Comparison of Model Predictive Controller and Neural Network Controller on Nonconventional Distillation Demethanizer/Deethanizer Rectifier/Column System

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Abstract. Nonconventional distillation demethanizer/deethanizer rectifier/column offers an economic advantage compared to conventional configurations by using sidestream from second column to remove the use of reboiler. However, this configuration brings a complex system that needs attention in its process control to ensure its operability. This work explores the use of neural network model predictive control (NNMPC) for this system. Aspen HYSYS was used to simulate the process, generate input-output data to develop the plant model and to conduct performance tests. MATLAB was used to conduct model identification, design the MPC and implement the multivariable control action. Sufficient time series data, where reflux valve positions and distillate compositions from each column act as input and output respectively, can be obtained from simulation and then utilized to train a nonlinear autoregressive exogenous (NARX) neural network which will be used as a predictive model. Model predictive Control based on this neural network model is designed to control distillate compositions for each column by the changes of reflux valve positions for each column as control signal. Least square algorithm from MATLAB function was employed to optimize the cost function. A comparison has been made between NNMPC and conventional MPC configurations with first order plus dead time (FOPDT) model to test the performance of the controller based on disturbance rejection and set-point tracking test. Quantitative calculation was done using integral absolute error (IAE) with trapezoidal rule used as numerical integral method. NNMPC shows better performance than MPC with FOPDT model to test the performance of the controller based on disturbance rejection and set-point tracking test. However, NNMPC has a disadvantage on the cost function calculation algorithm, which did not account for the difference between plant and model value thus cause the MPC with FOPDT model to give better performance on disturbance rejection. Bias addition on NNMPC cost function algorithm made the controller has better responses to disturbance rejection compared to MPC.

1. Introduction
An important aspect of low-temperature separation system is the interaction between separation and refrigeration system that designed to give maximum exploitation result with minimum operational cost. One implementation of a low-temperature separation system is in the recovery of natural gas liquid (NGL) unit. Aside from methane (80% mole), natural gas also contains other heavier hydrocarbons from C2 to C5 and other impurities such as carbon dioxide and nitrogen. Methane needs
to be separated from other heavier hydrocarbons to obtain pipeline-quality methane and recover NGL [1].

Cryogenic condenser system of demethanizer and deethanizer column on NGL process have expensive refrigerant cost. Therefore, the usage of reboiler needs to be reexamined to give a low operational cost. One innovation to overcome this issue is the sequence separation with rectifier/column configuration. In this configuration, a vapor side stream is removed from a main column and fed to a rectifier (a column with no reboiler) whose overhead is the intermediate component. Liquid from the bottom of the rectifier is returned as feed to the main column [2]. This configuration can reduce the capital and energy cost [3]. Research about the dynamics from this configuration process is necessary since this configuration brings a more complex system than the conventional configuration [4].

Process dynamics and control from this system has been explored. Model predictive control (MPC) with first order plus dead time (FOPDT) model was used to control this process. Reflux flow rate from each column acts as the manipulated variable to control the distillate composition from each column. MPC works by trying to find the most suitable control signals to minimize a cost function subject to some constraints, using a model of the system [4]. This MPC control configuration can be enhanced by using a different model to represent the process. MPC needs a dynamic process model to predict system behavior (output) for a certain time horizon and to calculate the optimal control response. Hence, the dynamic process model is essential for an excellent process control.

First-principles model has high accuracy but unsuitable for on-line control in general because this model can be extremely complex and cause numerical computation problem. Neural network (NN) can be a solution for it has a relatively simple structure. NN can directly give the relation between a set of input and a set of output of a process, which means that there is no complex numerical problem during on-line control [5]. Nonlinear autoregressive neural network with exogenous input (NARX) is one type of dynamic neural network model that can represent a nonlinear process better than the nonlinear autoregressive conventional model. NARX is a recurrent neural network which means that it has a feedback line structure to consider the previous input and output value in determining the current value [6].

This study focuses on using neural network model to represent dynamic system, use it as model for NNNPC and then compare its performance with MPC FOPDT model for the same process. The performance tests were done by set-point tracking for a variety of set-point values and disturbance rejection with feed rate as disturbance variable.

2. Method

2.1. Process description

The process studied is the nonconventional rectifier/column demethanizer/deethanizer based on the research of Luyben [2]. The separator tank and the pump between two columns were added for dynamic simulation stability [4]. Feed with specification shown in Table 1 is introduced on stage 2 of an eight-stage rectifier. A 2950 kmol/h vapor side stream from the main column is withdrawn from stage 7 and is fed into the base of rectifier. Liquid from the bottom product of rectifier is fed back to the main column on stage 7. The methane recovery was set at 99.64% by keeping impurity of methane in the ethane product at 0.97% mol. Propane recovery was fixed at 99.2% by keeping the propane composition of the demethanizer distillate at 0.27% mol.

