

# Multi-Model Predictive Control of a Distillation Column

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## ABSTRACT

Successful implementation of optimization-driven control techniques, such as model predictive control (MPC), is highly dependent on an accurate and detailed model of the process. As complexity in the system increases, linear approximation used in MPC may result in poor performance since a critical operating point is valid in only a small neighborhood of operation. To address this problem, this paper proposes a collaborative approach that combines linear and data-based models to predict state variables individually. The outputs of these models, along with constraints, are then incorporated into the MPC algorithm. For data-based process model, a multi-layered feed-forward network is used. Additionally, the offset-free technique is applied to eliminate steady-state errors resulting from model-process mismatch. To demonstrate the results, a binary distillation column process which is multivariable and inherently nonlinear is chosen as testbed. We compare the performance of the proposed method to MPC using the full nonlinear model and also to single-model MPC methods for both the linear model and neural network model. We show that the proposed method is only slightly suboptimal with respect to the best available performance and greatly improves over individual methods. In addition, the computational load is reduced when compared to the full nonlinear MPC.

**Keywords:** Distillation column, Multiple Models, Model Predictive Control, Data-based Modeling

## INTRODUCTION

Distillation column process constitutes a reasonably proper benchmark for a designer aiming superior control which finds solution to strongly coupled nonlinear multi-input multi-output (MIMO) system that is prone to input disturbances [1,2]. MPC is among the leading methods that provide control solutions for the plants with aforementioned challenges [3-6]. Due to the increasing demand for performance and rising complexity of systems, classical model predictive control (MPC) techniques are often inadequate and new applications often requires some modifications in predictive control mechanism [7-9]. The modifications frequently include reformulation of optimal control in order to cope with system uncertainties, external perturbations and adverse effect of rapid changes in operating points [10]. As complexity in the system increases, successful implementation of this optimization-driven control technique is highly dependent on an accurate and detailed model of the process.

However, the linear approximation at a critical point used in MPC may result in poor performance and remains valid in only a small neighborhood of operation. In such a case, nonlinear system model can be used for optimal control signal calculation but lack of reliable dynamic process model and high computational burden are major drawbacks in real time implementation of MPC schemes [11]. A multi model predictive controller (Multi-MPC) based on integration of linear system models may provide efficient control of nonlinear process with reduced computational complexity along with covering a large space of operating regions [12-15]. Alternatively, considering uncertainties in real-time operations, data-based models may complement linear approximation models for the prediction of MPC and enlarge the operational region of controller.

In this paper, we propose to employ multiple models that can describe the same process dynamics to a certain degree. In addition to the linear model, multi-layered feedforward network is used for data-based modeling

and constitutes an additional process model. A cost function formulation is proposed to enable both models to collaborate in predicting state variables individually, with their outputs and constraints incorporated into the MPC algorithm. The aim is to enhance efficiency and robustness in process control by compensating for the limitations of each individual model. Additionally, the offset-free technique is applied to eliminate steady-state errors resulting from model-process mismatch. To demonstrate the potential challenges addressed above, a binary distillation column process is chosen as testbed. The process is multivariable, inherently nonlinear and extremely sensitive to input uncertainty especially when LV configuration is selected [16]. We compare the performance of the proposed method to MPC using the full nonlinear model and also to single-model MPC methods for both the linear model and neural network model.

## PROCESS MODELING

A methanol-water binary distillation process schematic is depicted in Figure 1. Before giving the mathematical description of the system, the following assumptions are made:

- Heat losses are zero and temperature changes along the column are small.
- Constant liquid flow along the column.
- Liquid on every tray is well mixed.
- Each plate, which contains liquid and vapor leaving, is in equilibrium.
- There is no vapor holdup on trays.
- There is a constant liquid holdup on trays, reboiler, and condenser.
- The column operates at a constant pressure of 1 atm.
- Real liquid phase molar fraction equals the ideal liquid phase molar fraction,  $x = x^*$ .

