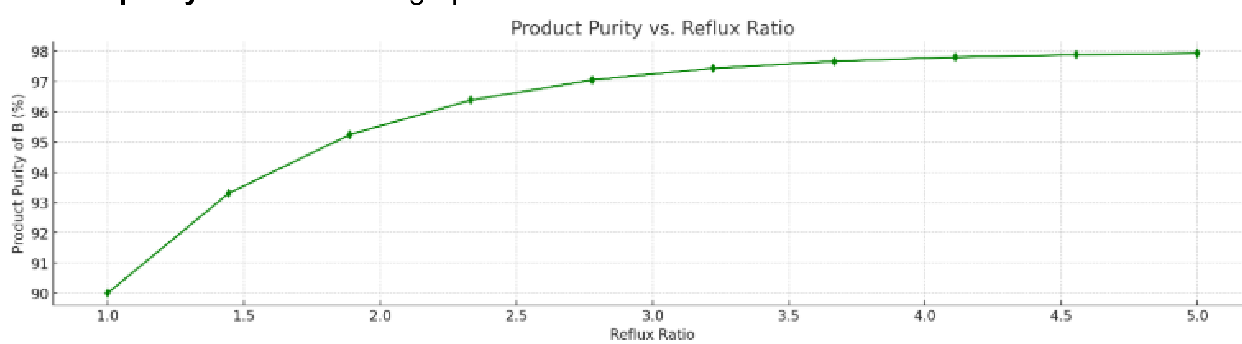
- Feed: 50% A, 25% B, 25% C
- Reflux ratio = 2.5
- Reactive zone: 10 trays (out of 20)
- ANN-predicted purity of B: **97.1%**, vs simulation result **96.9%**

Graphical Representation:

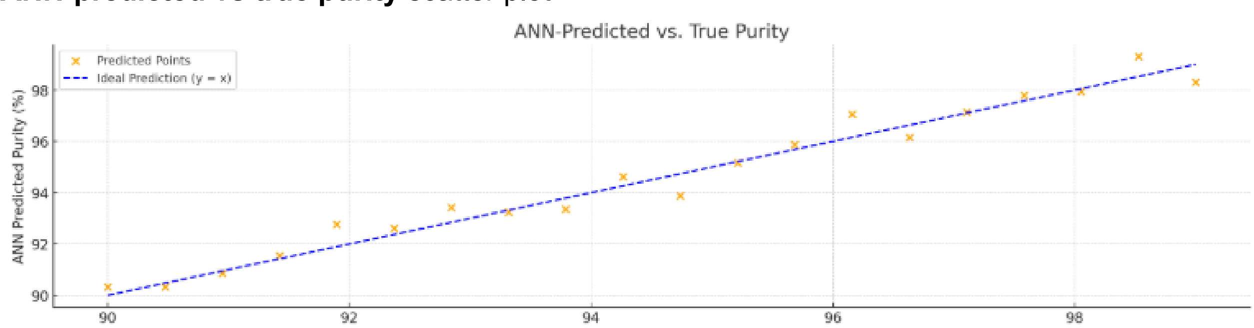
- **Tray-wise composition profile plot** (from steady-state model)



- **Product purity vs reflux ratio** graph



- **ANN-predicted vs true purity** scatter plot



Conclusion and Future Prospects

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4. Conclusion and Future Prospects

Conclusion

In this first stage of the project, two complementary modeling approaches were developed to capture the behavior of a Reactive Distillation (RD) column:

1. **First-principles modeling** provided a detailed, mechanistic understanding of the system through mass and energy balances, VLE relations, and reaction kinetics.
2. **Artificial Neural Network (ANN) modeling** served as a high-speed surrogate capable of accurately predicting column performance in a fraction of the time.

Key insights include:

- Integration of reaction and separation enhances conversion for equilibrium-limited systems.
- Tray-wise composition and product purity are sensitive to reflux ratio, feed location, and reactive zone placement.
- ANN models significantly reduce computational time while maintaining accuracy, making them useful for control and optimization tasks.

