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Neural-Wiener-based Model Predictive Control (NWMPC) for Methyl Tert-butyl Ether Catalytic Distillation

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Abstract: *The reactive distillation of methyl tert-butyl ether (MTBE) involves strong interactions between variables and is a highly nonlinear process. Here, a nonlinear model predictive control (MPC) was proposed to tackle the nonlinearity and the interaction involved in controlling the tray temperature in MTBE reactive distillation. To improve the performance of the MPC, an advanced nonlinear block-oriented model known as the neural Wiener model was employed. The control study was successfully simulated using Simulink (Matlab), which is integrated with the Aspen dynamic model. Set-point tracking, disturbance rejection and robustness tests were conducted to evaluate the neural-Wiener-based MPC (NWMPC) performance. The results achieved show that the NWMPC is able to maintain the product purity at its set-point of 99%, with isobutene conversion exceeding 99.98%. NWMPC is also able to reject disturbances, as shown in disturbance rejection study performed by changing the feed flowrate to 30% of the nominal value. This controller is also very robust and thus able to control the MTBE reactive distillation, even when the column efficiency was reduced to 80%.*

Keywords: Reactive distillation, NMPC, neural Wiener, sequential quadratic programming, nonlinear optimisation

1. INTRODUCTION

The main purpose of controlling the reactive distillation (RD) of methyl tert-butyl ether (MTBE) is to maintain the MTBE purity within a desired range. The desired MTBE purity can be obtained by controlling the tray temperature because the MTBE purity is correlated with tray temperature.[1] Temperature control is more economical than other approaches because the composition analyser can be omitted. Due to the highly variable interactions in RD and their nonlinearity, in this work, the nonlinear MPC is proposed to control this system. The neural Wiener (NW) model, a powerful block-oriented model capable of reducing the computational time, has been selected to be embedded in the MPC.[2–5] The proposed NW model consists of a state space as a linear dynamic block, followed by a neural network as a nonlinear static block. An MPC using the NW model and sequential quadratic programming (SQP) optimiser, called a neural-Wiener-based MPC (NWMPC), has been applied to control the MTBE RD.

2. DEVELOPMENT OF THE MTBE REACTIVE DISTILLATION PROCESS MODEL

The most promising technique for producing MTBE uses methanol and isobutene, where the liquid-phase reaction is catalysed by an ion exchange resin (heterogeneous reaction). The reaction scheme is:

$$i\text{-}C_4H_8 + CH_3\text{-}OH \quad \leftrightarrow \quad C_5H_{12}O \tag{1}$$

The butene feed for MTBE synthesis consists of approximately 40% isobutene and 60% n-butene, which the latter of which is inert. Methanol is usually fed in excess to improve the conversion of isobutene into MTBE. MTBE forms azeotropes with methanol and isobutene, making it difficult to separate MTBE from its impurities. However, in reactive distillation, the azeotropes are reacted in a reaction section.[6,7] The specifications for the MTBE RD considered here can be found in Sudibyo et al.[8]

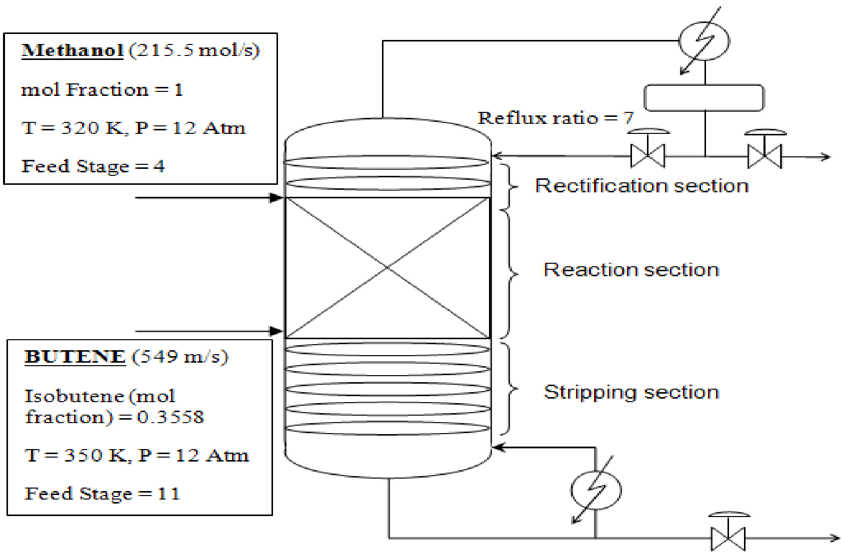

Figure 1: MTBE reactive distillation column.

