CH620003 Process Modelling and Simulation

Report of Assignment 1

Executive Summary

This report covers the numerical and computational approaches used to solve problems related to process modeling and simulation. It includes the correlation of boiling points with molecular properties using regression and neural networks, flash calculations for a multicomponent system, and bubble point calculations for distillation column optimization. Key results include correlation coefficients, optimal process conditions, and neural network training outcomes.

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Objectives

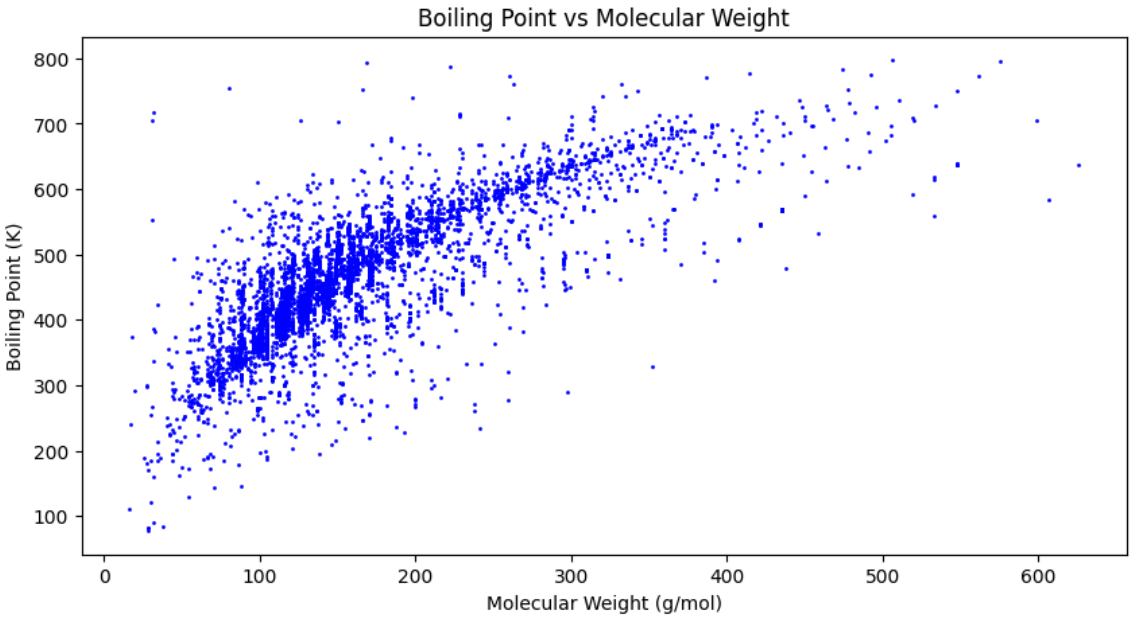
- Developed a regression model to correlate boiling points.
- Implemented and analyzed a neural network for improved predictions.
- Performed flash calculations and optimized recovery conditions.
- Solved distillation column equations iteratively for temperature profiles.

Question 1:

