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Novel Formulation and Application of Model Predictive Control.

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NOVEL FORMULATION AND APPLICATIONS OF MODEL PREDICTIVE CONTROL

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy

in

The Department of Chemical Engineering

by

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B.S. University of South Florida, 1996
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Abstract

Model predictive control (MPC) has been extensively studied in academia and widely accepted in industry. This research has focused on the novel formulation of model predictive controllers for systems that can be decomposed according to their nonlinearity properties and several novel MPC applications including bioreactors modeled by population balance equations (PBE), gas pipeline networks, and cryogenic distillation columns.

Two applications from air separation industries are studied. A representative gas pipeline network is modeled based on first principles. The full-order model is ill-conditioned, and reduced-order models are constructed using time-scale decomposition arguments. A linear model predictive control (LMPC) strategy is then developed based on the reduced-order model. The second application is a cryogenic distillation column. A low-order dynamic model based on nonlinear wave theory is developed by tracking the movement of the wave front. The low-order model is compared to a first-principles model developed with the commercial simulator HYSYS.Plant. On-line model adaptation is proposed to overcome the most restrictive modeling assumption. Extensions for multiple column modeling and nonlinear model predictive control (NMPC) also are discussed.

The third application is a continuous yeast bioreactor. The autonomous oscillations phenomenon is modeled by coupling PBE model of the cell mass distribution
to the rate limiting substrate mass balance. A controller design model is obtained by linearizing and temporally discretizing the ODEs derived from spatial discretization of the PBE model. The MPC controller regulate the discretized cell number distribution by manipulating the dilution rate and the feed substrate concentration.

A novel plant-wide control strategy is developed based on integration of LMPC and NMPC. It is motivated by the fact that most plants that can be decomposed into approximately linear subsystems and highly nonlinear subsystems. LMPCs and NMPCs are applied to the respective subsystems. A sequential solution algorithm is developed to minimize the amount of unknown information in the MPC design. Three coordination approaches are developed to reduce the amount of information unavailable due to the sequential MPC solution of the coupled subsystems and applied to a reaction/separation process. Furthermore, a multi-rate approach is developed to exploit time-scale differences in the subsystems.
Chapter 1

Introduction

1.1 Overview

Chemical processes are inherently nonlinear and highly interacting. Model predictive control (MPC) techniques were developed to overcome the inadequacies of single-loop controllers. MPC has been found to be beneficial for processes with the following characteristics [82]:

1. Multiple input and output variables.
2. Complex dynamics.
3. Constraints on input and/or output variables.

The underlying idea of MPC is the use of a process model to predict future outputs and to solve for inputs that minimize the difference between predicted outputs and their reference trajectories. The basic components of a MPC system include a plant model, an optimal control objective, constraint specifications, and a feedback structure that provides robustness. MPC is known for its multivariable formulation and ability to explicitly handle constraints, which are the most commonly encountered nonlinearity in chemical process industries.
Linear model predictive control (LMPC) utilizes linear models obtained from Jacobian linearization of first-principles models or step response models obtained from plant tests. The manipulated inputs are determined by differentiating the objective function with respect to input vectors if no constraints are considered. A quadratic programming problem can be solved if constraints are included. A wide range of LMPC formulations have been developed in industry and academia. Dynamic matrix control (DMC) [24], model algorithmic control (MAC, IDCOM) [49, 71] and quadratic dynamic matrix control (QDMC) [29] have led to successful applications in industry. Reviews of LMPC applications can be found in [82, 86].

Academia has contributed to the theoretical development of MPC by addressing issue such as stability [30, 56, 80].

While LMPC has been applied successfully to many processes in industry, there are some processes that are sufficiently nonlinear to require nonlinear compensation. This is necessary when the process is highly nonlinear or moderately nonlinear with a large operating range. Nonlinear model predictive control (NMPC) uses a nonlinear model for prediction and optimization, thus offering improved performance. At the same time, NMPC requires the solution of a nonlinear programming problem that has much higher computational requirements than linear programming or quadratic programming [14, 16, 89, 107]. Moreover, the non-convex nature of the NMPC optimization problem may result in a local minimum. Stability of NMPC can be established for the infinite horizon case or when a terminal equality constraint is
imposed [66, 69]. But these requirements increase the computational requirements. Some review papers of NMPC are presented in [39, 87].

1.2 Linear Model Predictive Control

Linear model predictive control (LMPC) involves the computation of a manipulated input profile into the future to optimize a performance index. The prediction is performed using a linear process model. The LMPC formulation presented by Muske and Rawling in 1993 [80] offers several advantages including:

1. State-space formulation for stable and unstable systems.
2. Nominal stability.
3. Extensions for output feedback.

This formulation is used for the LMPC designs in the following chapters.

Since most advanced control algorithms are implemented in digital computers, we consider a discrete-time form of the dynamic model:

\[ x(k + 1) = Ax(k) + Bu(k) \]  
\[ y(k) = Cx(k) \]  

where \( x(k) \) is a \( n \)-dimensional vector of state variables, \( u(k) \) is a \( p \)-dimensional vector of manipulated inputs, and \( y(k) \) is a \( m \)-dimensional vector of controlled outputs, and
$k$ is the discrete time index. The future input vector $U(k)$ is defined as:

$$U(k) = \begin{bmatrix} u(k|k) & u(k+1|k) & \ldots & u(k+N-1|k) \end{bmatrix}^T$$  \hspace{1cm} (1.2)$$

where $N$ the control horizon. $U(k)$ is calculated by minimizing an infinite horizon open-loop objective function. The problem can be reformulated with a finite prediction horizon [80]:

$$\min_{U(k)} \phi_k = [x(k+N|k) - x_s(k)]^T Q [x(k+N|k) - x_s(k)]$$

$$+ \Delta u(k+N|k)^T S \Delta u(k+N|k)$$

$$+ \sum_{j=0}^{N-1} \{ [x(k+j|k) - x_s(k)]^T C^T Q C [x(k+j|k) - x_s(k)]$$

$$+ [u(k+j|k) - u_s(k)]^T R [u(k+j|k) - u_s(k)]$$

$$+ \Delta u(k+j|k)^T S \Delta u(k+j|k) \}$$

where $Q$, $R$, $S$ are positive definite penalty matrices for the state vector, input vector and input change vector, respectively, and $\Delta u(k+j|k) = u(k+j|k) - u(k+j-1|k)$. The double indexed variables $x(k+j|k)$ and $u(k+j|k)$ represent the state and input variables, respectively, at time $k+j$ given by the model prediction based on information at time $k$. The subscript $s$ denotes the target values for the corresponding variables. This formulation accounts for the infinite prediction horizon via the terminal state penalty matrix ($Q$), which for stable systems is determined by the
solution of following discrete Lyapunov equation:

$$\overline{Q} = C^TQC + A^TQA$$

(1.4)

The LMPC solution is subject to the constraints:

\[ x(k + j|k) = Ax(k + j - 1|k) + Bu(k + j - 1|k) \quad j \in [1, N] \]
\[ u(k + j|k) = u_s(k) \quad \forall j \geq N \]
\[ u_{\text{min}} \leq u(k + j|k) \leq u_{\text{max}} \quad j \in [0, N - 1] \]
\[ \Delta u_{\text{min}} \leq \Delta u(k + j|k) \leq \Delta u_{\text{max}} \quad j \in [0, N] \]
\[ y_{\text{min}} \leq y(k + j|k) \leq y_{\text{max}} \quad j \in [1, \infty] \]

For unstable systems, an additional equality constraint is required [80]:

\[ z^u(k + N|k) = z^u_s(k) \]

(1.5)

where \( z^u(k + N|k) \) represents the unstable modes at the end of the control horizon and \( z^u_s(k) \) is the corresponding target values. A quadratic programming problem can be developed from the objective function and constraints. The detailed development can be found in [80].

The LMPC formulation presented above assumes that all state variables are measured. Even if full-state feedback is available, steady-state offset will result from disturbances and modeling errors if the measured state variables are simply used to reset the MPC calculation at each time step. An augmented state/disturbance
model is formulated as follows [80]:

\[
x(k + 1) = Ax(k) + Bu(k) \\
d(k + 1) = d(k) \\
y(k) = Cx(k) + d(k)
\]

where \(d\) is a vector of output disturbance variables. This model assumes that the difference between the model prediction and plant output at the current time is caused by a step output disturbance that remains constant in the future [80]. A linear observer has the form [80],

\[
\hat{x}(k + 1) = A\hat{x}(k) + Bu(k) + L_1[y(k) - C\hat{x}(k)] \\
\hat{d}(k + 1) = \hat{d}(k) + L_2[y(k) - C\hat{x}(k)]
\]

where \(\hat{x}(k)\) and \(\hat{d}(k)\) are the estimated state vector and output disturbances, respectively, at time \(k\), and \(L_1\) and \(L_2\) are the observer gains. The estimated state variables are used in the MPC calculation as the current state variables. The target vectors that eliminate steady state offset are found from the following quadratic programming problem [80]:

\[
\min_{[\hat{x}_s(k), u_s(k)]^T} [u_s(k) - u_{ref}]^T R_s [u_s(k) - u_{ref}]
\]
subject to:

\[
\begin{bmatrix}
    I - A & -B \\
    C & 0
\end{bmatrix}
\begin{bmatrix}
    x_s(k) \\
    u_s(k)
\end{bmatrix} = \begin{bmatrix}
    0 \\
    y_{ref} - \hat{d}(k)
\end{bmatrix}
\]

\[u_{min} \leq u_s(k) \leq u_{max}\]

where \(x_s(k)\) and \(u_s(k)\) are the state and input targets at time step \(k\), respectively, and \(u_{ref}\) and \(y_{ref}\) are the setpoint vectors for the input and output variables, respectively.

If the quadratic program (1.8) is infeasible or there are more outputs than inputs, the tracking error can be minimized by solving the following quadratic program [80]:

\[
\begin{bmatrix}
    y_{ref} - Cx_s(k) - \hat{d}(k)
\end{bmatrix}^T R_s \begin{bmatrix}
    y_{ref} - Cx_s(k) - \hat{d}(k)
\end{bmatrix} = \min_{[x_s(k), u_s(k)]^T}
\]

subject to:

\[
\begin{bmatrix}
    I - A & -B \\
    C & 0
\end{bmatrix}
\begin{bmatrix}
    x_s(k) \\
    u_s(k)
\end{bmatrix} = \begin{bmatrix}
    0 \\
    y_{ref} - \hat{d}(k)
\end{bmatrix}
\]

\[u_{min} \leq u_s(k) \leq u_{max}\]

A detailed proof that the output disturbance model eliminates offset is presented in [89].
1.3 Nonlinear Model Predictive Control

NMPC also involves the calculation of a sequence of control moves that minimize an objective function. In this case, the prediction of future behavior is performed using a nonlinear model of the system. The nonlinear model is assumed to have the following form:

\[
\begin{align*}
x(k + 1) &= f[x(k), u(k)] \quad (1.10) \\
y(k) &= h[x(k)]
\end{align*}
\]

where \(x\) is a \(n\)-dimensional vector of state variables, \(u\) is a \(m\)-dimensional vector of input variables, and \(y\) is a \(p\)-dimensional vector of output variables. The objective function in discrete form is [70]:

\[
\begin{align*}
&\min_{u(k), x(k)} \sum_{j=0}^{P} \{h[x(k + j|k)] - h[x_s(k)]\}^T Q \{h[x(k + j|k)] - h[x_s(k)]\} \\
&\quad + \sum_{j=0}^{N-1} \left\{[u(k + j|k) - u_s(k)]^T R[u(k + j|k) - u_s(k)] \right. \\
&\quad \left. + \Delta u(k + j|k)^T S \Delta u(k + j|k) \right\}
\end{align*}
\]

subject to:

\[
\begin{align*}
x(k + j|k) &= f[x(k + j - 1|k), u(k + j - 1|k)] \quad j \in [1, P] \\
u(k + j|k) &= u(k + N - 1|k) \quad j \geq N \\
\underline{u} \leq u(k + j|k) \leq \overline{u} \quad j \in [0, N - 1]
\end{align*}
\]