3. DEVELOPMENT OF THE NEURAL WIENER MODEL

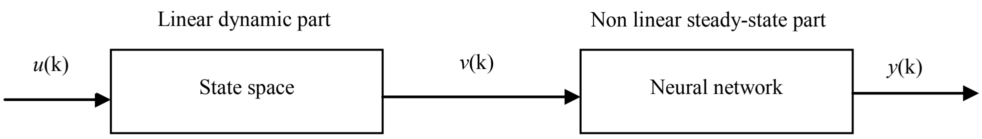

Figure 2: Neural Wiener model configuration.

The NW model consists of linear and nonlinear blocks, as shown in Figure 2. The linear block used in this work is a state space model. Using the Matlab identification toolbox, the state space model for multivariable MTBE reactive distillation can be identified as shown below:

$$x_{(k+1)} = A\, x_{(k)} + B\, u_{(k)} \tag{2}$$

$$v_{(k)} = C\, x_{(k)} + D\, u_{(k)} \tag{3}$$

where

$$A = \begin{bmatrix} 0.73897 & -0.042774 & 0.060387 & 0.02007 \\ -0.34542 & 0.7133 & -0.31961 & 0.30447 \\ -0.24956 & 0.44335 & -0.34634 & 0.7272 \\ -0.035443 & 0.059417 & -0.11259 & 0.61541 \end{bmatrix}$$

$$B = \begin{bmatrix} -1.3786 & 1.5398 \\ -4.2 & 4.1893 \\ 6.4984 & -5.8288 \\ 1.1353 & -0.38649 \end{bmatrix}$$

$$C = \begin{bmatrix} 0.20528 & 0.10429 & 0.10847 & -0.11637 \\ -0.0039021 & 0.0034986 & 0.0019554 & -0.00039005 \end{bmatrix}$$

D, u and x are zero matrices of size (2 × 2), (4 × 2) and (4 × 1), respectively, and G is a discrete-time model.

The neural Wiener nonlinear block used in this work is a neural network model used to represent the inverse of the nonlinear block in the N-W model. In this part, the MTBE reactive distillation was modelled using a multiple-input multiple-output (MIMO) feed-forward neural network model with 15 hidden nodes and one hidden layer. The output y(k) of the neural network is described as:

$$y_{(k)} = w_0 + \sum_{i=1}^{K} w_i^2 \varphi(w_{i,0}^1 + w_{i,1}^1 v_{(k)}) \tag{4}$$

where w_0 is the bias, $w_{i,j}$ is the weight of the first layer, w_i is the weight of the second layer, φ is a nonlinear transfer function (e.g., hyperbolic tangent sigmoid transfer function or tansig) and K is the number of hidden nodes.[5,9] The output of the N-W model can be defined by substituting Equation (3) into (4), as shown below:

$$y(k) = w_0 + \sum_{i=1}^{K} w_i^2 \varphi\{w_{i,0}^1 + w_{i,1}^1 [C\ x(k) + D\ u(k) + e(k)]\} \tag{5}$$

4. DEVELOPMENT OF THE NWMPC

The optimal control configurations with the most suitable control variable, manipulated variable and disturbances have been identified.[4,5] The empirical model developed and the optimisers proposed have been embedded in the NWMPC as shown in Figure 3. The accuracy of the controller is the main consideration in the design of the NWMPC.