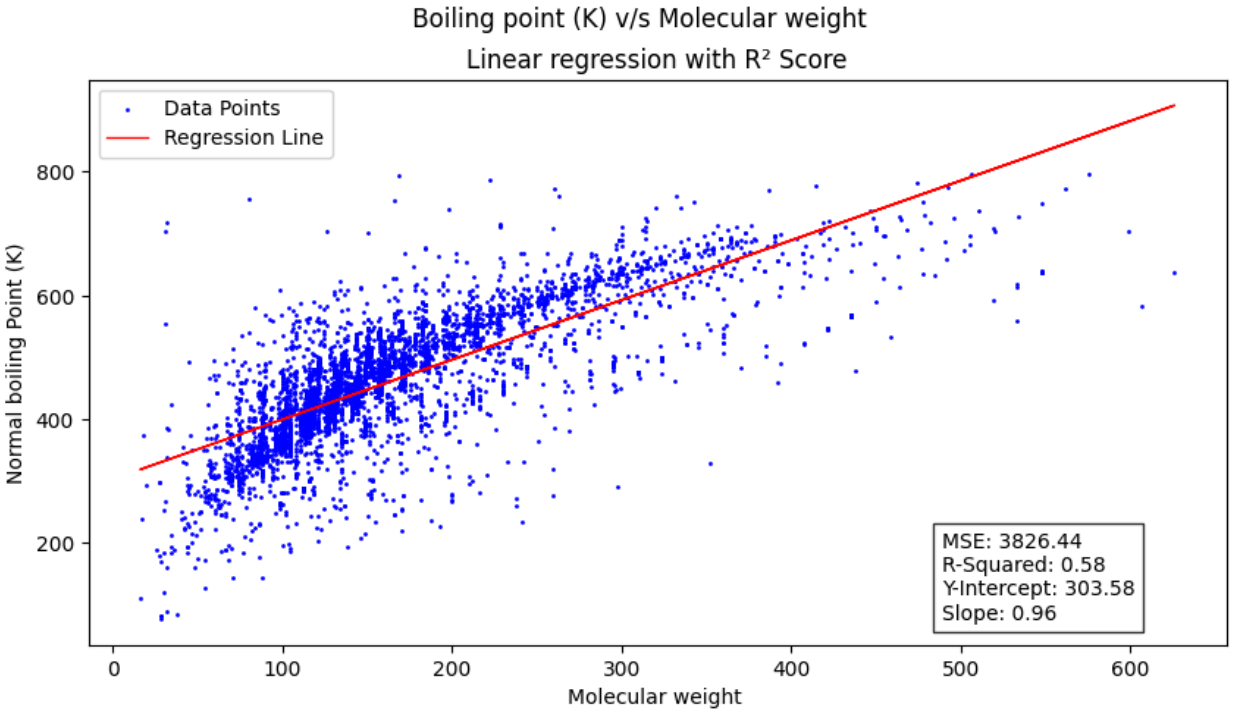
NN Correlation of Boiling Point with Chemical Properties

(a) Data Extraction and Preprocessing

- The dataset consists of columns for compound name, molecular weight, critical temperature, acentric factor, and normal boiling point.
- The entire dataset was extracted and stored in a matrix (AllData).
- The boiling points were extracted into a column vector.
- The molecular weights were extracted into another vector.
- The normal boiling point was plotted as a function of molecular weight.



- A linear regression line was fitted to the data, and the R^2 value was calculated to assess correlation strength.



Linear Regression Results:

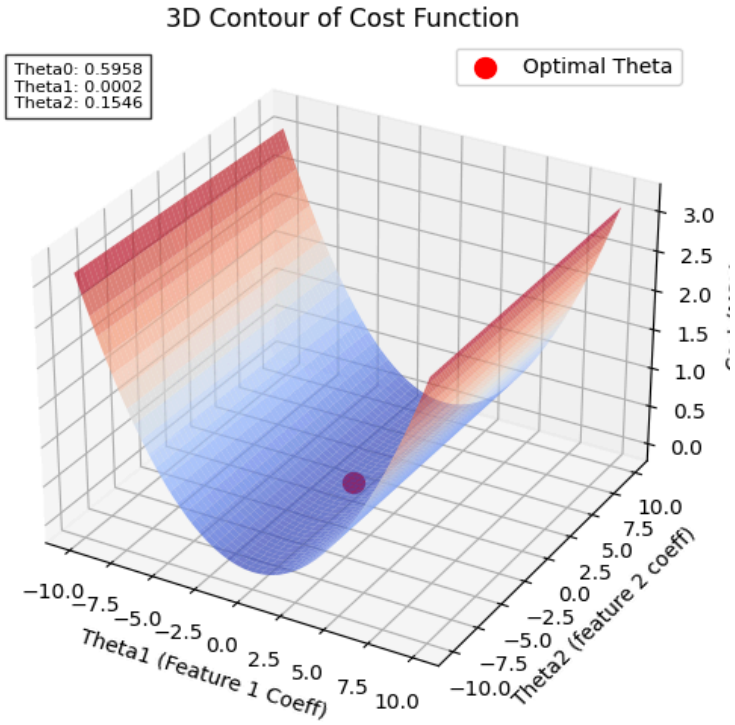
- Mean Squared Error: **3826.4377**
- R-Squared: **0.57998**
- Y-intercept: **303.5846**
- Slope: **0.9640**