Efficiency and vapor molar fractions are correlated with the following equation:

$$\eta_i = \frac{y_i - y_{i+1}}{y_i^* - y_{i+1}} \quad (1)$$

where  $y_i$  is real concentration of vapor phase on  $i$ -th tray and  $y^*$  is ideal concentration of vapor phase on  $i$ -th tray. The theoretical vapor and liquid molar fractions are correlated with the following empirical relation which is obtained by using a laboratory scale distillation column data:

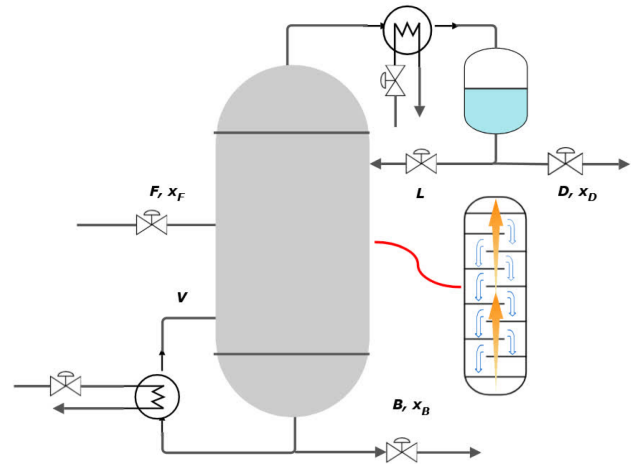


Figure 1. Distillation column schematic diagram.

$$y^* = -23.805x^6 + 82.142x^5 - 112.570x^4 + 78.529x^3 - 29.821x^2 + 6.524x + 0.003 \quad (2)$$

We consider 10 trays for the column, treating the condenser and reboiler as individual trays. Tray numbering starts from the top (tray 1) to the bottom (tray 10). The liquid mixture enters the column at tray 6. Considering mass balance for the entire column, the nonlinear state-space model is given by the following equations [17]:

$$\frac{dx_1}{dt} = -\frac{(D+L)}{N_1}x_1(t) + \frac{V}{N_1}y_2(t) \quad (3)$$

$$\frac{dx_i}{dt} = -\frac{L}{N_i}x_i(t) + \frac{L}{N_i}x_{i-1}(t) + \frac{V}{N_i}y_{i+1}(t) - \frac{V}{N_i}y_i(t), \quad i = 2, \dots, 5 \quad (4)$$

$$\frac{dx_6}{dt} = -\frac{L+F}{N_6}x_6(t) + \frac{L}{N_6}x_5(t) + \frac{F}{N_6}x_F(t) + \frac{V}{N_6}y_7(t) - \frac{V}{N_6}y_6(t) \quad (5)$$

$$\frac{dx_i}{dt} = -\frac{L+F}{N_i}x_i(t) + \frac{L+F}{N_i}x_{i-1}(t) + \frac{V}{N_i}y_{i+1}(t) - \frac{V}{N_i}y_i(t), \quad i = 7, \dots, 9 \quad (6)$$

$$\frac{dx_{10}}{dt} = -\frac{B}{N_{10}}x_{10}(t) + \frac{L+F}{N_{10}}x_9(t) - \frac{V}{N_{10}}y_{10}(t) \quad (7)$$

where  $N_i$  is holdup in  $i$ -th tray,  $x_F$  is the molar fraction of volatile component in feed,  $F$  is the molar flow of feed,  $D$  is the molar flow of distillate,  $V$  is the molar flow of vapor,  $L$  is the molar flow of reflux,  $B$  is the molar flow of bottom,  $x_i$  is the molar fraction of methanol in  $i$ -th tray in liquid phase,  $x_i^*$  is the ideal molar fraction of methanol in  $i$ -th tray in liquid phase,  $y_i$  is the molar fraction of methanol in  $i$ -th tray in vapor phase and  $y_i^*$  is the ideal molar fraction of methanol in  $i$ -th tray in vapor phase. Table 1 shows the process parameters.

The above equations including theoretical vapor and liquid molar fractions correlation imply that high purity distillation process has strong nonlinearity and any realistic study should take this into account. It is important to start control design with properly selected manipulated variables for the system of concern due to the system

complexity. There are various control variable pairings in practice such as LV, LB, DV, and LD where LV configuration is the most commonly used in industrial practice and chooses liquid and vapor flows as manipulated variables. In this study we select LV configuration for the optimal control application.

