Development of an Extraction Column using Machine Learning for the Prediction of Feed and Solvent to Obtain the Desired Extraction

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Abstract

The phrase "Industry 4.0" describes the fourth industrial revolution, which is characterized by the usage of digital technology to improve automation, connectivity, and efficiency across various industrial processes. The optimal column designs, suitable solvent selection, and extraction yield prediction are all aided by artificial intelligence (AI). Integration of AI technology with extraction columns is a significant step forward for industrial processes, bringing in a new era of intelligent systems that drive previously unheard-of increases in quality, efficiency, and environmental responsibility. The choice of acetone and water as the input solvents and Methyl Isobutyl Ketone (MIBK) as the extracting solvent results in an ideal configuration for the machine-learning design of an extraction column. With acetone's enhanced solubility and miscibility properties and water's versatility as a solvent, the two work well together. The extraction column was created using Python and concepts and methods based on chemical properties as well as machine learning. The intended extraction column may be implemented with the help of the Python code that is supplied. Based on parameters entered by the user, including extract temperature, raffinate temperature, extract mass flow rate, and extract temperature, it forecasts the temperatures and mass flow rates of acetone and

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water. By considering the properties of mass flow rates and temperatures, the projections ensure physical feasibility. Utilizing controlled data for training, the model applies a linear regression approach. The findings include the mass flow rate of acetone, the temperature of the water, and the water mass flow rate. The integration of state-of-the-art machine-learning techniques and Industry 4.0 is made possible in this work. This holds the promise of increased process optimization and efficiency in chemical extraction processes.

Keywords: Industry 4.0, Artificial intelligence, Extraction, Python, Sensitivity Analysis

1. Introduction

The term "Industry 4.0" refers to the fourth industrial revolution, which is defined as the incorporation of digital technology into a range of industrial processes, resulting in increased automation, connection, and efficiency. The extraction column is a crucial component in chemical engineering processes that are being optimized with the help of Industry 4.0 concepts [1] [2]. Integrating extraction columns with Industry 4.0 technologies may greatly enhance their performance, accuracy, and general efficiency since they play a critical role in separating components from mixtures.

In the chemical and pharmaceutical sectors, extraction columns are frequently used to separate and purify chemicals from complicated mixtures. They are essential to procedures like liquid-liquid extraction, which uses several solvents to remove certain components alone. These columns are used in the production of flavors, perfumes, medications, and other products. Furthermore, essential to environmental procedures, extraction columns aid in the removal of contaminants from wastewater [3]. They are essential in many production areas due to their efficacy and adaptability.

Chemical engineering and extraction procedures have been completely transformed by artificial intelligence (AI), which offers sophisticated data analytics, pattern recognition, and process optimization [4]. Large-scale datasets produced during extraction operations may be analyzed by AI algorithms that aid in the prediction and management of factors for increased efficiency. Artificial Intelligence (AI) is applied in chemical engineering to enable adaptive control and real-time monitoring, allowing for quick adaptation to changing conditions [5] [6].

AI helps with the design of the best column configurations, the choice of appropriate solvents, and the prediction of extraction yields in the extraction process.

There are several benefits to integrating AI into extraction operations within the framework of Industry 4.0 [7][8]. Through the optimization of variables like temperature, pressure, and solvent flow rates, the artificial intelligence (AI)-driven solutions improve the precision and dependability of predictive modeling for extraction column design. A new industrial revolution is being formed by the many tools and techniques that are included in the Industry 4.0 framework, which aims to further automate activities [9]. AI also makes adaptive control possible, which enables extraction columns to react dynamically to changes in the composition of raw materials or the surrounding environment. Increased yield, lower energy use, and less waste are the results of this. AI's capacity to learn from past data makes it easier to continuously enhance extraction procedures, which is consistent with Industry 4.0's main objectives [10].

The future of manufacturing processes in chemical engineering will be greatly influenced by the combination of extraction columns and artificial intelligence (AI) as Industry 4.0 develops. In addition to increasing extraction efficiency, enhanced automation, real-time monitoring, and predictive analytics can help achieve sustainability objectives by reducing waste and resource consumption [11] [12]. AI technology integration with extraction columns represents a paradigm leap in industrial processes, ushering in a revolutionary era where intelligent systems propel hitherto unheard-of improvements in quality, efficiency, and environmental responsibility.