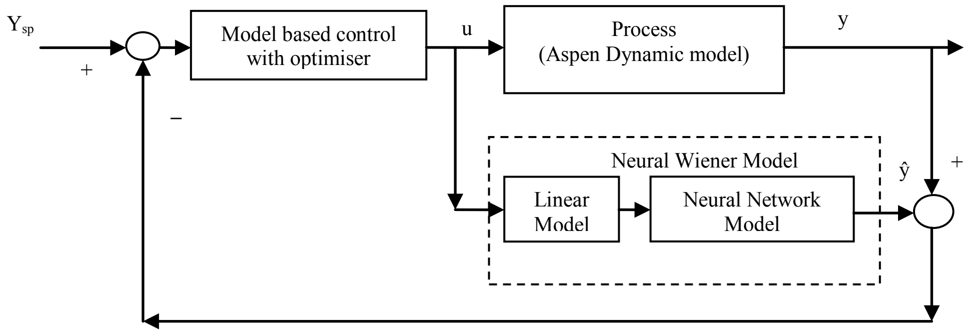

Figure 3: General structure of the NWMPC.

The NWMPC objective function for the MIMO case consists of the quadratic error between each controlled variable and its set-point and the quadratic change of each manipulated variable. The MPC objective function for the 2 × 2 system is defined as follows:

$$j_k = \sum_{i=1}^{P} \left((\mathrm{y}_{f1|k+i} - \mathrm{y}_{sp1|k+i})^2 Q_1 + (\mathrm{y}_{f2|k+i} - \mathrm{y}_{sp2|k+i})^2 Q_2 \right) + \left(\Delta\mu_{f1|k+i} \right)^2 .R_1 + \left(\Delta\mu_{f2|k+i} \right)^2 .R_2 \tag{6}$$

where y_f is the predicted future output, y_{sp} is the set-point, Q is the error penalty, R is the input change penalty, $\Delta\mu_f$ is the future input change and k is the current sampling time.

5. CONTROL STUDY

The controller performances have been evaluated based on the results obtained from set-point tracking, disturbance rejection and robustness tests. The performance criteria used are the integral absolute error (IAE), integral squared error (ISE) and integral time absolute error (ITAE).

5.1 Set-point Tracking Test

In this test, the set-point 1 values are 0, 5.4966, 4 and 5.4966, while the set point 2 values are 0, 0.424, 0.2708 and 0.424. These values were changed every 2 h to change the MTBE purity from 95% (low quality) to 99% (high quality) and then 97% (medium quality). The resulting CV profiles are shown in Figure 4. As observed in the figure, the CV_1 profile can be tracked very well, whereas the CV_2 profile slightly overshoots at the beginning of the step changes (t = 2 2.3). The CV_2 profile also shows small offset values, but the error calculated is still very small (ITAE = 1.55%).

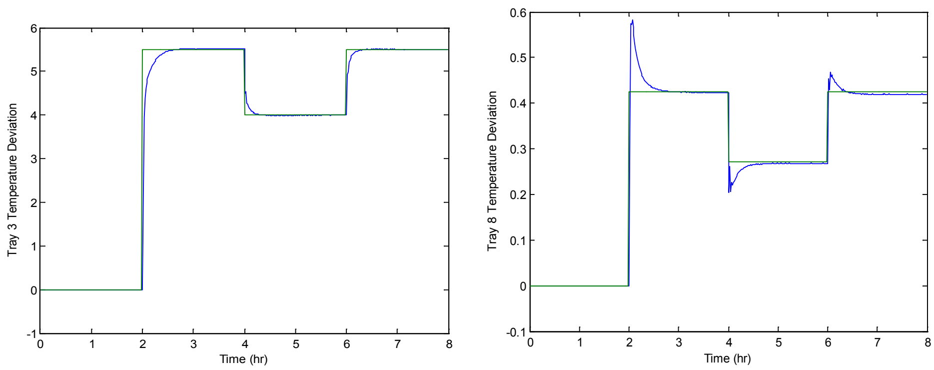

Figure 4: Set-point test profile of CV_1 and CV_2 using NWMPC.

5.2 Disturbance Rejection Test

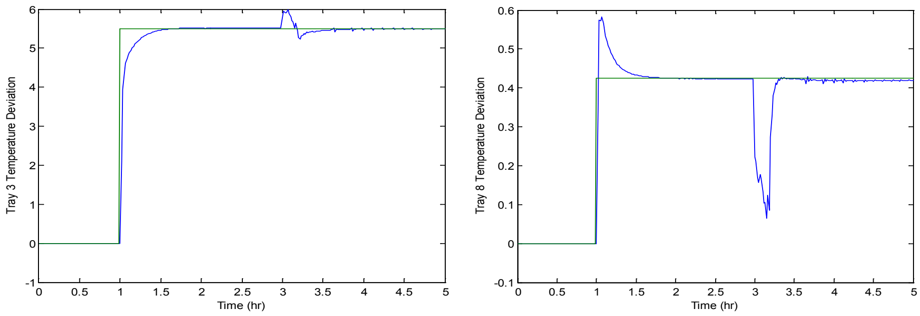

Figure 5: Disturbance rejection test profile of CV_1 and CV_2.