**Table 1:** Distillation column operating parameters.

Description	Variable	Unit	Value
Feed molar flow	$F$	$\text{kmolh}^{-1}$	0.300
Vapor molar flow	$V$	$\text{kmolh}^{-1}$	0.264
Reflux molar flow	$L$	$\text{kmolh}^{-1}$	0.104
Distillate molar flow	$D$	$\text{kmolh}^{-1}$	0.160
Feed molar fraction	$x_F$	-	0.650
Distillate molar fraction	$x_D$	-	0.904
Bottom molar fraction	$x_B$	-	0.164
Reboiler holdup	$N_{10}$	kmol	1
Tray/condenser holdup	$N_i$	kmol	0.2
Tray efficiency	$\eta_t$	-	0.8
Reboiler efficiency	$\eta_b$	-	1

## Linear System Model

A linear state-space model is used as the first approximation of the distillation process. System state variables represent concentrations in liquid phase for each tray,  $\mathbf{x} = (x_1, x_2, \dots, x_{10})^T$ , with initial conditions  $x_i(0) = x_{i0}$  for  $i = 1, 2, \dots, 10$ . The concentrations of interest are distillate fraction  $x_D = x_1(t)$  and bottom product  $x_B = x_{10}(t)$  which are considered as outputs of the process to be controlled by manipulated variables reflux  $L$  and boilup  $V$ . We assume that the process is in steady-state at  $t = 0$  where we start the system from operating point such that  $\mathbf{x}_{op} = (x_1(0), x_2(0), \dots, x_{10}(0))^T$  and  $\mathbf{u}_{op} = (u_1(0), u_2(0))^T = (L(0), V(0))^T$ . Then, the process is linearized in the steady-state with the assumption of small the deviation from operating point in the form of  $\mathbf{x}_{ss} = \mathbf{x}(t) - \mathbf{x}_{op}$ ,  $\mathbf{u}_{ss} = \mathbf{u}(t) - \mathbf{u}_{op}$ . The resulting multi-input multi-output (MIMO) state-space model in discrete time can be represented as follows:

$$\mathbf{x}_{ss}(k+1) = \mathbf{A}\mathbf{x}_{ss}(k) + \mathbf{B}\mathbf{u}_{ss}(k), \quad (8a)$$

$$\mathbf{y}_{ss}(k) = \mathbf{C}\mathbf{x}_{ss}(k) + \mathbf{D}\mathbf{u}_{ss}(k) \quad (8b)$$

## Neural Network Model

The second process model is created by acquiring system dynamics directly from data without using first principle models. A multi-layered feedforward neural network is used due to its effectiveness in process modeling and control. To construct data-driven model, datasets for training, testing, and validation are derived from a nonlinear simulation of a distillation process. Excitation signals are carefully designed to ensure the data encapsulates the system dynamic behavior across a wide range of operating conditions. Specifically, multilevel pseudorandom

step (MLPRS) signals are applied to the manipulated variables with a sampling interval of 0.5 s. These signals feature varying frequencies and amplitudes, constrained within the operational limits of the manipulated variables (e.g., reflux flow  $L$  and vapor molar flow  $V$ ), to excite the nonlinear dynamics sufficiently for accurate prediction and control. Since all system input/output variables change in range of (0, 1) preprocessing of raw data does not require scaling. The neural network (NN) model accepts current and previous values of system outputs plus current and previous values of manipulated variables as inputs and predicts two system outputs  $x_D$  and  $x_B$ . The model has 8 inputs and gives one-step ahead prediction of 2 outputs. We can write the discrete input-output model of NN in the following form

$$\mathbf{y}(k+1) = \mathbf{f}_{nn}(\mathbf{y}(k), \mathbf{y}(k+1), \mathbf{u}(k), \mathbf{u}(k-1)) \quad (9)$$

where  $\mathbf{y}(k) = (x_D(k), x_B(k))^T$  and  $\mathbf{u}(k) = (L(k), V(k))^T$ . In the NN design we use tanh activation function for nodes in the hidden layer and a linear activation in output layer. The defined NN is trained by using Levenberg-Marquardt algorithm for error convergence between predicted and actual target values. The dataset is split into training (70%), validation (15%), and testing (15%) subsets, ensuring no overlap in operating conditions between splits. The final architecture (16-8-16-8) is selected based on the lowest validation mean squared error (MSE) and satisfactory performance on the test set, achieving MSE =  $4.0 \times 10^{-7}$  for both outputs.

