Model Predictive Control of Interconnected Linear and Nonlinear Processes

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A plant-wide control strategy based on integration of linear model predictive control (LMPC) and nonlinear model predictive control (NMPC) is proposed. The design method is applicable to plants that can be decomposed according to the nonlinearity properties of the individual unit operations. The basic idea is to apply LMPC and NMPC controllers to the linear and nonlinear subsystems, respectively. A systematic procedure for performing the plant decomposition given nonlinearity information is presented. Because the subsystems are coupled via material and energy flows, a sequential solution procedure that aims to minimize the amount of unknown information in the MPC designs is developed. The plant decomposition and sequential MPC solution algorithms are applied to a large-scale styrene production flowsheet. Three controller coordination strategies are developed to handle the information-exchange problems caused by sequential MPC solution. The methods are shown to be nominally stabilizing for nonlinear plants with a certain triangular structure. A multi-rate extension for plants with time-scale separations is presented. A reaction/separation process with recycle is used to compare the different hybrid MPC approaches.

1. Introduction

The synthesis of plant-wide control structures is one of the most important problems in process control theory and practice.[1] The plant-wide control problem involves selection of controlled variables, manipulated variables, and measured variables; formulation of the control structure connecting the variables; and specification of the controller type.[2,3] The problem originally was studied by Buckley.[4] Considerable research has focused on decomposition of the plant into simpler subsystems based on functional and/or time-scale differences of the unit operations. In a series of papers by Stephanopoulos and co-workers,[2,5−7] the control structure formulation problem was posed as an optimization problem. The resulting structure was decomposed vertically on the basis of disturbance dynamics and horizontally on the basis of functional groups to yield a modular feedback optimizing control system. The same authors addressed the synthesis of regulatory loops, selection of secondary measurements, estimation of states, and synthesis of control structures for two representative chemical processes.

Price and Georgakis[8] proposed a tiered framework for solution of the plant-wide control problem. Control loops were grouped into multiple tiers on the basis of the relative importance of the associated control objectives. Zheng and co-workers[9] proposed a hierarchical procedure for formulating control structures on the basis of the minimization of economic penalties. Ng and Stephanopoulos[10] developed a hierarchical procedure that successively increases the resolution of the plant-wide control structure. Beginning with the optimizing feedback approach, Skogestad[3] developed a procedure for identifying controlled variables that allows near-optimal regulatory performance. Luyben et al.[11] proposed a heuristic design procedure for generating a decentralized control structure. These plant-wide control techniques are based on the use of decentralized control structures. An exception is the modular multivariable control structure[12] used in ref 10.

In principle, model predictive control (MPC) can be applied to very large plant-wide control problems. The multivariable and constraint-handling capabilities of MPC are very appealing compared to decentralized control. Linear model predictive control (LMPC) has been applied successfully to industrial processes with hundreds of input and output variables.[13] Process nonlinearities remain one of the most difficult problems associated with plant-wide MPC applications.[10] When strong nonlinearities preclude the successful application of LMPC, nonlinear model predictive control (NMPC) is required. Because NPMC utilizes a nonlinear dynamic model for prediction, a nonlinear programming problem must be solved at each sampling period to calculate the optimal input moves. Despite this difficulty, a NMPC controller has been developed for the Tennessee Eastman Challenge Process by the judicious use of modeling and controller simplifications.[14]

Motivated by the observation that highly nonlinear dynamical behavior is typically associated with a small number of unit operations, we have developed a hybrid model predictive control strategy for plant-wide control applications.[15] The advantage of the proposed approach is that NMPC is utilized only where necessary and LMPC is applied to the remaining unit operations. The plant is decomposed into a linear subsystem (the distillation column) and a nonlinear subsystem (the reactor) on the basis of the degree of nonlinearity. LMPC is applied to the column, and NMPC is applied to the

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reactor. Two controller coordination strategies are proposed to compensate for interconnections between the two subsystems. Simulation results for a reaction/separation process with recycle show that the hybrid MPC controller performance is comparable to that of a full NMPC controller and superior to that of a conventional LMPC controller. On the other hand, the computational time of the hybrid controller is less than 8% of the NMPC controller execution time.

Although our initial results are very promising, there remain several unresolved problems associated with the application of the hybrid LMPC−NMPC strategy to complex plants. A systematic procedure is needed to select the "optimal" plant decomposition from the large number of possible alternatives. The subsystem MPC controllers must be solved sequentially to achieve significant reductions in computational cost. This requires some type of approximation because the solution of a particular MPC subsystem problem requires information that is available only after the other MPC subsystem problems are solved. A systematic procedure is needed to determine the solution sequence of the MPC subsystem problems such that the amount of unavailable information is minimized. With the exception of certain triangular plant structures discussed below, couplings between the subsystems preclude exact solution of the MPC problems. Controller coordination strategies are needed to achieve acceptable closed-loop performance in the presence of such couplings. The class of nonlinear plants that can be stabilized with the hybrid MPC controller needs to be characterized. Finally, differences between subsystem time-scale properties can be exploited to further reduce on-line computational effort. All of these problems are investigated in this paper.

The remainder of the paper is organized as follows. In section 2, the plant decomposition algorithm is presented and applied to a styrene plant flowsheet. The hybrid MPC control strategy is developed in section 3. Simple plants, each comprising a single linear subsystem and a single nonlinear subsystem, are used to illustrate the development of controller coordination strategies. The remainder of the section is focused on more complex plants with multiple linear and/or nonlinear subsystems. A specific class of triangular nonlinear systems is shown to be asymptotically stabilized by the hybrid MPC controller. The MPC sequence selection algorithm is presented and applied to the decomposed styrene plant flowsheet. A multi-time-scale extension also is proposed. In section 4, the hybrid MPC control methods are applied to the reaction/separation process considered in ref 15. A summary and conclusion are given in section 5.

2. Plant Decomposition

The objective is to partition the plant into linear and nonlinear subsystems according to the nonlinearity properties of the individual unit operations. This approach requires a methodology for measuring the degree of process nonlinearity. Although rigorous nonlinearity measures have been proposed,[16,17] the requirement of a complete nonlinear plant model makes these techniques very difficult to apply to complex flowsheets. Data-driven methods such as coherence analysis[18,19] appear to represent a more promising framework for nonlinearity quantification. The development of such nonlinearity measures is beyond the scope of this paper. We believe that the relative nonlinearity of typical unit operations often can be determined a priori using process knowledge. This admittedly heuristic approach is pursued in this paper. The decomposition algorithm presented in section 2.1 is designed to produce the smallest number of subsystems. The algorithm is applied to a styrene plant flowsheet in section 2.2.

2.1. Plant Decomposition Algorithm. The required input data for the plant decomposition algorithm is a vector containing the nonlinearity properties of all unit operations and a matrix describing the unit connections, that is, unit operation nonlinearity vector n such that $n_i = 1$ if u_i is nonlinear and $n_i = 0$ if u_i is linear and unit operation connection matrix C such that $C_{i,j} = 1$ if u_i affects u_j and $C_{i,j} = 0$ otherwise, where u_i denotes the ith unit operation. If the total number of unit operations is denoted N, then n is an $N \times 1$ vector, and C is an $N \times N$ matrix. Solution of the decomposition problem yields (i) a decomposition matrix X that represent the resulting subsystems and their member unit operations, (ii) a subsystem nonlinearity vector Y that characterizes the nonlinearity property of each subsystem, and (iii) a subsystem connection matrix Γ that details the connections between the derived subsystems. These quantities are defined formally as follows:

decomposition matrix X

$$X_{i,j} = 1 \text{ if } u_i \text{ is contained in } g_j;\ X_{i,j} = 0 \text{ otherwise}$$

subsystem nonlinearity vector Y

$$Y_i = 1 \text{ if } g_i \text{ is nonlinear};\ Y_i = 0 \text{ otherwise}$$

subsystem connection matrix Γ

$$\Gamma_{i,j} = 1 \text{ if } g_i \text{ affects } g_j;\ \Gamma_{i,j} = 0 \text{ otherwise}$$

where g_j denotes the jth subsystem. The plant decomposition must satisfy the following constraints: (1) Every unit operation belongs to one and only one subsystem. (2) All unit operations in a given subsystem must have the same nonlinearity property. (3) Every unit in a given subsystem must be connected to at least one other unit in the same subsystem.

The decomposition problem can be formulated as an optimization problem in which the total number of subsystems is minimized. As shown in Appendix A, the optimization problem can be formulated as a binary polynomial programming problem. This problem can be transformed into a binary linear programming (LP) problem[20] with Z decision variables and $3N$ constraints, where

$$Z = \sum_{M=0}^{N} \frac{N}{M(N-M)!} \tag{1}$$

For the styrene plant flowsheet considered in the next section, $N = 16$, and the optimization problem involves 1 048 576 decision variables and 48 constraints. Below, we present an iterative algorithm that is more suitable for the plant-wide control problems typically encountered.

