NON-LINEAR PREDICTIVE CONTROL APPLIED TO DISTILLATION COLUMNS

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Abstract

This article presents an approximate alternative to non-linear predictive control. This alternative is based on an iterative linearisation of the response of the model, so that the responses from the closed loop are the same as those obtained with the non-linear method, but with a much lower computation delay and better optimisation tools.

In this case, this method has been applied to an ethanol distillation column.

For this purpose, the process has been developed in EcosimPro language, EL. The non-linear predictive control has been developed in C++ and it is called from EcosimPro.

Key words: simulation, non-linear predictive control, distillation columns, EcosimPro

1. INTRODUCTION

Model-based process control (MPC) is renowned worldwide as a tool capable of solving a great number of problems concerning multivariable controllers with restrictions. However, most of the industrial controllers are based on linear models, which limit the application of this type of control.

In recent years, non-linear model predictive control (NMPC) has been studied, both from the point of view of its properties (Chen *et al.* 1998) and of its implementation.

A comparison between MPC with NMPC shows that while the MPC with restrictions may solve an associated optimisation problem during each sampling period with QP or LP algorithms, the NMPC relies on non-linear programming methods (NPL) such as SQP, which require more CPU capacity.

Many solutions have been developed to deal with this problem, including the well-known simultaneous and sequential approximations.

The sequential solution solves the model by integrating it into each iteration of the optimisation routine. The only degree of freedom the NLP has are the control parameters. The simulation and optimisation calculations are performed sequentially (one after the other).

On the other hand, simultaneous solving of the model and optimisation consider the status model and the optimisation as decision variables, and the model equations are added to the optimisation problem as equality restrictions. This increases the size of the optimisation problem until a balance is struck between the two approaches.

In both cases the difficulty when implementing NMPC in a real process lies in the long computation delay.

Many alternatives have been proposed to conventional NMPC to solve this problem, including the NMPC techniques based on model linearisation.

This article also includes a second approximation (De Keyser, 1998), which applies a linear linearisation of the process in each sampling period to calculate an 'optimised response', similar to the 'forced response' of the linear MPC. This procedure is applied iteratively until the same non-linear solution is reached.

A description of the iterative linearisation is set out below, as well as a comparison between the NMPC that uses a sequential approach, and a version of the iterative linearisation. To do this, the control objectives of an ethanol distillation column have been used as a basis, and a description of the model developed has been included.

2. DESCRIPTION OF THE PROCESS

2.1 Distillation columns

Distillation is probably one of the most widespread operations in chemical industries. It can be used to separate different components in a current or to purify intermediate and end products. Its application ranges from alcohol distillation to petroleum cracking.

This study is centred on a high-purity ethanol distillation column which forms part of the distillation section of a sugar mill.

This case deals with the fermentation of sugars of which the end product is alcohol. The alcohol is subsequently separated from the rest of the components by means of a series of distillation processes.

Figure 1 shows a diagram of the rectifying column used as a basis for the study. The feed is a mix of three components: water, ethanol and propanol. Alcohol is obtained mainly from a side extraction at the top of the column.

There are also other secondary side extractions located several plates above the feed. These extractions are aimed at preventing isoamyl compounds from reaching the head of the column.

The column has a total of 82 plates, and the chemical compounds that are separated combine to form azeotropes, making the operation more complex.

The purpose of the controller is to maintain the molar fraction of ethanol at the bottom of the column and the molar fraction of water at the head as close as possible to their respective setpoints.

In order to achieve this, the flow of neutral alcohol from the side extraction and the flow of steam into the boiler have been selected as manipulated variables.

The levels at the bottom of the column and in the accumulator are also controlled, and the current at the bottom of the column and the reflux current are also manipulated in each case.

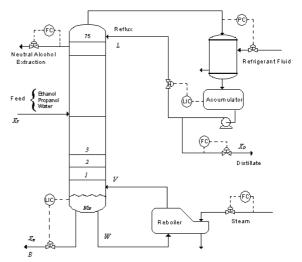


Fig. 1: Simplified diagram of a neutral alcohol distillation column

2.2 Process model

A detailed model of the process has been developed and the results have been compared with real plant data.

The mathematical model developed must represent the dynamic behaviour of the real process. A compromise must be reached between the accuracy in the approach of the model and the similarity between its response and the response of the process, as a function of the means available to solve the model.