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\[
\Delta u_{\text{min}} \leq \Delta u(k + j|k) \leq \Delta u_{\text{max}} \quad j \in [0, N - 1]
\]
\[
y_{\text{min}} \leq h[x(k + j|k)] \leq y_{\text{max}} \quad j \in [1, P]
\]

where \( P \) is the finite prediction horizon. \( N, Q, R, \) and \( S \) are defined similarly as those in the LMPC formulation. Both manipulated inputs and states are the decision variables of the optimization problem. The discretized model equations are equality constraints. \( X \) is defined as:

\[
X(k) = \begin{bmatrix}
x(k|k) & x(k + 1|k) & \cdots & x(k + P|k)
\end{bmatrix}^T
\]

\( U \) is defined as:

\[
U(k) = \begin{bmatrix}
u(k|k) & u(k + 1|k) & \cdots & u(k + P - 1|k)
\end{bmatrix}^T
\]

The nonlinear model equations lead to a nonlinear programming (NLP) problem. To guarantee stability, a terminal state constraint may be imposed [66]:

\[
x(k + P|k) = 0
\]

The NLP problem can be solved using nonlinear programming features of commercial software such as Matlab.
1.4 Discussion of Objectives

An accurate model is essential for successful application of model predictive control. However computational issues often are encountered with large dimensional models which are often obtained from first principles. The computational cost can be especially high for NMPC controllers. In Chapters 2–4 three novel applications, gas pipeline networks, cryogenic distillation columns, and oscillating yeast bioreactors that are characterized by high dimensional models are studied. A significant part of each chapter is dedicated to the development of nonlinear process models based on first principles and the subsequent model reduction. A LMPC controller is applied to the gas pipeline network in Chapter 2. In Chapter 3 a nonlinear wave theory based model is developed for a cryogenic distillation column. In Chapter 4 a population balance equation (PBE) model is developed for an oscillating yeast bioreactor. A LMPC controller is designed based on the PBE model to attenuate or induce oscillations. MPC application issues such as state estimation, unknown disturbance rejection, and infeasibilities caused by output constraints are addressed for each application.

The multivariable formulation and constraint handling ability of MPC make it an excellent candidate for plant-wide control applications. Two major challenges are the large dimensionality of the plant model and the strong nonlinearity associated with certain unit operations. It is not practical to implement a NMPC controller on the entire plant due to the excessive computational cost. Meanwhile
LMPC controllers often fail to address the plant nonlinearity effectively. A novel hybrid LMPC-NMPC approach is developed in Chapters 5 and 6 to overcome these difficulties. LMPC and NMPC controllers are applied to the linear and nonlinear subsystems, respectively, derived from a decomposition procedure based on the nonlinearity properties of the unit operations. A comprehensive approach is developed to address problems such as the plant decomposition, MPC solution sequence and MPC controller coordination.
Chapter 2

Dynamic Modeling and Linear Model Predictive Control of Gas Pipeline Networks

2.1 Introduction

The chemical and steel industries consume large quantities of purified nitrogen and oxygen. In regions highly concentrated with these industries, purified gases are produced by cryogenic air separation plants and supplied via extensive pipeline networks. The oxygen pipeline network considered in this paper is representation of those operated by Praxair. The pipeline is over 50 miles long and has approximately 15 customers. Pipeline pressures must be maintained near their desired values without violating constraints imposed by safety concerns and business contracts. The desired pressures may correspond to a certain economic optimum, such as the low pressure limits at all customer sites. When the pipeline pressure drops below the lower limit, vaporized liquid oxygen must be introduced to the pipeline to quickly increase the pressure. Emergency vents must be opened to release gas when the pressure exceeds the upper limit. Both situations result in economic penalties and should be prevented.

Heuristic operating guidelines for long distance natural gas transmission pipelines can be found in [12]. These pipelines have much longer pipes and simpler configura-
tions than the oxygen pipeline studied here. A partial differential equation (PDE) model of a natural gas pipeline is proposed by Guy [34]. Finite difference solution of this model is investigated by Lappus and Schmidt [57]. Commercial software packages for dynamic gas pipeline simulation include WinTran by Gregg Engineering [2] and PIPESYS by Hyprotech [1]. Based on the dynamic simulator GANESI [101], Marques and Morari [64] develop an optimization strategy based on quadratic programming to reduce compressor costs of natural gas pipelines. The literature on gas pipeline control is rather sparse. Sanada and Kitagawa [100] formulate a linear $H_{\infty}$ controller for a very simple gas pipeline described by ordinary differential equations that are obtained by discretizing a PDE model. Several articles [5, 18] suggest that the natural gas industry relies on simple regulatory control strategies and uses pipeline models primarily for early fault detection.

Current industrial practice for oxygen/nitrogen pipeline control involves regulatory control loops along with manual intervention by pipeline operators. Regulatory control loops are used to maintain certain pipeline pressures and flows. However, pipeline pressures are determined ultimately by the production rates of the cryogenic plants supplying the pipeline. Operators determine the production setpoint of each air separation plant manually by analyzing the current customer demands and pipeline pressures. This current practice is inadequate for achieving optimal operation of the pipeline. With the implementation of linear model predictive control (LMPC) on individual cryogenic plants, it is now possible to achieve closed-loop
control of the pipeline network by using the plant production rate setpoints as manipulated inputs. The pipeline LMPC controller proposed in this paper is designed to drive critical pressures to setpoints determined by the operations staff or a higher level steady-state optimizer. Important cryogenic plant constraints can be included explicitly when the pipeline controller computes the plant production setpoints.

LMPC has been widely accepted by the chemical industry due to its multivariable formulation and constraint handling abilities. The pipeline control problem is a good candidate for LMPC because it is a highly interacting and highly constrained process. A related application of LMPC to a combined sewer system is studied by Gelormino and Ricker [31]. According to their paper implementation of LMPC has achieved significant reduction of combined sewer overflows, which is a critical case of constraint violation. The LMPC controller utilized in this paper is the infinite horizon formulation proposed by Muske and Rawlings [80]. This formulation ensures nominal stability for stable and unstable systems subject to both input and output constraints [79, 91]. Output constraint infeasibilities are handled by completely removing the output constraints over a portion of the prediction horizon. The stability of infinite horizon LMPC with a soft output constraint handling method is examined by Zheng and Morari [123]. Both output constraint handling techniques are studied in [102] and in this chapter.

The remainder of the chapter is organized as follows. In Section 2.2, dynamic modeling of a representative oxygen pipeline network is discussed and open-loop
simulation results are presented. Formulation of the LMPC problem for the oxygen pipeline is described in Section 2.3. Section 2.4 contains closed-loop simulation results for the oxygen pipeline example. Finally, a summary and conclusions are given in Section 2.5.

2.2 Dynamic Modeling of Gas Pipeline Networks

Figure 2.1 is a schematic of the oxygen pipeline considered in this paper. Each number indicates a production site, a customer site or a pipe junction. They are called "nodes" in the sequel. The control valve that divides the high pressure and low pressure sides of the pipeline is known as the "let-down station". The let-down station offers an additional manipulated variable that is especially effective for controlling the low pressure side pressure of the pipeline. The let-down station also is important for extreme conditions such as a plant shutdown on the high pressure side of the pipeline. When this occurs, the let-down station valve can be closed to maintain pressure on the high pressure side.

A first-principles model is derived to describe the pressure dynamics of the oxygen pipeline. We are primarily interested in pressure changes at each node rather than a detailed description of the spatial pressure gradients. While a PDE model offers accurate description of the gas transmission dynamics and is suitable for infrequent on-line optimization, it is unnecessarily complex for model-based control solved at the frequency of minutes. Therefore we construct an ordinary differential equation (ODE) model that only describes the pressure changes at the nodes.
Although not discussed here for proprietary reasons, the proposed model compares favorably with Praxair's internal dynamic model derived from plant tests.

The complete pipeline model is composed of three groups of equations: (i) node pressure equations; (ii) let-down station pressure control loop equations; and (iii) cryogenic plant production and constraint variable equations. The second set of equations describe the pressure control loop for the let-down station. The third set of equations represent the closed-loop cryogenic plant production dynamics and dynamic relations between other plant constraint variables and the production rates.
Approximate closed-loop dynamics of the LMPC controlled cryogenic plants are
included to eliminate the need for detailed modeling.

2.2.1 Full-order Nonlinear Model

Node pressure equations are derived from molar balances at each node. Energy bal­
ances are not needed because the temperature changes in the pipeline are negligible.
The molar balance for node $i$ is:

$$
\dot{N}_i = \rho_{sc} \left[ \sum_k F_{i,k} + \sum_j f_1(P_i, P_j, \theta) \right]
$$

(2.1)

where $N_i$ is the gas molar holdup at node $i$, $\rho_{sc}$ is the molar density of oxygen at
standard conditions (1 atm and 60 °F), $F_{i,k}$ is the volumetric gas flow rate from
a production plant (positive flow) or to a customer (negative flow) at node $i$. A
complete set of nomenclature is shown in Appendix A.1. The subscript $k$ denotes
the production plant $k$ at nodes $i = 10, 24, \text{and } 29$; $k = 1$ for customer withdraws
at all other nodes. The function $f_1(P_i, P_j, \theta)$ represents the volumetric flow rate
between node $i$ and node $j$. The flow depends on the associated pressures ($P_i$ and
$P_j$) and the pipeline leg parameters ($\theta$). A leg connects two nodes and can be a pipe
or a valve. For a pipe $f_1$ takes the form of the Weymouth equation [3], which can
be derived from a momentum balance and is used extensively in the gas industry.
for modeling compressible flows:

\[
\begin{align*}
f_1(P_i, P_j) &= 114.2 \sqrt{ \frac{(P_i^2 - P_j^2)d_p^5}{f_r L T S_g Z_m}} & P_i \geq P_j \\
&= -114.2 \sqrt{ \frac{(P_j^2 - P_i^2)d_p^5}{f_r L T S_g Z_m}} & P_i < P_j
\end{align*}
\]

where \(d_p\) is the pipe diameter, \(f_r\) is the friction factor, \(L\) is the pipe length, \(T\) is the temperature, \(S_g\) is the specific gravity of the gas, \(E_f\) is the efficiency factor and \(Z_m\) is the mean compressibility of the gas. The friction factor \((f_r)\) is estimated using the formula [3]:

\[
f_r = \frac{0.032}{d_p^{1/3}}
\]

The efficiency factor \((E_f)\) is assumed to be one. For the let-down station, linear valve dynamics are assumed and the flow equation is:

\[
f_1(P_i, P_j, l) = C_v \frac{l}{100} \sqrt{ \frac{P_i - P_j}{S_g}}
\]

where \(l\) is the percentage of valve opening and \(C_v\) is the valve characteristic constant. This equation is appropriate because the let-down station pressure does not change significantly from the nominal value and the pressure drop across the valve is only around 10% of \(P_i\).