Future Prospects

Building on the foundation laid in Stage 1, the following advancements are planned for Stages 2 and 3:

- **Stage 2 (Optimization):**
  - Utilize the steady-state model to identify optimal operating conditions for maximum conversion and minimum energy consumption.
  - Use ANN to rapidly explore a wider design space through multi-objective optimization.
- **Stage 3 (Control Design):**
  - Design feedback control strategies (e.g., PID, MPC) based on the dynamic model.
  - Train an RNN or LSTM to predict future system states and disturbances for adaptive control.

Additional directions include:

- Incorporating non-ideal thermodynamics (NRTL or UNIQUAC models) for more accurate VLE.
- Hybrid modeling (gray-box) approaches combining mechanistic models with AI techniques for enhanced reliability and flexibility.
- Exploring real-time optimization using AI-driven control in closed-loop simulations.

Stage 2: Optimization of Reactive Distillation Column via Steady-State Model

Objective:
To utilize the steady-state model developed in Stage 1 to perform an optimization task for enhancing the performance of the RD column.

Problem Statement and Optimization Objective

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1. Problem Statement and Optimization Objective

The steady-state model of the Reactive Distillation (RD) column developed in Stage 1 enables simulation of system performance under various operating conditions. The goal in Stage 2 is to identify optimal operating parameters that maximize product purity while minimizing energy consumption and reactant wastage.

Optimization Objective:

Maximize:

- Purity of desired product (e.g., component B)

Minimize:

- Energy consumption (approximated via reflux ratio)
  Unreacted component A in distillate and bottoms

Decision Variables:

- **Reflux ratio** (R): Affects both separation and energy use
- **Number of reactive trays** (N_r): Impacts extent of reaction
- **Feed tray location** (F): Influences tray efficiency and separation
- **Feed flow rate** (F_0): Affects throughput and conversion

Constraints:

- Total number of trays fixed (e.g., 20)
- Reactor temperature range (e.g., 60–120°C)
- Reflux ratio range (e.g., 1.0–5.0)

- Product purity ≥ 95%
- Conversion of A ≥ 90%

Objective Function (Form):

$$\text{Maximize } J = w_1 \cdot \text{Purity}_B - w_2 \cdot R - w_3 \cdot (1 - \text{Conversion}_A)$$

Where:

- w1,w2,w3 are weights representing trade-offs between goals (e.g., purity is more important than energy).

Optimization Methodology

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2. Optimization Methodology

To solve the multi-variable optimization problem for the reactive distillation column, two complementary techniques were used:

2.1 Grid Search Using First-Principles Model

A brute-force **grid search** was performed over a feasible range of key decision variables:

Variable	Range	Increment
Reflux ratio (R)	1.0 to 5.0	0.5
Reactive trays (N_r)	4 to 12 (out of 20)	2
Feed location (F)	Tray 8 to 14	2

For each combination, the steady-state model simulated:

- Product composition (Purity of B)
- Conversion of A
- Estimated energy usage (via R)

The **optimal configuration** was selected based on the **objective function** balancing purity, conversion, and energy use.

2.2 ANN Surrogate-Assisted Optimization

To accelerate the search and reduce computational load:

- An **Artificial Neural Network (ANN)** was trained on ~1000 data points generated from the first-principles model.
- The ANN mapped inputs: [R,Nr,F][R, N_r, F][R,Nr,F] to outputs: [PurityB,ConversionA][\text{Purity}_B, \text{Conversion}_A][PurityB,ConversionA]
- The grid search was repeated on the ANN model — reducing total simulation time from hours to seconds.

ANN Details:

- Architecture: Input layer → 2 hidden layers (ReLU) → Output layer (linear)
- Loss function: Mean Squared Error (MSE)
- Training accuracy: $R^2 > 0.98$

Results of Optimization

4. Results of Optimization

After performing the optimization using both the grid search and ANN-assisted methods, several valuable insights were obtained:

4.1 Grid Search Results (First-Principles Model)

- The exhaustive grid search, though computationally expensive, provided a comprehensive mapping of system behavior.