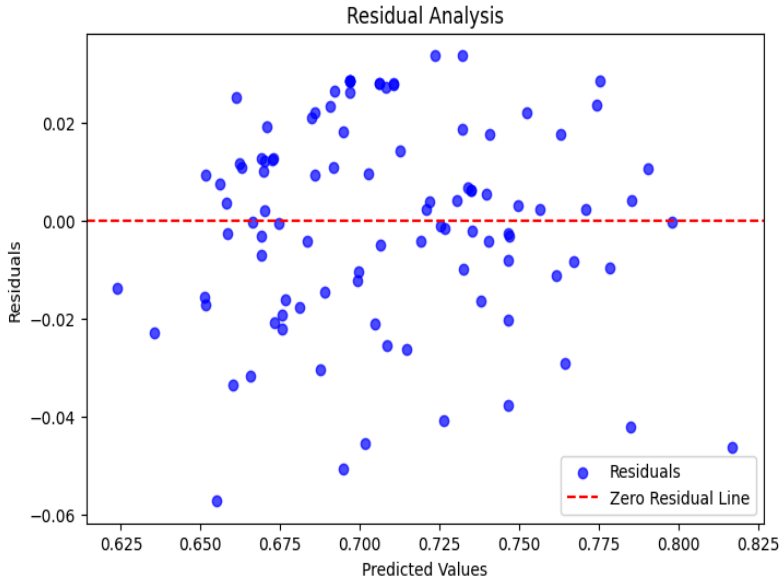
(b) Machine Learning Correlation (Linear Regression)

- 100 random compounds were selected as the training set.
- Constructed input matrix X:
  - First column: Bias term (ones)
  - Second column: Molecular weight
  - Third column: Acentric factor
- Constructed the output vector y, containing reduced boiling point (Tb/Tc).
- The solution to the linear regression equation was computed using:

$$\theta=(X^TX)^{-1}X^Ty$$

- The values of coefficients were obtained, assessing the quality of the correlation.
- Optimal Theta values: $\theta 0 = 0.5958$, $\theta 1 = 0.0002$, $\theta 2 = 0.1546$
- Linear Regression Results:
  - Mean Squared Error: **0.0004**
  - R-Squared: **0.7861**





(c) Neural Network Model

- Extracted two input columns (MW, acentric factor) and one output column (Tb/Tc).
- Standardized the input features using **StandardScaler**.
- Split the dataset into 10% training and 90% testing sets.
- Built a neural network with:
    - Input layer: **2** neurons (MW and acentric factor)
    - Hidden layers: **3** layers, **16** neurons each, ReLU activation
    - Output layer: **1** neuron (linear activation)

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Best Parameters:

Hidden Layers: 3

Neurons per Layer: 16

Minimum Loss: 0.0005707242526113987

Minimum MAE: 0.01662134937942028
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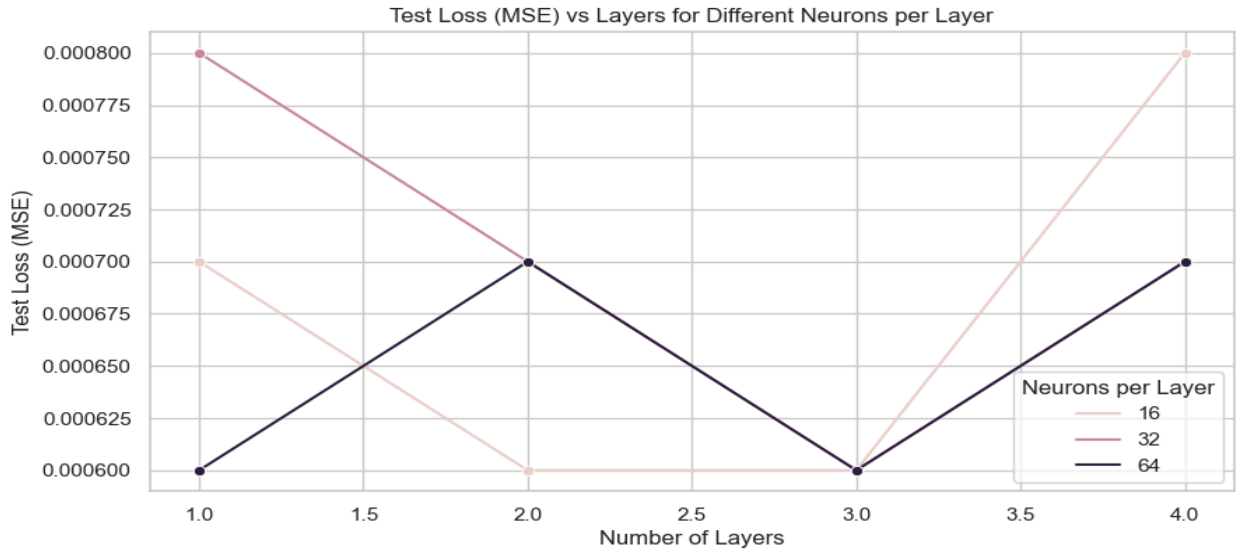
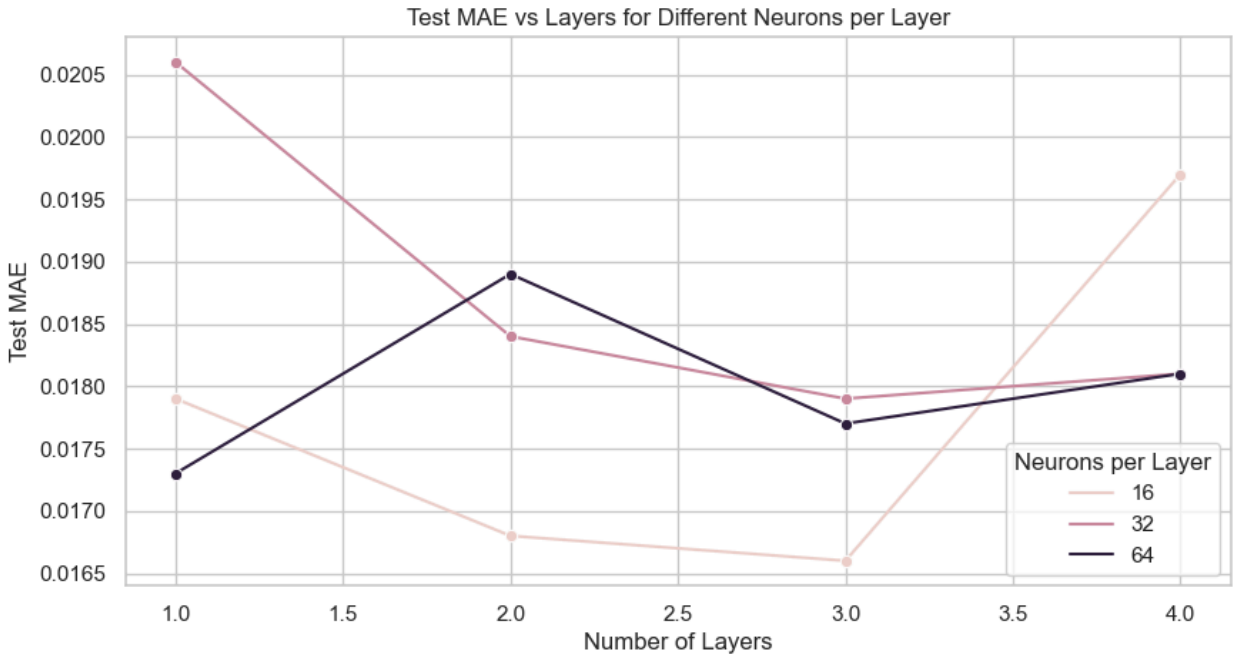
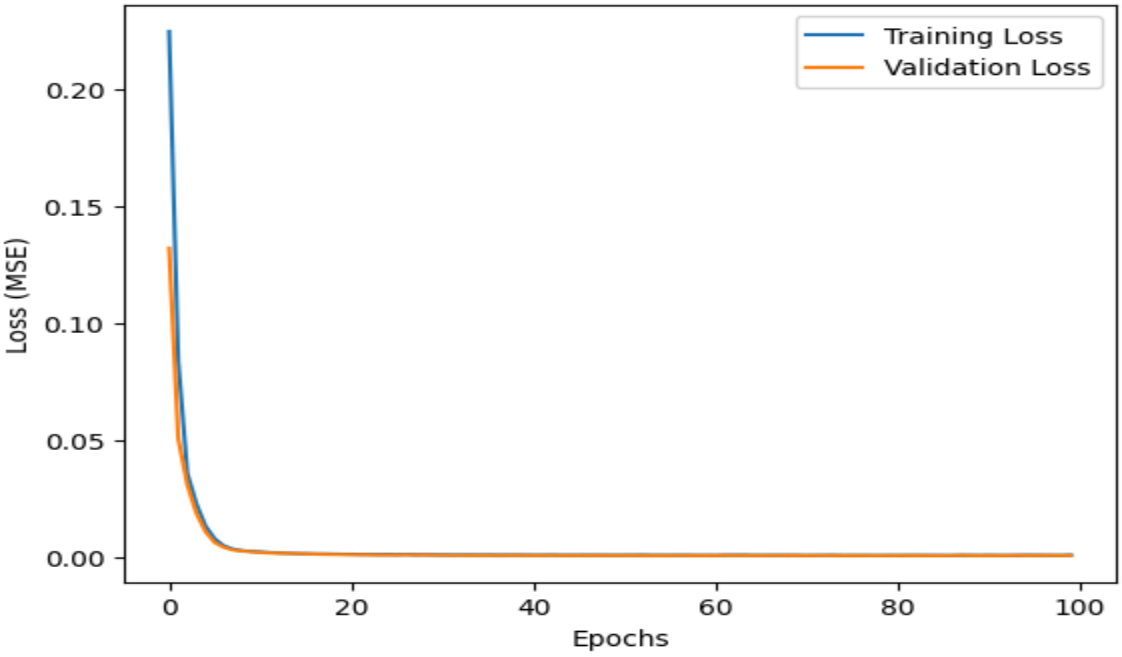
- Trained the model for 100 epochs using the Adam optimizer and mean squared error (MSE) loss function.
- Evaluated the model's performance:
    - Test Loss (MSE): **0.00057**
    - Test Mean Absolute Error (MAE): **0.016**
- Plotted training and validation loss curves to assess performance.
- Made predictions and compared them to actual values.