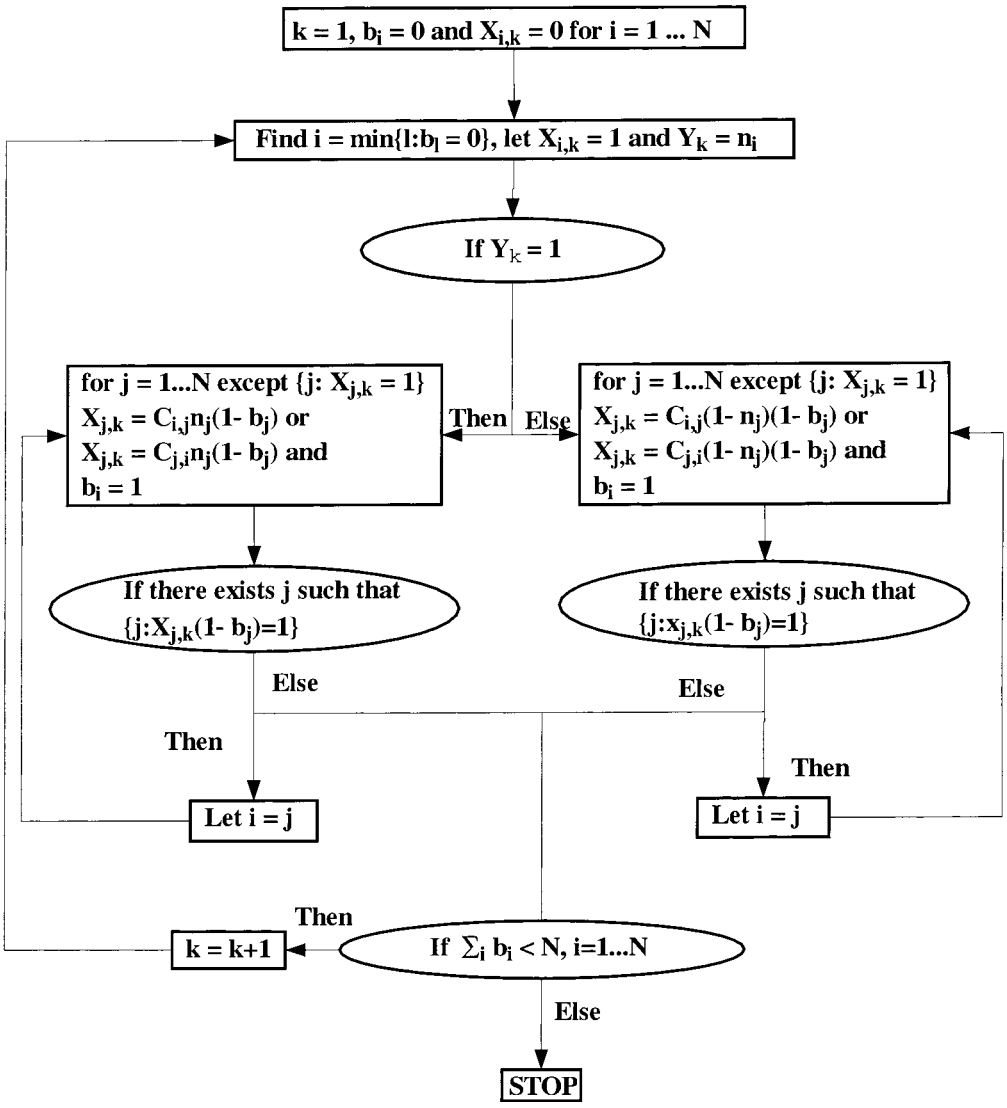

Figure 1. Schematic representation of the iterative plant decomposition algorithm.

A schematic representation of the decomposition algorithm is shown in Figure 1. Here, k is the subsystem index, and b is an $N \times 1$ vector whose ith element is set to unity when unit i and all connected units with the same nonlinearity property as unit i are assigned to the same subsystem. The decomposition algorithm is designed to construct the decomposition matrix X such that the total number of subsystems M is minimized. The algorithm involves three loops. The inner loop assigns to the subsystem k all units j that have the same nonlinearity property as and are connected directly to a given unit i already in subsystem k. The middle loop simply repeats the first loop until no additional units can be added to the current subsystem. The outer loop creates additional subsystems if any units remain unassigned. The subsystem connection matrix Γ is computed as follows:

$$\Gamma_{i,j} = \begin{cases} 1 & \text{if } X_i^{\mathrm{T}} C X_j \geq 1 \\ 0 & \text{otherwise} \end{cases} \qquad (2)$$

where X_i denotes the ith column of X corresponding to the ith subsystem. The scalar $X_i^{\mathrm{T}} C X_j$ is a positive integer if any units in subsystem i affect any units in subsystem j.

2.2. Application to a Styrene Plant Flowsheet. The styrene plant flowsheet shown in Figure 2 was chosen to illustrate the decomposition algorithm because it contains a large number of unit operations and several recycle streams. Ethylene and benzene are fed to the first reactor, where ethylbenzene (EB) is formed. The effluent from the first reactor is fed to a benzene recovery section from which both benzene and polyethylbenzene (PEB) are recycled. High-purity EB is produced from one of the four columns and fed to a second reactor, where styrene is formed. The products from the second reactor are fed to a series of columns to produce high-purity styrene and EB for recycle back to the styrene reactor. Operational experience[21,22] suggests that the EB reactor, the high-purity EB column (overhead EB purity of 99.6%), and the EB/styrene splitter (overhead styrene purity of 99.9%) are sufficiently nonlinear to warrant NMPC. The remainder of the 16 unit operations are considered to be approximately linear. Therefore, the nonzero elements of the unit operation nonlinearity vector n are n_4, n_6, and n_{13}. The nonzero elements of the connection matrix C are $C_{1,2}$, $C_{2,1}$, $C_{2,3}$, $C_{2,5}$, $C_{3,4}$, $C_{4,2}$, $C_{5,2}$, $C_{5,6}$, $C_{6,7}$, $C_{6,9}$, $C_{7,3}$, $C_{8,9}$, $C_{9,10}$, $C_{10,11}$, $C_{11,12}$, $C_{11,13}$, $C_{12,11}$, $C_{13,14}$, $C_{13,15}$, $C_{14,9}$, and $C_{14,16}$.

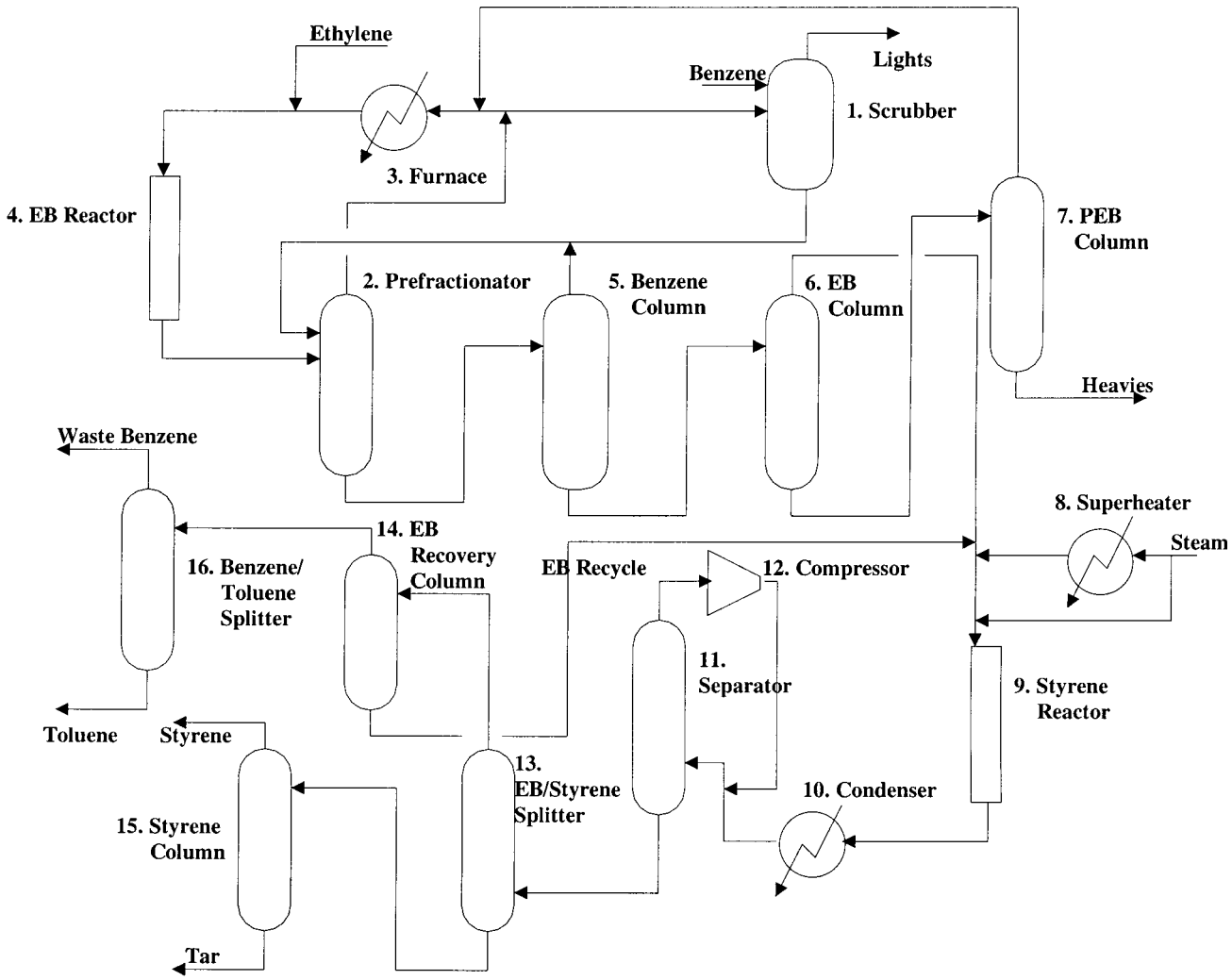

Figure 2. Styrene plant flowsheet.

From this information, the decomposition algorithm generates the following connection matrix X, subsystem nonlinearity property vector Y, and subsystem connection matrix Γ:

$$X^{T} = \begin{bmatrix} 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

$$Y = [0 \;\; 1 \;\; 1 \;\; 0 \;\; 1 \;\; 0]$$

$$\Gamma = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The decomposed styrene plant flowsheet is shown in Figure 3. Subsystem 1 consists of a large group of linear unit operations including all EB production units except for the EB reactor and EB column, which comprise nonlinear subsystems 2 and 3, respectively. Most of the styrene production units are contained in linear subsystem 4. The EB/styrene column is contained in nonlinear subsystem 5. Because the styrene column is connected only to the EB/styrene column, it forms a single-unit linear subsystem 6. The subsystem connections characterized by the matrix Γ are also shown in Figure 3. It is important to emphasize that engineering judgment can be applied to the plant decomposition to obtain the final solution. For the styrene flowsheet, it might be desirable to reduce the number of subsystems by combining subsystems 5 and 6 to produce a single nonlinear subsystem.