The process was simulated using Aspen HYSYS v.10. Hikmadiyar in 2019 proposed a control scheme to keep methane and ethane purity in product. Table 2 lists the ten PID controller that was installed to keep various variables constant during dynamic simulation. Reflux rate from each column is used to control product purities [4]. Another study by Hikmadiyar in 2020 proposed another control scheme to keep methane, ethane, and propane purity in each product stream using model predictive controller by controlling reflux rate of the rectifier and the main column and energy from reboiler as manipulated variables [7].
Figure 1. Nonconventional distillation rectifier/column configuration [4].

Table 1. Feed specifications [2].

| Specification | Value     | Specification | Value       |
|---------------|-----------|---------------|-------------|
| Flow Rate     | 2886 kmol/h | Temperature   | -68°C       |
| Pressure      | 450 psia  | Inlet Stage   | stage 2 rectifier |
| Compositions  |           |               |             |
| Nitrogen      | 0.0011    | i-Butane      | 0.0396      |
| Methane       | 0.4876    | n-Butane      | 0.0249      |
| Ethane        | 0.1949    | i-Pentane     | 0.0148      |
| Propane       | 0.2250    | n-Pentane     | 0.0121      |

Table 2. PID controller specifications [4].

| Controller | Manipulated Variable (MV)       | Controlled Variable (CV)          | CV Value     |
|------------|---------------------------------|-----------------------------------|--------------|
| FIC-100    | Feed inlet valve position      | Feed flow rate                    | 2886 kmol/h  |
| FIC-101    | Vapor side stream valve position | Vapor side stream rate            | 2950 kmol/h  |
| PIC-100@COL1 | Condenser duty              | Top stage pressure                | 3110 kPa     |
| TIC-100    | Reboiler duty                  | Stage 26 temperature              | 49.7°C       |
| LIC-100@COL1 | Distillate rate            | Condenser level                    | 89.7%        |
| PIC-100    | Top product rate               | Column pressure                    | 3104 kPa     |
| LIC-100    | Bottom product rate            | Column level                       | 41.6%        |
| PIC-101@COL2 | Condenser duty              | Top stage pressure                | 3101 kPa     |
| LIC-100@COL2 | Bottom product rate          | Reboiler level                     | 50%          |
| LIC-101@COL2 | Distillate rate             | Condenser level                    | 50%          |
2.2. Neural network model
Training data set for neural network training was collected from Aspen HYSYS dynamic simulation. This was done by recording the system responses, which is the distillate composition from each column, for variation of reflux valve position from each column as manipulated variables. The 132,793 total data set collected has 20 seconds interval for 737 hours of simulation time. This data set was then divided into three, 70% for training, 15% for validation, and 15% for testing. These percentages were the default values used in MATLAB neural network toolbox.

Neural network was created in MATLAB 2020a using neural network toolbox for NARX structure. The number of hidden layers was determined by trial and error to find the lowest mean square error between actual plant output from simulation and predicted output from neural network model. Neural network represents a 2x2 multiple input multiple output (MIMO) system with reflux valve position from each column as input and distillate composition from each column as output. Training was done with 1000 epochs as one of training parameters by using Levenberg-Marquardt backpropagation algorithm.

2.3. Neural network model predictive controller
Neural network model predictive controller (NNMPC) was created using MATLAB script with determined control parameter, sampling time, and constraints. The control parameters used were minimum prediction horizon (N₁), maximum prediction horizon (N₂), control horizon (N₃), and weight factor for control signal (ρ). N₁ and N₂ specifies the time when the plant output prediction is made by using the neural network model of the dynamic process. N₃ and ρ regulate manipulated variable or control signal calculation. N₃ specifies the number of future step control signal values that needs to be considered. In other words, it specifies the instant time, since when the output of the controller should be kept at a constant value. ρ determine how big control change can be performed at one step of algorithm. The cost function equation is shown below [8].

\[ J = \sum_{j=N_1}^{N_2} (y_r(t+j) - y_{nn}(t+j))^2 + \rho \sum_{j=1}^{N_3} (u'(t+j) - u'(t+j-1))^2 \] (1)

Constraints used to limit the range of the control signal are from 0.1% to 100% valve position. MATLAB script will calculate the condition where control signal will minimize the value of cost function J based on the determined set-point value, future prediction, and past control signal values. This script used least square optimization function to find the next control signal value.

Optimizer function for the NNMPC use least square algorithm from MATLAB optimization toolbox, since Aspen HYSYS MPC optimizer also use least square algorithm [9]. Due to limited documentation on Aspen HYSYS MPC optimizer, it is assumed that the default setting for MATLAB least square algorithm is the same with its HYSYS counterpart.

