Artificial Neural Network based Model Predictive Control of Batch Distillation Column

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1 Introduction

Batch distillation is a widely used separation process in various industries. However, controlling batch distillation columns presents a challenge due to their dynamic nature and continuously changing compositions. Traditional PID control methods struggle to handle these complexities. Model Predictive Control (MPC) offers advantages over PID control by incorporating a dynamic model of the system. However, traditional mathematical models for batch distillation can be computationally expensive and time-consuming to solve, creating limitations for real-time control.

This research proposes an Artificial Neural Network (ANN)-based approach to address the limitations of traditional models for MPC in batch distillation control for composition control of the top product. This research will investigate the development and implementation of an ANN model to predict key variables in a batch distillation column, enabling real-time control by overcoming the computational time limitation and improved process efficiency.

2 Methodology

2.1 Model Acquisition

This research leverages a pre-built mathematical model of a batch distillation column obtained from a published research paper by Bonsfills and Puigjaner [1]. This model captures the non-linear dynamics of the system and serves as the foundation for developing the ANN-based control strategy. This model is based on the following assumptions:

- Adiabatic column with total condenser
- Constant liquid and Vapor molar flow rates
- Constant liquid holdup with negligible vapor holdup for each tray and condenser
- Theoretical trays

Vapor liquid equilibrium data is calculated assuming a constant relative volatility value.

The model is adjusted to run with externally supplied reflux ratio as an input that can change during the operating period. Here reflux ratio is the only manipulated variable in the system. Top product purity is the controlled variable. Other variables like feed temperature and pressure are kept constant.

2.2 Simulation and Data Generation

The acquired model was implemented and simulated using Simulink software. This simulation allowed is employed to generate datasets encompassing a wide range of practical operating conditions and process variables. These datasets provide the necessary training data for the ANN model.

Determining the distribution of the operating reflux ratio set requires extra attention. It is important that the values cover the total range of operating reflux ratios of the distillation column. Using a smaller range, and a smaller step size shows the best results.

The simulated distillation column is operated under a constant reflux ratio for the set of reflux ratio values that is pre-determined. Compositions of distillate and still are monitored throughout the operation of the distillation column. These values are then entered into the training dataset with format shown in **Table *1***.

Table 1: Sample data for training dataset

Still Composition	Distillate Composition	Reflux Ratio
0.2	0.80	0.1
0.1	0.70	0.1
0.2	0.85	0.2
0.1	0.75	0.2
0.2	0.89	0.3

This set of training data is fed into the neural network for the training.

2.3 Artificial Neural Network Development

A pre-built ANN architecture, inspired by an ANN utilized for model predictive control for improving purity [4], was employed for this research. This pre-built architecture serves as a starting point for the development. Architecture is adapted to output reflux ratio as the sole output of the neural network using compositions as inputs. TensorFlow framework is utilized to train the ANN models on the generated datasets. **Table *2*** shows the architecture of the neural network. ANN model is compiled using "Adam" as the optimizer, mean squared error (MSE) as loss function, and mean absolute error (MAE) as evaluation metric.

Table 2: Architecture of the Artificial Neural Network

Number of Layer	Number of Nodes	Activation function
0 (Input layer)	2	
1	256	Rectified Linear Unit (ReLU)
2	128	Rectified Linear Unit (ReLU)
3 (Output layer)	1	Linear

2.4 ANN-based Control Simulation

A separate simulation environment will be developed to integrate the trained ANN model for real-time control of the batch distillation column. This simulation is utilized to evaluate the effectiveness of the ANN-based approach in controlling the process variables and achieving desired product purities. Control Block diagram for control structure is shown in **Fig. *1***.