3. Model Predictive Control Strategy

The plant decomposition allows linear model predictive control (LMPC) to be applied to the linear subsystems and nonlinear model predictive control (NMPC) to be applied to the nonlinear subsystems. Little reduction in on-line computation time as compared to plant-wide NMPC will be realized if a single optimization problem is formulated for the entire plant using linear and nonlinear subsystem models. A reasonable alternative is to solve the individual MPC subsystem problems in a sequential fashion. Sequential solution is not straightforward when subsystems are coupled by mass and energy flows. In this case, the solution of a particular MPC subsystem problem might require the

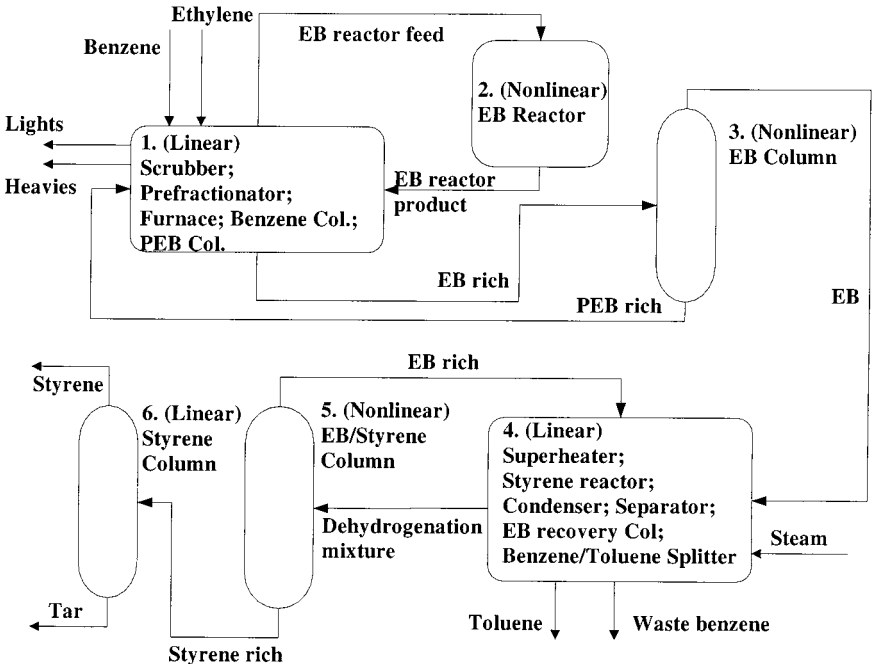

Figure 3. Decomposed styrene plant flowsheet.

solution of other subsystem problems. The optimal MPC solution sequence can be viewed as the sequence that minimizes the amount of unknown information from unsolved MPC subsystem problems. For most plants of practical interest, an ideal solution sequence for which the subsystem MPC problems can be solved without the application of certain approximations does not exist. In section 3.1, controller coordination methods that compensate for unknown subsystem information are presented for plants consisting of a single linear subsystem and a single nonlinear subsystem. In section 3.2, plants comprising multiple linear and/or nonlinear subsystems are investigated. We show that nonlinear systems with a certain triangular structure that makes solution of the MPC solution sequence problem trivial can be asymptotically stabilized by hybrid MPC control. For more general plants, an algorithm for determining the optimal MPC solution sequence is presented and applied to the decomposed styrene plant flowsheet. In section 3.3, an extension of the hybrid MPC strategy that exploits differences between subsystem time-scale properties to further reduce the on-line computational effort is presented.

Before proceeding to the detailed development, it is important to emphasize that the plant decomposition and MPC solution sequence problems are not independent. A poorly conceived decomposition can lead to considerable difficulties in determining an acceptable solution sequence. Our approach is based on decoupling these two problems to achieve a reasonably simple but suboptimal solution. We believe that combining this approach with sound engineering judgment will lead to the development of effective plant-wide control structures.

3.1 Two Subsystem Problems. *Plant Configurations.* The simplest possible plant decomposition consists of a single linear subsystem and a single nonlinear subsystem. The state-space model equations for

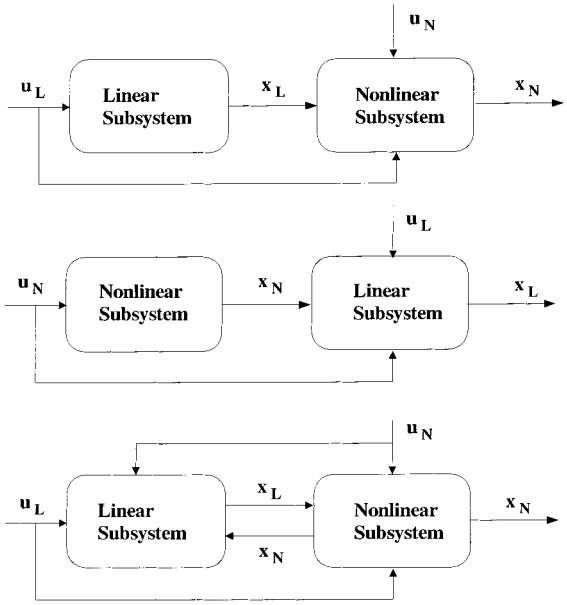

Figure 4. Two subsystem plant configurations.

the two subsystems can be written as

$$x_L(k+1) = A_L x_L(k) + A_N x_N(k) + B_L u_L(k) + B_N u_N(k) \quad (3)$$

$$y_L(k) = C_L x_L(k) + C_N x_N(k) \quad (4)$$

$$x_N(k+1) = f[x_L(k), x_N(k), u_L(k), u_N(k)] \quad (5)$$

$$y_N(k) = h[x_L(k), x_N(k)] \quad (6)$$

where the subscripts L and N denote the linear and nonlinear subsystems, respectively; x_L and x_N are state vectors; u_L and u_N are input vectors; y_L and y_N are output vectors; A_L, A_N, B_L, B_N, C_L, and C_N are constant matrices; and f and h are nonlinear functions. Figure 4 shows the three possible plant configurations: (1) The linear subsystem is unaffected by the nonlinear sub-

system, so that $A_N = B_N = C_N = 0$. (2) The nonlinear subsystem is unaffected by the linear subsystem, so that

$$\frac{\partial f}{\partial x_L} = \frac{\partial f}{\partial u_L} = \frac{\partial h}{\partial x_L} = 0$$

(3) The linear and nonlinear subsystem are fully coupled.

Clearly, different MPC solution sequences are appropriate for the three plant configurations. In the first two configurations, the MPC controller for the subsystem that unidirectionally affects the other subsystem is solved first, and then the MPC controller for the other subsystem is solved. The necessary information from the first subsystem can be generated even if the control horizon of the first MPC controller is shorter than that of the second MPC controller because the first subsystem can be iterated in an open-loop fashion with constant input to yield the future state variables needed. Brief descriptions of the LMPC and NMPC formulations used in this paper are presented in Appendices B and C, respectively. The third configuration in Figure 4 is more challenging, as the two subsystems are fully coupled. In this case, some type of approximation is required to develop an implementable sequential solution strategy.

Global Controller Coordination Method. In our previous work,[15] we developed a solution approximation strategy in which a LMPC controller is designed for the entire plant by linear approximation of the nonlinear subsystem. The LMPC problem is solved first, and then the NMPC problem for the nonlinear subsystem is solved using the LMPC solution for the linear subsystem only. We call this the global controller coordination method. It can be viewed as a transformation of the third configuration to the first configuration in Figure 4 because the entire plant is, by definition, unidirectionally connected to the nonlinear subsystem. Using the reaction/separation process introduced in section 4, we showed that the closed-loop performance obtained with this coordination method is comparable to that of a full NMPC controller and superior to that of a conventional LMPC controller.[15] As compared to the alternative strategies discussed below, shortcomings of this method include an increase in the LMPC problem size and approximation of the nonlinear subsystem by a linear model in the LMPC problem.

Local Steady-State Controller Coordination Method. Another controller coordination method briefly discussed in ref 15 utilizes the MPC problem solutions at the previous time step to solve the MPC problems at the current time step. This method eliminates the problem of unknown subsystem information and allows the LMPC and NMPC problems to be formulated separately for each subsystem. We pursue here a simplified version of this method in which the current state and input variables from the first subsystem are assumed to remain constant in the future for solution of the second MPC problem. This is called the local steady-state controller coordination method. Consider the case where the LMPC subsystem problem is solved first. The nonlinear subsystem variables are treated as constant disturbances in the LMPC steady-state target calculation

$$\min_{x_L^s(k),u_L^s(k)} = [u_L^{ref}(k) - u_L^s(k)]^T R_s [u_L^{ref}(k) - u_L^s(k)] \quad (7)$$

subject to

$$x_L^s(k) = A_L x_L^s(k) + B_L u_L^s(k) + A_N x_N(k|k) + B_N u_N(k|k-1)$$

$$y_L^{ref}(k) = C_L x_L^s(k) + C_N x_N(k|k) + \hat{d}_L(k)$$

$$u_{L,min} \le u_L^s(k) \le u_{L,max}$$

$$y_{L,min} \le C_L x_L^s(k) + C_N x_N(k|k) + \hat{d}_L(k) \le y_{L,max}$$

where $x_L^s(k)$ and $u_L^s(k)$ are the steady-state and input targets, respectively, for the linear subsystem and $\hat{d}_L(k)$ is an estimated step output disturbance. The targets are calculated by minimizing the difference between the desired input, u_L^{ref}, and the input target subject to steady-state equality and inequality constraints involving the desired output, y_L^{ref}. If the NMPC subsystem problem is solved first, the NMPC steady-state targets can be calculated analogously using $x_L(k|k)$ and $u_L(k|k-1)$ from the previous LMPC solution.

Local Dynamic Controller Coordination Method. A more sophisticated controller coordination strategy proposed in ref 15 involves the use of predicted variable trajectories from previously solved MPC problems for solution of the current MPC problem. The technique differs from the local steady-state coordination method in that variables from the first subsystem are allowed to vary over the control horizon of the second MPC controller. This method is called the local dynamic controller coordination method because dynamic information from each subsystem is used in the MPC calculations.