## MULTI-MODEL PREDICTIVE CONTROL

The control goal is to utilize linear system model and NN model to predict future states and maintain the system covering a broader space of operating points. Since the scenario is to use linear model in (8) and data-based model in (9) as MPC predictors, plant-model mismatch is likely to occur when a large deviation from operating point is started. In order to overcome this problem, the value of the state disturbance is estimated using the measurement of current process states and linear system states as follows [18]

$$\mathbf{d}_{ss}(k) = (\mathbf{x}(k) - \mathbf{x}_{op}) - (\mathbf{A}\mathbf{x}_{ss}(k-1) + \mathbf{B}\mathbf{u}_{ss}(k-1)) \quad (10)$$

Then the state and output predictions for linear MPC are calculated with the help of (10) and can be rewritten as

$$\mathbf{x}_{ss}(k+i|k) = \mathbf{A}\mathbf{x}_{ss}(k+i-1|k) + \mathbf{B}\mathbf{u}_{ss}(k+i-1|k) + \mathbf{d}_{ss}(k), \quad i = 1, \dots, p, \quad (11a)$$

$$\mathbf{y}_{ss}(k+i|k) = (x_{ss,D}(k+i|k), x_{ss,B}(k+i|k))^T, \quad i = 1, \dots, p. \quad (11b)$$

where  $p$  is the length of the prediction horizon and the notation  $\mathbf{x}_{ss}(k+i|k)$  denotes variable  $\mathbf{x}$  predicted for a

future sample  $k + i$ , but calculated at the current sample time  $k$ . The same mechanism for output disturbance estimation can be applied to the NN model. Off-set values between NN model outputs and actual process outputs are estimated with the following formulation

$$\mathbf{d}_{nn}(k) = \mathbf{y}(k) - \mathbf{f}_{nn}(\mathbf{y}(k-1), \mathbf{y}(k-2), \mathbf{u}(k-1), \mathbf{u}(k-2)) \quad (12)$$

Considering (12), the output predictions are then be calculated as follows

$$\mathbf{y}_{nn}(k+i|k) = \mathbf{f}_{nn}(\mathbf{y}_{nn}(k+i-1|k), \mathbf{y}_{nn}(k+i-2|k), \mathbf{u}(k+i-1|k), \mathbf{u}(k+i-2|k)) + \mathbf{d}_{nn}(k), \quad i = 1, \dots, p. \quad (13)$$

## Predictive Control Formulation

Control design aims to combine precision of each model over prediction horizon of MPC to obtain process outputs  $\mathbf{y}(k+i|k) = (x_D(k+i|k), x_B(k+i|k))^T$  using the calculated present and future control  $\mathbf{u}(k+m-1|k) = L(k|k), \dots, L(k+m-1|k), V(k|k), \dots, V(k+m-1|k)^T$  where  $m$  is the control horizon. Subsequently, optimization problem for reference tracking with partial costs can be represented as

$$J_{ss}(k) = \sum_{i=1}^p \mathbf{e}_{ss}(k+i|k)^T \mathbf{Q}_y \mathbf{e}_{ss}(k+i|k) + \sum_{i=0}^{m-1} \Delta \mathbf{u}(k+i|k)^T \mathbf{Q}_u \Delta \mathbf{u}(k+i|k) \quad (14a)$$

$$J_{nn}(k) = \sum_{i=1}^p \mathbf{e}_{nn}(k+i|k)^T \mathbf{Q}_y \mathbf{e}_{nn}(k+i|k) + \sum_{i=0}^{m-1} \Delta \mathbf{u}(k+i|k)^T \mathbf{Q}_u \Delta \mathbf{u}(k+i|k) \quad (14b)$$