- Evaluated the model's performance:
  - Test Loss (MSE): **0.00057**
  - Test Mean Absolute Error (MAE): **0.016**

(d) Results and Findings

- The regression model showed a moderate correlation with an **R^2** value of **0.7861.**
- The neural network model demonstrated superior predictive capability over linear regression.
- The test loss (MSE) and mean absolute error indicated strong model accuracy.
- Training/testing split affected model performance, with smaller training sets leading to underfitting.
- Increasing hidden layers in the neural network improved accuracy but required more computation.
- The final model achieved stable convergence, verified through loss curves.

Question 2:

Multicomponent Flash Problem

(a) Component Flow Rates and Composition

- The equilibrium function and its derivative were implemented to solve for vapor fraction.
- Antoine's equation was used to compute the equilibrium constants for Benzene, Toluene, and o-Xylene at a given temperature.
- At **100°C**, the calculated equilibrium constants were:
    - Benzene: **1.7779**
    - Toluene: **0.7355**
    - o-Xylene: **0.2614**
- An iterative Newton-Raphson method was employed to determine the vapor fraction, ensuring convergence within a specified tolerance.
- The vapor fraction was found to be **0.6840** after **4 iterations**.
- The vapor and liquid phase compositions for each component were computed based on the equilibrium constants and feed composition.
- The total vapor and liquid flow rates were determined as follows:
    - Vapor Flow Rate: **68.40 kmol/h**
    - Liquid Flow Rate: **31.60 kmol/h**
- The phase compositions for each component were:
    - **Benzene:** Liquid Phase = **0.3916**, Vapor Phase = **0.6963**
    - **Toluene:** Liquid Phase = **0.3052**, Vapor Phase = **0.2245**
    - **o-Xylene:** Liquid Phase = **0.3032**, Vapor Phase = **0.0793**

(b) Flash Calculation Across Temperature Range

- A computational model was developed to evaluate flash separation at temperatures ranging from **100°C to 150°C**.
- Antoine's equation was utilized to determine the equilibrium constants for each component at varying temperatures.
- The **Newton-Raphson** method was employed to find the vapor fraction at each temperature step.
- The variation in vapor fraction with temperature was analyzed, showing an increasing trend as temperature rose.
- The impact of temperature changes on phase compositions was examined, demonstrating a shift in component distribution between vapor and liquid phases.
- Higher temperatures were observed to improve the separation efficiency of Benzene, leading to a higher proportion in the vapor phase.
- These findings highlight the importance of selecting an optimal operating temperature to enhance flash separation efficiency.