Consider the case where the LMPC subsystem problem is solved first. At time k, estimates of the future nonlinear state and input variables are available from the NMPC solution at time $k-1$

$$X_N(k-1) =$$

$$[x_N^T(k|k-1) \ \cdots \ x_N^T(k+P_N-1|k-1) \ \cdots \ x_N^T(k+N_L-1|k-1)]^T$$

$$U_N(k-1) =$$

$$[u_N^T(k|k-1) \ \cdots \ u_N^T(k+N_N-2|k-1) \ \cdots \ x_N^T(k+N_L-1|k-1)]^T$$

where it has been assumed that the LMPC control horizon (N_L) is larger than the NMPC control horizon (N_N) and the NMPC prediction horizon (P_N). In this case, the last $N_L - P_N$ elements of $X_N(k-1)$ can be obtained by open-loop simulation of the nonlinear subsystem with constant input $u_N(k+j|k-1) = u_N(k+N_N-2|k-1) \ \forall \ j \ge N_N - 1$. A simpler approach is to assume that $x_N(k+j|k-1) = x_N(k+P_N-1|k-1) \ \forall \ j \ge P_N$. The quadratic program (QP) formulation of the LMPC problem must be modified from that given in ref 23 to incorporate $X_N(k-1)$ and $U_N(k-1)$. The modified QP matrices are presented in Appendix D. The steady-state target calculation in

eq 10 is modified by replacing $x_N(k)$ and $u_N(k|k-1)$ with $x_N(k+N_L-1|\ k-1)$ and $u_N(k+N_L-1|k-1)$, respectively. The following information is available to the NMPC controller after the LMPC problem is solved at time k:

$$X_L(k) = [x_L^T(k|k)\ x_L^T(k+1|k)\ \cdots\ x_L^T(k+N_L|k)]^T$$

$$U_L(k) = [u_L^T(k|k)\ u_L^T(k+1|k)\ \cdots\ u_L^T(k+N_L-1|k)]^T$$

These predicted values can be incorporated directly into the equality constraints representing the discretized nonlinear model equations in the NMPC problem. Extension of these controller coordination methods to plant decompositions with multiple linear and/or nonlinear subsystems is tedious but conceptually straightforward.

3.2 Multiple Subsystem Problems. *Triangular Plant Decompositions.* As discussed below, the determination of an appropriate MPC solution sequence for plant decompositions with multiple linear and/or nonlinear subsystems can be difficult. The solution sequence problem is solved trivially for the following class of plant decompositions

$$x_1(k+1) = f_1[x_1(k), u_1(k)]$$

$$x_2(k+1) = f_1[x_1(k), x_2(k), u_1(k), u_2(k)]$$

$$\vdots$$

$$x_{M-1}(k+1) = f_{M-1}[x_1(k), ..., x_{M-1}(k), u_1(k), ..., u_{M-1}(k)]$$

$$x_M(k+1) = f_{M-1}[x_1(k), ..., x_M(k), u_1(k), ..., u_M(k)] \quad (8)$$

where M is the total number of linear and nonlinear subsystems; $x_i(k)$ and $u_i(k)$ are the state and input vectors of the ith subsystem, respectively; and $f_i(\cdot)$ are (possibly) nonlinear functions. This is called a triangular decomposition because the ith subsystem depends only on variables from the first i subsystems. Because of the triangular structure, the optimal MPC solution sequence is $\{g_1, g_2, ..., g_{n-1}, g_n\}$ where g_i represents the ith subsystem. In this case, each MPC problem can be solved exactly without any approximations about the other subsystems.

Such triangular decompositions represent the class of nonlinear systems for which we are able to verify that hybrid LMPC−NMPC control is stabilizing. The proof of the following result, which is based on the theorems in ref 24, is omitted for the sake of brevity. Assume that each MPC problem is feasible and that the resulting nonlinear feedback control laws are represented by

$$u_i(k+j|k) = h_j^i[x_1(k), ..., x_i(k)] \qquad j \in [0, N_i - 1],\ i \in [1, M] \quad (9)$$

where N_i is the control horizon of the ith MPC controller and $h_j^i(\cdot)$ are nonlinear functions. If the assumptions (1) $f_i(x_1, ..., x_i, u_1, ..., u_i)$ is Lipschitz in its arguments $\forall i \in [1, M]$ and (2) $h_j^i(x_1, ..., x_i)$ is Lipschitz in its arguments $\forall j \in [0, N_i - 1]$, $\forall i \in [1, M]$ hold, then $x(k) = [x_1^T(k) \cdots x_M^T(k)]^T = 0$ is a locally asymptotically stable fixed point of the closed-loop system

$$x_i(k+1) = f_i[x_1(k), ..., x_i(k), h_0^1[x_1(k)], ..., h_0^i[x_1(k), ..., x_i(k)]], \qquad i \in [1, M]$$

Note that the functions $f_i(\cdot)$ and $h_i^j(\cdot)$ are guaranteed to be Lipschitz if the ith subsystem is linear.[25]

Although hybrid LMPC−NMPC control is stabilizing for this class of nonlinear systems, sequential solution of subsystem MPC problems typically will result in a loss of performance compared to that obtained via plant-wide NMPC control. The motivation for decomposing the plant into subsystems is that an intractable plant-wide NMPC problem can be transformed into a set of smaller LMPC and NMPC problems. It is expected that performance will degrade as the number of subsystems increases. Consequently, plant decomposition should be pursued only to the extent necessary to produce a computationally tractable set of MPC problems.

MPC Solution Sequence Algorithm. The determination of an appropriate MPC solution sequence is more difficult for complex decompositions with highly interconnected subsystems. The styrene plant flowsheet shown in Figure 3 is an example of such a nontrivial decomposition. Clearly, the amount of unknown information from other subsystems required by each MPC controller depends on the solution sequence. The optimization problem presented in Appendix E yields a MPC solution sequence with the least amount of information required from unsolved subsystems. Although it might be possible to solve the optimization problem using methods developed for the traveling salesman problem,[26] the inherent computational complexity motivated us to investigate alternative approaches. For the decomposed styrene plant problem, it is feasible to enumerate and evaluate all 6! possible solution sequences. This approach might not be tractable for more complex plant decompositions.

Below, we present an iterative algorithm for determining the optimal MPC solution sequence using the subsystem connection matrix Γ and the subsystem nonlinearity property vector Y derived from the plant decomposition. The algorithm produces a solution sequence represented by the $M \times M$ matrix Ψ with elements $\Psi_{i,j} = 1$ if the jth subsystem is the ith subsystem solved. The algorithm shown schematically in Figure 5 consists of two loops. The outer loop simply increments the solution sequence index, whereas the inner loop determines the next subsystem to be solved. Three vectors are introduced and evaluated during every iteration of the outer loop on the basis of the updated Ψ matrix. The vector A represents the total number of subsystems that affect a given subsystem, the vector B represents the total number of subsystems that are affected by a given subsystem, and the vector C represents the subsystems chosen in previous iterations. The criteria for determining which subsystem to select are ranked below according to priority: (1) The subsystem is affected by the least number of other subsystems not yet selected. (2) The subsystem affects the greatest number of other subsystems not yet selected. (3) The subsystem is linear. (4) The subsystem has the lowest number in the flowsheet.

The results obtained by applying the MPC sequence selection algorithm to the decomposed styrene flowsheet (Figure 3) are shown in Figure 6. Both the EB column

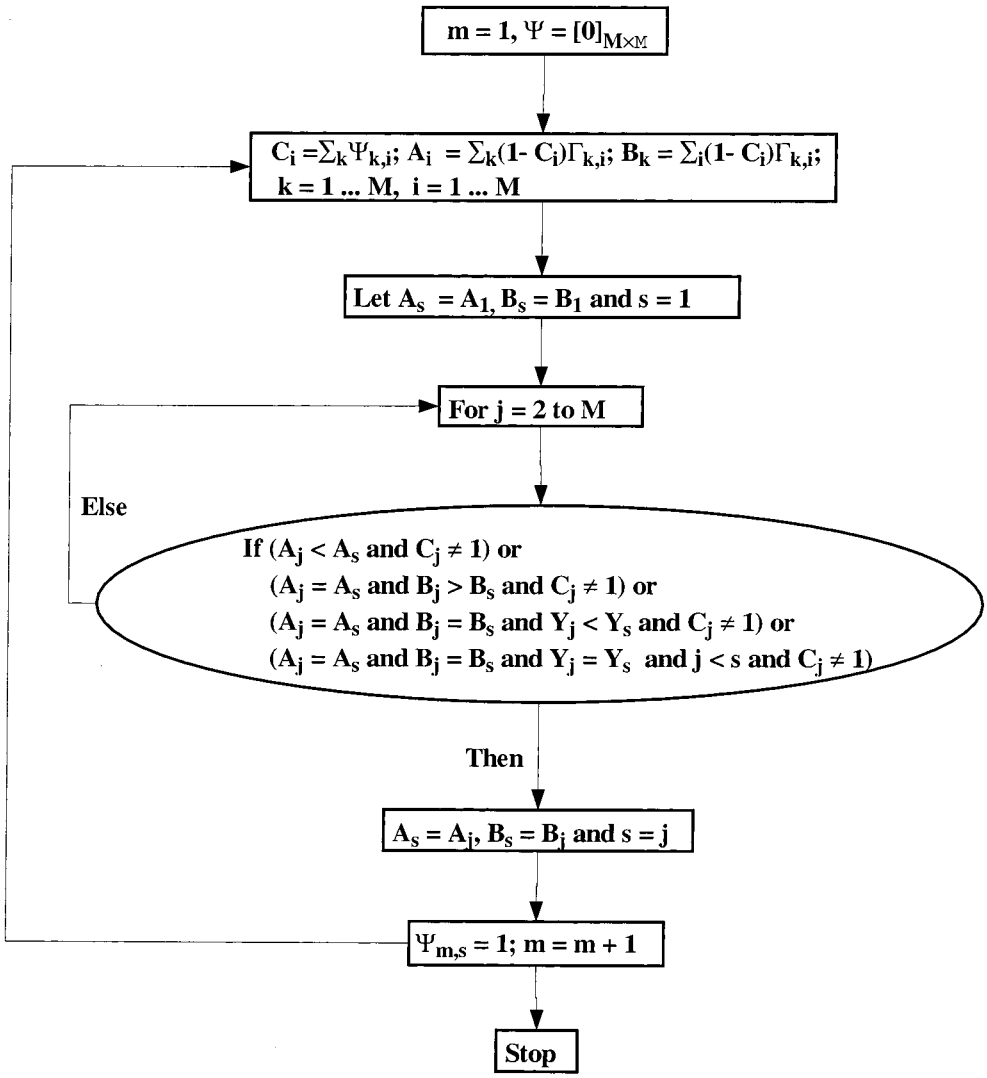

Figure 5. Iterative MPC selection sequence algorithm.