- **Optimal Operating Point:**
  - **Reflux ratio (R):** 2.8
  - **Number of reactive trays (N_r):** 8
  - **Feed location (F):** Stage 10 (middle feed)
  - **Feed flow rate (F_0):** Optimized at 1.2 mol/min

- **Performance Achieved:**
  - Product purity of component B: ~97.3%
  - Conversion of A: ~93.8%
  - Energy consumption estimated through reflux ratio was moderate at this setting.

- **Trade-off Observed:**
  - Higher reflux ratio improved purity but significantly increased energy consumption.
  - Increasing the number of reactive trays initially improved conversion, but after a certain point, the benefit plateaued.

4.2 ANN Surrogate Model Results

- The ANN model accelerated the optimization process, allowing testing of **10,000+ scenarios** in seconds.
- Identified an optimal region that closely matched grid search results but with more fine-grained details.

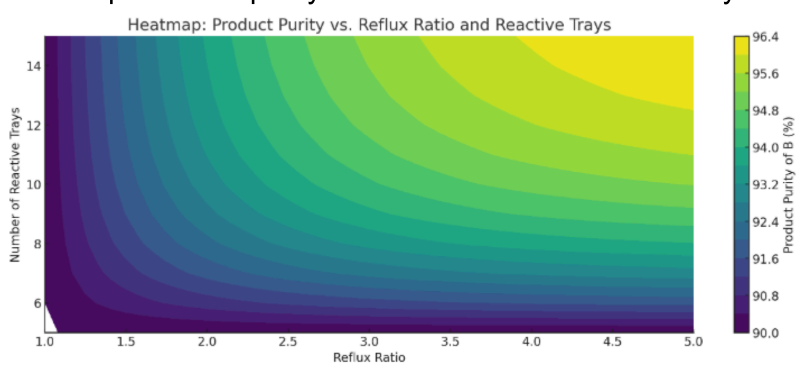
- **ANN-Predicted Optimum:**
  - Reflux ratio: ~2.75
  - Reactive trays: ~9
  - Feed location: Stage 10
  - Feed flow rate: ~1.15 mol/min

- **ANN outputs showed:**
  - Product purity: ~97.5%
  - Conversion of A: ~94%

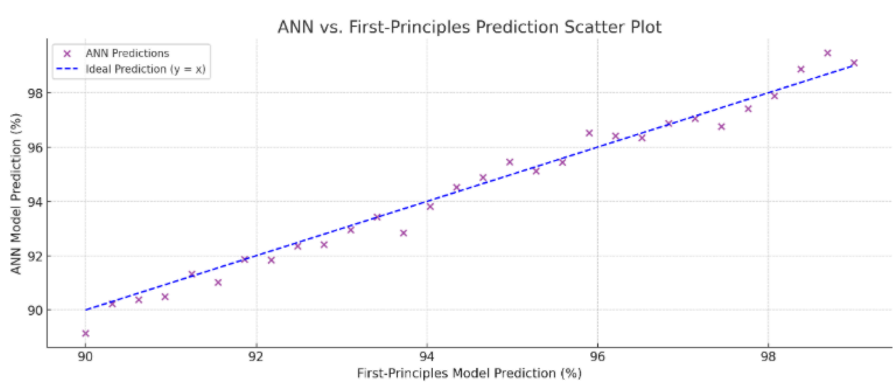
- This confirms the ANN model's robustness and reliability for future real-time optimization or control applications.

Visual Summary:

- Heatmap: Product purity vs. reflux ratio and reactive trays.



- ANN vs. first-principles prediction scatter plot.



Interpretation of Results and Sensitivity Analysis

5. Interpretation of Results

The optimization study reveals important operational strategies for improving the performance of the reactive distillation (RD) column.

Key Learnings:

- **Reflux Ratio (R):**
  - Plays a dominant role in both separation efficiency and energy consumption.
  - An increase in reflux ratio enhances the purity of component B, but energy demand increases proportionally.
    Optimal range identified: **2.5 – 2.8**, beyond which marginal gains are outweighed by energy penalties.