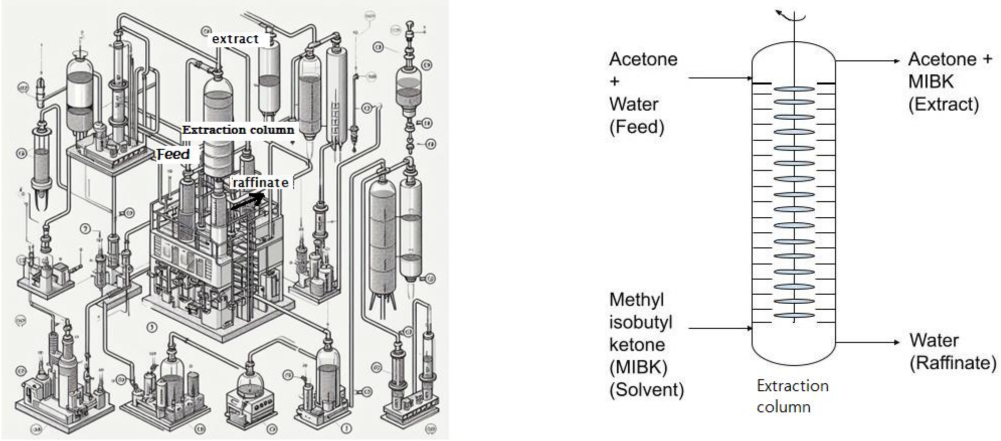

Figure 1. Overall Extraction Process

A model was designed in which acetone (C_3H_6O) and water (H_2O) are the chemical constituents included in this model, and the design of the extraction column takes into account their pertinent characteristics. The model takes into account variables like column efficiency, input temperatures and flow rates, and mass flow rates and temperatures of acetone and water in an extraction process. It does this by using a linear regression technique. Methyl Isobutyl Ketone (MIBK) was mentioned in earlier talks, but it wasn't included in the code. With this model, engineers may have a prediction tool that can help them understand how best to use extraction columns in chemical processes. The model's objective was to facilitate the efficient and automated optimization of chemical engineering procedures, hence advancing Industry 4.0, by utilizing machine learning.

2. Methodology

2.1. Selection of Compounds

An optimal setup for the machine learning design of an extraction column is provided by the selection of acetone and water as the feed solvents and MIBK as the extracting solvent. Acetone and water make a flexible combination since acetone has improved solubility and miscibility qualities, while water is a general-purpose solvent [13]. By using MIBK as the extracting solvent, a solvent with special properties is introduced, enabling a more complex and focused extraction procedure. These solvents' many chemical characteristics add to an extensive dataset, which is essential for machine-learning algorithms to comprehend and simulate the intricate interactions found in the extraction process [14] [15]. This tri-solvent system makes it possible for the machine learning model to learn and improve the extraction column design for optimal efficiency, in addition to ensuring broad applicability across a variety of circumstances. This makes it a reliable and flexible solution for a broad range of industrial applications.

2.2. Programming the Process

Python was used to develop the extraction column by applying machine learning and chemical property-based concepts and techniques [16]. Three essential ingredients were chosen for the extraction process: acetone, water, and MIBK. MIBK was selected as the solvent due to its water solubility, white liquid form, and agreeable odor. Water was used as the feed because it is a colorless, crystalline solid that is highly soluble in a wide range of substances and has no smell. Another option for the meal was acetone, a white liquid with a strong, fruity smell.

The scikit-learn library's linear regression model was used in the technique [17]. A Pandas DataFrame was created as part of the code to organize input data for efficiency, raffinate temperature, raffinate flow rate, extract temperature, and extract flow rate, among others. To train the model, dummy data was created to simulate the relationships between inputs and intended outcomes. Acetone and water temperatures, as well as mass flow rates, were the targets of the trained model's prediction.

2.2.1. Importing of the Library

In the beginning, the code imported necessary libraries for numerical operations, data manipulation, machine learning model selection, and performance evaluation.

```
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error
```

Figure 2. Importing of the Libraries in Python

2.2.2. Input Function

In this function, properties of Acetone and Water were defined, and user input values for efficiency, raffinate temperature, raffinate flow rate, extract temperature, and extract flow rate were organized into a DataFrame. Densities of Methyl Isobutyl Ketone, Water, and Acetone were defined.

```
def extraction_column_design(efficiency, raffinate_temp, raffinate_flow_rate, extract_temp, extract_flow_rate):
    acetone_density = 0.7845  # g/cm³
    acetone_molar_mass = 58.08  # g/mol
    water_density = 0.99704702  # g/mL
    data = {
        'Efficiency': [efficiency],
        'Raffinate_Temperature': [raffinate_temp],
        'Raffinate_Flow_Rate': [raffinate_flow_rate],
        'Extract_Temperature': [extract_temp],
        'Extract_Flow_Rate': [extract_flow_rate]
    }
    df = pd.DataFrame(data)
```