The following hypotheses have been proposed:

- 1. Feed on a single plate
- 2. The feed enters as saturated liquid, although thought is given to the possibility of it being partially or totally vaporised
- 3. Neutral alcohol is extracted from the side of the penultimate plate
- 4. There are no heat losses. The column is adiabatic
- 5. The condenser is total, so the composition of the steam exiting the column through the head will be the same as that of the reflux and distillate current
- 6. There is no boiler, but a direct water vapour injection instead
- 7. A non-constant steam flow is considered, calculated on the basis of the energy balance established for each of the plates
- 8. The total loss of pressure from the column is distributed linearly amongst all the plates
- 9. The flow of liquid is calculated on the basis of the Francis formula for spillways
- 10. The liquid accumulated in each plate cannot be compressed. Furthermore, it it is a perfect mix (the composition will be the same at all points)

- 11. The liquid and steam exiting the plate have thermal equilibrium and are at the same temperature and pressure
- 12. The liquid and steam phases exiting the plate do not have phase equilibrium because a Murphree efficiency has been defined
- 13. The liquid-steam equilibrium is represented taking the following into consideration:
 - Ideal steam phase
 - Non-ideal liquid phase: the Wilson model is used to calculate the activity coefficient
- 14. The dead time in the steam current from the last plate of the column to the condenser is disregarded, as is the dead time in the return current of the reflux at the head of the column
- 15. The dynamics of the condenser are considered in the development of the model of the distillation column
- 16. No steam accumulation is considered throughout the system

The equations that represent the behaviour of a generic plate are the same for the whole column.

♦ Overall mass balance:

$$\frac{dM_n}{dt} = L_{n+1} + V_{n-1} + F_n - L_n - V_n - S_n \quad (1)$$

where:

 M_n = mass of liquid accumulated on plate n (kg)

 L_{n+1} = liquid that falls onto plate n from plate n+1 (kg/s)

- V_{n-1} = steam flow from plate n-1 (kg/s)
- L_n = liquid that exits plate n (kg/s)
- V_n = steam flow that exits plate n (kg/s)
- F_n = feed flow from plate n (kg/s)
- S_n = side extraction onto plate n (kg/s)
- \heartsuit Overall mass balance at component (j-1):

$$\frac{d(M_n x_n^j)}{dt} = L_{n+1} x_{n+1}^j + V_{n-1} y_{n-1}^j + F_n z_n - L_n x_n^j - V_n y_n^j - S_n x_n^j$$
(2)

where:

 x_n^j = molar fraction of component j in the liquid on plate n

- x_{n+1}^{j} = molar fraction of component j in the liquid flow of plate n+1
- y_{n-1}^{j} = molar fraction of component j in the steam flow of plate n-1
- y_n^y = molar fraction of component j in the steam flow of plate n
- $z_n^j =$ molar fraction of component j in the feed flow of plate n

The above balance is established for all components except one, which is calculated on the basis of:

$$x_N^j = 1 - \sum_{j=1}^{j=n-1} x_N^j$$
(3)

♦ Overall energy balance:

$$\frac{d(M_nh_n)}{dt} = L_{n+1}h_{n+1} + V_{n-1}H_{n-1} + F_nh_f - L_nh_n - V_nH_n - S_nh_n$$
(4)

where:

 h_n = enthalpy of the liquid on plate n (kJ/kg) h_{n+1} = enthalpy of the liquid on plate n+1 (kJ/kg) H_n = enthalpy of the steam on plate n (kJ/kg)

 H_{n-1} =enthalpy of the steam on plate n-1 (kJ/kg)

The changes in the specific enthalpy of the liquid phase are generally very small in comparison with the total enthalpy of the plate. This means that the energy balance may be normally reduced to an algebraic equation used as a basis for the calculation of the steam flow that exits the plate. The final energy balance is therefore as follows:

$$L_{n+1}h_{n+1} + V_{n-1}H_{n-1} + F_nh_{f,n} - L_nh_n - V_nH_n - S_nh_n = 0$$
(5)

Solution of the temperature.

The temperature in each plate is not obtained on the basis of the energy balance, as is the case at the bottom of the column. Instead, the temperature of the bubble (the temperature which is in equilibrium with a known composition of the liquid at a certain pressure, also known) is calculated.