Since the molar holdup at each node cannot be measured, it is desirable to have the node pressures as dependent variables in the model equations. This is achieved...
by assuming each node has a constant volume. The node volumes are determined by dividing the pipe volumes equally among the adjacent nodes. Each node molar volume is related to its associated node pressure by an equation of state. Commonly used cubic equations of state (e.g. Peng-Robinson [110]) yield very complicated expressions for the pressure derivatives. For the pressure range of a typical oxygen pipeline, the Virial equation of state [110] provides good prediction of gas properties and makes the resulting model much simpler. Using the truncated Virial equation, the molar holdup at node \( i \) can be expressed as:

\[
N_i = \frac{V_i P_i}{Z_i RT} = \frac{V_i P_i}{RT + B_i P_i}
\]  

(2.4)

where \( R \) is the gas constant, \( B_i \) is the second Virial coefficient for node \( i \) and \( V_i \) is the node volume. Taking time derivatives on both sides of (2.4) yields:

\[
\frac{dN_i}{dt} = \frac{V_i RT}{(RT + B_i P_i)^2} \frac{dP_i}{dt}
\]  

(2.5)

Substituting (2.5) into the node molar balance equation (2.1) yields:

\[
\frac{dP_i}{dt} = \rho_{sc} f_2(P_i) \left[ \sum_j f_1(P_i, P_j) + \sum_k F_{ik} \right]
\]  

(2.6)

where the function \( f_2 \) is defined as:

\[
f_2(P_i) = \frac{(RT + B_i P_i)^2}{V_i RT}
\]
The let-down station pressure control loop is described by following equations:

\[
I = I_{ss} + K_c e_f + \frac{K_c}{\tau_I} \eta_f \quad (2.7)
\]

\[
\dot{\eta} = P_{sp} - P \quad (2.8)
\]

\[
\dot{e}_f = \frac{1}{\tau_f} [(P_{sp} - P) - e_f] \quad (2.9)
\]

\[
\dot{\eta}_f = \frac{1}{\tau_f} (\eta - \eta_f) \quad (2.10)
\]

where \( I \) and \( I_{ss} \) are the valve position and steady-state valve position, respectively; \( K_c \) and \( \tau_I \) are tuning parameters for the PI regulator; \( e_f \) is a filtered value of the difference between the pressure \( (P) \) and its setpoint \( (P_{sp}) \); \( \eta \) is the integrated error; and \( \eta_f \) is the filtered value of \( \eta \). The error signals are filtered to reduce large valve movements which can cause numerical problems when the full-order model is simulated. The pressure control loop equations are included explicitly in the model because the LMPC controller manipulates the let-down pressure setpoint \( (P_{sp}) \).

The production rates \( (F_i) \) of the LMPC controlled cryogenic plants are modeled empirically as first-order-plus-deadtime (FOPDT) systems:

\[
\frac{dF_i}{dt} = \frac{1}{\tau_i} [F_{req}(t - t_d) - F_i(t)] \quad (2.11)
\]

where \( \tau_i \) is the closed-loop time constant for the \( i \)th production plant and \( F_{req} \) is the production request (setpoint). All the cryogenic plant models have the same deadtime \( t_d \). The FOPDT model parameters are obtained from closed-loop plant
data. The dynamics of the other constraint variables ($\Gamma \in R^{10}$) associated with individual cryogenic plants are described by a set of ordinary differential equations and algebraic equations derived from the empirical relations (2.11). These constraint variables includes air flow rates, liquid nitrogen production rates, total compressor flow rates and power consumptions. These plant constraints must be honored because of equipment limits and business contracts. The associated equations are not shown there for proprietary reasons. While the plant constraints are included in the subsequent simulations, it should be noted that the constraints are not active during any of the simulation tests. Thus, identical results will be obtained if the plant constraints are omitted. A complete set of model equations excluding the plant constraint variables is included in Appendix A.2.

2.2.2 Reduced-order Nonlinear Models

The full-order model of the oxygen pipeline is comprised of 43 ordinary differential equations and 7 algebraic equations. Thirty differential equations describe the node pressure changes along the pipeline. The node pressure dynamics are determined primarily by the physical dimensions of the adjacent legs. Due to large differences in leg lengths (50 ft to 161,200 ft), the full-order model exhibits multiple time scales. As discussed below, the pipeline network is an integrating system and therefore the linearized system matrix $A$ has a zero singular value. The large difference in time scales is exemplified by the very wide range of nonzero singular values.
(0.1705 to 3.083 × 10^7). As a result, numerical problems are encountered when the full-order model is used as the basis for LMPC design.

One approach for improving the conditioning of the model is to combine adjacent nodes with small pressure drops. This eliminates short pipes with fast dynamics and also reduces the total number of model equations. To construct reduced-order pipeline models, the following guidelines are followed:

1. The new pipe lengths are the sum of the combined pipe lengths.

2. The new pipe diameters are determined such that the total volume of the combined legs is preserved.

3. The pipe efficiency factors are adjusted such that the difference between the steady-state solutions of the full-order and reduced-order models are minimized in a least-squares sense.

4. The volumes corresponding to eliminated nodes are distributed between adjacent nodes to achieve more uniform time scales.

The full-order pipeline model first is reduced from 30 nodes to 19 nodes by eliminating short lateral legs. As shown later, there is very little difference between the reduced-order and full-order model predictions. But the reduced-order model is better conditioned as shown by the range of non-zero singular values (0.1884 to 4.168 × 10^5). This reduced-order model serves as the plant in closed-loop simulations. The model is reduced further to only 10 nodes to generate the
model used for LMPC design. This reduction is performed such that the node pressures subsequently defined as controlled outputs remain explicitly in the model. The non-zero singular value range (0.0987 to $5.1401 \times 10^4$) shows that the controller model is slightly better conditioned than the plant model. Figures 2.1-2.3 show the pipeline layouts corresponding to the three models. Table 2.1 shows the definition of the reduced-order model nodes in terms of the full-order model nodes.

Figure 2.2: Reduced-order pipeline network for the plant model (19 nodes).
Table 2.1: Node reduction: full-order model, plant model and controller model.

<table>
<thead>
<tr>
<th>Node</th>
<th>Full $R^{43}$</th>
<th>Plant $R^{32}$</th>
<th>Control $R^{23}$</th>
<th>Node</th>
<th>Full $R^{43}$</th>
<th>Plant $R^{32}$</th>
<th>Control $R^{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$P_1$</td>
<td>$P_1$</td>
<td>$P_{1-4}$</td>
<td>21</td>
<td>$P_{21}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>$P_2$</td>
<td>$P_{2,4}$</td>
<td>$P_{5-9}$</td>
<td>22</td>
<td>$P_{22}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>$P_3$</td>
<td>$P_3$</td>
<td>$P_{10}$</td>
<td>23</td>
<td>$P_{23}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$P_4$</td>
<td>$P_{5,6}$</td>
<td>$P_{11,12}$</td>
<td>24</td>
<td>$P_{24}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>$P_5$</td>
<td>$P_7$</td>
<td>$P_{13-17}$</td>
<td>25</td>
<td>$P_{25}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>$P_6$</td>
<td>$P_{8,9}$</td>
<td>$P_{18-21}$</td>
<td>26</td>
<td>$P_{26}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>$P_7$</td>
<td>$P_{10}$</td>
<td>$P_{22,23}$</td>
<td>27</td>
<td>$P_{27}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>$P_8$</td>
<td>$P_{11}$</td>
<td>$P_{24}$</td>
<td>28</td>
<td>$P_{28}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>$P_9$</td>
<td>$P_{12}$</td>
<td>$P_{25,26}$</td>
<td>29</td>
<td>$P_{29}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>$P_{10}$</td>
<td>$P_{13}$</td>
<td>$P_{27-30}$</td>
<td>30</td>
<td>$P_{30}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>$P_{11}$</td>
<td>$P_{14}$</td>
<td>$F_{10,2}$</td>
<td></td>
<td>$F_{10,2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>$P_{12}$</td>
<td>$P_{15-17}$</td>
<td>$F_{10,3}$</td>
<td></td>
<td>$F_{10,3}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>$P_{13}$</td>
<td>$P_{18-21}$</td>
<td>$F_{24,1}$</td>
<td></td>
<td>$F_{24,1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>$P_{14}$</td>
<td>$P_{22}$</td>
<td>$F_{24,2}$</td>
<td></td>
<td>$F_{24,2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>$P_{15}$</td>
<td>$P_{23}$</td>
<td>$F_{29,1}$</td>
<td></td>
<td>$F_{29,1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>$P_{16}$</td>
<td>$P_{24}$</td>
<td>$\eta$</td>
<td></td>
<td>$\eta$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>$P_{17}$</td>
<td>$P_{25,26}$</td>
<td>$\eta_f$</td>
<td></td>
<td>$\eta_f$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>$P_{18}$</td>
<td>$P_{27,28}$</td>
<td>$\eta_f$</td>
<td></td>
<td>$\eta_f$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>$P_{19}$</td>
<td>$P_{29,30}$</td>
<td>$\Gamma_x$</td>
<td></td>
<td>$\Gamma_x$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>$P_{20}$</td>
<td></td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>
The linear model used for LMPC design is obtained by linearizing the nonlinear controller model at a steady-state operating point. The pipeline network is an integrating system because it contains an inventory of gas. Consequently, for any set of inputs there exists an equilibrium space rather than isolated equilibrium points. The steady-state values used for linearization correspond to the nominal operating condition for the pipeline. The resulting linear controller design model has the form:

\[ x(k+1) = Ax(k) + Bu(k) + B_d(k) \]
\[ y(k) = Cx(k) \]
\[ y_c(k) = C_c x(k) + D_d(k) \]
where $x \in \mathbb{R}^{23}$ is the vector of state variables shown in Table 2.1, $u \in \mathbb{R}^{6}$ is a vector of manipulated inputs, $d \in \mathbb{R}^{10}$ is a vector of measured disturbances, $y \in \mathbb{R}^{3}$ is a vector of controlled outputs, $y_c \in \mathbb{R}^{14}$ is a vector of constrained outputs and $k$ is the discrete time index. The sampling time is 2 minutes.

The state vector consists of the node pressures, the cryogenic plant production rates, the let-down station control loop variables, and plant constraint variables:

$$x = \left[ P_{1-4} \ P_{5-9} \ P_{10} \ P_{11,12} \ P_{13-17} \ P_{18-21} \ P_{22,23} \ P_{24} \ P_{25,26} \ P_{27-30} \ F_{10,2} \ F_{10,3} \ F_{24,1} \ F_{24,2} \ F_{29,1} \ \eta \ e_f \ \eta_f \ \Gamma^T_x \right]^T$$

where the subscripted $P$ terms denote node pressures for the controller model based on Figure 2.3 and $\Gamma_x \in \mathbb{R}^5$ is the subset of plant constraint variables contained in the state vector. The input vector is comprised of the production requests for the five LMPC controlled cryogenic plants and the pressure setpoint for the let-down station:

$$u = \left[ Frq_{10,2} \ Frq_{10,3} \ Frq_{24,1} \ Frq_{24,2} \ Frq_{29,1} \ P_{sp} \right]^T$$

It is assumed that the production requests are delayed by one sampling time ($t_d = 2$ min). Therefore, an augmented state vector is defined as:

$$\tilde{x}(k) = \left[ x_1(k) \ \ldots \ x_{23}(k) \ u_1(k-1) \ \ldots \ u_5(k-1) \right]^T$$
and the system matrices $A$, $B$, $B_d$, $C$, $C_c$ and $D_d$ are modified accordingly [28].