$$\text{s.t. } \mathbf{e}_{ss}(k+i|k) = \mathbf{y}_{ref}(k+i|k) - \mathbf{y}_{ss}(k+i|k) \quad (14c)$$

$$\mathbf{e}_{nn}(k+i|k) = \mathbf{y}_{ref}(k+i|k) - \mathbf{y}_{nn}(k+i|k) \quad (14d)$$

$$\mathbf{y}_{min} \leq \mathbf{y}_{ss}(k+i|k) \leq \mathbf{y}_{max}, \quad (14e)$$

$$\mathbf{y}_{min} \leq \mathbf{y}_{nn}(k+i|k) \leq \mathbf{y}_{max}, \quad (14f)$$

$$\mathbf{u}_{min} \leq \mathbf{u}(k-1+i|k) \leq \mathbf{u}_{max}, \quad (14g)$$

$$i = 1, \dots, p,$$

where  $\mathbf{y}_{ref}(k+i|k)$  denotes the future reference,  $\mathbf{Q}_y$  and  $\mathbf{Q}_u$ , are the penalizations on outputs and control increments, respectively. There are lower/upper constraints on the manipulated variables ( $\mathbf{u}_{min}, \mathbf{u}_{max}$ ) and outputs ( $\mathbf{y}_{min}, \mathbf{y}_{max}$ ). The state and output disturbance,  $\mathbf{d}_{ss}$  and  $\mathbf{d}_{nn}$ , for each model plays a crucial role in multi-model MPC and the proposed control configuration uses weighted costs for optimization problem which is defined as:

$$\min_{\mathbf{u}(k)} \{ \omega(k) J_{ss}(k) + (1 - \omega(k)) J_{nn}(k) \}, \text{ s.t. (14)} \quad (15)$$

where  $\omega(k)$  represents weighting parameter of performance functions at each sampling instant  $k$ , which depends on the values of modeling errors. Using the Euclidean norm for vectors of estimated off-set values of models, it can be calculated as follows:

$$\omega(k) = 1 - \frac{\|\mathbf{d}_{ss}(k)\|}{\|\mathbf{d}_{ss}(k)\| + \|\mathbf{d}_{nn}(k)\|} \quad (16)$$

## RESULTS AND DISCUSSION

Nonlinear system simulations are conducted on a workstation equipped with an i7 10750H Intel 6-core CPU (base clock speed of 2.60 Ghz up to 4.8 GHz) and 16 GB of RAM. The simulations are performed in the MATLAB environment by utilizing ode15s solver with a relative tolerance of  $1 \times 10^{-6}$  and simulation step size of 0.5 s. The calculation of optimal control inputs for predictive control is performed using the `fmincon` function.

For MPC setup, all controllers run with  $\mathbf{Q}_y = \text{diag}(1,1)$  and  $\mathbf{Q}_u = \text{diag}(0.05,0.05)$ , the prediction horizon and control horizon are set to  $p = 10, m = 3$ . The control inputs of the plant,  $\mathbf{u}(k) = (L(k), V(k))^T$  i.e, reflux liquid flow rate and vapor flow rate are constrained such that distillate flow rate must be kept in the interval of  $0.01 < D < 0.200$  kmol/h as well as having the physical constraints. The controlled outputs  $\mathbf{y}(k) = (x_D(k), x_B(k))^T$  are constrained as well

$$\begin{bmatrix} 0.01 \\ 0.01 \end{bmatrix} \leq \mathbf{u}(k) \leq \begin{bmatrix} 0.3874 \\ 0.5874 \end{bmatrix}, \quad \begin{bmatrix} 0.8973 \\ 0.0600 \end{bmatrix} \leq \mathbf{y}(k) \leq \begin{bmatrix} 0.9663 \\ 0.2261 \end{bmatrix} \quad (17)$$