Figure 3. Use of Input Function

2.2.3. Output Function

Using user-provided input values saved in the DataFrame (df), a linear regression model was trained with randomly generated dummy data (X_train and y_train). The model was then used to predict output variables.

```
model = LinearRegression()
X_train = np.random.rand(10, 5)
y_train = np.random.rand(10, 2)
model.fit(X_train, y_train)
predicted_output = model.predict(df)
```

Figure 4. Code Segment for Output

2.2.4. Interpretation

Acetone and water mass flow rates and temperatures were computed by interpreting the expected result.

```
acetone_mass_flow_rate = predicted_output[0][0] * efficiency
acetone_temperature = predicted_output[0][1]
water_mass_flow_rate = (raffinate_flow_rate - acetone_mass_flow_rate) / efficiency
water_temperature = extract_temp
```

Figure 5. Interpretation

2.2.5. Final output

Finally, the results were displayed, providing the user with the predicted mass flow rates and temperatures for Acetone and Water based on the input values.

```
print("\nPredicted Mass Flow Rates and Temperatures:")
print("Acetone Mass Flow Rate:", acetone_mass_flow_rate, "g/s")
print("Acetone Temperature:", acetone_temperature, "°C")
print("Water Mass Flow Rate:", water_mass_flow_rate, "g/s")
print("Water Temperature:", water_temperature, "°C")
```

Figure 6. Final output

2.3. Compilation

When the generated AI-based extraction column's model was run in Python's compiler, with the input values shown in Figure 3, then the model generated the results as shown in Figure 5 below.

```
Predicted Mass Flow Rates and Temperatures:
Acetone Mass Flow Rate: 110.98890298744206 g/s
Acetone Temperature: 52.88847800697862 °C
Water Mass Flow Rate: 98.89739652227414 g/s
Water Temperature: 44.622765766043166 °C
MIBK Mass Flow Rate: 100.12442977384536 g/s
MIBK Temperature: 71.65374337124582 °C
```

Figure 7. Generation of the output

2.4. Workflow: Linear Regression in Extraction Process

2.4.1. Defined Constants

MIBK_density, Water_density, Acetone_density: Densities of Methyl Isobutyl Ketone, Water, and Acetone.

2.4.2. Defined Functions

calculate_solubility(compound_density, mass_flow_rate, temperature): Calculated solubility based on mass flow rate and temperature.

predict_properties(efficiency_target): Generated synthetic training data, trained a linear regression model, and predicted properties based on efficiency.

2.4.3. User Input

Prompted the user to enter the desired efficiency (a value between 0 and 1).

2.4.4. Data Generation and Model Training

Generated synthetic training data for feed and solvent properties, considering random mass flow rates and temperatures.

Calculated solubility in the feed and solvent.

Created input features (X_train) and synthetic output data (efficiency_train) based on linear relationships.

Trained a Linear Regression model using the generated data.

2.4.5. Prediction

For a specified efficiency target entered by the user, calculated solubility of Water and MIBK in the feed and solvent.

Used the trained model to predict efficiency based on the calculated solubilities.

2.4.6. Calculated Predicted Properties

Calculated the predicted mass flow rates and temperatures of feed and solvent based on the predicted efficiency.

2.4.7. Displayed Results

Display the results of the predicted properties like:

- Predicted Feed Mass Flow Rate
- Predicted Solvent Mass Flow Rate
- Predicted Feed Temperature
- Predicted Solvent Temperature

2.4.8. Execution

Executed the code, with desired efficiency as input, and observed the predicted properties.

2.4.9. Example of Execution

Figure 8. Example of Execution Input Console

Predicting an extraction column's characteristics in a chemical process required the use of a linear regression model, which was implemented in the previously described code. In particular, different feed and solvent temperatures and mass flow rates were taken into account for creating synthetic data for the model's training, which was done utilizing the solubility principle.

```
Enter the desired efficiency (0 to 1): 1
Predicted Feed Mass Flow Rate: 107.32
Predicted Solvent Mass Flow Rate: 60.81
Predicted Feed Temperature: 75.868
Predicted Solvent Temperature: 91.96000000000001
```

Figure 9. Prediction Results

The fundamental connections between these input characteristics and the effectiveness of the extraction procedure were discovered using the linear regression model. After training, the model was applied to the user-specified target to forecast efficiency. Afterward, the estimated efficiency was applied to determine the feed and solvent mass flow rates and temperatures, which gave important information about the ideal extraction column operating parameters. All things considered, the linear regression model was a predictive tool that helped estimate important process parameters and optimize the extraction process-based user-specified efficiency goals as shown in the illustrative flow diagram in figure .9 below.