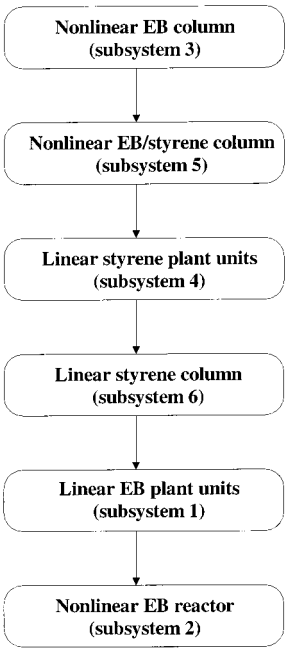

Figure 6. MPC solution sequence for the decomposed styrene plant.

and EB/styrene column are affected by one other subsystem, affect two other subsystems, and are nonlinear. The EB column is solved first because it is further upstream. The EB/styrene column is selected second. Both the styrene plant units (subsystem 4) and the styrene column (subsystem 6) are affected by zero unselected subsystems, affect zero unselected subsystems, and are linear. The styrene plant subsystem is solved third because it is further upstream. The styrene column is solved fourth. The EB plant units (subsystem 1) are solved before the EB reactor because subsystem 1 is linear. Although the iterative algorithm generates a unique solution, alternative sequences that yield an equally acceptable solution might exist. For example, solution of subsystems 1 and 2 before subsystems 4 and 6 yields a solution sequence that is identical to that in Figure 6 with regard to unknown information. Therefore, engineering judgment should be used to determine the final solution sequence.

3.3. Multi-Rate Problems. Plant decompositions based on nonlinearity properties of the unit operations can produce subsystems with significant differences in their characteristic time scales. For example, a reaction/separation process in which the reactor has much faster dynamics than the distillation column is considered in the next section. For such plant decompositions, computational efficiency can be further enhanced by solving the MPC controllers for the slow subsystems at a lower frequency than the MPC controllers for the fast sub-

systems. This approach is particularly beneficial if the nonlinear subsystems have slower dynamics as it allows less frequent solution of the NMPC problems. Below, we present a multi-rate formulation of the hybrid LMPC−NMPC strategy for two subsystem problems based on the local dynamic coordination method discussed previously. Furthermore, the development is restricted to the case where the linear subsystem dynamics are slower because the solution is applicable to the reaction/separation example. Extensions for other types of decompositions are conceptually straightforward.

Let the sampling rate of the NMPC controller be denoted Δt_N and that of LMPC problem be denoted Δt_L such that $\Delta t_L = n\Delta t_N$ where n is an integer. The time index is denoted k_N for the NMPC problem and k_L for the LMPC problem. At time step k_L, where $t = k_L\Delta t_L$, the LMPC problem is solved using the current linear state variables $x_L(k_L)$ and the nonlinear state and input variables available from the NMPC solution at time step $k_N - 1$ where $k_N = nk_L$

$$X_N(k_N-1) =$$
$$[x_N^T(k_L|k_N-1) \ \cdots \ x_N^T(k_L+\tilde{P}_N|k_N-1) \ \cdots \ x_N^T(k_L+N_L-1|k_N-1)]^T$$

$$U_N(k_N-1) =$$
$$[u_N^T(k_L|k_N-1) \ \cdots \ u_N^T(k_L+\tilde{N}_N|k_N-1) \ \cdots \ x_N^T(k_L+N_L-1|k_N-1)]^T$$

Here, $\tilde{P}_N$ and $\tilde{N}_N$ are the NMPC prediction and control horizons, respectively, expressed as integer multiples of the linear sampling time Δt_L, such that

$$\tilde{P}_N = \text{int}\left(\frac{P_N - 1}{n}\right)$$

and

$$\tilde{N}_N = \text{int}\left(\frac{N_N - 2}{n}\right)$$

If necessary, x_N beyond the NMPC prediction horizon can be obtained via open-loop simulation of the nonlinear subsystem with constant u_N. The LMPC solution at time k_L is implemented, and it is not recalculated until time $k_L + 1$. The NMPC problem is solved n times at time steps k_N, $k_N + 1$, ..., $k_N + n - 1$ between the two LMPC solutions. At time step $k_N + j$ the NMPC solution is determined using the linear state and input predictions available at time k_L

$$X_L(k_L) =$$
$$[x_L^T(k_N+j|k_L) \ \ x_L^T(k_N+j+1|k_L) \ \cdots \ x_L^T(k_N+j+nN_L|k_L)]^T$$

$$U_L(k_L) =$$
$$[u_L^T(k_N+j|k_L) \ \ u_L^T(k_N+j+1|k_L) \ \cdots \ u_L^T(k_N+j+n(N_L-1)|k_L)]^T$$

where $j \in [0, n - 1]$. The NMPC solution is recomputed and implemented every Δt_N time units.

4. Simulation Example

Given the plant decomposition and MPC solution sequence shown in Figures 3 and 6, respectively, it is possible to develop a hybrid LMPC−NMPC control strategy for the styrene plant. This would require the design of three LMPC controllers and three NMPC controllers along with development of the associated subsystem models. Such an effort is beyond the scope of this paper. Instead, the reaction/separation process studied in ref 15 is used to evaluate the MPC controller coordination methods in section 3. This example offers the advantage that plant decomposition yields a single linear subsystem and a single nonlinear subsystem.

Table 1. Nominal Operating Conditions for the Reaction/Separation Process

variable	value	variable	value	variable	value
F	45.022 L/min	E/R	8750 K	X_{A1}	0.95
F_R	54.978 L/min	k_0	5.14×10^{10} 1/min	X_{A2}	0.826
C_{Af}	1 mol/L	UA	5×10^4 J/(min K)	X_{A3}	0.709
T_f	350 K	T_c	309.480 K	X_{A4}	0.619
V_r	100 L	C_A	0.567 mol/L	X_{A5}	0.559
ρ	1000 g/L	T	350 K	X_{A6}	0.506
C_p	0.239 J/(g K)	M_1, M_9	200 mol	X_{A7}	0.394
$(-\Delta H)$	5×10^4 J/mol	M_2, ..., M_8	50 mol	X_{A8}	0.235
ρ_m	1 mol/L	L	29.2 mol/min	X_{A9}	0.1
α	4	V	84.2 mol/min		

4.1. Process Model. The process consists of continuous stirred tank reactor that is used to manufacture a product B by irreversible reaction of a reactant A. The reactor is modeled by assuming first-order kinetics, constant-volume operation, and negligible coolant jacket dynamics. Furthermore, the reactor feed stream, which is obtained by mixing a fresh feed stream with a recycle stream from a downstream distillation column, is assumed to be maintained at a constant temperature and flow rate by fast regulatory control loops. As shown in Appendix F, the reactor model consists of two highly nonlinear differential equations for the temperature and the component concentration. The reactor control objective is to regulate the reactor temperature by manipulation of the cooling jacket temperature. The effluent from the reactor is introduced into the fourth tray of a distillation column that consists of seven trays, a partial condenser, and a reboiler. The overhead stream enriched in A is recycled to the reactor, while the bottom stream enriched in B is recovered as the product. Standard assumptions such as equimolar overflow are used to derive the distillation column model.[27] As shown in Appendix F, a component balance on an equilibrium stage yields a moderately nonlinear model consisting of nine differential equations. The column control objective is to regulate the overhead and bottom compositions by manipulation of the vapor and reflux rates.

For this simple process, the linear subsystem (column) and the nonlinear subsystem (reactor) are easily determined. The combined model can be represented as in eqs 6−9 where

$$x_L = [X_{A1} \ \ X_{A2} \ \ X_{A3} \ \ X_{A4} \ \ X_{A5} \ \ X_{A6} \ \ X_{A7} \ \ X_{A8} \ \ X_{A9}]^T$$

$$u_L = [L \ \ V]^T, \quad y_L = [X_{A1} \ \ X_{A9}]^T$$

$$x_N = [T \ \ C_A]^T, \quad u_N = T_c, \quad y_N = T$$

where X_{An} and Y_{An} are the mole fractions of component A on tray n in the liquid and vapor phases, respectively; V and L are the molar flow rates in the column of the vapor and liquid streams, respectively; C_A and T are the concentration of A and the temperature of the reactor effluent stream, respectively; and T_c is the temperature of the reactor coolant stream. Nominal values of the model parameters are given in Table 1.

4.2. Controller Design. The global controller coordination method presented above is applied to this

reaction/separation process in ref 15. When compared to conventional LMPC controller, the hybrid LMPC−NMPC controller is shown to provide vastly superior performance for operation at an unstable operating point of the reactor. The hybrid controller provides performance comparable to that of a conventional NMPC controller with less than 10% of the computing effort. In this section, all three controller coordination methods and the multi-rate controller formulation discussed in section 3 are evaluated using the reaction/separation example. The controller tuning parameters for each coordination method are listed below, where the sampling rate $\Delta t = 10$ s.

Global coordination method

LMPC: $N_L = 15$, $P_L = \infty$

$$Q = \begin{bmatrix} 0.1 & 0 & 0 \\ 0 & 5 \times 10^4 & 0 \\ 0 & 0 & 5 \times 10^4 \end{bmatrix}$$

$$R = \begin{bmatrix} 0.01 & 0 & 0 \\ 0 & 0.01 & 0 \\ 0 & 0 & 0.01 \end{bmatrix}$$

$$S = \begin{bmatrix} 50 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

NMPC:

$$N_N = 1,\ P_N = 4,\ Q = 2,\ R = 0.001,\ S = 0.001$$

Local steady-state coordination method

LMPC: $N_L = 15$, $P_L = \infty$

$$Q = \begin{bmatrix} 5 \times 10^4 & 0 \\ 0 & 5 \times 10^4 \end{bmatrix}$$

$$R = \begin{bmatrix} 0.01 & 0 \\ 0 & 0.01 \end{bmatrix}$$

$$S = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

NMPC:

$$N_N = 1,\ P_N = 5,\ Q = 2,\ R = 0.001,\ S = 0.001$$

Local dynamic coordination approach

All tuning parameters are identical to those for the local steady-state coordination method.

