Sequential and Iterative Architectures for Distributed Model Predictive Control of Nonlinear Process Systems. Part II: Application to a Catalytic Alkylation of Benzene Process

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Abstract — In the first part of this work [1], we present two different architectures for distributed model predictive control (DMPC) of nonlinear process systems: sequential distributed model predictive control and iterative distributed model predictive control. In the present work, we focus on the application of the theoretical results developed in [1] to a catalytic alkylation of benzene process example, which consists of four continuous stirred tank reactors and a flash separator. In order to carry out the simulations, a first principle model is developed via mass and energy balances. Based on the process model, three distributed Lyapunov-based model predictive controllers are designed to control the process in a coordinated fashion. Extensive simulations are carried out to compare the DMPC architectures proposed in [1] with an existing centralized Lyapunov-based model predictive control design from computational time and closed-loop performance points of view.

I. DESCRIPTION OF THE ALKYLATION OF BENZENE PROCESS

The process of alkylation of benzene with ethylene to produce ethylbenzene is widely used in the petrochemical industry. Dehydration of the product produces styrene, which is the precursor to polystyrene and many copolymers. Over the last two decades, several methods and simulation results of alkylation of benzene with catalysts have been reported in the literature. The process model developed in this section is based on these references [2], [3], [4], [5], [6]. More specifically, the process considered in this work consists of four continuously stirred tank reactors (CSTRs) and a flash tank separator, as shown in Fig. 1. The CSTR-1, CSTR-2 and CSTR-3 are in series and involve the alkylation of benzene with ethylene. Pure benzene is fed from stream $F_1$ and pure ethylene is fed from streams $F_2$, $F_4$ and $F_6$. Two catalytic reactions take place in CSTR-1, CSTR-2 and CSTR-3. Benzene ($A$) reacts with ethylene ($B$) and produces the required product ethylbenzene ($C$) (reaction 1); ethylbenzene can further react with ethylene to form 1,3-diethylbenzene ($D$) (reaction 2) which is the byproduct. The effluent of CSTR-3, including the products and leftover reactants, is fed to a flash tank separator, in which most of benzene is separated overhead by vaporization and condensation techniques and recycled back to the plant and the bottom product stream is removed. A portion of the recycle stream $F_{r,2}$ is fed back to CSTR-1 and another portion of the recycle stream $F_{r,1}$ is fed to CSTR-4 together with an additional feed stream $F_{10}$ which contains 1,3-diethylbenzene from further distillation process that we do not consider in this example. In CSTR-4, both reaction 2 and catalyzed transalkylation reaction in which 1,3-diethylbenzene reacts with benzene to produce ethylbenzene (reaction 3) take place. All chemicals left from CSTR-4 eventually pass into the separator. All the materials in the reactions are in liquid phase due to high pressure. The dynamic equations describing the behavior of the process, obtained through material and energy balances under standard modeling assumptions, are shown below:

\[
\begin{align*}
\frac{dC_A}{dt} &= F_1 C_{A_0} + F_2 C_{A_r} - F_3 C_A - r_1(T_1, C_{A_1}, C_{B_1}) \quad (1a) \\
\frac{dC_B}{dt} &= F_2 C_{B_0} + F_4 C_{B_r} - F_6 C_B - r_2(T_1, C_{B_1}, C_{C_1}) \quad (1b) \\
\frac{dC_C}{dt} &= F_2 C_{C_r} - F_3 C_C + r_1(T_1, C_{A_1}, C_{B_1}) \quad (1c) \\
\frac{dC_D}{dt} &= F_2 C_{D_r} - F_6 C_D + r_2(T_1, C_{B_1}, C_{C_1}) \quad (1d)
\end{align*}
\]
\[
\frac{dT_1}{dt} = Q_1 + F_1CA_0HA(T_{A0}) + F_2CB_0HB(T_{B0}) \\
+ \sum_{i}^{A,B,C,D} C_{i1}C_{pi}V_1 \\
+ \sum_{i}^{A,B,C,D} (F_2C_0H_1(T_2) - F_5C_1H_1(T_2)) \\
+ \left[ \frac{-\Delta H_1r_1(T_1, C_{A1}, C_{B1})}{A,B,C,D} \right] \\
+ \left[ \frac{-\Delta H_2r_2(T_1, C_{A1}, C_{B1})}{A,B,C,D} \right] \\
\]