The calculation algorithm in each plate therefore iterates on the temperature until the sum of the compositions of the steam phase of plate N equals 1.

$$1 - \sum_{j=1}^{n} y_{j}^{N} = 0 \tag{6}$$

Equilibrium ratio between the liquid-steam phases:

$$y_{n,j}^{*} = \frac{\gamma_{n}^{j} P_{n,j}^{sat}}{P_{n}} x_{n}^{j}$$
(7)

where:

 $y_{n,j}^*$ = molar fraction of component j on plate n in equilibrium with x_n^j

 γ_n^j = activity coefficient of component j on plate n

 $P_{n,j}^{sat}$ = steam pressure of component j on plate n (bar)

 P_n = total pressure on plate n (bar)

 x_n^j = molar fraction of component j in the liquid on plate n

 \clubsuit Total pressure on plate n:

$$P_n = P_{n+1} + \Delta P \tag{8}$$

where:

 P_n = total pressure on plate n (bar) P_{n+1} = total pressure on plate n+1 (bar) ΔP_n = pressure loss between plate n and n+1 (bar)

 \clubsuit Pressure loss on the plate

The distribution of the pressure loss is considered linear throughout the whole column, and directly proportional to the flow of superheated steam.

$$\Delta P = \left(\frac{V_0}{K}\right)^2 \tag{9}$$

where:

 V_0 = flow of superheated steam (m³/h) K = proportionality constant (m³/bar·h)

✤ Flow of liquid that exits plate n:

Calculated on the basis of the Francis formula for segmented spillways:

$$h_{ow} = 664 \cdot \left(\frac{Q}{L_w}\right)^{2/3} \tag{10}$$

where:

 h_{ow} = height of liquid over spillway crest (mm) Q = liquid that falls from the spillway (m³/s) L_w = length of the spillway (m)

The flow of liquid that falls onto a lower plate is thus:

$$Q_n = 1.8482L_w (h_{ow,n})^{1.5} \tag{11}$$

where:

 Q_n = liquid that exits plate n (m³/s) L_w = length of the spillway (m) $h_{ow,n}$ = height of liquid over spillway crest (m) Calculated using the following expression:

$$h_{ow,n} = \frac{Vol_n - V_{plato}}{A_{plato}}$$
(12)

where:

 Vol_n = volume of liquid on plate n (m³) V_{plato} = volume of plate (m³) A_{plato} = active area of the plate (m²)

 \clubsuit Steam flow exiting plate n:

As mentioned above, the steam flow to the next plate is calculated using the energy balance in steady state.

$$V_n = \frac{L_{n+1}h_{n+1} + V_{n-1}H_{n-1} + F_nh_{f,n} - L_nh_n - S_nh_n}{H_n}$$
(13)

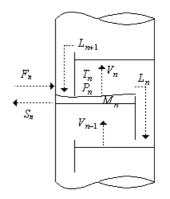


Fig. 2: Diagram of a generic plate

The mathematical characteristics of the model once it is implemented in the EcosimPro modelling language are the following:

No. of equations: 7217 No. of subsystems of coupled equations: 85 - Linear: 0 - Non-linear: 85 No. of explicit variables: 6870 No. of derived variables: 264 No. of algebraic variables: 83 No. of boundary variables: 11 No. status variables: 347 Size of the Jacobian matrix: 347×347 Spreading f. of the Jacobian matrix: 62.2088%

3. NON-LINEAR PREDICTIVE CONTROL

Non-linear model-based predictive control (NMPC) is a natural progression of the linear model-based predictive control technique (MPC). In NMPC, the

algorithm is also based on the use of an internal process model that includes the main characteristics of the process.

As mentioned in the introduction, two different formulae of the NMPC are going to be compared. One is the algorithm of the pure NMPC, and the other is an iterative linearisation technique.

3.1 NMPC Controller

The purpose of non-linear model-based predictive control (NMPC) is to find the optimum sequence of the values of the manipulated variables so that a function is minimised. This function is calculated on the basis of a desired trajectory of the outlet output??? variables along a prediction horizon.