The disturbance rejection study is performed by changing the feed flowrate by 30% of the nominal value. The duration of the change is 0.2 h (from 3 h to 3.2 h). The resulting CV_1 shows that the NWMPC is able to reject the disturbance (within 0.5 h) and return the CV_1 to its original set-point, as shown in Figure 5. On the other hand, for CV_2, the NWMPC takes longer to reject the disturbance imposed. It can also be observed in Figure 5 that the deviation for the CV_2 profile is quite large, which is due to the reaction and separation process in this tray.[1]

5.3 Robustness Test

In this test, the column efficiency was changed to 80% without changing the NMPC parameter. Under the new initial conditions resulting from this efficiency change, at the steady-state, the MTBE purity is 95.24%, while the temperatures of tray numbers 3 and 8 are 93.92°C and 126.96°C, respectively. In this test, the set-point steps were 0, 7, 4 and 7 for CV_1 and 0, 0.75, 0.39 and 0.75 for CV_2, which were varied with a switching time of 2 h. For the T_3 (CV_1) profiles, the NWMPC controller managed to force the CV_1 to follow the set-point despite the reduced tray efficiency of the column, as shown in Figure 8. Meanwhile, the CV_2 profile shows an overshoot at the beginning of the set-point change, eventually converging to the steady-state. The performance criteria (error information) for CV_1 and CV_2 are tabulated in Table 1. The table shows that, overall, the NWMPC managed to control the tray temperature of MTBE RD very well.

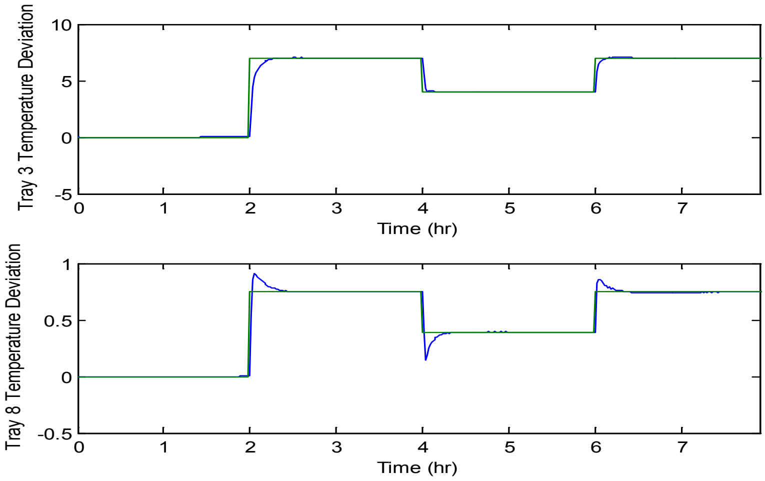

Figure 6: Robustness test profile of CV_1 and CV_2.

Table 1: Error calculation for the set-point change, disturbance rejection and robustness tests.

	NWMPC					
	Set-point change test		Disturbance rejection test		Robustness test	
	Y_1	Y_2	Y_1	Y_2	Y_1	Y_2
IAE	0.5009	0.4958	0.4511	0.1072	0.6529	0.1029
ISE	0.6740	0.4872	0.2601	0.1986	0.3979	0.0570
ITAE	1.5627	1.5479	0.7502	0.2684	2.3473	0.4184

6. CONCLUSION

An NWMPC using an SQP optimiser has been successfully applied to control the tray temperatures in MTBE reactive distillation. The NWMPC was then evaluated based on set-point tracking, disturbance rejection and robustness tests. The results showed that the NWMPC is able to control the CV_1 and CV_2 effectively, with small error values.

7. ACKNOWLEDGEMENT

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