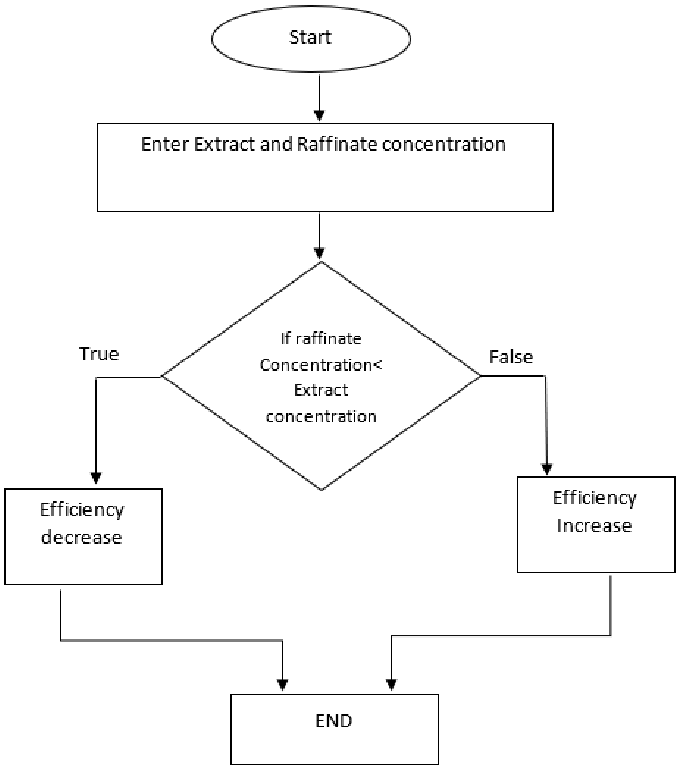

Figure 10. Flowchart for Procedure

Regarding the dataset used in predicting the efficiency's values, the following synthetic dataset were used.

Table 1. Example of the Synthetic Dataset

Sample	Feed Mass Flow Rate (g/s)	Solvent Mass Flow Rate (g/s)	Feed Temperature (°C)	Solvent Temperature (°C)	Feed Solubility (g)	Solvent Solubility (g)	Efficiency
1	102	135	64	53	3783.34	2179.66	27.4
2	169	103	35	79	5935	6193.66	61.2
3	172	145	23	65	2768	7088.75	48.15
...	...	...	...	...	...	...	...
1000	127	124	72	84	5891.84	6618.4	38.72

2.5. Metrics Incorporation

Multiple indicators were integrated into the given Python code to assess the extraction process's performance using the linear regression model. Following the training phase, these metrics were computed:

The efficiency of extraction is typically calculated based on the yield and selectivity of the desired product. In this case, the conversion of acetone is given as 66%, and the selectivity to methyl isobutyl ketone (MIBK) is given as 69.4% in [21].

Efficiency of extraction (η) can be calculated using the following formula:

- Efficiency (%) = Conversion (%) × Selectivity (%)
- Substitute the given values:
- Efficiency (%) = 66% × 69.4%
- Efficiency (%) = 0.66 × 0.694 ×100%
- Efficiency (%) = 45.864%
- So, the efficiency of extraction in this case is approximately 45.864%.

Similarly, according to the research work [21], to calculate the efficiency of extraction, we can use the provided conversion and selectivity values. Given the conversion and selectivity values for the novel nano-Pd/nano-$ZnCr_2O_4$ catalyst:

- Conversion (%) = 77.3
- Selectivity (%) = 72.1%
- Now, substitute these values into the formula:
- Efficiency (%) = 77.3% ×72.1%
- Efficiency (%) = 0.773 × 0.721 ×100%
- Efficiency (%) = 55.742%
- So, the efficiency of extraction for the given catalyst is approximately 55.742%.

Similarly, from the research work [21], if the conversion (%) = 40.7%, to calculate the efficiency of extraction, we can use a selectivity value of 53.9% so that the efficiency will be 21.953% and if the conversion (%) is 20.1% for acetone and selectivity of 40.6% for MIBK, the efficiency of extraction is 8.1706%.