To simplify the notation, the model form (2.12) will continue to be used in the subsequent development. The measured disturbance vector includes the customer withdraw rates at each node and the production rate of plant 10-1 where LMPC is not implemented:

$$d = \begin{bmatrix}
\sum_{i=1}^{4} F_i, & \sum_{i=5}^{9} F_i, & F_{10}, & \sum_{i=11}^{12} F_i, & \sum_{i=13}^{17} F_i, \\
\sum_{i=18}^{21} F_i, & \sum_{i=22}^{26} F_i, & \sum_{i=27}^{30} F_i, & \sum_{i=31}^{33} F_i
\end{bmatrix}^T$$

where the $F_{i,j}$ denote gas flow rates for the full-order model derived from Figure 2.1 and each term in the vector corresponds to the gas flow rate at a node of the controller model derived from Figure 2.3. The pressures at nodes 4, 8 and 10 (see Figure 2.3) are controlled to setpoints because these pressures largely determine the entire pipeline pressure distribution:

$$y = \begin{bmatrix}
P_{11,12}, & P_{24}, & P_{27-30}
\end{bmatrix}^T$$

There also are 14 output constraint variables which include the three controlled outputs defined above. Additional constrained outputs are the let-down station valve position and the plant constraint variables discussed earlier.

To further establish the need for multivariable control, it is useful to obtain the relative gain array (RGA) for the LMPC design model. The RGA can be used to
determine if interactions between single-loop controllers will be problematic. The linear model used for this analysis excludes the let-down station control loop since the let-down control valve position is used as an input in the RGA analysis. The outputs are chosen as the pressures defined above \((P_{11,12}, P_{24}, P_{27-30})\) as well as the pressure downstream of the let-down station \((P_{18-21})\). The inputs are the total production requests at nodes 10, 24 and 29 of the full-order model (see Figure 2.1) and the let-down station valve position. The gain matrix is generated using a method specifically designed for integrating systems [7]:

\[
K = \begin{bmatrix}
0.0378 & 0.0378 & 0.0378 & 0.5879 \\
0.0375 & 0.0375 & 0.0375 & 0.5827 \\
0.0370 & 0.0370 & 0.0370 & -0.2443 \\
0.0382 & 0.0382 & 0.0382 & -0.2519 \\
\end{bmatrix}
\]

The first three columns contain integrating gains (slopes) between the node pressures and the production requests. The last column contains steady-state gains between the node pressures and the valve position.

The relative gain between controlled variable \(Y_i\) and manipulated variable \(U_j\) is defined as [104]:

\[
\lambda_{i,j} = \frac{(\partial Y_i/\partial U_j)_u}{(\partial Y_i/\partial U_j)_Y} \tag{2.13}
\]
Because the gain matrix is singular, the RGA cannot be computed. For this system the closed-loop gain \((\partial Y_i / \partial U_j)_Y\) is always zero because the pressure at a given node does not change if the other pressures are held constant. The RGA analysis suggests that single-loop controllers designed using these inputs and outputs will be highly interacting. While it has been shown that LMPC can exhibit robustness problems when applied to systems with large RGA values [109], we have not observed any such problems in our simulations. Therefore, LMPC appears to be an appropriate control strategy for this problem.

2.2.4 Open-loop Simulation

The dynamic models are solved in MATLAB using the SIMULINK integration routine ODE15s [4]. Open-loop responses of the full-order model (Figure 2.1) and the plant model (Figure 2.2) are compared in Figure 2.4 for a positive step change of 50 kcfh in the plant 10-1 product request. All pressures are plotted as deviations from the let-down station pressure, which is controlled at a constant setpoint. This test confirms that the dimensionality reduction used to generate the plant model does not significantly affect the dynamic behavior. The full-order model simulation requires about 20 minutes for an eight hour simulation on a DEC Alpha 433 workstation, while the plant model simulation takes less than 3 minutes. The “spikes” observed in the full-order model response are indicative of numerical instability caused by ill-conditioning.
Figure 2.5 shows the open-loop responses obtained when the plant model, non-linear controller model and linear controller model are subjected to the following changes:

1. $-25$ kcfh change in plant 10-1 production request at $t = 1$ hr.
2. $+25$ kcfh change in plant 10-1 production request at $t = 2.5$ hr.
3. $+50$ kcfh change in node 26 customer withdraw at $t = 5$ hr.
4. $-50$ kcfh change in node 26 customer withdraw at $t = 7.5$ hr.
The node pressures on the low pressure side converge to constant values close to the initial steady state because the let-down station pressure is controlled at its setpoint. On the high pressure side, the node pressures increase or decrease with constant slopes after some initial dynamics. The three models show similar trends, so the linear controller model appears to adequately capture the important dynamics of this "slightly" nonlinear process.
2.3 Linear Model Predictive Control Strategy

The infinite horizon LMPC formulation proposed by Muske and Rawlings [80] is applied to the oxygen pipeline. Because this formulation provides nominal stability for unstable systems, it is not necessary to pre-stabilize the pipeline with a conventional controller prior to applying LMPC. Other advantages of the formulation include flexible use of alternative feedback structures to handle measured and unmeasured disturbances, as well as the explicit incorporation of input and output constraints. Below the LMPC strategy is presented with an emphasis on the specific formulation for the pipeline network.

2.3.1 LMPC Regulator

A necessary condition for LMPC to be applicable is that the linear model is stabilizable. It is easy to show that the augmented linear controller model (2.12) satisfies this condition. A vector of future inputs, $U(k)$ defined in (1.2), is calculated by solving the open-loop optimization problem (1.3).

The linearized pipeline model has one eigenvalue on the unit disk. For such unstable systems, the matrix $A$ is partitioned into stable and unstable parts. This is necessary because the unstable modes must be driven to their targets by the end of the control horizon so the infinite horizon objective function has a finite value.
Partitioning is performed by finding the Jordan form of $A$ [80]:

$$A = V J V^{-1} = \begin{bmatrix} V_u & V_s \end{bmatrix} \begin{bmatrix} J_u & 0 \\ 0 & J_s \end{bmatrix} \begin{bmatrix} \tilde{V}_u \\ \tilde{V}_s \end{bmatrix}$$

(2.14)

where the diagonal matrices $J_u$ and $J_s$ contain the unstable and stable eigenvalues, respectively, and $V_u$ and $V_s$ are comprised of the corresponding eigenvectors. The state vector is transformed into decoupled unstable ($z^u$) and stable ($z^s$) modes as follows:

$$\begin{bmatrix} z^u \\ z^s \end{bmatrix} = \begin{bmatrix} \tilde{V}_u \\ \tilde{V}_s \end{bmatrix} x$$

(2.15)

The following terminal equality constraint is appended to the optimization problem:

$$z^u(k + N|k) = \tilde{V}_u x_s$$

(2.16)

where $x_s$ is the state target vector obtained from (1.8)–(1.9). The terminal penalty matrix $\bar{Q}$ is computed by solving the Lyapunov equation using only the stable modes [80]:

$$\bar{Q} = \tilde{V}_s^T \Sigma \tilde{V}_s$$

(2.17)

$$\Sigma = V_s^T C^T QC V_s + J_s^T \Sigma J_s$$

(2.18)
With some algebraic manipulation, the optimization problem (1.3) can be formulated as a quadratic program (QP) for $u^N$:

$$
\min_{u^N} \phi_k = (u^N)^T H u^N + 2(u^N)^T [G x(k) - F u(k-1)]
$$

(2.19)

The form of the matrices $H$, $G$, and $F$ can be found in [80]. It is possible to include measured disturbances in the state predictions with some modification of the QP problem (see Appendix D.2). Because customer withdraw rates cannot be forecasted accurately, we utilize an alternative feedforward control strategy in which the measured disturbances are used to shift the target values [80]. This is discussed below. The following input and output constraints also are considered:

$$
\begin{align*}
    u_{\min} & \leq u(k+j|k) \leq u_{\max} & j = 1 \ldots N \\
    y_{\min} & \leq y_c(k+j|k) \leq y_{\max} & j = 1 \ldots \infty
\end{align*}
$$

(2.20)

Note that the output constraints are to be enforced over the infinite prediction horizon. In some situations, it is necessary to relax the output constraints to achieve feasibility of the QP. The feasibility issue is discussed later in this section.

### 2.3.2 Disturbance Estimation and Steady-state Target Calculation

The output disturbance model is the most common paradigm for estimating unknown disturbances in LMPC applications. Offset-free tracking performance can be
achieved only if there are sufficient degrees of freedom [80]; that is, the number of un-
constrained inputs is greater than or equal to the number of outputs. When choosing
a feedback structure for the gas pipeline system, the following characteristics need
to be considered: (i) there are only six inputs; (ii) 14 outputs must be maintained
within constraints, but only three outputs need to be controlled to setpoints; (iii)
all the state variables are measurable because they are node pressures, flow rates
and controller signals; (iv) the customer withdraw rates are measurable; and (v)
the pair \((C,A)\) of the LMPC design model is not observable. A custom disturbance
modeling approach is developed to fully exploit these system characteristics.

Instead of a more conventional output or input disturbance model, we take ad-
vantage of the fact that all the state variables are measurable and propose a state
disturbance model. The difference between the estimated and measured state vec-
tors is assumed to be attributable to a constant step disturbance vector \(\zeta\). Therefore,
the augmented process model takes the following form:

\[
\begin{align*}
x(k+1) &= Ax(k) + Bu(k) + B_d d(k) + \zeta(k) \\
\zeta(k+1) &= \zeta(k)
\end{align*}
\]  

Estimates of the disturbance vector are generated using the deadbeat observer:

\[
\begin{align*}
\hat{\zeta}(k-1|k) &= x(k) - Ax(k-1) - Bu(k-1) - B_d d(k-1) \\
\hat{\zeta}(k|k) &= \hat{\zeta}(k-1|k)
\end{align*}
\]
Once the disturbance estimates are available, the new steady-state targets for the state and input variables are determined by solving a slight modification of QP problem (1.8):

\[
\min_{x_s(k), u_s(k)} \left[ u_s(k) - u_{ref} \right]^T R_s \left[ u_s(k) - u_{ref} \right]
\]  

subject to:

\[
\begin{bmatrix}
I - A & -B \\
C & 0 \\
\end{bmatrix}
\begin{bmatrix}
x_s(k) \\
u_s(k) \\
\end{bmatrix}
= \begin{bmatrix}
B_d d(k) + \zeta(k|k) \\
y_{ref} \\
\end{bmatrix}
\]

\[u_{min} \leq u_s(k) \leq u_{max}\]

where \(R_s\) is a positive definite weighting matrix, and \(y_{ref}\) and \(u_{ref}\) are output and input setpoints, respectively. For the pipeline system, this problem can become infeasible when the number of active input constraints exceeds three. In this case, an alternative QP problem is solved which minimizes the difference between the outputs and their setpoints:

\[
\min_{x_s(k), u_s(k)} \left[ y_{ref} - C x_s(k) \right]^T Q_s \left[ y_{ref} - C x_s(k) \right]
\]  

subject to:

\[
\begin{bmatrix}
I - A & -B \\
C & 0 \\
\end{bmatrix}
\begin{bmatrix}
x_s(k) \\
u_s(k) \\
\end{bmatrix}
= \begin{bmatrix}
B_d d(k) + \zeta(k|k) \\
y_{ref} \\
\end{bmatrix}
\]
\[ u_{\min} \leq u_s(k) \leq u_{\max} \]

where \( Q_s \) is a positive definite weighting matrix. A necessary condition for the target calculation to be feasible is that the measured disturbances satisfy:

\[
\sum_{i=1}^{10} d_i(k) \leq \sum_{j=1}^{5} u_{\max j}
\]

which mathematically states the obvious condition that the system does not have a steady-state solution if the combined customer withdraws exceeds the total capacity of the cryogenic plants.