We also consider slack variables of outputs at constraints for SSMPC and NNMPC so as to ensure feasibility of the optimization problem in a case of unknown disturbances such that

$$\mathbf{y}_{min} - \boldsymbol{\varepsilon}(i) \leq \mathbf{y}_{ss}(k+i|k) \leq \mathbf{y}_{max} + \boldsymbol{\varepsilon}(i) \quad (18a)$$

$$\mathbf{y}_{min} - \boldsymbol{\varepsilon}(i) \leq \mathbf{y}_{nn}(k+i|k) \leq \mathbf{y}_{max} + \boldsymbol{\varepsilon}(i) \quad (18b)$$

where slack variable  $\boldsymbol{\varepsilon}(i)$  is subject to the constraint  $\boldsymbol{\varepsilon}(i) \geq 0$ . Consequently, cost of optimization problem given in (14a) and (14b) is updated with slack variable as

$$J(k) = \sum_{i=1}^p [\mathbf{e}(k+i|k)^T \mathbf{Q}_y \mathbf{e}(k+i|k) + \boldsymbol{\varepsilon}(i)^T \mathbf{Q}_\varepsilon \boldsymbol{\varepsilon}(i)] + \sum_{i=0}^{m-1} \Delta \mathbf{u}(k+i|k)^T \mathbf{Q}_u \Delta \mathbf{u}(k+i|k) \quad (19)$$

The penalization of new variable is set to  $\mathbf{Q}_\varepsilon = \text{diag}(0.5,0.5)$  for both NN-MPC and SS-MPC. The parameters listed in Table 1 are used to derive linear process model of distillation column. The operating point, for this steady state data, corresponds to a lower purity of compositions  $x_D$  and  $x_B$ . Here, it is desired to drive the system to another operating point with high purity of top product, which implies that large perturbations from steady state are expected. Therefore, a linear state-space model may not be adequate to give sufficiently accurate predictions for MPC mechanism. It should be noted that the nonlinear process accepts  $x_F$  and  $F$  as disturbance inputs in addition to manipulated variables  $L$  and  $V$  in the selected control setup, and they are assumed to be constant for all simulation scenarios. Simulations are started with an initial condition selected in the vicinity of steady-state data

which is used to linearize nonlinear column model. To evaluate the reference tracking performance of all controllers, the following four distinct step changes in the setpoints are applied to both outputs

$$\mathbf{y}_{\text{ref},1} = \begin{bmatrix} 0.928 \\ 0.190 \end{bmatrix}, \mathbf{y}_{\text{ref},2} = \begin{bmatrix} 0.897 \\ 0.226 \end{bmatrix}, \mathbf{y}_{\text{ref},3} = \begin{bmatrix} 0.941 \\ 0.126 \end{bmatrix}, \\ \mathbf{y}_{\text{ref},4} = \begin{bmatrix} 0.966 \\ 0.060 \end{bmatrix}$$

A predictive control employing exact nonlinear process model, which is referred to as Nonlinear-MPC in this context, is selected as benchmark for time response performance evaluation. The optimization problem in (19) subject to the constraints given in (17) and (18) is also valid for Nonlinear-MPC case. Single-model approaches, including Nonlinear-MPC, NN-MPC, and SSMPC, are compared with Multi-MPC. Their reference tracking capabilities are demonstrated in Figure 2. It can be seen from the figure that both SS-MPC and NN-MPC approaches are prone to exhibit large overshoots especially when the plant is forced to run in a high purity point coinciding with output constraints. NN-MPC approach has slightly better time response whereas it generates more aggressive control inputs. On the other hand, controlled process using Multi-MPC formulations exhibits better reference tracking performance along with reduced control effort. Nonlinear-MPC, which is base control for simulations, exhibits the best performance among the controllers.