The cost function is the integral of the squares of the waste resulting from the difference between the predicted model **outlets [outputs???]** (y_{pred}) and the reference values (r) during prediction time $N_2\tau$ (where N_2 is the prediction horizon and τ is the sampling period).

The following is a standard formula:

$$\min_{u(k/k),\dots,u(k+N_u-1/k)} J = \int_{t_k}^{t_k+N_2\cdot\tau} \gamma \left[(y_{pred}(t) - r(t)) \right]^2 dt + \sum_{j=0}^{N_u-1} \beta \left[\Delta u(k+j|t) \right]^2$$
(14)

The change in manipulated variable u is also included in the minimisation function.

Parametrisation of the manipulated variables is necessary because an infinite number of decision variables could otherwise appear for the problem.

A common solution is the discretisation of the manipulated variable u along the control horizon (N_u) when the input variables remain constant during a τ sampling period:

$$u(t) = u(k), \ k\tau \le t < (k+1)\tau$$

$$u(k) = u(N_u - 1) \qquad \text{for all } k > N_u - 1$$

The minimisation of equation (14) is subject to the continuous model equations and the common restrictions that apply both to manipulated and controlled variables:

$$u_{\min} \le u(k) \le u_{\max}$$
$$\Delta u_{\min} \le \Delta u(k) \le \Delta u_{\max}$$
(15)

$$y_{\min} \le y(k) \le y_{\max}$$

Only the first of the control movements is implemented out of all the sequence along the control horizon.

Within this schema, the process model is used to calculate the predictions of the outlet [output???] variables $(y_{pred}(t))$, required to minimise equation 14 (Fig. 3).

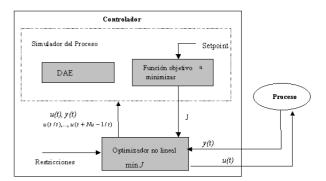


Fig. 3: Implementation of the non-linear controller

In this formula, the model equations are not considered explicit restrictions within the optimisation problem, and the only decision variables are the manipulated variables.

The function of the process simulation is to integrate the model equations along the prediction horizon taking the current state of the process as input conditions and to evaluate the target function formulated at the end of each integration.

All of the above enables a non-linear problem to be programmed with a generic formula, such as the minimisation in real time of a non-linear target function with restrictions.

3.2 Formulation of a non-linear iterative predictive controller (EPSAC)

The main idea behind this formula is to draw non-linear predictions closer by means of iterative linearisation around future trajectories so that this **linearisation** reaches the same optimum non-linear solution.

In order to achieve this, the sequence of future values of the manipulated variables is considered the sum of *base* future control actions $u_{base}(t+k/t), k \ge 0$, and *optimised* future control actions, $\delta u(t+k/t), 0 \le k \le N_u - 1$:

$$u(t+k/t) = u_{base}(t+k/t) + \delta u(t+k/t) \quad (16)$$

The predictions of the output variables can therefore be considered as the sum of two effects:

$$y(t+k/t) \approx y_{base}(t+k/t) + y_{ontimize}(t+k/t)$$
(17)

The first component, $y_{base}(t + k/t)$, is calculated by using the non-linear model together with the known sequence of the manipulated variable, $u_{base}(t + k/t)$ as inputs for the model.

The second component, $y_{optimize}(t + k/t)$, is the result of a series of impulse and step inputs (De Keyser, 1998):

$$y_{optimize}(t+k/t) = h_k \delta u(t/t) + h_{k-1} \delta u(t+1/t) + \dots + g_{k-N_u+1} \delta u(t+N_u-1/t)$$
(18)

where parameters $h_1, h_2, ..., h_k, ..., h_{N_2}$ are the coefficients of the responses of the system to a single impulse in the current operating conditions.

The values of g_k are the coefficients of the response to a single step.