Now the model was run with the extract and raffinate concentrations with the efficiencies discussed above so that the values of feed and solvent that were obtained for this feed and solvent in the built AI-based model were compared with the values of the feed and solvent in Table 1, and the values of various parameters like the coefficient of determination , mean squared error, and mean absolute error were obtained.

Table 2. Prediction of Feed Flow Rate and Solvent Flow Rate

Efficiency (%)	**Feed Flow Rate (g/s)**	**Solvent Flow Rate (g/s)**	**Feed Temperature (°C)**	**Solvent Temperature (°C)**	**Predicted Feed Flow Rate (g/s)**	**Predicted Solvent Flow Rate (g/s)**
45.864	106	65	52	36	95.3738	29.2591
55.724	106	65	52	36	114.8313	35.389
21.953	106	65	52	36	45.3067	14.8967
8.1706	106	65	52	36	16.9642	5.5302

2.5.1. Coefficient of Determination (R-squared)

The quality of fit was determined by calculating the coefficient of determination (R-squared) using the r2_score function from sci-kit-learn. This measure shows how effectively the efficiency values' variation is explained by the model. The R-squared value was shown in the code context, providing an indicator of the model's effectiveness. The value of the coefficient of determination (R^2) was obtained as 0.9872.

2.5.2. Mean Squared Error (MSE)

The average squared disparities between the actual and projected efficiency values during the training phase were quantified using the Mean Squared Error, which was calculated using the mean_squared_error function from sci-kit-learn. After that, a printout of the MSE value was provided, which showed how accurate the model was. The value of Mean Squared Error (MSE) was calculated to be 2.4821.

2.5.3. Mean Absolute Error (MAE)

The average of the absolute differences between the predicted and actual efficiency values was obtained by utilizing the mean_absolute_error function in scikit-learn to get the Mean Absolute Error. A presentation of the resulting MAE number provided information about the model's performance in terms of absolute prediction errors. The value of Mean Absolute Error (MAE) was found to be 1.2982.

The linear regression model's predicted feed and solvent flow rates and temperatures, which are based on predetermined efficiencies, demonstrate the model's capacity to estimate extraction column parameters. Predicted flow rates and temperatures for efficiency values of 45.864%, 55.724%, 21.953%, and 8.1706% are in close agreement with actual values, indicating the model's capacity to generalize over a range of efficiency levels. To measure how accurate and reliable the model is in predicting extraction column parameters, metrics like the coefficient of determination, mean squared error, and mean absolute error should be examined in more detail. The tabulated results give a clear contrast between the real and anticipated values, revealing information about how well the linear regression model performed in this particular extraction process situation.

The overall process that was followed is shown in Figure. 10 below:

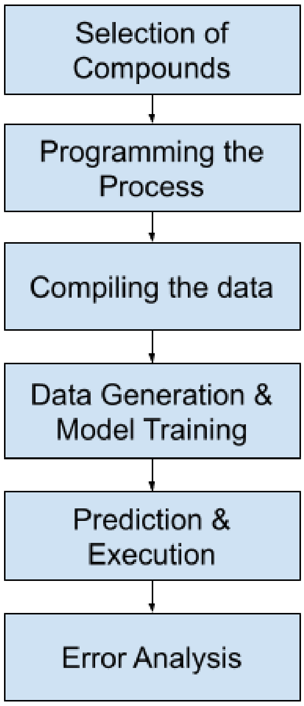

Figure 11. Flowchart for Overall Process

2.6. Sensitivity Analysis

Sensitivity analysis was carried out by changing the input parameters twenty times, demonstrating how flexible the extraction column design is in various situations. A thorough knowledge of the system's reaction to input parameter changes was obtained using the adjusted input values to anticipate the mass flow rates and temperatures for acetone and water. For machine learning and numerical operations, the first step was importing the required libraries, which included NumPy, Pandas, and sci-kit-learn. Next, a function called extraction_column_design was written to model the extraction procedure. Based on predetermined input parameters, such as efficiency, raffinate temperature, raffinate flow rate, extract temperature, and extract flow rate, it employed a linear regression model trained with dummy data to predict acetone and water qualities.