4.3. Results. In Figure 7, the three controller coordination methods are compared for a +10-K change in the reactor temperature setpoint. All three controller rapidly bring the reactor temperature to the new setpoint while rejecting the disturbance that propagates through the distillation column. The closed-loop reactor dynamics are slightly improved for the second and third methods because of the longer prediction horizons used. Note that the input moves generated by the three controllers for the nonlinear subsystem are virtually identical. More significant differences are observed in column performance, as the global and local dynamic coordination methods yield much better disturbance rejection than does the local steady-state method. This result can be attributed to the steady-state approximation for future state and input variables used in the steady-state method. The global method yields slightly better control of the column compositions than does the local dynamic method. This might be a result of the assumption in the local dynamic method that the nonlinear subsystem variables are constant beyond the relatively short NMPC horizon.

In Figure 8, the three methods are compared for an unmeasured +5-K disturbance in the reactor feed temperature. The global method yields the smallest overshoot in the reactor temperature. The local dynamic method provides very similar performance, whereas the local steady-state method yields relatively poor column performance.

In Figure 9, a multi-rate hybrid MPC controller is compared to a single-rate hybrid MPC controller when the local dynamic method is used for controller coordination. The single-rate controller is executed for 10 s. Because the column dynamics are significantly slower than the reactor dynamics, the multi-rate LMPC controller is executed at a frequency of 60 s, while the multi-rate NMPC controller is executed every 10 s (i.e., $n = 6$). As expected, the two hybrid controllers yield very similar performances for the reactor. The column performance obtained with the multi-rate controller is slightly degraded because of the larger sampling time used for the multi-rate LMPC controller. Note that $\tilde{P}_N = 0$ and $\tilde{N}_N = 0$ because both P_N and N_N are less than $n = 6$. Therefore, the multi-rate controller is equivalent to a local steady-state controller except that the multi-rate LMPC controller is solved at a lower frequency with a longer control horizon because of the larger sampling period. Note that the multi-rate controller outperforms the single-rate local steady-state controller (compare Figures 7 and 9). This might be a result of the longer control horizon used for the multi-rate LMPC controller. The multi-rate controller provides only a modest improvement in computation time as compared to the single-rate controllers. More significant reductions in computational effort are expected when NMPC controllers can be executed less frequently than LMPC controllers.

5. Summary and Conclusions

A systematic methodology for integrating linear model predictive control (LMPC) and nonlinear model predictive control (NMPC) for plant-wide control applications has been presented. The method is applicable to plants that can be decomposed into a number of linear and nonlinear subsystems on the basis of the nonlinearity properties and interconnections of the individual unit operations. An iterative decomposition algorithm was developed and applied to a complex styrene plant flowsheet. The plant decomposition enables LMPC and NMPC to be applied selectively to subsystems according to their degrees of nonlinearity. An iterative algorithm designed to minimize the amount of unknown information resulting from sequential solution of the MPC problems was developed and applied to the decomposed styrene flowsheet. The hybrid LMPC−NMPC controller was shown to be stabilizing for a class of triangular nonlinear systems for which the MPC solution sequence problem is trivially solved. Three controller coordination strategies were presented to handle plants with more complex interconnections. An extension for multi-rate control was presented for plants that can be decomposed into subsystems with different characteristic time scales.

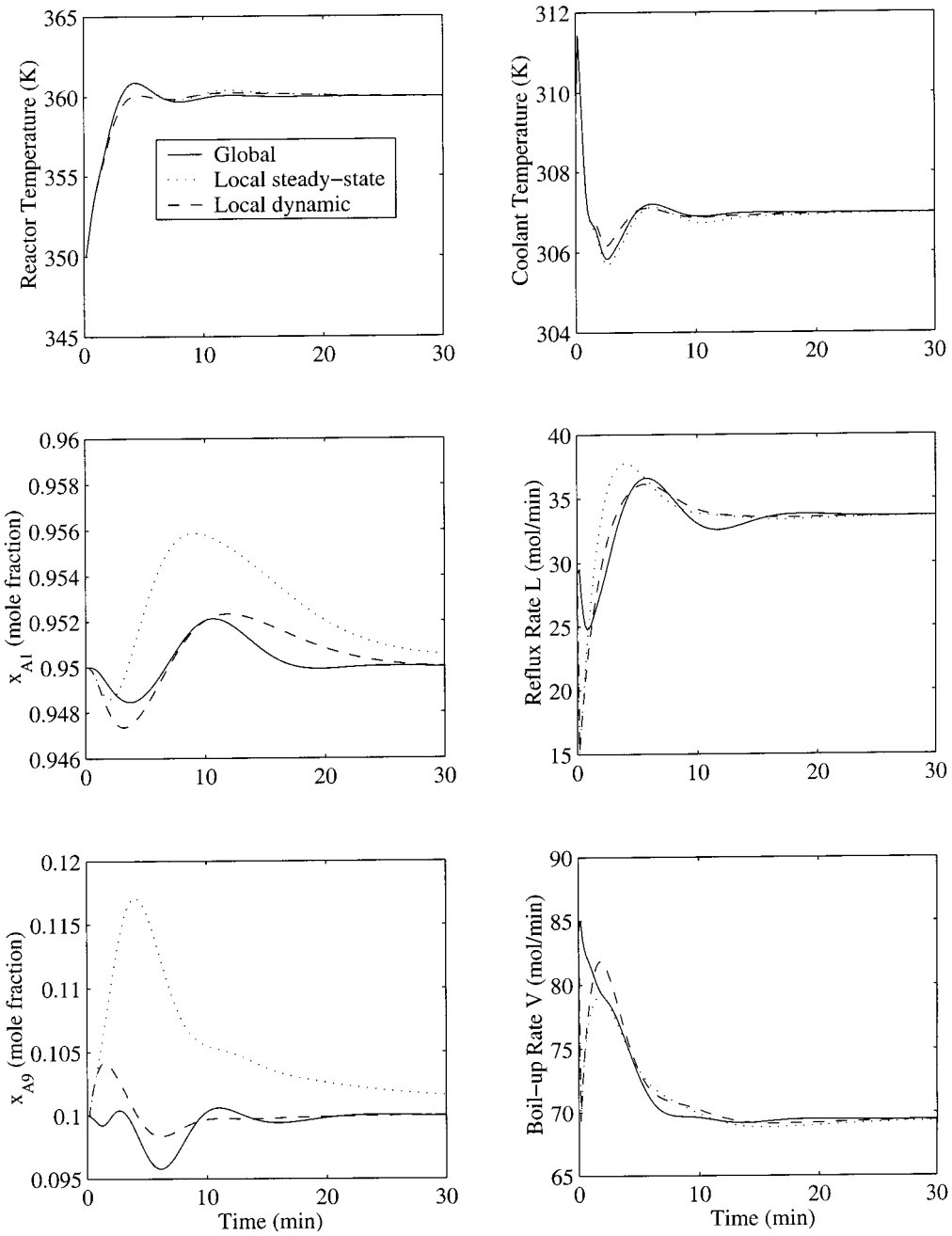

Figure 7. Closed-loop simulation for +10-K change in reactor temperature setpoint.

A reaction/separation process was used to evaluate the various hybrid LMPC−NMPC controller design strategies.

Acknowledgment

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Appendix A: Optimization Formulation of the Plant Decomposition Problem

The plant decomposition problem can be formulated as the following optimization problem

$$\max_{\tilde{X},\tilde{Y}} \sum_{k=1}^{N} [\prod_{i=1}^{N}(1 - \tilde{X}_{i,k})] + \sum_{k=1}^{N}(1 - \tilde{Y}_k) \qquad (10)$$

subject to

$$\sum_{k=1}^{N} \tilde{X}_{i,k} = 1 \quad i \in [1, N]$$

$$\sum_{i=1}^{N} n_i \tilde{X}_{i,k} = \tilde{Y}_k \sum_{i=1}^{N} X_{i,k} \quad k \in [1, N]$$

$$\sum_{i=2}^{N} \sum_{j=1}^{i-1} (1 - C_{i,j})(1 - C_{j,i}) \tilde{X}_{i,k} \tilde{X}_{j,k} = 0 \quad k \in [1, N]$$

Because the number of subsystems M is unknown until the problem is solved, it is necessary to introduce the $N \times N$ matrix $\tilde{X}$ and the $N \times 1$ vector $\tilde{Y}$. The elements of $\tilde{X}$ and $\tilde{Y}$ are defined identically to the elements of the matrix X and vector Y, respectively, introduced in section 2 except that the number of subsystems is assumed to be N instead of M. There is a total of (N +