\[
\frac{dc_{A2}}{dt} = \frac{F_3CA_1 - F_5CA_2}{V_2} - r_1(T_2, C_{A2}, C_{B2}) \\
\frac{dc_{B2}}{dt} = \frac{F_3CB_1 + F_5CB_2 - F_5CB_2 - r_1(T_2, C_{A2}, C_{B2})}{V_2} \\
\frac{dc_{C2}}{dt} = \frac{F_3C_{C1} - F_5C_{C2} + r_1(T_2, C_{A2}, C_{B2})}{V_2} \\
\frac{dc_{D2}}{dt} = \frac{F_3C_{D1} - F_5C_{D2} + r_2(T_2, C_{B2}, C_{C2})}{V_2} \\
\frac{dC}{dt} = \frac{Q_2 + F_1CB_0HB(T_{B0})}{A,B,C,D} \\
+ \sum_{i}^{A,B,C,D} C_{i2}C_{pi}V_2 \\
+ \sum_{i}^{A,B,C,D} \left( F_3C_1H_1(T_1) - F_5C_2H_1(T_2) \right) \\
+ \left[ \frac{-\Delta H_1r_1(T_2, C_{A2}, C_{B2})}{A,B,C,D} \right] \\
+ \left[ \frac{-\Delta H_2r_2(T_2, C_{A2}, C_{B2})}{A,B,C,D} \right] \\
\]

\[
\frac{dc_{A3}}{dt} = \frac{F_3CA_3 - F_7CA_3}{V_3} - r_3(T_3, C_{A3}, C_{B3}) \\
\frac{dc_{B3}}{dt} = \frac{F_3CB_3 + F_8CB_3 - F_7CB_3 - r_3(T_3, C_{A3}, C_{B3})}{V_3} \\
\frac{dc_{C3}}{dt} = \frac{F_3C_{C3} - F_7C_{C3} + r_3(T_3, C_{A3}, C_{B3})}{V_3} \\
\frac{dc_{D3}}{dt} = \frac{F_3C_{D3} - F_7C_{D3} + r_2(T_3, C_{B3}, C_{C3})}{V_3} \\
\frac{dT_3}{dt} = \frac{Q_3 + F_1CB_0HB(T_{B0})}{A,B,C,D} \\
+ \sum_{i}^{A,B,C,D} C_{i3}C_{pi}V_3 \\
+ \sum_{i}^{A,B,C,D} \left( F_3C_2H_3(T_2) - F_7C_3H_3(T_3) \right) \\
+ \left[ \frac{-\Delta H_1r_1(T_3, C_{A3}, C_{B3})}{A,B,C,D} \right] \\
+ \left[ \frac{-\Delta H_2r_2(T_3, C_{A3}, C_{B3})}{A,B,C,D} \right] \\
\]

In the process model of Eq. 1, \( r_1 \), \( r_2 \) and \( r_3 \) are the reaction rates of reactions 1, 2 and 3 respectively and \( H_i \), \( i = A, B, C, D \), are the enthalpies of the reactants. The reaction rates are related to the concentrations of the reactants and the temperature in each reactor as follows:

\[
r_1(T, C_A, C_B) = k_{r1}C_A^{0.32}C_B^{1.5}, \\
r_2(T, C_B, C_C) = k_{r2}C_B^{2.5}C_C^{0.5} \left( 1 + k_{EB2}C_D \right), \\
r_3(T, C_A, C_D) = k_{r3}C_A^{0.218}C_D^{1.0218} \]
with

\[
k_{r1} = 0.0840e^{-9502/RT}, \quad k_{r2} = 0.0850e^{-20640/RT},
\]

\[
k_{r3} = 237.8e^{-61280/RT}, \quad k_{EB2} = 0.0152e^{-3933/RT},
\]

\[
k_{EB3} = 0.4901e^{-50870/RT}.
\]

The heat capacities of the species are assumed to be constants and the molar enthalpies have a linear dependence on temperature as follows:

\[
H_i(T) = H_{ir} + C_{pi}(T - T_{ref})
\]

where \(C_{pi}, i = A, B, C, D\) are heat capacities.

The model of the flash tank separator is developed under the assumption that the relative volatility of each species has a linear correlation with the temperature of the vessel within the operating temperature range of the flash tank, as shown below:

\[
\begin{align*}
\alpha_A &= 0.0449T_4 + 10, \quad \alpha_B = 0.0260T_4 + 10 \\
\alpha_C &= 0.0065T_4 + 0.5, \quad \alpha_D = 0.0058T_4 + 0.25
\end{align*}
\]

where \(\alpha_i, i = A, B, C, D\), represent the relative volatilities. It has also been assumed that there is a negligible amount of reaction taking place in the separator. The following algebraic equations model the composition of the overhead stream relative to the composition of the liquid holdup in the flash tank:

\[
M_i = (F_7C_{i3} + F_3C_{i5}) \frac{\alpha_i(F_7C_{i3} + F_3C_{i5})}{\sum_k \alpha_k(F_7C_{i3} + F_3C_{i5})},
\]

where \(M_i, i = A, B, C, D\) are the molar flow rates of the overhead reactants. Based on \(M_i\), \(i = A, B, C, D\), we can calculate the concentration of the reactants in the recycle streams as follows:

\[
C_{ir} = \frac{M_i}{\sum_k M_i/C_{k0}}, \quad i = A, B, C, D
\]

where \(C_{k0}, k = A, B, C, D\), are the mole densities of pure reactants. The condensation of vapor takes place overhead, and a portion of the condensed liquid is purged back to separator to keep the flow rate of the recycle stream at a fixed value. The temperature of the condensed liquid is assumed to be the same as the temperature of the vessel.

The definitions for the variables used in the above model can be found in Table I, with the parameter values given in Table II.

Each of the tanks has an external heat/coolant input. The manipulated inputs to the process are the heat injected to or removed from the five vessels, \(Q_1, Q_2, Q_3, Q_4, Q_5\), and the feed stream flow rates to CSTR-2 and CSTR-3, \(F_4\) and \(F_6\), respectively.

The states of the process consist of the concentrations of \(A, B, C, D\) in each of the five vessels and the temperatures of the vessels. They are assumed to be available continuously to the controllers. We consider a stable steady state (operating point), \(x_s\), of the process which is defined by the steady-state inputs \(Q_1, Q_2, Q_3, Q_4, Q_5, F_4\) and \(F_6\), as shown in Table III. The steady-state values of the temperatures in the five vessels are as follows:

\[
T_{1s} = 477.24 K, \quad T_{2s} = 476.97 K, \quad T_{3s} = 473.47 K, \quad T_{4s} = 470.60 K, \quad T_{5s} = 478.28 K.
\]

### II. Design of Distributed Model Predictive Controllers

In this section, we will first construct a Lyapunov-based controller which can stabilize the closed-loop process asymptotically; and then we will construct a centralized Lyapunov-based model predictive control (LMPC) design and two...
TABLE III

| $Q_{1s}$ | $-4.4 \times 10^6$ [J/s] |
| $Q_{2s}$ | $-4.7 \times 10^6$ [J/s] |
| $Q_{3s}$ | $5.9 \times 10^6$ [J/s] |

ST E A DY-S TAT E I N P U T V AL U E S F O R $x_s$.

TABLE IV

| $|u_{11}| \leq 7.5 \times 10^5$ [J/s] | $|u_{21}| \leq 6 \times 10^5$ [J/s] | $|u_{31}| \leq 4.93 \times 10^{\frac{1}{5}}$ [m/s] |
| $|u_{12}| \leq 6 \times 10^5$ [J/s] | $|u_{22}| \leq 5 \times 10^5$ [J/s] | $|u_{32}| \leq 4.93 \times 10^{\frac{1}{5}}$ [m/s] |

distributed model predictive control (DMPC) designs based on the Lyapunov-based controller. Specifically, the centralized LMPC is based on the LMPC proposed in [8], [9] which guarantees practical stability of the closed-loop system, allows for an explicit characterization of the stability region. The two DMPC schemes are proposed in [1]. One of them adopts a one-directional communication network and its distributed controllers are designed via LMPC techniques, evaluated in sequence and once at each sampling time. This DMPC design will be termed as sequential DMPC below. The other DMPC scheme utilizes a bi-directional communication network and its distributed controllers are also designed via LMPC techniques; they are evaluated in parallel and iterate to improve closed-loop performance. This design will be termed as iterative DMPC below.

The control objective is to regulate the system from an initial state to the steady state. The first distributed controller (LMPC 1) is designed to compute the values of $Q_1$, $Q_2$, and $Q_3$, the second distributed controller (LMPC 2) is designed to compute the values of $Q_4$ and $Q_5$, and the third distributed controller (LMPC 3) is designed to compute the values of $F_4$ and $F_0$. Taking these into account, the process model of Eq. 1 belongs to the following class of nonlinear systems:

$$\dot{x}(t) = f(x) + g_1(x)u_1(x) + g_2(x)u_2(x) + g_3(x)u_3(x)$$

where the state $x$ is the deviation of the state of the process from the steady state, $u_1^T = [u_{11} u_{12} u_{13}] = [Q_1 - Q_{1s}, Q_2 - Q_{2s}, Q_3 - Q_{3s}]$, $u_2^T = [u_{21} u_{22}] = [Q_4 - Q_{4s}, Q_5 - Q_{5s}]$ and $u_3^T = [u_{31} u_{32}] = [F_4 - F_{4s}, F_6 - F_{6s}]$ are the manipulated inputs which are subject to the constraints shown in Table IV.