### 2.3.3 Output Constraint Handling

As discussed previously, output constraints of the following form are considered:

\[
y_{\min} \leq y_c(k + j|k) \leq y_{\max} \quad j = 1 \ldots \infty \tag{2.28}
\]

The output constraints can be reformulated as [91]:

\[
\hat{H}x(k + j|k) \leq h \quad j = 1 \ldots \infty \tag{2.29}
\]

where \( \hat{H} \) is a constant matrix and the vector \( h \) has all positive elements. A key feature of any LMPC strategy is the method used to relax the output constraints to achieve feasibility of the QP. While other techniques are available [102], only the three output handling methods discussed below are considered here.
Rawlings and Muske [91] propose the relaxation of output constraints during the initial portion of the prediction horizon when an infeasibility is encountered. They show the existence of a finite number $k_1$ such that the output constraints are guaranteed to be feasible for all $k > k_1$. For unstable systems, $k_1$ can be computed as [91]:

$$
k_1 = N + \max \left\{ \ln \left( \frac{h_{\min}}{\| F \| \| V_s \| z^*(k + N \| k \|)} \right) / \ln(\lambda_{max}), 1 \right\}
$$

(2.30)

where $\lambda_{max}$ is the largest eigenvalue of $J_s$ and $h_{\min}$ is the smallest element of vector $h$. Rawlings and Muske [91] also show the existence of a finite $k_2$ such that the output constraints are enforced over the rest of the infinite horizon if they are satisfied between $k_1$ and $k_2$. This is called the hard constraint handling method. For the pipeline system, the values of $k_1$ and $k_2$ calculated from these formulas can be very large (> 1000) because the largest stable eigenvalue (0.995) is very close to unity. This makes the constraint handling method rather difficult to implement.

To address this limitation, we propose an alternative hard constraint handling method. When an infeasibility occurs, the output constraints are removed at the first time step in the horizon and the QP is resolved. If the QP remains infeasible, then the output constraints at the second time step also are removed and the QP is resolved. This procedure is continued until the QP problem is feasible. The advantage of this approach is that the output constraints are relaxed the minimum number of times required to obtain feasibility. A shortcoming is that a potentially large number of QP problems must be solved at a single time step. For the pipeline

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system, we have found that the constraints must be removed only at the first one or two steps in the horizon. The problem of large $k_2$ values is circumvented by enforcing the output constraints only up to the control horizon $N$. Clearly, this approach does not guarantee that the constraints are satisfied over the entire horizon.

Zheng and Morari [123] propose an output constraint handling method in which slack variables are introduced to soften the output constraints. The slack variables are penalized by a positive definite weighting matrix $P_s$ in the objective function. The following LMPC problem is obtained:

$$\min_{U(k),s(k)} \phi_k = [x(k + N|k) - x_s]^{T}Q[x(k + N|k) - x_s]$$

$$+ \Delta u(k + N|k)^{T}S \Delta u(k + N|k)$$

$$+ \sum_{j=0}^{N-1} \{[x(k + j|k) - x_s]^{T}C^{T}QC[x(k + j|k) - x_s]$$

$$+ [u(k + j|k) - u_s]^{T}R[u(k + j|k) - u_s]$$

$$+ \Delta u(k + j|k)^{T}S \Delta u(k + j|k) + s(k)^{T}P_s s(k)\}$$

subject to:

$$y_{\min} - s(k) \leq y_c(k + j|k) \leq y_{\max} + s(k) \quad j = 1, \ldots, N$$

where $s(k)$ is a vector of slack variables. Again the output constraints are only enforced over the control horizon $N$. To formulate the QP, the output constraints
are written as inequality constraints in terms of $u^N$ and $s(k)$:

$$
\begin{bmatrix}
  D \\
  -D
\end{bmatrix}
\begin{bmatrix}
  u^N \\
  s(k)
\end{bmatrix}
\leq
\begin{bmatrix}
  d_1 \\
  d_2
\end{bmatrix}
$$

(2.32)

The formulation of $D$, $d_1$ and $d_2$ can be found in [80].

2.4 Simulation Results and Discussion

We now apply the LMPC controller to the simulated oxygen pipeline network. The reduced-order nonlinear plant model (see Figure 2.2) is used to represent the pipeline network. The control horizon is $N = 15$, and the quadratic weighting matrices in the objective function are chosen as: $Q = I_{3 \times 3}$, $R = 0.1 I_{6 \times 6}$, $S = 100 I_{6 \times 6}$. When the soft output constraint handling method is used, the penalty matrix $P_s$ on the slack variables is chosen as $50 I_{14 \times 14}$. These tuning parameters were determined via closed-loop simulation. Except for the let-down station valve position, the input and output constraints in deviations from the nominal steady states are:

\[
\begin{bmatrix}
  -200 \text{ kcfh} \\
  -150 \text{ kcfh} \\
  -200 \text{ kcfh} \\
  -200 \text{ kcfh} \\
  -210 \text{ kcfh} \\
  -14.9 \text{ psig}
\end{bmatrix}
\leq u(k) \leq
\begin{bmatrix}
  150 \text{ kcfh} \\
  150 \text{ kcfh} \\
  100 \text{ kcfh} \\
  100 \text{ kcfh} \\
  190 \text{ kcfh} \\
  25.1 \text{ psig}
\end{bmatrix}
\]

\[
\begin{bmatrix}
  -5.2 \text{ psig} \\
  -23 \text{ psig} \\
  -35.1 \text{ psig} \\
  0 \% \\
  \Gamma_{\min}
\end{bmatrix}
\leq y_{e}(k) \leq
\begin{bmatrix}
  29.8 \text{ psig} \\
  17 \text{ psig} \\
  24.9 \text{ psig} \\
  90 \% \\
  \Gamma_{\max}
\end{bmatrix}
\]
The limits $\Gamma_{\text{max}}$ and $\Gamma_{\text{min}}$ for the plant constraint variables are not reported for proprietary reasons. However, it is important to emphasize that none of these constraints are active during any of the following simulation tests. All simulations are performed in MATLAB on a DEC Alpha 433 workstation. A typical closed-loop simulation of 8 hours requires approximately 5 minutes of CPU time.

Figure 2.6 shows stabilization of the pipeline network at the nominal steady state. The figure includes the first four constrained outputs (including the three pressures controlled to setpoints) and the six manipulated inputs. The dotted lines represent the setpoints for the outputs and the actual flow rates corresponding to the first five inputs. For the last input, the dotted line represents the actual letdown station pressure. Because the controller design model is a reduced-order linear approximation of the plant model, there is plant/model mismatch even at steady state. This test shows that the LMPC controller is capable of handling the mismatch as the pressures are maintained within one psig of the desired steady-state values.

Figure 2.7 shows the closed-loop response for +10 psig setpoint changes in the node 24 and 29 pressures (see Figure 2.1) at $t = 3$ hr. Setpoint changes of the same magnitude are introduced since these two pressures should have a relatively constant pressure difference. This test simulates a desired pressure build-up on the high pressure side of the network to take advantage of low utility costs at off-peak hours. The initial transient is due to plant/model mismatch as discussed above. The new setpoints are achieved about two hours after the requests are issued, and
the pressure at node 12 is kept very close to its setpoint. The let-down valve is closed about 10 percent because the pressure drop across the valve is increased. For the first five inputs, the production requests (solid lines) increase rapidly when the
setpoint changes are implemented. The production requests for two plants reach their upper limits for a brief period of time. The actual production rates (dotted lines) follow the flow requests according to the first-order-plus-deadtime models used to model the closed-loop cryogenic plant dynamics.

The results obtained for two measured customer withdraw rate changes are shown in Figure 2.8. At \( t = 3 \) hr the customer withdraw rate at node 24 is increased by 100 kcfh, then at \( t = 8 \) hr the customer withdraw rate at node 1 is increased by 150 kcfh. This test models a combination of smaller customer withdraw rate changes near these nodes. Both disturbances are rejected with only small deviations of the outputs from their setpoints. The same test has been performed with the withdraw rates considered as unmeasured disturbances. Since a deadbeat observer is used to generate the disturbance estimates, and the entire state vector is measured, the controller responds very quickly to the demand changes. As a result, the closed-loop response is virtually identical to Figure 2.8 and is not shown here.

First-order-plus-dead-time (FOPDT) models obtained from plant tests are used to model the dynamics of the LMPC controlled cryogenic plants. In practice, the actual closed-loop plant behavior will deviate from the FOPDT model predictions. To examine the ability of the LMPC controller to handle this uncertainty, the time constant of each FOPDT model in the simulated plant is increased by 15 minutes (60% – 100% increases) while the controller design model is unchanged. The closed-loop response for the same disturbance sequence as in Figure 2.8 is shown in Figure
The controller rejects the measured disturbances quite effectively despite the modeling error. Although slightly larger production request changes are observed,
Figure 2.8: Disturbance rejection for known changes in customer withdraw.

the output responses are very similar to those obtained for a perfect model (Figure 2.8).
Figure 2.9: Disturbance rejection for known changes in customer withdraws with modeling errors in the cryogenic plant responses.

The complete shut-down of plant 10-1 represents a very large measured disturbance that is simulated to test the constraint handling abilities of the LMPC.
Figure 2.10: Disturbance rejection for known plant shutdown using the soft constraint handling method: $P_s = 50I$ (---) and $P_s = I$ (——).

controller. The upper constraint for the let-down valve position is reduced to 85% to allow output constraint violations to be examined more easily. Figure 2.10 shows
the results obtained with the soft output constraint handling method [123]. When the plant shut-down occurs at \( t = 3 \text{ hr} \), the pipeline pressures on the low pressure side drop rapidly. Production requests are driven to their upper limits to compensate for the pressure loss. Note that the node 29 pressure exhibits a large overshoot immediately after the initial pressure drop. This can be explained by noting that node 29 is on the high pressure side of the let-down valve while plant 10-1 is on the low pressure side. The plant 29-1 production rate responds quickly to the disturbance and causes the node pressures on the high pressure side to increase. Two different slack variable penalty matrices have been evaluated. When \( P_s = 50I \), the valve position (solid line) barely violates its upper limit. When \( P_s = I \), the valve position (dashed line) exhibits a significant violation of the upper constraint. The responses of the other variables are nearly identical. Clearly the tuning of \( P_s \) plays a critical role in the constraint handling behavior of the LMPC controller.

The hard output constraint method is not evaluated because the large \( k_1 \) values calculated from (2.30) effectively eliminates the output constraints over the entire horizon. In Figure 2.11, the alternative hard output constraint method described earlier is evaluated for the same disturbance and output constraints as in Figure 2.10. The output and input responses are very similar to those obtained with the soft constraint handling method (Figure 2.10). The QP remains feasible except at a few time steps where the upper valve position constraint is violated. At those time steps, feasibility is established by removing the output constraints only at the first
Figure 2.11: Disturbance rejection for known plant shutdown using the alternative hard constraint handling method.

time step and enforcing the constraints over the rest of the horizon \( j \in [k + 1, N] \).