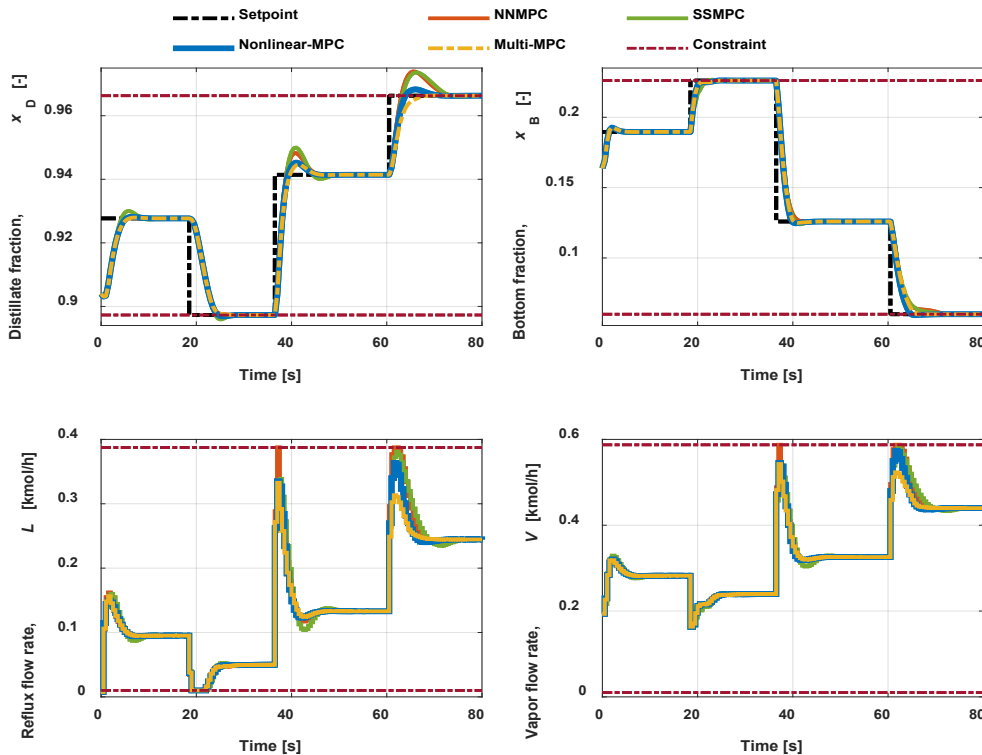
**Table 2:** Performance indicators of MPC methods

Controller	$J$ (%)	Average CPU Time (sec)
NN-MPC	107	4.802
SS-MPC	107	3.378
Multi-MPC	102	4.157
Nonlinear-MPC	100	5.106

For the purpose of better understanding of results, the performance of controllers are also evaluated by using closed-loop objective function with the following formulation

$$J = \sum_{i=1}^N \mathbf{e}(i)^T \mathbf{Q}_x \mathbf{e}(i) + \Delta \mathbf{u}(i)^T \mathbf{Q}_u \Delta \mathbf{u}(i) \quad (20)$$

where  $N$  is the number of sampling instants within the total simulation time. The closed-loop performance costs in Table 2 are normalized with respect to the benchmark Nonlinear-MPC. In the case of using approximate models as predictors, Multi-MPC achieves superior reference tracking for both process outputs while generating less aggressive control signals. It also performs better compared with SS-MPC and NN-MPC in terms of the performance cost. Multi-MPC requires slightly less computational effort compared to Nonlinear-MPC, as indicated by the average CPU time. Note that CPU time for SS-MPC was found using the default NLP solver and it would be significantly reduced using a QP solver.



**Figure 2:** Setpoint tracking results of controlled system outputs (top two plots) and manipulated variables



## CONCLUSION

This study represents an implementation of multi-model predictive control to a distillation column process which constitutes a notably proper benchmark for multi-input interacting nonlinear MIMO systems. Time responses of both single-model and multi-model MPC formulations are demonstrated via computer simulations under various control scenarios including operational limits as well as input and output constraints. Running the system in a large space operating regions allows us to observe that multi-model MPC outperforms linear and data-based single model approaches. The results are validated with closed-loop performance cost values of all controllers. In addition, time response and performance indicators show that offset-free technique successfully eliminates steady state errors resulting from model-process mismatch for all control methods. The proposed multi-model MPC formulation demonstrates that collaboration of linear and data-based models might be an acceptable candidate instead of full nonlinear MPC with less computational time.

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