If a matrix notation is used, equation 17 would be as follows:

$$\mathbf{Y} = \overline{\mathbf{Y}} + \mathbf{G}\mathbf{U} \tag{19}$$

where:

$$\mathbf{Y} = \begin{bmatrix} y_{base}(t + N_1 / t) & \dots & y_{base}(t + N_2 / t) \end{bmatrix}^T \quad (20)$$
$$\mathbf{U} = \begin{bmatrix} \delta u(t / t) & \dots & \delta u(t + N_u - 1 / t) \end{bmatrix}^T$$
$$\mathbf{G} = \begin{bmatrix} h_{N_1} & h_{N_1 - 1} & h_{N_1 - 2} & \dots & g_{N_1 - N_u + 1} \\ h_{N_1 + 1} & h_{N_1} & h_{N_1 - 1} & \dots & g_{N_1 - N_u + 2} \\ \dots & \dots & \dots & \dots & \dots \\ h_{N2} & h_{N_2 - 1} & h_{N_2 - 2} & \dots & g_{N_2 - N_u + 1} \end{bmatrix}$$

The ratio between control actions Δu and δu is as follows:

$$\begin{bmatrix} \Delta u(t/t) \\ \Delta u(t+1/t) \\ \dots \\ \Delta u(t+N_u-1/t) \end{bmatrix} = \mathbf{A} \begin{bmatrix} \delta u(t/t) \\ \delta u(t+1/t) \\ \dots \\ \delta u(t+N_u-1/t) \end{bmatrix} + \mathbf{b}$$
(21)

where matrix A and vector b are provided by:

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ -1 & 1 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & -1 & 1 \end{bmatrix},$$
(22)
$$\mathbf{b} = \begin{bmatrix} u_{base}(t/t) - u(t-1) \\ u_{base}(t+1/t) - u_{base}(t/t) \\ \dots \\ u_{base}(t+N_u - 1/t) - u_{base}(t+N_u - 2/t) \end{bmatrix}$$

The coefficients of matrix G are calculated using the linearised model on the current status for each sampling period.

However, it is difficult to obtain model linearisation for a complex dynamic process. Thus, a possible alternative has been developed, consisting in the use of the non-linear model to calculate coefficients h_k and g_k by means of model simulation.

Taking equation 21 into consideration, and keeping in mind that $h_k = g_k - g_{k-1}$, equation 18 may be rewritten as follows:

$$y_{optimize}(t+k/t) = g_k [u(t-1) + \Delta u(t) - u_{base}(t)] + \sum_{i=1}^{N_u-1} g_{k-i} [\Delta u(t+i) + u_{base}(t+i-1) - u_{base}(t+i)]$$
(23)

The step response coefficients may be calculated for a sampling period by simulating the non-linear process model with a specific sequence of control actions, $u^{*}(t + k/t)$, taking the current state of the process as an initial condition and evaluating the predictions as well, $y^{*}(t + k/t)$.

The following is a sequence of control actions that could be selected: $u(t-1) + \Delta u^*(t)$.

With this sequence, and taking into consideration that

$$y^{*}(t+k/t) = y_{base}(t+k/t) + y^{*}_{optimize}(t+k/t)$$
(24)

the g_k coefficients verify the following expression:

$$c_0 g_k = y^* (t + k/t) - y_{base} (t + k/t) - g_{k-1} c_1 - g_{k-2} c_2 - \dots - g_{k-N_u+1} c_{N_u-1}$$
(25)

where:

$$g_{0} = 0$$

$$c_{0} = u(t-1) + \Delta u^{*}(t) - u_{base}(t) \qquad (26)$$

$$c_{j} = u_{base}(t+j-1) - u_{base}(t+j), j \ge 1$$

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Finally, the cost function, which needs to be minimised, turns out to be a U square function.

$$J = \gamma \sum_{k=N_1}^{N_2} [y(t+k/t) - r(t+k/t)]^2 + \beta \sum_{k=0}^{N_u-1} [\Delta u(t+k/t)]^2$$
$$\gamma (\mathbf{R} - \overline{\mathbf{Y}} - \mathbf{GU})^T (\mathbf{R} - \overline{\mathbf{Y}} - \mathbf{GU}) + \beta (\mathbf{AU} + \mathbf{b})^T (\mathbf{AU} + \mathbf{b})$$
(27)

As regards the optimisation, the minimisation of J is subjected to the restrictions of (10). This problem is solved with simple techniques of quadratic programming (QP).

controls

ile $\delta u(t+k/t) \neq 0$,

 $u(t + k/t) = u_{base}(t + k/t) + \delta u(t + k/t)$ are suboptimum, because approximation is based on the principle of overlapping (12). However, they may converge in the optimum controls by iteratively redefining $u_{base}(t + k/t) \equiv u(t + k/t)$ and recalculating $\delta u(t + k/t)$ and u(t + k/t) until $\delta u(t + k/t) \approx 0$, so that $y_{optimize}(t + k/t)$ is practically zero.