This procedure allows the valve position constraint to be violated only very slightly.
Because this output constraint handling method may require the solution of a large number of QP problems when an infeasibility is encountered, careful tuning of the soft output constraint handling method appears to be preferred for this problem.

2.5 Summary and Conclusions

Effective control of large-scale gas pipeline networks is required to ensure safe and profitable operation. While pipelines are critical in the air separation and natural gas industries, the application of advanced control to such systems is not currently practiced. We have developed and evaluated a linear model predictive control (LMPC) strategy for a simulated industrial-scale oxygen pipeline network. A first-principles nonlinear model for the node pressures is derived from mass balances and the Virial equation of state. The LMPC design is based on a linearized model derived from a reduced-order nonlinear pipeline model. Both measured and unmeasured disturbances are systematically incorporated in the LMPC target calculations. The LMPC controller provides excellent closed-loop performance for a wide variety of setpoint changes and disturbances. Three output constraint handling techniques to resolve infeasibilities in the LMPC quadratic program have been examined. The proposed LMPC strategy can significantly improve the operability of large-scale gas pipeline networks and can enable gas suppliers to take full advantage of the deregulation of the utility industry.
Chapter 3

Lower-Order Dynamic Modeling of Cryogenic Distillation Columns Based on Nonlinear Wave Phenomenon

3.1 Introduction

Cryogenic distillation is used to produce large quantities of purified nitrogen, oxygen and argon for consumption in the steel, chemical, food processing, semiconductor and health care industries. Cryogenic distillation columns are operated at extremely low temperatures (-170 to -190 °C) to separate air components according to their different boiling temperatures. The purified streams are produced in liquid and/or gaseous states for transportation to end users. The major operational cost associated with cryogenic air separation plants is electricity. The domestic consumption of electricity by industrial gas producers is over $700 million per year. Therefore small improvements in process control have the potential to result in substantial economic benefits. Current control practice in the air separation industry involves the use of linear dynamic models and linear model predictive control. This approach has proven adequate because production rates are changed infrequently and startups/shutdowns are uncommon.

Deregulation of the electric utility industry is expected to lead to frequent and unpredictable changes in the cost of electricity. This will dictate fundamental
changes in the operating philosophy of air separation plants. Large changes in production rate and more frequent startups/shutdowns will be required to take full advantage of time-varying utility rates. Process nonlinearities will become much more pronounced, and some type of nonlinear control will be required to achieve satisfactory operation. The availability of a suitable nonlinear dynamic model is a prerequisite for the development of a nonlinear model-based controller. Because a typical nitrogen purification column has approximately 40 theoretical stages, a rigorous nonlinear model comprised of mass and energy balances for each stage is too complex for on-line control applications.

A number of researchers have investigated the formulation of low-order distillation column models and the use of these models for controller design [13, 32, 59]. Benallou et al. [13] achieve order reduction by combining a number of stages into a single equivalent stage. Levine and Rouchon [59] propose a similar approach based on singular perturbation techniques [53] to generate a reduced-order model that accounts only for the slow column dynamics. Gilles and Retzbach [32] propose a low-order dynamic model for distillation columns with sharp temperature profiles based on nonlinear wave theory and utilize the model for temperature profile position control.

Nonlinear wave theory was developed for multicomponent chromatography [38, 95]. The propagation of temperature and composition profiles in high-purity distillation columns was studied by Luyben [61]. Later Marquardt [62] derived expressions
for the wave propagation velocity and the shape of the wave profile in distillation columns from differential material balances. Meanwhile Hwang and Helfferich [46, 48] developed a distributed wave model for general counterflow separation processes. The model was used to capture the propagation, reflection, superposition and self-sharpening behaviors of concentration waves in nonlinear distillation columns [47]. More recently, a number of papers illustrating the use of wave models for distillation column control have appeared [10, 11, 35, 36, 93].

In this chapter, a low-order wave model for a nitrogen purification column is derived and compared to a first-principles model developed with the commercial dynamic simulator HYSYS.Plant (Hyprotech). As compared to previous work on nonlinear wave modeling of distillation columns, the major contributions of the current work include the application of wave modeling to cryogenic air separation columns, rigorous modeling of the combined reboiler/condenser assembly and the use of a rigorous dynamic simulator for model verification. The remainder of the chapter is organized in four sections. Section 3.2 provides a brief review of nonlinear wave theory for distillation column modeling. In Section 3.3 the low-order wave model for a nitrogen column is developed and a brief description of the HYSYS simulation model is presented. The low-order model is compared with the HYSYS model in Section 3.4. Section 3.5 concludes the chapter with a discussion of potential modeling enhancements and future control application.
3.2 Nonlinear Wave Models for Distillation Columns

The basic idea of the nonlinear wave model is that the concentration or temperature profile of a distillation column can be described by a wavefront with constant pattern. Column disturbances such as feed concentration and flow rate changes can be described by the movement and distortion of this profile. A number of assumptions are necessary to formulate simple mathematical expressions for the wave phenomenon. This allows the nonlinear wave model to be derived from differential material balances and equilibrium relations that characterize the wave profile and velocity.

3.2.1 Assumptions

Nonlinear wave models for distillation columns typically are based on the following assumptions:

1. Constant molar overflow
2. Constant molar holdup
3. Constant relative volatility
4. Perfect tray efficiency
5. Constant wave pattern
6. Binary mixture
The first two assumptions are used to simplify the wave velocity equation. The implication of the first assumption is that the heat of vaporization of the mixture does not change with composition. This holds if the components have similar heats of vaporization. From the HYSYS nitrogen column model described later, we observe that the top stage vapor and liquid flow rates are approximately 10% larger than the bottom flow rates due to heat of vaporization differences between pure nitrogen (1336 cal/mol) and pure oxygen (1629 cal/mol) [84]. The molar holdup is related to the column pressure and the molar volume of the mixture. In the HYSYS model the vapor phase holdups are approximately constant along the column, but the top stage liquid phase holdup is about 15% smaller than that of the bottom stage. Consequently the liquid molar holdup is assumed to be the average value over all stages. The constant relative volatility assumption is needed to derive the composition profile expression. The relative volatility between nitrogen and oxygen in the HYSYS model varies from 2.97 at the bottom of the column to 2.74 at the top of the column. Instead of calculating the composition profile parameters from the relative volatility and mass transfer coefficient [52], the parameters are estimated from HYSYS steady-state data as shown in the next section. Assumption 4 often is invoked in distillation modeling and also is used in the HYSYS model.

The constant wave pattern assumption is unique to nonlinear wave models. It is necessary to achieve the desired order reduction and works well for highly pinched separations in which the composition profile is flat at both sides of the column. As
shown later, the identification of an appropriate wave pattern is critical for generating accurate predictions. The limitation of this assumption is evaluated more carefully in Section 3.4. By considering oxygen and argon as a single lumped component, the problem is reduced to separation of a binary nitrogen/oxygen mixture. This assumption will be eliminated when a triple column system is considered. Assumptions used in the modeling of other equipment such as the combined reboiler/condenser are stated separately in Section 3.3.

3.2.2 Nonlinear Wave Theory

A nonlinear wave is defined in mathematical physics as a structure moving along a spatial coordinate with constant propagation velocity and constant shape. The high-order dynamics of distillation columns can be approximated by modeling the composition and temperature profiles as traveling nonlinear waves. To obtain the concentration profile and wavefront velocity equations, we start from the following differential material balance equations [62]:

\[
\frac{\partial x}{\partial \tau} - \frac{\partial x}{\partial z} = -B[y^* - y] \tag{3.1}
\]

\[
\frac{n_v \partial y}{n_l \partial \tau} + \frac{V \partial y}{L \partial z} = B[y^* - y] \tag{3.2}
\]

where: \(y\) and \(x\) are the vapor and liquid compositions, respectively; \(y^*\) is the vapor composition in equilibrium with \(x\); \(n_v\) and \(n_l\) are the vapor and liquid holdups on each tray, respectively; \(V\) and \(L\) are the vapor and liquid molar flow rates, respec-
tively; \( B \) is a dimensionless mass transfer coefficient; and the independent variables \( \tau \) and \( z \) are dimensionless time and spatial coordinates, respectively. The composition profile can be derived from the differential material balances if the vapor-liquid equilibrium relation \( y^* = f(x) \) is known [52, 62]. The wavefront propagation velocity can be derived from an overall material balance [63] or a material balance across the discontinuous shock wave front [95].

By assuming local equilibrium, \( y = y^* = f(x) \), the propagation velocity \( v \) of a specific concentration \( x_i \) can be derived from (3.1) and (3.2) [48]:

\[
\left( \frac{dz}{d\tau} \right)_{x_i} = \frac{-1 + \frac{V}{L} \left[ \frac{dy}{dx} \right]_{x_i}}{1 + \frac{n_c}{n_i} \left[ \frac{dy}{dx} \right]_{x_i}}
\]

(3.3)

It has been shown [95] that the wave is self-sharpening and will result in a discontinuity (shock wave formation) when the equilibrium relationship satisfies \( \frac{d^2 y}{dx^2} < 0 \). In practice, there always is a finite mass transfer rate and the boundary effect also will counteract the self-sharpening tendency of the wave [48]. Therefore a constant pattern wave is observed instead of a shock wave.

Nevertheless the wave propagation velocity can be approximated as the velocity of the idealized shock wave. The shock wave velocity equation can be derived using a component balance from the standpoint of an observer on the discontinuity [95] or from an overall component balance on the column with a discontinuous composition profile [63]. The velocity \( (w) \) expressed in actual time and normalized column height
is:

$$w = \frac{1}{N} \left( -L(x_{in} - x_{out}) + V(y_{out} - y_{in}) \right)$$

(3.4)

where: $N$ is the total number of theoretical stages; $x_{in}$ and $x_{out}$ are the liquid compositions entering and exiting the column, respectively; and $y_{in}$ and $y_{out}$ are the vapor compositions entering and exiting the column, respectively. Two distinct wave fronts with different wave velocities exist in the rectifying and stripping sections when the feed enters in the middle of the column. For the nitrogen column, there only is a rectifying section as all theoretical stages are located above the feed stage. Marquardt and Amrhein [63] have derived the velocity of the wave front when the concentration profile has varying shape. They note that the effect on the wave velocity is small.

The derivation of the composition profile for binary columns is attributable to Marquardt [62]. The material balance equations are transformed by introducing the wave coordinate $\xi$:

$$\xi = z - \nu \tau$$

(3.5)

where the $\nu$ is the wave velocity based on dimensionless time $\tau$ and is defined as $\nu = \frac{Nm}{L}w$. Then (3.1) and (3.2) take the form:

$$-(1 + \nu) \frac{dx}{d\xi} = -B[y^* - y]$$

(3.6)

$$\left(-\frac{n_v}{n_i} \nu + \frac{V}{L}\right) \frac{dy}{d\xi} = B[y^* - y]$$

(3.7)
The composition profile expression can be derived from (3.6) and (3.7) given the equilibrium relation \( y^* = f(x) \). For a quadratic equilibrium relation, the composition can be expressed explicitly in terms of the spatial position along the column:

\[
y(z) = y_{\min} + \frac{y_{\max} - y_{\min}}{1 + \exp[-\gamma(z - s)]}
\]

(3.8)

where: \( y_{\min} \) and \( y_{\max} \) are the concentration limits as \( z \to -\infty \) and \( z \to +\infty \), respectively; \( \gamma \) is the maximum slope of the profile; and \( s \) is the location of the wave front. The column dynamics are predicted by tracking the wave position \( s \) using the velocity equation (3.4). When an equilibrium relation with a constant volatility \( \alpha \) is used:

\[
y^*(x) = \frac{\alpha x}{1 + (\alpha - 1)x}
\]

(3.9)

only an implicit solution to (3.6) and (3.7) can be found [62]. In a recent paper by Kienle [52], the composition profile (3.8) is derived from the implicit solution under certain additional assumptions. Despite these limitations, the expression (3.8) is used in most nonlinear wave models due to its simplicity and the physical significance of its parameters.