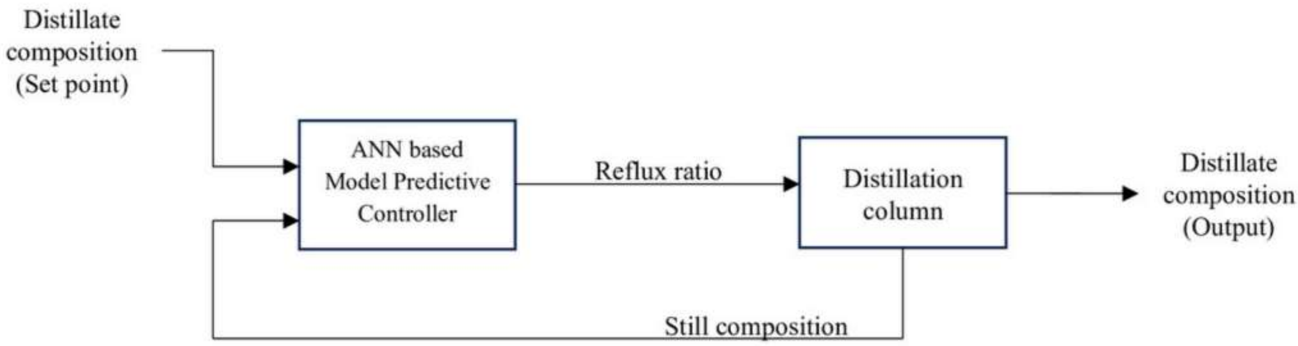

Fig. 1: Control structure

2.5 Performance Evaluation

The performance of each ANN model with varying node configurations will be evaluated by monitoring key metrics such as control stability, product purity, and separation efficiency within the simulated control environment. The results will be visualized to identify the optimal network architecture for effective control of the batch distillation column.

3 Results and Discussion

The distillation column initially starts with total reflux and is allowed to reach steady state and held in the steady state for 1000 seconds. From the results, this seems to be more than enough time for every plate to reach a steady state. **Table *3*** summarizes parameters for the distillation column. Target of the controller is to keep the molar composition of the top product as close as possible to the given set point which is 0.9 for the experiment.

Table 3: Distillation column specification

Parameter	Value
Number of ideal trays	15
Vapor boil-up rate (mol / hr)	72
Feed charge (mol)	1000
Tray liquid holdup (mol)	0.175
Condenser holdup (mol)	0.175
Feed composition (methanol mole fraction)	0.20

Running the simulated distillation column with the neural network-based Model Predictive Controller directly using the output from the neural network gives promising results (see **Fig. *2***).

These results can be improved using an error correction on the prediction. Experimenting with few different methods of correction shows that the best results with minimal effort can be obtained through correction method shown in equation 1.

$$Operating\ Reflux\ Ratio = Predicted\ Reflux\ Ratio \times (1 + k \times Predicted\ Reflux\ Ratio) \quad (1)$$

Here k is a factor of correction determined empirically. Dependencies for the value of k include number of plates, liquid hold up in plate, and boiler heat load. Experiments reveal that $k = 0.32$ gives results for the designed batch distillation column used in this experiment (see **Fig. *2***).

Without error correction　　　　With error correction (k = 0.32)