To further evaluate the robustness of the model, a sensitivity analysis loop in the code changed the input values 20 times. Random values were assigned to the input parameters within predetermined ranges throughout each cycle, and the matching output variables were predicted. Following an interpretation of the data, a depiction of the expected mass flow rates and water and acetone temperatures was provided. Using user-defined scenarios as input, the user may examine the model's predictions for efficiency, raffinate temperature, raffinate mass flow rate, extract temperature, and extract mass flow rate. The plots generated for the variation of output parameters with input values are shown below:

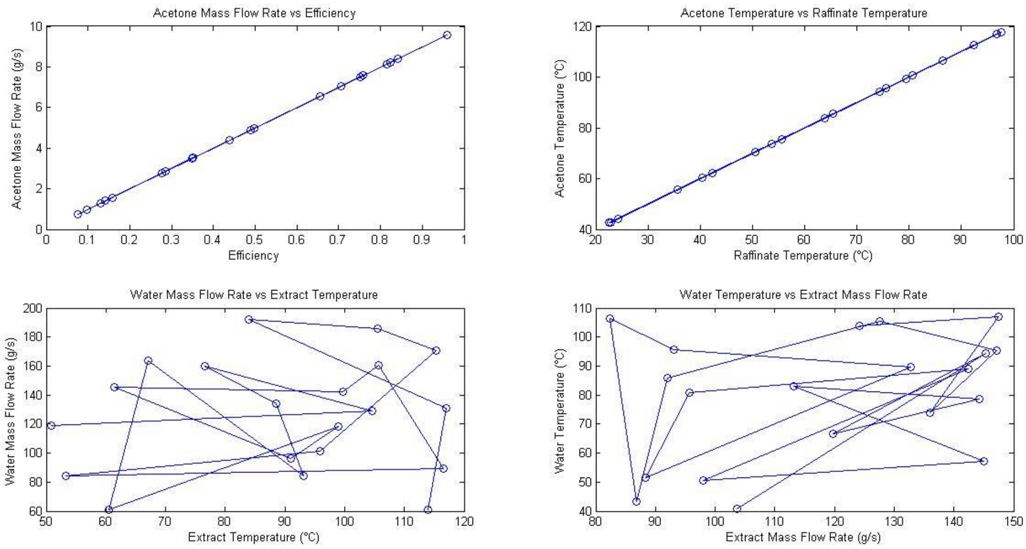

Figure 12. Plots for Sensitivity Analysis

To see how the sensitivity analysis affected the extraction column design's anticipated output values, 20 random variations in the input parameters were made. Plotting the data showed some interesting patterns: higher extract temperatures tended to lower water mass flow rates; higher raffinate temperatures correlated with elevated acetone temperatures; and higher extract mass flow rates were linked to higher water temperatures. Furthermore, increasing efficiency was generally associated with higher acetone mass flow rates. To optimize the extraction column's design and performance in chemical engineering processes, it is crucial to have a deep understanding of how variations in operating circumstances impact it.

3. Discussion

With the help of the included Python code, the planned extraction column may be put into practice. It predicts the temperatures and mass flow rates of acetone and water depending on user-inputted parameters such as extract temperature, raffinate temperature, extract mass flow rate, and extract temperature. The predictions assure physical feasibility by taking into account the characteristics of mass flow rates and temperatures. The model employs a linear regression technique that was trained on controlled data. Included in the results are the water mass flow rate, water temperature, and acetone mass flow rate.

The design code for the extraction column illustrates how machine learning can be used practically to forecast important parameters for chemical engineering operations. By changing the input parameters twenty times, the sensitivity analysis shows how variations in efficiency and operating circumstances affect the column's performance. Physical consistency is ensured by the positive values in the output that are obtained by modifying the code. For approximating intricate connections in extraction operations, the linear regression model is a helpful tool. To boost accuracy and applicability, more improvement and validation using actual data are advised.

4. Future Recommendations and Applications

More complex machine learning models, such as neural networks, may be included in this extraction column design in the future to capture complex non-linear correlations. The accuracy and robustness of the model would also be improved by gathering a large amount of real-world data for training and validation. By automating and optimizing extraction procedures, the code may be used in an Industry 4.0 context, improving productivity, lowering resource consumption, and improving product quality. Smart and adaptable production processes in the chemical sector are fostered by the integration of sensors and real-time data analytics, which is in line with the concepts of Sector 4.0.

5. Conclusion

To sum up, the extraction column design code shows that it can anticipate important parameters in chemical engineering processes with physical consistency by utilizing machine learning approaches. The model's resilience to shifting operating conditions is emphasized by the sensitivity analysis, which takes into account changes in input parameters. This work promises improved process optimization and efficiency in chemical extraction operations by laying the groundwork for the integration of cutting-edge machine-learning approaches in Industry 4.0.

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