The wave parameters \( y_{\min}, y_{\max} \) and \( \gamma \) are estimated from steady-state composition profile data and are assumed to be constant in the subsequent dynamic simulations. Due to the self-sharpening tendency discussed previously, it is important to note that the parameter \( \gamma \) actually is time varying. This behavior becomes quite pronounced for columns that are not highly pinched [62]. To account for time-
varying $\gamma$, multiple points on the composition profile must be tracked to describe different velocities along the spatial coordinate. This can be accomplished by discretizing the profile with respect to the spatial coordinate [48]. However a large number of ordinary differential equations are generated and the resulting model is rather complex. Balasubramhanya and Doyle [10] propose the use of a Kalman filter for on-line estimation of parameter $\gamma$. Their simulation results show close agreement between the adapted wave model and a full-order model with time-varying $\gamma$. We intend to utilize such an on-line parameter estimation scheme in our future closed-loop simulation studies. However in this paper an estimator is not used to allow the possible deficiencies of the nonlinear wave model to be investigated.

3.3 Low-Order Dynamic Model for Nitrogen Columns

The major process equipment for a nitrogen production plant are shown schematically in Figure 3.1. The feed air stream is first compressed to a pressure of 4-8 bars. Impurities such as water and carbon dioxide are removed from the feed stream via adsorption. The purified air stream is cooled by the waste and product streams in a multi-pass heat exchanger. A portion of the feed stream is expanded to provide additional cooling. The combined feed stream is fed to the bottom of a column with 42 theoretical stages. There is a sump below the feed stage where bottom liquid is accumulated. The liquid distributor improves the flow characteristics of the liquid moving down the column. Part of the column overhead stream is withdrawn as
the high-purity gaseous nitrogen product. The bottom liquid stream is expanded through a valve and partially liquefied. The resulting two-phase stream has a lower temperature than the overhead stream. In the combined condenser/reboiler, the partially liquefied bottom stream is vaporized and the gaseous nitrogen stream is condensed to produce the reflux stream and the liquid nitrogen product stream. Since the main focus of this paper is cryogenic column modeling, only the equipment inside the dashed line in Figure 3.1 are modeled. This includes the cryogenic column, the combined condenser/reboiler, and the expansion valve.

3.3.1 Nonlinear Column Modeling

The first step in formulating the nonlinear wave model is to find the parameters \( y_{\text{max}}, y_{\text{min}}, \) and \( \gamma \) associated with the composition equation (3.8). These parameters are generated from steady-state composition profile data by least-squares estimation subject to boundary conditions and constraints on \( y_{\text{min}} \) and \( y_{\text{max}} \):

\[
\min_{y_{\text{min}}, y_{\text{max}}, \gamma} \sum_{i=1}^{N} [\hat{y}(z_i) - y(z_i)]^2
\]

subject to:

\[
\hat{y}(z_1) = y(z_1)
\]

\[
\hat{y}(z_N) = y(z_N)
\]

\[0 \leq y_{\text{max}} \leq 1\]

\[0 \leq y_{\text{min}} \leq 1\]
where: $z_i$ is the normalized distance of stage $i$ from the bottom of the column; 
$\hat{y}(z_i)$ denotes the vapor phase composition estimate at stage $i$ from (3.8); and $y(z_i)$ is the vapor phase composition at stage $i$ obtained from steady-state solution of
the HYSYS model. Note that the column section includes all the theoretical stages above the feed. The boundary conditions guarantee that both models have the same concentrations at the column section entrance and exit. The lower and upper limits maintain $y_{\text{min}}$ and $y_{\text{max}}$ within a physically meaningful region. It will shown later that the parameter values obtained are strongly affected by the steady-state profile used for estimation.

The model equations shown below include the wave description of the column dynamics and a steady-state material balance for the feed stage. The steady-state approximation is justified because the feed stage dynamics are much faster than the overall column dynamics.

$$ w = \frac{ds}{dt} = \frac{1}{N} \frac{-L(x_{\text{in}} - x_{\text{out}}) + qF(y_{\text{out}} - y_{\text{in}})}{n_{\text{i}}(x_{\text{in}} - x_{\text{out}}) + n_{\text{v}}(y_{\text{out}} - y_{\text{in}})} $$  \hspace{1cm} (3.11)

$$ y_{\text{out}} = y_{\text{min}} + \frac{y_{\text{max}} - y_{\text{min}}}{1 + \exp[-\gamma(1 - s)]]} $$  \hspace{1cm} (3.12)

$$ y(0) = y_{\text{min}} + \frac{y_{\text{max}} - y_{\text{min}}}{1 + \exp(\gamma s)} $$ \hspace{1cm} (3.13)

$$ x_{\text{out}} = \frac{y(0)}{\alpha - (\alpha - 1)y(0)} $$  \hspace{1cm} (3.14)

$$ y_{\text{in}} = \frac{\alpha x_f}{1 + (\alpha - 1)x_f} $$  \hspace{1cm} (3.15)

$$ Fz_f + Lx_{\text{out}} = qFy_{\text{in}} + [(1 - q)F + L]x_f $$  \hspace{1cm} (3.16)

where: $F$, $q$ and $z_f$ are the flow rate, vapor fraction and nitrogen composition of the feed air, respectively; and $x_f$ is the feed stage liquid nitrogen composition. The wave front position $s$ is described by the velocity equation (3.11) which is identical
to (3.4). Note that the liquid distributor holdup is split equally among all the stages to account its dynamic effect. The composition of the overhead vapor stream \(y_{out}\) is calculated from the composition profile equation (3.8) at the top of the column \(z = 1\). The vapor composition at the bottom of the column \(z = 0\) is calculated analogously. The composition of the exiting liquid stream \(x_{out}\) is determined from (3.9) based on the assumption that \(x_{out}\) and \(y(0)\) are equilibrium concentrations. The composition of the vapor stream entering the column \(y_{in}\) is determined from (3.15)–(3.16) where the feed stage is assumed to be in equilibrium and at steady state. The reflux stream composition \(x_{in}\) is calculated from the condenser balances presented below. The equations (3.15)–(3.16) associated with \(y_{in}\) and \(x_{f}\) can be combined to yield a single quadratic equation that can be solved for \(x_{f}\). It can be shown that one root always violates a physical constraint. The \(y_{in}\) value corresponding to \(x_{f}\) can be substituted into the velocity equation (3.11). The vapor composition at each stage can be found from the profile equation (3.8), while the corresponding liquid compositions can be determined from the equilibrium relation (3.9). Therefore the model equations (3.11)–(3.16) can be reduced to a single nonlinear ordinary differential equation.

The top stage column pressure is equal to the condenser pressure, which is determined from the condenser model presented below. The column pressure profile is specified by assuming a constant, linear pressure drop between the top and bottom of the column. Because the composition and pressure of each stage are known, the
stage temperatures can be determined from the vapor-liquid equilibrium relationship. For example, the feed stage temperature \( T_f \) can be calculated from Raoult's law since the solution is ideal and the pressure is moderate:

\[
y_{in}P_f = x_f P_{N_2}^{sat}(T_f)
\]  

(3.17)

where \( P_f \) is the feed stage pressure and \( P_{N_2}^{sat}(T_f) \) is the nitrogen vapor pressure estimated from Wagner's equation [94].

### 3.3.2 Dynamic Modeling of Associated Equipment

The remaining model equations describe the column sump, the expansion valve and the combined condenser/reboiler. A dynamic model is required for this equipment to predict the overhead pressure and reflux composition. The liquid composition of liquid in the column sump is assumed to be equal to the feed stage liquid composition \( x_f \) for simplicity. The sump level is described by the following material balance equation:

\[
\frac{dH_s}{dt} = \frac{1}{\rho(x_f)V_s} [L + (1 - q)F - F_s]
\]  

(3.18)

where \( H_s \), \( V_s \) and \( F_s \) denote the sump level, sump volume and sump outlet flow, respectively. The sump outlet flow is manipulated by a proportional-integral (PI) controller to regulate the sump level. The liquid density \( \rho(x_f) \) is estimated from the
pure component density, using following mixing rule:

\[
\frac{1}{\rho(x_f)} = \frac{x_f}{\rho_{N_2}} + \frac{(1-x_f)}{\rho_{O_2}}
\]  

(3.19)

The bottom stream temperature is reduced by the expansion valve. The properties of the resulting two-phase stream are determined from a flash calculation across the expansion valve:

\[
y_{N_2}^v P_r = P_{N_2}^{sat}(T_v)x_{N_2}^v
\]  

(3.20)

\[
y_{O_2}^v P_r = P_{O_2}^{sat}(T_v)x_{O_2}^v
\]  

(3.21)

\[
x_f F_s = y_{N_2}^v F_s q_v - x_{N_2}^v F_s(1 - q_v)
\]  

(3.22)

\[
(1-x_f) F_s = y_{O_2}^v F_s q_v - x_{O_2}^v F_s(1 - q_v)
\]  

(3.23)

\[
x_{N_2}^v + x_{O_2}^v = 1
\]  

(3.24)

\[
h_l(T_f, x_f) F_s = h_l(T_v, x_{N_2}^v) F_s(1 - q_v) + h_v(T_v, y_{N_2}^v) F_s q_v
\]  

(3.25)

where: the superscript/subscript \( v \) represents properties associated with the expansion valve exit stream; \( y_{N_2}^v, x_{N_2}^v, y_{O_2}^v \) and \( x_{O_2}^v \) are the vapor and liquid phase compositions of nitrogen and oxygen; \( q_v \) is the vapor fraction; \( T_v \) is the stream temperature; \( P_{N_2}^{sat} \) and \( P_{O_2}^{sat} \) are the nitrogen and oxygen vapor pressures, respectively; \( h_l \) and \( h_v \) are the liquid and vapor enthalpies, respectively; and the stream pressure is equal to the reboiler pressure \( P_r \). While more sophisticated enthalpy correlations are available [94], both liquid and vapor enthalpies are assumed to be a function.
only of temperature and composition:

\[ h(T, x_i) = \sum_{i=1}^{2} x_i(h_i^o + \int_{T^o}^{T} C_p_i dT) \]  

(3.26)

\[ C_{p_i} = C_{p_{iA}} + C_{p_{iB}} T + C_{p_{iC}} T^2 \]  

(3.27)

where \( h_i^o \) is the enthalpy of pure component \( i \) at the reference temperature \( T^o \) and \( C_{p_i} \) is chosen as a second order polynomial in \( T \). The correlation parameters \((C_{p_{iA}}, C_{p_{iB}}, C_{p_{iC}})\) for the liquid and vapor phases are estimated from enthalpy data generated using HYSYS at the pressure \( P_r \) and over a reasonable range of operating temperatures. The enthalpy calculation is performed at constant pressure because the reboiler pressure is regulated by a PI controller and should not vary significantly from its setpoint.