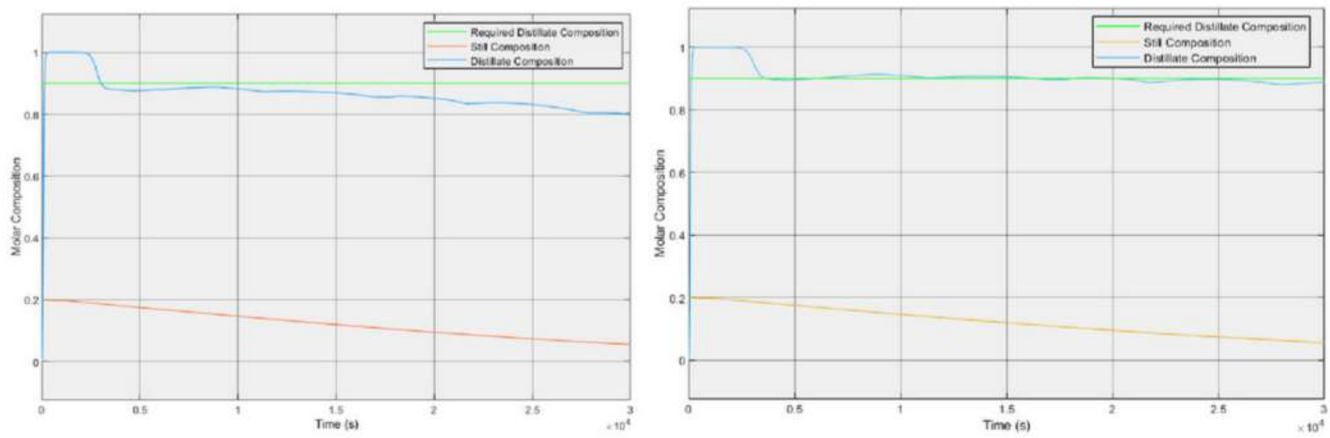

Fig. 2: Molar compositions of distillate and still using neural network-based Model Predictive Controller

Required top composition is 0.9. The minimum value obtained for the top composition while in operation is 0.8993, and the maximum is 0.9005. Maximum error for the operating period is 0.078%.

With the error correction factor, mean absolute error for top composition for the operating duration of the distillation column is less than 0.001. This indicates that the control system is adequate for the operating duration of the distillation column for controlling the distillate composition.

As expected, difference between predicted reflux ratio and operating reflux ratio with this error correction is significant when the reflux ratio is high (see **Fig. *3***). This is the result of vapor molecules taking longer to reach the top as the reflux ratio increases.

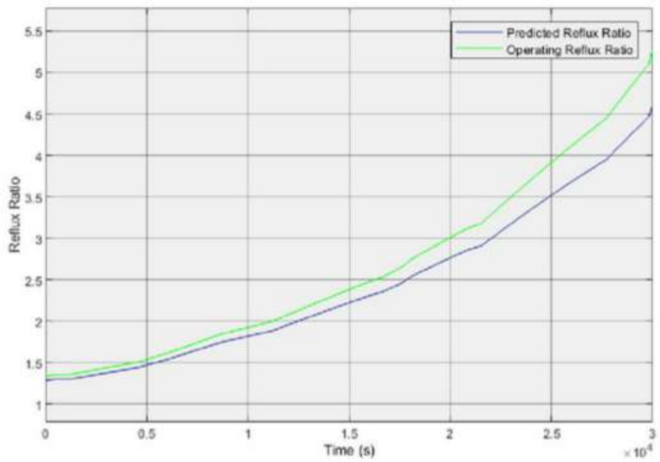

Fig. 3: Predicted reflux ratio vs. Operating reflux ratio with error correction using k=0.32

4 Future Work

4.1 Error correction in the preprocessing stage

Error correction factor in the controller has 3 dependent factors.

1. Number of plates
2. Liquid holdup in plate
3. Boiler heat load

These dependencies can be condensed into a single variable that indicates the residence time of the distillation column (the time it takes a vapor particle to reach the top). Using this value data in the training set can be adjusted to include an offset where the offset is the residence time.

This correction in the preprocessing stage of the training data could eliminate the requirement for the error correction factor in the control stage.

Conclusion

This research investigated the feasibility of using Artificial Neural Networks (ANNs) for model-based control of batch distillation columns, aiming to address limitations of traditional models in Model Predictive Control (MPC). By leveraging a pre-built mathematical model and Simulink simulations, we developed and trained ANN models to predict the reflux ratio for optimal product composition control. The results demonstrate promising performance of the ANN-based Model Predictive Control (MPC) strategy. A simple error correction method further improves the control accuracy. Future work will explore incorporating residence time information into the training data to potentially eliminate the need for the external error correction factor. This research highlights the potential of ANNs to address the limitations of traditional models for MPC in batch distillation control, paving the way for improved process efficiency and product quality.

Keywords: Batch Distillation, Artificial Neural Network, Model Predictive Control, Composition Control

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