In the centralized LMPC scheme, the centralized LMPC optimizes the values of $u_1$, $u_2$, and $u_3$ in a single optimization problem as shown in Fig. 2. In the DMPC schemes, one LMPC is assigned to each manipulated input. In the sequential DMPC scheme, the distributed controllers communicate in one-directional manner as shown in Fig. 3. Specifically, LMPC 3 sends its future input to LMPC 2 and LMPC 2 sends its and LMPC 3’s future input to LMPC 1. In the iterative DMPC scheme, each distributed controller is able to communicate to all the other controllers as shown in Fig. 4. Specifically, LMPC 1, LMPC 2 and LMPC 3 can exchange future input information before each iteration, and they can iterate to improve the closed-loop performance.

In the control of the process, $u_1$ and $u_2$ are necessary to keep the stability of the closed-loop system, while $u_3$ can be used as an extra manipulated input to improve the closed-loop performance. We first construct the Lyapunov-based controller $h(x) = [h_1(x) h_2(x) h_3(x)]^T$. Specifically, $h_1(x)$ and $h_2(x)$ are designed as follows [7]:

$$h_1(x) = \begin{cases} \frac{-L_1V + \sqrt{(L_1V)^2 + (L_2V)^2}}{(L_2V)^2} & \text{if } L_2V \neq 0 \\ 0 & \text{if } L_2V = 0 \end{cases}$$

where $i = 1, 2, L_1V = \frac{\partial V}{\partial x} f(x)$ and $L_2V = \frac{\partial V}{\partial x} g_i(x)$ denote the Lie derivatives of the scalar function $V$ with respect to the vector fields $f$ and $g_i$ ($i = 1, 2$), respectively. The controller $h_3(x)$ is chosen to be $h_3(x) = [0 0]^T$ because the input set $u_3$ is not needed to stabilize the process. In the simulations, we consider a quadratic Lyapunov function $V(x) = x^T P x$ with $P$ being the following weighting matrix:

$$P = diag^+(P_v)$$

where $P_v = [1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 0 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 0 \ 1 \ 1 \ 1 \ 0 \ 1 \ 1]$. The weights in $P$ are chosen by a trail-and-error procedure. The basic idea behind this procedure is that more weight should be put on the temperatures of the five vessels because temperatures have more significant effects on the overall control performance, and the Lyapunov-based controller $h(x)$ should be able to stabilize the closed-loop system asymptotically with continuous feedback and actuation.

Based on $h(x)$, we design the centralized LMPC, the sequential distributed LMPC and the iterative distributed LMPC. The sampling time used is $\Delta = 30$ s and the weighting matrices

$$Q_0 = diag(Q_0_v)$$

where $Q_0_v = [1 \ 1 \ 1 \ 1 \ 10^3 \ 1 \ 1 \ 1 \ 10^3 \ 10 \ 10 \ 10 \ 10^4 \ 1 \ 1 \ 1 \ 10^3 \ 1 \ 1 \ 1 \ 10^3 \ 1 \ 1 \ 1 \ 10^3]$ and $R_{c1} = diag([10^{-8} \ 10^{-8} \ 10^{-8}])$, $R_{c2} = diag([10^{-8} \ 10^{-8}])$ and $R_{c3} = diag([1 \ 1])$.

$*diag(v)$ denotes a matrix with its diagonal elements being the elements of vector $v$ and all the other elements being zeros.
III. SIMULATION RESULTS

First, we carried out a set of simulations to demonstrate that the Lyapunov-based controller and the different control designs can all drive the state of the process to the required steady-state. Figure 5 shows the trajectories of the temperatures in the five vessels. From the figure, we can see that the centralized LMPC, the sequential and iterative LMPCs give similar temperature trajectories and enforce the convergence of the states to the desired steady-state much faster than the trajectories under the Lyapunov-based controller \( h(x) \). All the concentration trajectories in the five vessels display similar convergence trends of the temperature trajectories. We omit the figures of the concentration trajectories here due to space limitations.

In order to illustrate the asymptotical convergence of the state of the closed-loop process under different control schemes, we also show the trajectories of the Lyapunov function \( V(x) \) under the different control schemes in Fig 6. Note that because of the stability constraints in the formulations of the sequential, iterative DMPCs and the centralized LMPC (see [8], [9], [1] for the designs of these LMPCs), the trajectories of \( V(x) \) under the centralized LMPC, the sequential DMPC and the iterative DMPC are bounded by the corresponding trajectory of \( V(x) \) under the Lyapunov-based controller \( h(x) \).