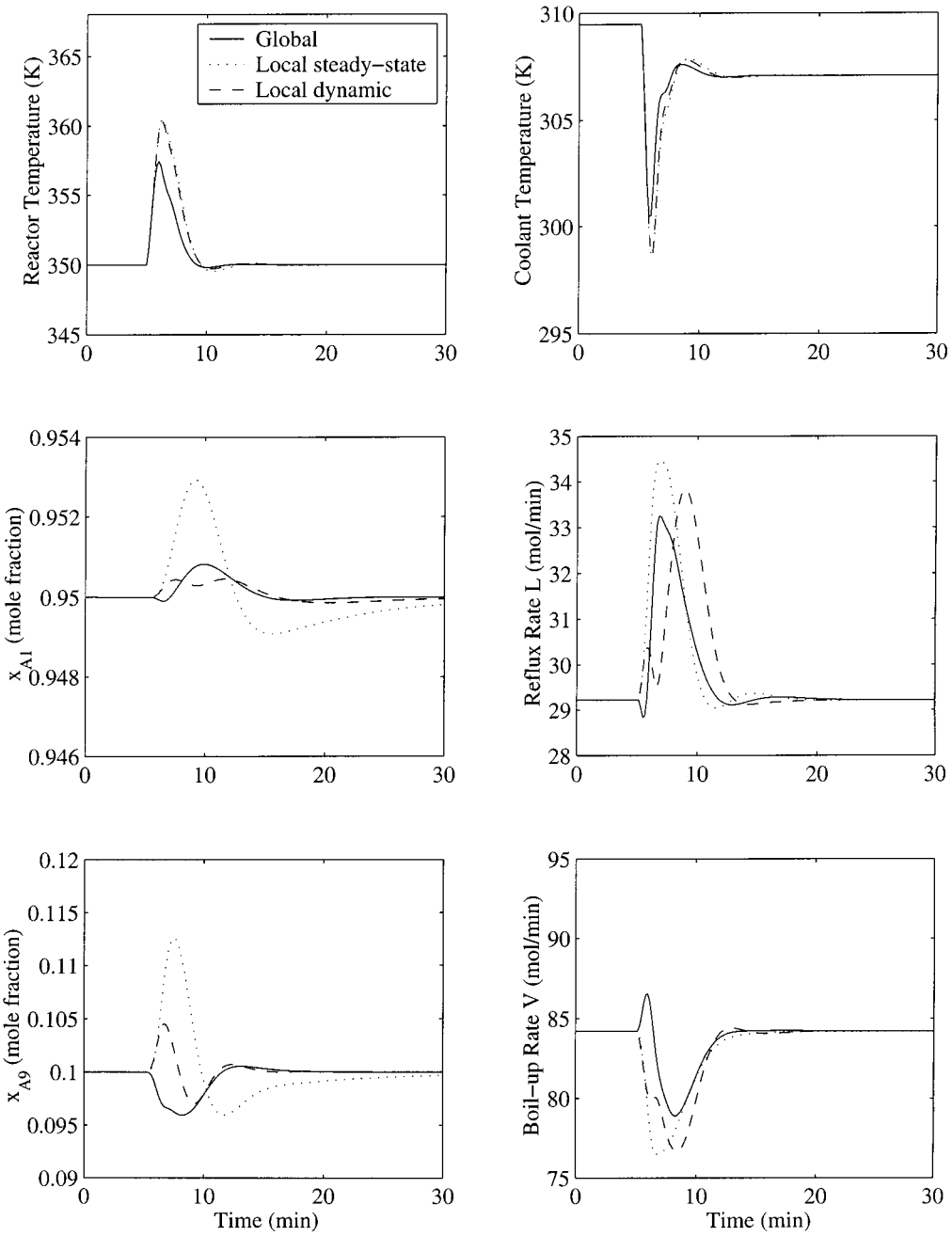

Figure 8. Closed-loop simulation for +5-K disturbance in reactor feed temperature.

1)N decision variables corresponding to the elements of $\tilde{X}$ and $\tilde{Y}$. The term $\sum_{i=1}^{N}(1 - \tilde{X}_{i,k})$ for a given column k is 1 if and only if every element of column k is 0; this corresponds to an empty subsystem. Thus, the first term in the objective function represents the total number of empty subsystems. If the subsystem k is empty, then $\tilde{Y}_k$ can be either 0 or 1. The second term in the objective function ensures that each empty subsystem k is assigned $\tilde{Y}_k = 0$. The first constraint ensures that each unit operation is allocated to one and only one subsystem. The second constraint guarantees that all unit operations in a given subsystem have the same nonlinearity property (i.e., linear or nonlinear). The third constraint ensures that every unit operation in a given subsystem is connected to at least one other unit operation in the same subsystem. The matrices X and Y are constructed from $\tilde{X}$ and $\tilde{Y}$, respectively, by eliminating zero columns that correspond to empty subsystems.

Appendix B: LMPC Controller Formulation

The formulation of the LMPC controller for the case in which the linear and nonlinear subsystems in eqs 6−9 are uncoupled is briefly outlined here. The objective function is a quadratic function of the future state and input variables given by[23]

$$\min_{U_L(k)} [x_L(k+N_L|k) - x_L^s(k)]^T \bar{Q}[x_L(k+N_L|k) - x_L^s(k)] + \Delta u_L^T(k+N_L|k) S \Delta u_L(k+N_L|k) + \sum_{j=0}^{N_L-1} \{[x_L(k+j|k) - x_L^s(k)]^T C_L^T Q C_L [x_L(k+j|k) - x_L^s(k)] + \Delta u_L^T(k+j|k) S \Delta u_L(k+j|k) + [u_L(k+j|k) - u_L^s(k)]^T R [u_L(k+j|k) - u_L^s(k)]\} \quad (11)$$

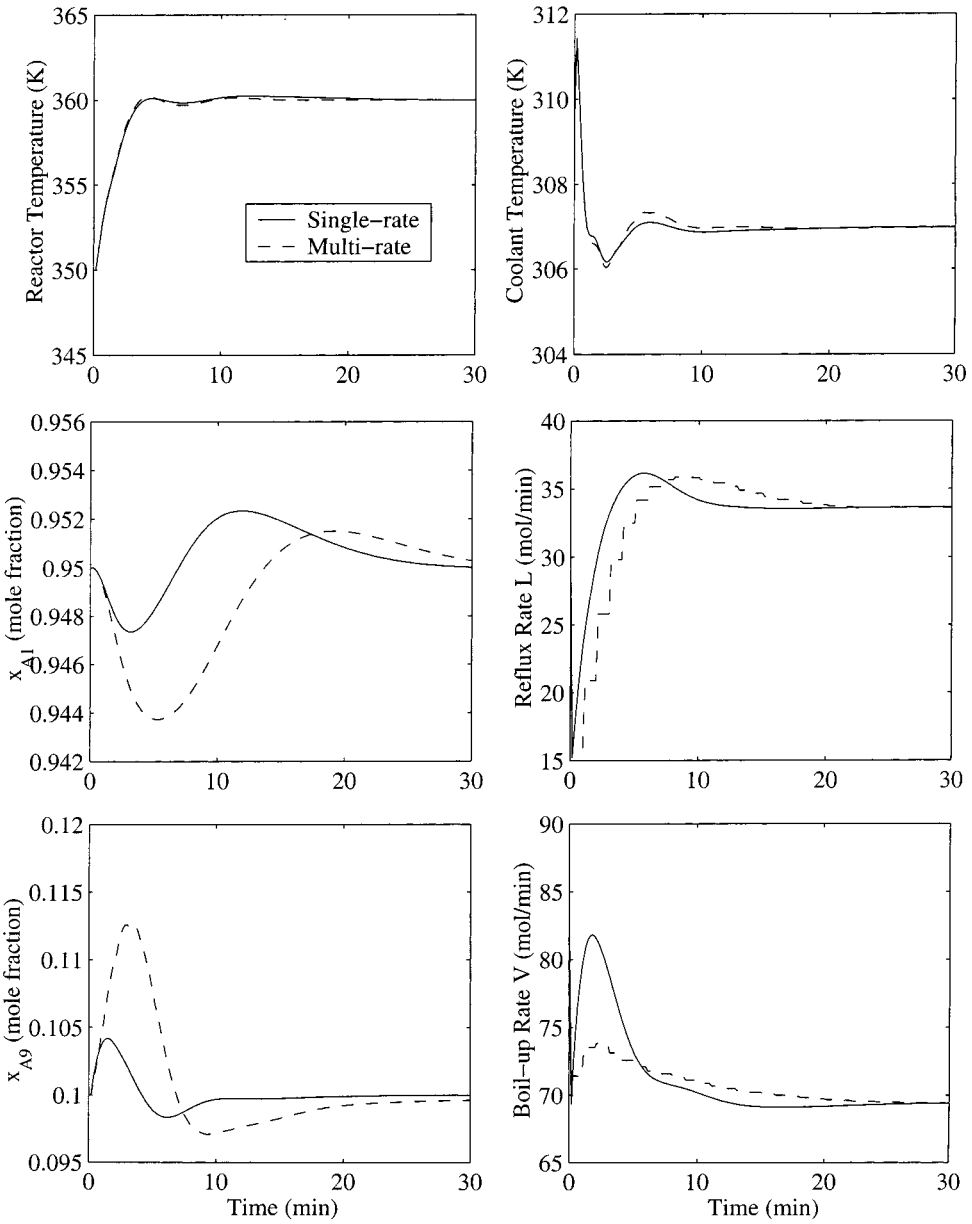

Figure 9. Single-rate and multi-rate control for +10-K change in reactor temperature setpoint.

subject to

$$x_L(k+j|k) = A_L x_L(k+j-1|k) + B_L u_L(k+j-1|k) \qquad j \in [1, N_L]$$

$$u_L(k+j|k) = u_L(k+N_L-1|k) \quad \forall\, j \geq N_L$$

$$u_{L,\min} \leq u_L(k+j|k) \leq u_{L,\max}$$

$$\Delta u_{L,\min} \leq \Delta u_L(k+j|k) \leq \Delta u_{L,\max}$$

$$y_{L,\min} \leq C_L x_L(k+j|k) \leq y_{L,\max}$$

where $x_L(k+j|k)$ and $u_L(k+j|k)$ are predicted state and input vectors, respectively; $x_L^s(k)$ and $u_L^s(k)$ are state and input target vectors, respectively; $\Delta u_L(k+j|k) = u_L(k+j|k) - u_L(k+j-1|k)$; Q, R, and S are weighting matrices; $u_{L,\min}$, $\Delta u_{L,\min}$, and $y_{L,\min}$ are lower limits; and $u_{L,\max}$, $\Delta u_{L,\max}$, and $y_{L,\max}$ are upper limits. An infinite prediction horizon is realized by determining the penalty matrix $\bar{Q}$ by solution of a Lyapunov equation.[23] The decision variables are future values of the input vector over the control horizon N_L

$$U_L(k) = [u_L(k|k)\ \ u_L(k+1|k)\ \cdots\ u_L(k+N_L-1|k)]^T \quad (12)$$

Future values of the state variables are predicted from the linear model eqs 6 and 7. The objective function in eq 24 can be manipulated to yield a quadratic programming problem that is well-suited for real-time solution.[23]

Appendix C: NMPC Controller Formulation

The formulation of the NMPC controller for the case in which the linear and nonlinear subsystems in eqs 6−9 are uncoupled is briefly outlined here. The NMPC

optimization problem is posed as

$$\min_{U_N(k),X_N(k)} \sum_{j=0}^{P_N} \{h[x_N(k+j|k)] - h[x_N^s(k)]\}^T Q\{h[x_N(k+j|k)] - h[x_N^s(k)]\} + \sum_{j=0}^{N_N-1} \{[u_N(k+j|k) - u_N^s(k)]^T R[u_N(k+j|k) - u_N^s(k)] + \Delta u_N(k+j|k)^T S \Delta u_N(k+j|k)\} \quad (13)$$

subject to

$$x_N(k+j|k) = f[x_N(k+j-1|k), u_N(k+j-1|\ k)] \quad j \in [1, P_N]$$

$$u_N(k+j|k) = u_N(k+N_N-1|k) \quad \forall\, j \geq N_N$$

$$u_{N,\min} \leq u_N(k+j|k) \leq u_{N,\max}$$

$$\Delta u_{N,\min} \leq \Delta u_N(k+j|k) \leq \Delta u_{N,\max}$$

$$y_{N,\min} \leq h[x_N(k+j|k)] \leq y_{N,\max}$$

where the nonlinear subsystem variables are defined similarly to the linear subsystem variables in the LMPC problem. Note that NMPC controller has a finite prediction horizon P_N. The decision variables are future values of the state and input vectors, respectively

$$X_N(k) = [x_N(k|k)\ \ x_N(k+1|k)\ \ \cdots\ \ x_N(k+P_N|k)]^T$$

$$U_N(k) = [u_N(k|k)\ \ u_N(k+1|k)\ \ \cdots\ \ u_N(k+N_N-1|k)]^T$$

Because of the nonlinear constraints arising from the model equations, the NMPC formulation leads to a nonlinear programming problem that is very difficult to solve on-line for plants of reasonable complexity.