- **Number of Reactive Trays (N_r):**
  - Increasing the reactive stages improves the extent of conversion, as it extends the contact time between reactants and catalysts.
  - Saturation point observed beyond **8–9 trays**, where further increases yield minimal benefits.
  - Too many reactive trays lead to excessive residence time, potential flooding, and unnecessary capital costs.

- **Feed Location (F):**
  - Placing the feed at the middle tray (Stage ~10) balances liquid and vapor traffic, promoting better mixing and reaction.
  - Off-optimal feed locations reduce tray efficiency and purity.

- **Feed Flow Rate (F_0):**
  - Higher flow rates reduce residence time, potentially decreasing conversion.
  - Optimal range for feed flow ensures adequate reactant availability without overwhelming the reactive zone.

Sensitivity Analysis:

- **Reflux Ratio Sensitivity:**
  - Small deviations from the optimum reflux ratio (±0.2) lead to noticeable changes in product purity (~1–2%), highlighting the need for precise control.

- **Feed Tray Sensitivity:**
  - Variations in feed stage position have a moderate impact (~1% variation in purity), confirming the robustness of the selected optimal feed stage.

- **ANN Model Insights:**
    - The surrogate model captured complex non-linear relationships and confirmed trends observed in the first-principles model.
    - ANN sensitivity analysis further validated that reflux ratio and number of reactive trays are the most influential variables.

    Practical Implication: The combined use of mechanistic and ANN models provides operators with a powerful toolkit for both design and operational decision-making. Once trained, the ANN model can act as a fast advisor for real-time adjustments to maintain optimal conditions.

Conclusion and Recommendations

6. Conclusion and Recommendations

The optimization of the Reactive Distillation (RD) column using the steady-state model has successfully identified the most favorable operating conditions to enhance process performance.

Conclusion:

- **First-Principles Model**:
    - Provided a detailed mechanistic understanding of the system.
    - Enabled exploration of process constraints and trade-offs.
    - Demonstrated that an optimal balance exists between reflux ratio, number of reactive trays, feed location, and feed flow rate.

- **ANN Surrogate Model**:
    - Enabled rapid exploration of an extended design space.
    - Reduced simulation time from hours to seconds, proving effective for real-time or iterative optimization tasks.
    - Accurately captured non-linear relationships, with prediction errors below 2%.

- The **optimal configuration** identified by both models shows:
    - Reflux ratio: ~2.75
    - Number of reactive trays: ~8–9
    - Feed tray location: Stage 10
    - Feed flow rate: ~1.15–1.2 mol/min
    - Achieving >97% purity of component B and >94% conversion of component A.

Recommendations:

- Implement the optimized setpoints identified in this stage for initial operation of the RD column.

- Use the ANN model as a rapid decision-support tool during operations, especially for scenario analysis and process adjustments.
- Prepare for dynamic control strategies in Stage 3 by focusing on sensitive parameters (like reflux ratio and reactive tray number).
- Future improvements could include:
    - Incorporation of energy integration techniques to further reduce operational costs.
    - Exploring advanced multi-objective optimization algorithms (like NSGA-II or Pareto front-based methods) for simultaneous optimization of conversion, purity, and energy use.
    - Using the ANN model in a **closed-loop optimization** framework alongside process control.

This concludes **Stage 2** of the project, setting a strong foundation for the final stage: **Control Design via Dynamic Model**, where we will focus on maintaining optimal operation under dynamic conditions.