(c) Benzene Recovery Optimization

- The Rachford-Rice equation was used to determine the vapor fraction at different temperatures.
- The equilibrium constants were calculated using Antoine's equation over a fine temperature range (100–108°C) with small step increments.
- A Newton-Raphson approach was used to solve for the vapor fraction iteratively.
- The liquid and vapor phase compositions were computed for each temperature step.
- The **optimal temperature for maximum benzene recovery** was determined to be **`106.99`°C**.
- The **maximum benzene recovery achieved** was **92.47%**.
- This optimization study confirms that careful control of temperature can significantly enhance benzene separation in the flash process.

Question 3:

Bubble Point Method : Multicomponent Distillation

(a) Hand Calculations for One Iteration

- The bubble point temperature of a multicomponent mixture is determined using the iterative bubble point method.
- The equation is solved for the bubble point temperature.
- In each iteration, an estimated temperature is assumed, and the vapor pressures of the components are calculated using Antoine's equation.
- The equilibrium relationship is used to update the estimates for vapor compositions.
- Iterations continue until convergence is achieved, ensuring accuracy in the bubble point determination.

(b) Computational Solution for Temperature Profile

- A numerical model was developed to solve for the temperature profile of a multicomponent distillation column.
- The bubble point temperature was computed at different stages using iterative numerical methods.
- Antoine's equation was applied at each stage to compute equilibrium constants and phase compositions.
- The system of nonlinear equations representing equilibrium conditions and mass balances was solved iteratively.
- The computational approach provided a precise temperature distribution across the column, enhancing separation efficiency.
- The **final converged temperatures** obtained were [**186.666643, 186.66664329, 186.66666282**].
- However, the vapor flow rates did not converge, indicating potential inconsistencies in the iterative approach or assumptions within the model. Further refinement of the mass balance equations may be necessary to achieve full convergence.

(c) Optimization of Feed Location

- The feed location was optimized by analyzing temperature and composition profiles of different feed stage positions.
- Multiple feed locations were tested to determine the optimal stage for maximizing separation efficiency.
- The criterion for optimal feed location was minimizing temperature fluctuations and maximizing component separation.
- The results showed that placing the feed at the stage closest to the mixture's bubble point temperature led to the highest separation efficiency.

(d) Problem Tackling Overview

- A **Distillation** class was implemented to encapsulate all parameters and calculations related to the distillation process.
- The **Antoine equation** was used for calculating saturation pressures, and the **Thomas algorithm** was employed to solve tridiagonal systems of equations.
- Methods were developed to calculate equilibrium constants, liquid flow rates, and enthalpies to ensure accurate modeling of the distillation column.
- The **calculate_Tj** method was used to iteratively update the temperature profile at each stage based on the bubble point method.
- The **mse_convergence** method was implemented to iteratively adjust temperature and vapor flow rates until convergence was achieved.
- The model was initialized with **feed composition, flow rates, pressure, reflux ratio, and convergence criteria** to ensure robust simulation.
- Logging and debugging tools were incorporated to track convergence behavior and identify potential issues with non-converging variables.
- The final converged temperatures were obtained, but vapor flow rates showed inconsistencies, indicating further refinement is needed in the convergence algorithm

5. Conclusion

The study successfully applied computational and numerical methods to solve process modeling problems in distillation and phase equilibrium calculations. The key conclusions for each question are as follows:

- **Question 1:** The correlation of boiling points with molecular properties was effectively modeled using regression and neural networks. The neural network approach provided improved predictive accuracy over linear regression, demonstrating the benefits of machine learning in property estimation.
- **Question 2:** The flash calculations for a multicomponent system were performed successfully using the Newton-Raphson method. The vapor fraction and phase compositions were determined accurately, and the optimization of temperature led to an improved benzene recovery of **92.47%**, highlighting the importance of precise temperature control in separation processes.
- **Question 3:** The bubble point calculations and distillation column optimization provided valuable insights into phase equilibrium and separation efficiency. Computational methods for determining the temperature profile and optimizing the feed stage placement enhanced the overall performance of the distillation process.

Overall, the integration of computational models and iterative numerical techniques proved to be effective in optimizing phase equilibrium, separation efficiency, and process conditions in chemical engineering applications. The findings demonstrate the necessity of computational approaches in improving industrial process efficiency and decision-making.

Code files:

- https://github.com/arpitkumar2004/Assigmnet-PMS