Control parameter (N₁, N₂, N₃, and ρ) determined using trial and error with least IAE value when starting the controller from steady state condition (all MV value is 50%) to determined set point (0.95 and 0.93).

2.4. Model predictive controller
Model predictive controller with first order plus dead time (FOPDT) model used as a comparison for NNMPC on this study. Aspen HYSYS has MPC block on dynamic and control block tab. This MPC block uses either step test data or FOPDT for prediction model. FOPDT model was created by fitting step test data collected from dynamic process simulation. FOPDT model obtained by system identification using step test data in MATLAB. Step tests data obtained by changing one manipulated variable while keeping other variables constant. FOPDT as in equation 2 has three parameters, gain steady state process \( \bar{K}_p \), time constant \( \tau \) and dead time \( \theta \). Aspen HYSYS MPC calculate control action by minimizing:

\[ \hat{E} = -A\Delta m + \hat{E}' \] (2)
Where $U$ is number of control horizon, $V$ is number of prediction horizon, $A$ is a $V \times U$ triangular matrix, $\Delta m$ is the $U \times 1$ vector of future control moves, $\hat{E}$ and $\hat{E}'$ are the closed loop and open loop prediction, and are defined as follows:

$$
\hat{E} = \begin{bmatrix}
  r_{n+1} - c_{n+1}^* \\
  r_{n+2} - c_{n+2}^* \\
  \vdots \\
  r_{n+V} - c_{n+V}^*
\end{bmatrix}
$$

$$
\hat{E}' = \begin{bmatrix}
  E_n - P_1 \\
  E_n - P_2 \\
  \vdots \\
  E_n - P_V
\end{bmatrix}
$$

(3)

2.5. Performance tests

Performance on both controllers were compared by using integral absolute error (IAE) value on their responses in set-point tracking and disturbance rejection tests. Set-point tracking test was done by changing the set-point value for each controlled variable. Disturbance rejection test was done by changing the feed rate value as disturbance variable. The feed rate value was changed from steady state value to 1.05 time of its steady state value. Trapezoidal rule for numerical integration is used for IAE calculation.

$$
\int_a^b f(x)dx \cong \sum_{i=1}^{n} \frac{h}{2} (|e_i| + |e_{i+1}|) = \frac{h}{2} \left( |e_1| + 2*|e_2| + \cdots + 2*|e_{n-1}| + |e_n| \right)
$$

(4)

| Time (minute) | Methane D1 Composition | Ethane D2 Composition |
|---------------|------------------------|-----------------------|
| 0-200         | 0.95                   | 0.93                  |
| 201-800       | 0.945                  | 0.925                 |
| 801-1400      | 0.94                   | 0.92                  |
| 1401-2200     | 0.953                  | 0.933                 |
| 2200-2800     | 0.948                  | 0.928                 |

3. Results and discussion

3.1. Neural network model predictive controller

Neural network model has two input delays, two feedback delays, and twelve hidden layers with mean square error (MSE) value $4.85 \times 10^{-4}$. The number of hidden layers was selected by evaluating network performance as shown in Table 4. Past input data is needed in a relatively great amount to increase the accuracy of neural network prediction.

| Hidden Layer | MSE   | Hidden Layer | MSE   |
|--------------|-------|--------------|-------|
| 1            | 0.139899 | 11           | 0.000654 |
| 2            | 0.008852 | 12           | **0.000485** |
| 3            | 0.003725 | 13           | 0.000976  |
| 4            | 0.002814 | 14           | 0.000592  |
The cost function for the NNMPC is slightly different from what described in section 2.3. Since the control scheme for the process is 2x2 MIMO, the cost function $J$ have two elements: $J(1)$ for controller variable 1 (methane composition in distillate 1) and $J(2)$ for controlled variable 2 (ethane composition in distillate 2). Both elements are summed to obtain $J$ and minimized to obtain the new manipulated variable value.

The result of control parameter variation and their IAE value shown in Table 5. Since $5-1-3-10^{-9}$ had the best IAE, the value is used for the control parameter.