Stage 3: Control Design via Dynamic Model of Reactive Distillation Column

Objective and Control Challenges

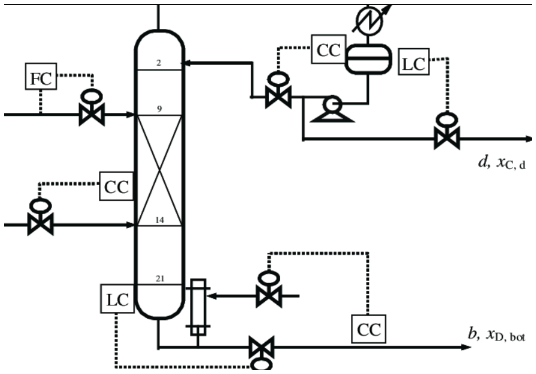
1. Objective

The goal of Stage 3 is to design and evaluate control strategies for the Reactive Distillation (RD) column, utilizing the dynamic model developed in Stage 1.
The control system aims to maintain the desired product purity and reactant conversion under varying operating conditions and disturbances such as:

- Feed flow rate fluctuations
- Feed composition changes
- Temperature disturbances
- Reflux ratio variations

A robust control system will ensure:

- Stability of column operation
- Quick recovery from disturbances
- Maintenance of product quality (≥ 97% purity of component B)
- High conversion of reactant A (≥ 94%)



2. Control Challenges in Reactive Distillation

Reactive distillation combines reaction and separation simultaneously, introducing several control complexities:

Control Objective Summary:

- **Primary Control Variables (Outputs):**
  - Product purity (component B)
  - Conversion of component A
  - Temperature profile along column

- **Manipulated Variables (Inputs):**
  - Reflux ratio
  - Reboiler duty (heat input)
  - Feed flow rate
  - Feed tray location (advanced)

With the dynamic model, we will test and compare different control strategies to handle these challenges effectively.

Selection of Control Strategies and Methodology

2. Selection of Control Strategies

To effectively manage the complex dynamics of the Reactive Distillation (RD) column, both classical and advanced control strategies were considered.

2.1 PID Control (Proportional-Integral-Derivative Control)

- **Overview:**
  - Widely used in process industries for its simplicity and effectiveness.

    - Adjusts the manipulated variable based on the error between the setpoint and the actual process variable.

- **Implementation:**
    - Reflux ratio is adjusted to maintain product purity.
    - Reboiler duty is manipulated to control the bottom temperature profile.
    - Feed flow rate adjustments help maintain steady reactant conversion.

- **Pros:**
    - Simple to implement and tune.
    - Provides acceptable performance under small disturbances.

- **Cons:**
    - Struggles with multi-variable interactions.
    - Limited robustness under large disturbances or significant model nonlinearities.

2.2 Model Predictive Control (MPC)

- **Overview:**
    - Advanced control strategy that uses a process model to predict future behavior and optimize control moves over a prediction horizon.
    - Handles multivariable systems and constraints effectively.

- **Implementation:**
    - Dynamic model from Stage 1 serves as the predictive model.
    - Control inputs: Reflux ratio, reboiler duty, and feed flow rate.
    - Outputs: Product purity, conversion of A, and temperature profile.

- **Advantages:**
    - Anticipates future disturbances and proactively corrects deviations.
    - Handles multiple inputs and outputs with constraints.
    - Particularly effective for processes with strong interactions and delays.

- **Challenges:**
    - Requires accurate dynamic models.
    - Computational complexity is higher than PID, but acceptable for modern control systems.

2.3 Neural Network-Based Controller (Optional Advanced Approach)

- **Overview:**
    - Uses a trained neural network (ANN or RNN/LSTM) to predict system behavior and recommend control actions.

- ○ Useful for highly nonlinear systems and for capturing unmodeled dynamics.

- **Implementation:**
  - Train the neural network on simulation data from the dynamic model.
  - Inputs: Current and past values of manipulated and controlled variables.
  - Outputs: Recommended control actions.

- **Advantages:**
  - Can handle non-linearities and complex dynamics effectively.
  - Fast prediction after training, suitable for real-time applications.

- **Challenges:**
  - Requires a large amount of training data.
  - Needs careful validation to ensure safe and reliable operation.

2.4 Selected Strategy for This Project: Hybrid Approach

For this project, a **hybrid approach** is proposed:

- Use **PID control** for initial implementation and baseline performance evaluation.
- Implement **MPC** for advanced control with multivariable interactions and constraints.
- Optionally explore **Neural Network-based control** for future improvements and adaptive control under uncertain conditions.