In order to reduce the number of iterations, the initial value of $u_{base}(t + k/t)$ is important. A simple and effective choice (De Keyser, 1998) is to start with the optimum control policy derived from the previous step $u_{base}(t + k/t) \equiv u(t + k/t - 1)$. This strategy has been applied in this article.

4. **RESULTS OF THE SIMULATION**

Extensive testing has been performed to compare the standard NMPC with the non-linear EPSAC, both from the point of view of computation delay and efficiency.

The sampling period is 5 minutes, while the rest of the parameters are $N_2=\{15,15\}$, $N_u=\{1,1\}$, $\gamma=\{5,1\}$, $\beta=\{0,0\}$.

The restrictions of the manipulated variables were set at $\mathbf{u}_{\min} = \{2000, 7000\}$, $\mathbf{u}_{\max} = \{5000, 13000\}$ and their changes limited to $\Delta \mathbf{u}_{\min} = \{-150, -1500\}$; $\Delta \mathbf{u}_{\max} = \{150, 1500\}$.

Additionally, the restrictions for the controlled variables are $\mathbf{y}_{min} = \{0,0\}$ and $\mathbf{y}_{max} = \{0.05, 0.4\}$.

In these simulations it is assumed that measurable process statuses are available at t_k , for example, and that the initial condition is known in each iteration.

Changes in the reference of the controlled variables

Variations for both controlled variables have been simulated over a period of 4.5 hours, and the behaviour obtained by both controllers was similar. Fig. 4 shows how the controller tries to make the ethanol concentration at the bottom of the column follow the change in the setpoint from 0.0225 to 0.0246 at t=0.2 hours.

Fig. 5 shows the response of the second controlled variable (concentration of water at the top of the column) with respect to the change in the reference from 0.1809 to 0.1654 at t=1.8 hours.

The two manipulated variables are shown in Figs. 6 and 7.

However, analysis of the calculations indicates a clear advantage of the EPSAC controller. The calculation time for the whole of the simulated experiment was almost 12 hours in this case.

In the case of standard non-linear models, the calculation time was 53 hours. The simulation was run with EcosimPro in a PentiumIII PC with 800 MHz processing speed and 512 Mbytes RAM.

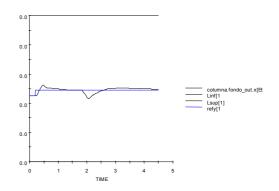


Fig. 4 Reference changes of the first controlled variable (ethanol concentration at bottom of column)

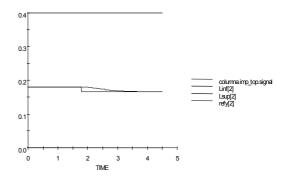


Fig. 5 Reference changes in 2^{nd} controlled variable (molar concentration of water at head of column).

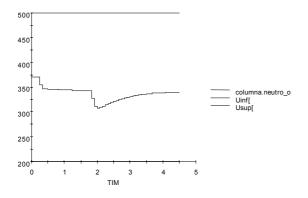


Fig. 6. The 1st manipulated variable (flow of neutral alcohol).

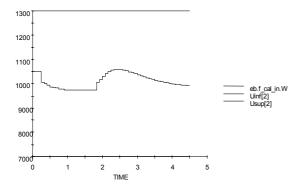


Fig. 7. The 2nd manipulated variable (steam introduced into the evaporator)

5. CONCLUSIONS

Two non-linear predictive control models have been compared taking a distillation column modelled in EcosimPro as a basis.

One of them (non-linear EPSAC, based on an iterative linearisation approach) has proved to be a promising technique to reduce the computation time by up to 25%.

However, in the process considered here the time required to solve the problem of predictive control in each sampling period is still too long to implement the controller in real time.

The model proposed does not require that the nonlinear model be linearised; itonly requires calculation of its impulse response, which may store a large number of calculations in cases such as the one presented above.

A further advantage of non-linear EPSAC is the use of more efficient codes such as QP instead of SQP methods. Greater effort is required to put NMPC into practice when it is based on complex models such as the one presented in this article.

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