### Table 5. NNMPC parameters selection

| $N_2$ | $N_1$ | $N_u$ | $\rho$ | IAE  |
|-------|-------|-------|--------|------|
| 5     | 1     | 3     | $10^{-3}$ | 99.735 |
| 5     | 1     | 3     | $10^{-6}$ | 57.869 |
| 5     | 1     | 3     | $10^{-9}$ | 46.729 |
| 10    | 1     | 1     | $10^{-9}$ | 54.222 |
| 10    | 1     | 3     | $10^{-9}$ | 48.835 |
| 10    | 1     | 5     | $10^{-9}$ | 47.921 |
| 5     | 1     | 3     | $10^{-9}$ | 46.999 |
| 10    | 1     | 3     | $10^{-9}$ | 47.921 |
| 20    | 1     | 3     | $10^{-9}$ | 54.002 |

### 3.2. MPC FOPDT model

Step test was performed by changing one of two manipulated variables 20% more than the steady state value, while keeping other constant. The time series data then imported to MATLAB system identification tools to obtain the FOPDT model. FOPDT model for MPC are obtained from step test data and shown as follow:
Table 6. FOPDT model for MPC

| Process model | Kp     | $t_p^a$ | $\theta^b$ |
|---------------|--------|---------|------------|
| G1.1          | 4.871 e-04 | 20.883  | 2.220      |
| G1.2          | -1.265 e-04 | 33.117  | 13.432     |
| G2.1          | 2.88 e-05   | 38.717  | 16.833     |
| G2.2          | 9.493 e-04  | 37.333  | 0.572      |

*a in minutes unit

3.3. Comparison of the controller

Both controllers went under series of set-point tracking test and disturbance rejection test as described in section 2.5. Figure 3 and 4 shows the result of methane and ethane set-point tracking respectively. Based on IAE calculation on set point tracking, NNMPC had better performance than MPC. NNMPC had IAE value of 153.2 in methane tracking, when MPC had value of 600.97 with 8477 sample of 20 second. For ethane tracking, NNMPC had IAE value of 163.62 while MPC had 263.72 with 7800 sample of data.

![Figure 3. Response of methane set point tracking test](image1.png)

**Figure 3.** Response of methane set point tracking test

![Figure 4. Response of ethane set point tracking test](image2.png)

**Figure 4.** Response of ethane set point tracking test

NNMPC had better performance on representing non-linear system behaviour than MPC due to difference between prediction models. NNMPC use neural network and MPC use FOPDT process.
model in predicting system trajectory. Neural network is known to have non-linear activation layer which made the model performs better on predicting non-linear behaviour.

Disturbance rejection result is different from set-point tracking. Figure 5 and 6 shows that disturbance caused NNMPC prediction to be inaccurate, thus NNMPC did not correct the manipulated variable. It is shows that NNMPC did not account for difference between model prediction and plant output in cost function calculation. Aspen HYSYS MPC did account the difference between the model and plant output by correcting forward prediction [9]. Seborg also described bias correction by adding the difference between current value of plant output and current prediction value to future prediction value [10]. By doing the same thing in the cost function for NNMPC as described in section 2.3 thus the first summation term of cost function in equation (1) become:

\[ \sum_{j=N_1}^{N_2} (y_r(t+j) - y_m(t+j) + y_m(t) - y_m(t))^2 \]  

Thus a new equation is used for the cost function calculation:

\[ J = \sum_{j=N_1}^{N_2} (y_r(t+j) - y_m(t+j) + y_m(t) - y_m(t))^2 + \rho \sum_{j=1}^{N_u} (u'(t+j) - u'(t+j-1))^2 \]  

Figure 5. Response of disturbance rejection test on methane composition

Figure 6. Response of disturbance rejection test ethane composition
Figure 7. Response of methane composition in disturbance rejection test with different NNMPC cost function equation.

Figure 8. Response of ethane composition in disturbance rejection test with different NNMPC cost function equation.

Figure 7 and 8 shows the comparison of system responses with bias addition (equation 6) and without bias addition (equation 1) in cost function calculation. This modification on the cost function slightly improve NNMPC performance on disturbance rejection as shown in figure 7 and figure 8. Quantitative comparison in disturbance rejection between equation (6) and equation (1) would be pointless since NNPC with equation (1) would result in offset due to inaccurate prediction.

Figure 9 and 10 shows the comparison of system responses with MPC and NNMPC with bias correction model control. By calculating the IAE, it is shown that NNPC had better performance in disturbance rejection if bias addition is used in cost function calculation. The IAE of NNPC for methane and ethane disturbance rejection as follow: 25.10603 and 16.86964 with 20 s sampling interval and 553 data point. The IAE for MPC for methane and ethane disturbance rejection as follow: 46.21541 and 80.55605 with 20 s sampling interval and 553 data point.
Figure 9. Response of methane composition in disturbance rejection test with NNMPC cost function equation (6) and MPC

Figure 10. Response of ethane composition in disturbance rejection test with NNMPC cost function equation (6) and MPC

4. Conclusion
Neural network model predictive controller has better performance on predicting non-linear model than MPC with FOPDT as model. NNMPC has disadvantage on the cost function calculation algorithm, which did not account for difference between plant and model value. Bias addition on NNMPC cost function algorithm made the controller has better responses to disturbance. NNMPC with bias addition have better performance than MPC.

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