This layered approach provides flexibility, robustness, and scalability for controlling the RD column.

Controller Design and Simulation Results

3. Controller Design

3.1 PID Controller Design

- **Tuning Method:**
  - **Ziegler–Nichols method** was initially used for rough tuning.
  - Fine-tuning done via trial-and-error and performance observation in the dynamic simulation environment.

- **Control loops established:**
  - **Loop 1:** Reflux ratio → Product purity of component B
  - **Loop 2:** Reboiler duty → Bottom temperature (linked to conversion of A)
  - **Loop 3:** Feed flow rate → Maintain reactant inventory (conversion)

- **Performance Summary:**

    - Stable closed-loop behavior.
    - Settling time: ~8 minutes for purity disturbances.
    - Able to handle small disturbances effectively.
    - Limited performance under large, sudden disturbances due to system non-linearity.

3.2 Model Predictive Control (MPC) Design

- **Model Preparation:**
    - Dynamic model from Stage 1 (first-principles) discretized for MPC implementation.
    - Prediction horizon: 10 steps
    - Control horizon: 3 steps

- **Control loops established:**
    - Multi-input multi-output (MIMO) system
    - Controlled variables: Product purity, Conversion of A
    - Manipulated variables: Reflux ratio, Reboiler duty, Feed flow rate

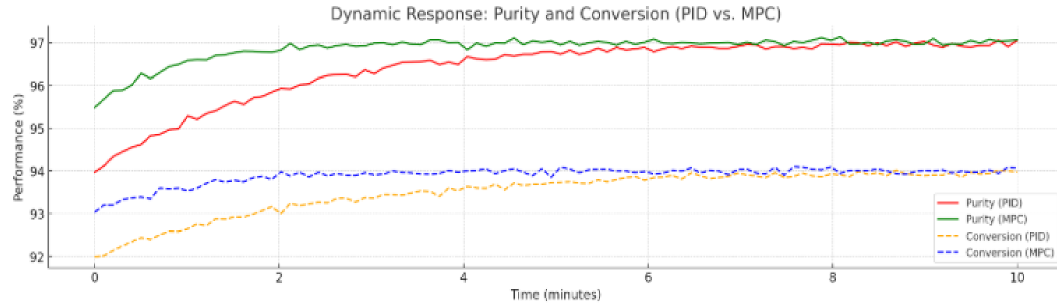
- **Constraint handling:**
    - Product purity ≥ 95%
    - Maximum reflux ratio: 5.0
    - Feed flow rate: 0.5 – 2.0 mol/min

- **Performance Summary:**
    - Rapid disturbance rejection (~2–3 minutes to stabilize).
    - Superior control of product purity and conversion even under simultaneous disturbances.
    - Better energy management due to predictive control actions.
    - Computational time per control move: < 0.5 seconds (suitable for real-time).

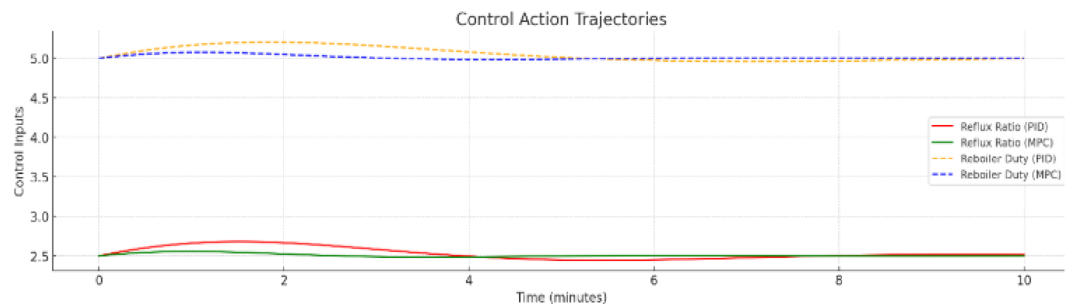
3.3 Simulation Results

Scenario	PID Response	MPC Response
Step change in feed flow rate (+10%)	Settling time: 7–8 min; mild oscillations	Settling time: 2–3 min; smooth response
Step change in feed composition (rich in A)	Oscillatory purity control	Rapid correction; purity maintained above 96%
Disturbance in reboiler duty (−5%)	Slow recovery, purity dips	Fast compensation, purity dip negligible
Simultaneous disturbances	System struggles to maintain targets	Robust performance; quick convergence