Appendix D: QP Formulation of LMPC for Local Dynamic Controller Coordination

Below, we show that the LMPC problem can be formulated as a quadratic programming (QP) problem even though the coupled linear system (eq 6) depends on the nonlinear subsystem state and input variables. The LMPC objective function in eq 11 can be algebraically manipulated to yield the following QP problem

$$\min_{U_L(k)} [U_L(k)]^T H U_L(k) + 2[U_L(k)]^T [G_1 X_N(k) + G_2 U_N(k) + G_3 x_L(k) - F u_L(k-1)] \quad (14)$$

where $U_L(k)$, $X_N(k)$, and $U_N(k)$ are defined as

$$U_L(k) = [u_L(k|k)\ u_L(k+1|k)\ \cdots\ u_L(k+N_L-1|k)]^T$$

$$X_N(k) = [x_N(k|k)\ x_N(k+1|k)\ \cdots\ x_N(k+P_N|k)\ \cdots\ x_N(k+N_L-1|k)]^T$$

$$U_N(k) = [u_N(k|k)\ u_N(k+1|k)\ \cdots\ u_N(k+N_N-1|k)\ \cdots\ x_N(k+N_L-1|k)]^T$$

The NMPC prediction horizon (P_N) and control horizon (N_N) typically are chosen to be shorter than the LMPC control horizon (N_L). As discussed in section 3.1, the last $N_L - P_N - 1$ elements of $X_N(k)$ can be obtained by iterating the nonlinear subsystem model in open-loop fashion with constant input vector $u_N(k+N_N-1|k)$ or by assuming that the state vector remains constant at $x_N(k+P_N|k)$. The last $N_L - N_N$ elements of $U_N(k)$ are assumed to be equal to $u_N(k+N_N-1|k)$. The matrices H, G_1, G_2, G_3, and F in eq 14 can be determined from the linear model and tuning matrices as follows:

$$H = \begin{bmatrix} B_L^T\bar{Q}B_L + R + 2S & B_L^T A_L^T\bar{Q}B_L - S & \cdots & B_L^T(A_L^T)^{N_L-1}\bar{Q}B_L \\ B_L^T\bar{Q}A_L B_L - S & B_L^T\bar{Q}B_L + R + 2S & \cdots & B_L^T(A_L^T)^{N_L-2}\bar{Q}B_L \\ \vdots & \vdots & \ddots & \vdots \\ B_L^T\bar{Q}(A_L)^{N_L-1}B_L & B_L^T\bar{Q}(A_L)^{N_L-2}B_L & \cdots & B_L^T\bar{Q}B_L + R + 2S \end{bmatrix}$$

$$G_1 = \begin{bmatrix} B_L^T\bar{Q}A_N & B_L^T A_L^T\bar{Q}A_N & \cdots & B_L^T(A_L^T)^{N_L-1}\bar{Q}A_N \\ B_L^T\bar{Q}A_L A_N & B_L^T\bar{Q}A_N & \cdots & B_L^T(A_L^T)^{N_L-2}\bar{Q}A_N \\ \vdots & \vdots & \ddots & \vdots \\ B_L^T\bar{Q}(A_L)^{N_L-1}A_N & B_L^T\bar{Q}(A_L)^{N_L-2}A_N & \cdots & B_L^T\bar{Q}A_N \end{bmatrix}$$

$$G_2 = \begin{bmatrix} B_L^T\bar{Q}B_N & B_L^T A_L^T\bar{Q}B_N & \cdots & B_L^T(A_L^T)^{N_L-1}\bar{Q}B_N \\ B_L^T\bar{Q}A_L B_N & B_L^T\bar{Q}B_N & \cdots & B_L^T(A_L^T)^{N_L-2}\bar{Q}B_N \\ \vdots & \vdots & \ddots & \vdots \\ B_L^T\bar{Q}(A_L)^{N_L-1}B_N & B_L^T\bar{Q}(A_L)^{N_L-2}B_N & \cdots & B_L^T\bar{Q}B_N \end{bmatrix}$$

$$G_3 = \begin{bmatrix} B_L^T\bar{Q}A_L \\ B_L^T\bar{Q}(A_L)^2 \\ \vdots \\ B_L^T\bar{Q}(A_L)^N \end{bmatrix}$$

$$F = \begin{bmatrix} S \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

where $\bar{Q}$ is defined as follows for stable systems[23]

$$\bar{Q} = \sum_{i=0}^{\infty} [A_L^T]^i C_L^T Q C_L A_L^i \quad (15)$$

For unstable systems, the QP matrices can be obtained by a similar extension of the development in ref 23.

Appendix E: Optimization Formulation of the MPC Solution Sequence Problem

The subsystem connection matrix Γ is required for solution of the MPC sequence problem. Recall that $\Gamma_{i,j} = 1$ if subsystem i affects subsystem j and $\Gamma_{i,j} = 0$ otherwise. We define a vector d such that $d_j = \sum_{i=1}^{M} \Gamma_{i,j}$ for $j = 1, \ldots, M$ where M is the total number of subsystems. The decision variables are elements of the $M \times M$ matrix Ψ, where $\Psi_{k,j} = 1$ if and only if subsystem j is the kth subsystem solved. An optimization problem that yields a MPC solution sequence with the least amount of information required from unsolved sub-

systems is formulated as

$$\min_{\psi} \sum_{k=1}^{M} \sum_{j=1}^{M} [d_j - \sum_{l=1}^{k-1} \sum_{i=1}^{M} \Psi_{l,i} \Gamma_{i,j}] \Psi_{k,j} \qquad (16)$$

subject to

$$\sum_{k=1}^{M} \Psi_{k,j} = 1$$

$$\sum_{j=1}^{M} \Psi_{k,j} = 1$$

The first constraint guarantees that subsystem j is solved only once, and the second constraint allows only one system to be solved at a given time.

Appendix F: Model Equations for the Reaction/Separation Process

$$\dot{C}_A = \frac{1}{V_r}[FC_{Af} + \rho_m F_R X_{Ar} - (F + F_R)C_A] - k_0 \exp\left(-\frac{E}{RT}\right)C_A \qquad (17)$$

$$\dot{T} = \frac{(F + F_R)}{V_r}(T_f - T) + \frac{-\Delta H}{\rho C_p} k_0 \exp\left(-\frac{E}{RT}\right)C_A + \frac{UA}{V\rho C_p}(T_c - T) \qquad (18)$$

$$\dot{X}_{A1} = \frac{1}{M_1}(VY_{A2} - LX_{A1} - \rho_m F_R X_{A1}) \qquad (19)$$

$$\dot{X}_{A2} = \frac{1}{M_2}[L(X_{A1} - X_{A2}) + V(Y_{A3} - Y_{A2})] \qquad (20)$$

$$\dot{X}_{A3} = \frac{1}{M_3}[L(X_{A2} - X_{A3}) + V(Y_{A4} - Y_{A3})] \qquad (21)$$

$$\dot{X}_{A4} = \frac{1}{M_4}[L(X_{A3} - X_{A4}) + V(Y_{A5} - Y_{A4})] \qquad (22)$$

$$X_{A5} = \frac{1}{M_5}\{(F + F_R)C_A + LX_{A4} - [L + \rho_m(F + F_R)]X_{A5} + V(Y_{A6} - Y_{A5})\} \qquad (23)$$

$$\dot{X}_{A6} = \frac{1}{M_6}\{[L + \rho_m(F + F_R)](X_{A5} - X_{A6}) + V(Y_{A7} - Y_{A6})\} \qquad (24)$$

$$\dot{X}_{A7} = \frac{1}{M_7}\{[L + \rho_m(F + F_R)](X_{A6} - X_{A7}) + V(Y_{A8} - Y_{A7})\} \qquad (25)$$

$$\dot{X}_{A8} = \frac{1}{M_8}\{[L + \rho_m(F + F_R)](X_{A7} - X_{A8}) + V(Y_{A9} - Y_{A8})\} \qquad (26)$$

$$\dot{X}_{A9} = \frac{1}{M_9}\{[L + \rho_m(F + F_R)]X_{A9} - VY_{A9} - [L + \rho_m(F + F_R) - V]X_{A9}\} \qquad (27)$$

where F, C_{Af}, and T_f are the volumetric flow rate, concentration of A, and temperature, respectively, of the reactor feed stream; F_R, X_{A1}, and ρ_m are the volumetric flow rate, mole fraction of A, and molar density, respectively, of the recycle stream; $(F + F_R)$, C_A, and T are the volumetric flow rate, concentration of A, and temperature, respectively, of the effluent stream; T_c is the temperature of the coolant stream in the jacket surrounding the reactor; the condenser and reboiler are denoted as trays 1 and 9, respectively; X_{An} and Y_{An} are the mole fractions of A in the liquid and vapor phases, respectively, on tray n; M_n is the liquid molar holdup on tray n; and V and L are the molar flow rates of the vapor and liquid streams, respectively, in the column. The vapor−liquid equilibrium on each tray is described by

$$Y_{An} = \frac{\alpha X_{An}}{1 + (\alpha - 1)X_{An}} \qquad (28)$$

where α is the relative volatility.

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