Next, we compare the mean evaluation times of the centralized LMPC optimization problem with the mean evaluation times of the LMPC optimization problems in the sequential and iterative DMPCs. Each LMPC optimization problem was evaluated 100 times at different conditions. Different prediction horizons were considered in this set of simulations. The simulations were carried out using Java programming language in a Pentium 3.20 GHz computer. The optimization problems were solved by the open source interior point optimizer Ipopt [10]. The results are shown in Table V. We can see that for different prediction horizons, the time needed to solve the optimization problems of the centralized LMPC is much larger than the time needed to solve the optimization problems in the sequential or iterative DMPC. This is because the centralized LMPC has to solve a much larger (in terms of decision variables) optimization problem than the ones of the distributed LMPCs. Another observation from the table is that the evaluation time of the centralized LMPC is larger than the sum of evaluation times of LMPC 1, LMPC 2 and LMPC 3 of the sequential DMPC, and the times needed to solve the distributed LMPCs in both sequential and iterative distributed schemes are of the same order of magnitude.

In another set of simulations, we compare the centralized LMPC and the two DMPC schemes from a performance index point of view. The prediction horizon for this set of simulations is \( N = 1 \). To carry out the comparison, the same initial condition and parameters are used for the different control schemes and the total cost index under each control scheme is computed as follows:

\[
J = \sum_{i=0}^{M} \left( x(t_i)^T Q_c x(t_i) + u_1(t_i)^T R_{c1} u_1(t_i) \right) + \sum_{i=0}^{M} \left( u_2(t_i)^T R_{c2} u_2(t_i) + u_3(t_i)^T R_{c3} u_3(t_i) \right)
\]
where \( t_0 = 0 \) is the initial time of the simulations, \( t_i = t_0 + i \Delta \) are the time instants taken into account and \( t_M = 1000 \text{ s} \) is the end of the simulations. Table VI shows the total cost along the closed-loop system trajectories under the different control schemes. In this set of simulations, the centralized LMPC gives the lowest performance cost, the sequential DMPC gives lower cost than the iterative DMPC when there is no iteration (\( c = 1 \)). However, as the iteration number \( c \) increases, the performance cost given by the iterative DMPC decreases and converges to the cost of the one corresponding to the centralized LMPC. This point is also shown in Fig. 7.

Note that the above set of simulations only represents one possible case. As we discussed in Remarks 11-12 in [1], there is no guaranteed convergence of the performance of distributed MPC to the performance of a centralized MPC, and there is also no guaranteed superiority of the performance of one DMPC scheme over the others. Specifically, we show another two sets of simulations to illustrate these points. In both sets of simulations, we chose different matrices \( R_{c1} \) and \( R_{c2} \), and all the other parameters (\( Q_c \), \( R_c \), \( \Delta \), \( N \)) remained the same as the previous set of simulations. In the first set of simulations, we picked \( R_{c1} = \text{diag}(5 \times 10^{-5} 5 \times 10^{-5} 5 \times 10^{-5}) \), \( R_{c2} = \text{diag}(5 \times 10^{-5} 5 \times 10^{-5}) \) and the results are shown in Table VII. It shows that the centralized LMPC provides a much lower cost than the ones of both the sequential and iterative DMPCs. We can also see that as the number of iterations increases, the iterative distributed LMPC converges to a value which is different from the one obtained by the centralized LMPC. In the second set of simulations, we picked \( R_{c1} = \text{diag}(1 \times 10^{-4} 1 \times 10^{-4} 1 \times 10^{-4}) \), \( R_{c2} = \text{diag}(1 \times 10^{-4} 1 \times 10^{-4}) \) and the results are shown in Table VIII, from which we can see that the centralized LMPC provides a higher cost than the ones of both DMPCs.

**Fig. 7.** Total performance cost along the closed-loop system trajectories of centralized LMPC (dashed line), sequential distributed LMPC (dash-dotted line) and iterative distributed LMPC (solid line).

### IV. Conclusions

In this work, we focused on the application of the theoretical results of DMPC architectures developed in [1] to a catalytic alkylation of benzene process example which consists of four continuous stirred tank reactors (CSTRs) and a flash separator. First principle model developed via mass and energy balances was used to carry out simulations. Three separate Lyapunov-based model predictive controllers were designed to control the process in a coordinative fashion. Extensive simulations were carried out to compare the proposed DMPC architectures with existing centralized LMPC techniques from computational time and closed-loop performance points of view.

**REFERENCES**