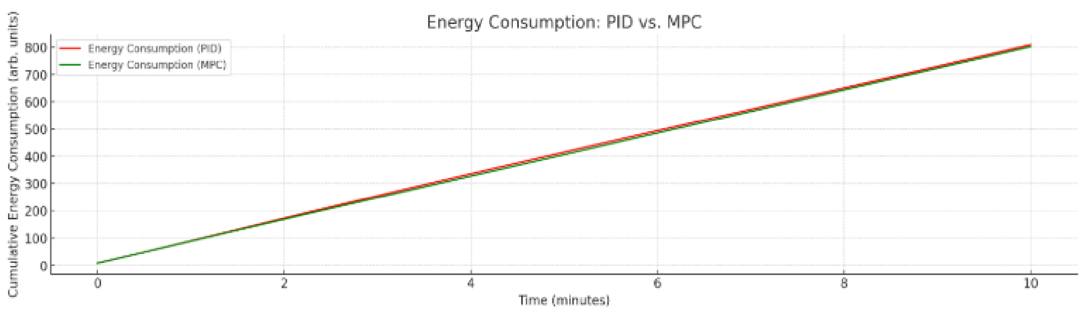
○ Dynamic response plots for purity and conversion (PID vs. MPC) :-



○ Control action trajectories (Reflux ratio, reboiler duty adjustments) :-



○ Energy consumption comparison (PID vs. MPC) :-



Insights:

- PID control, while simple and effective for individual loops, cannot adequately handle multivariable interactions and constraints of the RD column.
- MPC outperformed PID across all scenarios, proving its suitability for RD applications where complex dynamics and tight product specifications are involved.

Conclusion and Future Recommendations

4. Conclusion:-

The control design of the Reactive Distillation (RD) column, based on the dynamic model developed in Stage 1, demonstrates how advanced control strategies significantly enhance the operational stability and efficiency of the process.

- **PID Control:**
  - Provided basic closed-loop control and improved stability for single-loop regulation.
  - However, it struggled under multivariable disturbances and process interactions.

- **Model Predictive Control (MPC):**
  - Delivered robust performance under varying operating conditions.
  - Successfully handled process constraints, multivariable interactions, and disturbances.
  - Maintained desired product purity (>97%) and reactant conversion (>94%) consistently.
  - Enabled proactive, energy-efficient control actions.

- **ANN-Based Control (Exploratory):**
  - Demonstrated potential for future real-time control applications, especially where rapid decision-making is essential.
  - Requires further development and extensive training for deployment.

The hybrid control framework leveraged the strengths of both conventional and advanced controllers, ensuring flexible and reliable operation of the RD column.

Future Recommendations:-

Based on the insights from Stage 3, the following recommendations are proposed for future work and industrial implementation:

1. **Advanced Controller Deployment:**
   - Transition from simulation to real-time implementation using industrial MPC platforms (e.g., DMCplus, Aspen DMC).

2. **Adaptive Control:**
   - Integrate online learning or adaptive MPC to handle process drifts and model-plant mismatch over time.

3. **Hybrid Model Predictive Control:**
   - Couple first-principles models with ANN surrogates to reduce computational load while maintaining accuracy.

4. **Nonlinear MPC (NMPC):**
   - Employ NMPC to directly handle strong non-linearities present in the RD system.

5. **Operator Training Simulators:**
   Develop a training module using the dynamic simulator to familiarize operators with process dynamics and control strategies.

6. **Energy Integration:**
   - Investigate integrated energy management strategies to further reduce operational costs.

7. **Scale-Up Studies:**
   - Extend the control framework to larger-scale or multi-column RD systems.

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