After exiting the expansion valve, the bottom stream is fed to the reboiler. Expansion causes the bottom stream temperature to become lower than the temperature of the vapor exiting the top of the column. Thus the bottom stream inside the reboiler can be used to condense the overhead vapor stream in the condenser. Figure 3.2 illustrates the configuration of the combined condenser/reboiler. In the reboiler, a large amount of liquid is vaporized \((F_v)\) and significant amount of the liquid \((F_L)\) is carried away from the pool by the vaporizing stream. The liquid stream spills over the side of the condenser and then is returned to the liquid pool. Since the bulk of the reboiler liquid and vapor phases are not in direct contact, they cannot be assumed to be in equilibrium. However the vaporizing stream and the
returning liquid stream are in equilibrium. Therefore the reboiler can be modeled by separate balance equations for each phase coupled with a flash calculation for the vaporizing stream.

Three assumptions are invoked for the combined condenser/reboiler to reduce the complexity of the resulting model. The first assumption is that the ratio of the reboiler vaporizing stream flow rate \((F_V)\) and returning liquid stream flow rate \((F_L)\) is constant. This allows variables such as the reboiler temperature, the flow rates \(F_V\) and \(F_L\), and the associated compositions to be determined from a flash calculation and a liquid phase energy balance. The second assumption is that the temperature...
difference between the reboiler and condenser is constant. This assumption eliminates the need for an additional condenser energy balance and is supported by plant data. The third assumption is that the condenser liquid is saturated. This allows the condenser pressure to be solved directly from the component vapor pressures and the liquid composition. The reboiler model equations are:

\[
\frac{dM_l}{dt} = (1 - q_v)F_s - F_V - F_{rl} 
\]

(3.28)

\[
\frac{dM_v}{dt} = q_v F_s + F_V - F_{rv} 
\]

(3.29)

\[
\frac{dM_l x_r}{dt} = (1 - q_v)F_s x_{N_2}^L - (F_V + F_L)x_r + F_L x_{N_2}^L - F_{rl} x_r 
\]

(3.30)

\[
\frac{dM_v y_r}{dt} = q_v F_s y_{N_2}^V + (F_V + F_L)x_r - F_L x_{N_2}^L - F_{rv} y_r 
\]

(3.31)

\[
\frac{dM_l h_l(T_r, x_r)}{dt} = (1 - q_v)F_s h_l(T_v, x_{N_2}^V) - F_V h_v(T_r, x_r) - F_L h_l(T_r, x_r) + Q 
\]

(3.32)

\[
y_{N_2}^V P_r = P_{N_2}^{\text{sat}}(T_r) x_{N_2}^L 
\]

(3.33)

\[
y_{O_2}^V P_r = P_{O_2}^{\text{sat}}(T_r) x_{O_2}^L 
\]

(3.34)

\[
x_r(F_L + F_V) = F_V y_{N_2}^V - F_L x_{N_2}^L 
\]

(3.35)

\[
(1 - x_r)F_s = F_V y_{O_2}^V - F_L x_{O_2}^L 
\]

(3.36)

\[
x_{N_2}^L + x_{O_2}^L = 1 
\]

(3.37)

\[
\frac{F_L}{F_V} = r 
\]

(3.38)

where: \( M_l \) and \( M_v \) are the liquid and vapor molar holdups in the reboiler, respectively; \( F_{rl} \) and \( F_{rv} \) are the liquid and vapor flow rates leaving the reboiler, respec-
tively; the nitrogen compositions of these two streams are denoted \( x_r \) and \( y_r \); the nitrogen and oxygen compositions associated with the flows \( F_V \) and \( F_L \) are denoted \( y_{N_2}^V, y_{O_2}^V, x_{N_2}^L \), and \( x_{O_2}^L \); \( T_r \) is the reboiler temperature; \( Q \) is the heat transfer rate between the condenser and reboiler; and \( r \) is called the priming ratio and is assumed to be constant.

Equations (3.28)–(3.31) can be manipulated to yield nonlinear ordinary differential equations for the reboiler level \((H_r)\), the reboiler pressure \((P_r)\), and the reboiler liquid and vapor phase compositions \((x_r, y_r)\):

\[
\frac{dH_r}{dt} = \frac{(1 - q_v)F_s - F_V - F_{rl}}{\rho(x_r)V_r} - \frac{\rho N_2 - \rho O_2}{[\rho(x_r)]^2 V_r} [(1 - q_v)F_s(x_{N_2}^V - x_r) + F_L(x_{N_2}^L - x_r)]
\]

\[
\frac{dP_r}{dt} = \frac{RT_r}{V_r(1 - H_r)} (V + q_v F_s - F_{rv} + P_r V_r \frac{dH_r}{dt})
\]

\[
\frac{dx_r}{dt} = \frac{(1 - q_v)F_s(x_{N_2}^V - x_r) + F_L(x_{N_2}^L - x_r)}{\rho(x_r)H_r V_r}
\]

\[
\frac{dy_r}{dt} = \frac{RT_r}{P_r V_r (1 - H_r)} [q_v F_s(y_{N_2}^V - y_r) + F_V(y_r - y_r) + F_L(x_r - x_{N_2}^L)]
\]

where \( V_r \) is the reboiler volume and \( R \) is the gas constant. Here the ideal gas law has been used to calculate the pressure from the vapor phase molar holdup. The reboiler pressure and level are controlled by PI controllers which manipulate the reboiler vapor and liquid exit flows, respectively. The liquid phase energy balance (3.32) can be transformed into an algebraic equation by substitution of the derivatives \( dM_t/dt \) (3.28), \( dx_r/dt \) (3.41) and \( dT_r/dt \). We invoke the quasi-steady-state
assumption for the reboiler temperature; \((dT_r/dt \approx 0)\), because the temperature dynamics are much faster than the level and composition dynamics. A rigorous description of the temperature dynamics based on an overall energy balance on the reboiler is not pursued because the resulting model equations are complex. The reboiler temperature along with the vaporizing and returning liquid stream flow rates and compositions are calculated from the liquid phase energy balance and the flash equations (3.32)-(3.38).

The condenser temperature is approximated as \(T_c = T_r + \Delta T\), where \(\Delta T\) is a constant temperature difference between the reboiler and condenser. Since the condenser liquid is assumed to be saturated, the condenser pressure \(P_c\) can be calculated as:

\[
P_c = x_c P_{N_2}^{\text{sat}}(T_c) + (1 - x_c) P_{O_2}^{\text{sat}}(T_c)
\]

(3.43)

where \(x_c\) is the condenser liquid composition. In the limit as the condenser liquid is pure nitrogen, this equation reduces to \(P_c = P_{N_2}^{\text{sat}}(T_c)\). The condenser level \((H_c)\) and liquid composition \((x_c)\) are described by following equations:

\[
\frac{dH_c}{dt} = \frac{qF - F_{LN2} - F_{GN2} - L}{\rho(x_c)V_c}
\]

(3.44)

\[
\frac{dx_c}{dt} = \frac{(qF - F_{GN2})(y_{out} - x_c)}{\rho(x_c)V_cH_c}
\]

(3.45)

where: \(V_c\) is the condenser volume; and \(F_{LN2}\) and \(F_{GN2}\) are the liquid and gas nitrogen production rates, respectively.
The complete nitrogen column model is comprised of eight ordinary differential equations (3.11, 3.18, 3.39, 3.40, 3.41, 3.42, 3.44, 3.45) and fifteen algebraic equations (3.17, 3.20, 3.21, 3.22, 3.23, 3.24, 3.25, 3.32, 3.33, 3.34, 3.35, 3.36, 3.37, 3.38, 3.43). The majority of the equations are associated with the expansion valve and the combined condenser/reboiler. The dependent variables in the differential equations are: \( s, H_s, H_r, P_r, x_r, y_r, H_c \) and \( x_c \). The variables determined from the algebraic equations are: \( T_f, T_v, y_{N_2}, y_{O_2}, x_{N_2}, x_{O_2}, q_v, T_r, y_{N_2}, y_{O_2}, x_{N_2}, x_{O_2}, F_v, F_L \) and \( P_c \). A list of variables can be found in Appendix B.1.

The differential-algebraic equation model is solved in MATLAB. In addition to the model equations described above, four PI control loops are included for regulation of the column sump level \( (H_s) \), reboiler level \( (H_r) \), reboiler pressure \( (P_r) \), and condenser level \( (H_c) \). The manipulated variables for these controllers are the sump exit flow \( (F_s) \), reboiler liquid exit flow \( (F_{rl}) \), reboiler vapor exit flow \( (F_{rv}) \) and reflux rate \( (L) \). The PI controllers are tuned to have similar closed-loop responses as observed in the HYSYS model. Although both the HYSYS and low-order models include an explicit control loop for the condenser level, this variable is self-regulating in real plants.

### 3.4 Simulation Study

Possible disturbances encountered during normal operation of a nitrogen column include changes in the feed air rate, feed air vapor fraction, and the desired gaseous and liquid nitrogen production rates. The liquid and vapor flow rates inside the
column will change transiently as a result of these disturbances. The composition profile will move up or down the column until a new steady-state position is established. Since we are interested in the dynamic behavior of the nitrogen column during startups and shutdowns, large disturbances that cause the wave front to move over a wide range are introduced. First a set of wave model parameters must be estimated from a representative steady-state composition profile.

### 3.4.1 Parameter Estimation Using Steady-State Data

During normal operation, the cryogenic distillation column produces gaseous and liquid nitrogen products with 1 ppm oxygen and 1000 ppm argon. A HYSYS steady state corresponding to a high purity nitrogen product is listed in Table 3.1 as HYSYS SS1. Also shown in Table 3.1 is a steady-state corresponding to a lower product purity which is referred to as HYSYS SS2.

The wave model parameters \((y_{\text{min}}, y_{\text{max}}, \gamma)\) are estimated for each HYSYS steady state by solving the optimization problem (3.10). The results are:

- **SS1:** \(y_{\text{min}} = 0.7367, y_{\text{max}} = 1, \gamma = 6.6154\).
- **SS2:** \(y_{\text{min}} = 0.7894, y_{\text{max}} = 1, \gamma = 11.1578\).

Figure 3.3 shows the vapor phase \(N_2\) composition along the column for the two HYSYS steady states and the estimated profiles from the low-order wave model. While the composition profile can be approximated accurately with the function (3.8), the optimal parameters \(y_{\text{min}}\) and \(\gamma\) are different for the two steady states.
The wave front slope ($\gamma$) changes as the wave propagates through the column due to the self-sharpening tendency described in Section 3.2. Under the constant pattern assumption, the performance of the nonlinear wave model depends strongly on the selection of the steady-state profile used for estimation. It is important to note that the value of $y_{\min}$ should not change unless the feed composition changes. We have found that SS2 yields a better estimate of $y_{\min}$ because the bottom composition is very close to the pinched lower column composition. The other steady state SS1 yields a lower $y_{\min}$ estimate than the true value because the nitrogen composition is not pinched at the column bottom. Therefore although SS1 is the more desirable
Table 3.1: Nitrogen plant steady-state operating conditions.

<table>
<thead>
<tr>
<th>Variables</th>
<th>HYSYS SS1</th>
<th>Low-order SS1</th>
<th>HYSYS SS2</th>
<th>Low-order SS2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F$ (kmol/hr)</td>
<td>100.8</td>
<td>100.8</td>
<td>98.5</td>
<td>98.5</td>
</tr>
<tr>
<td>$q$</td>
<td>0.969</td>
<td>0.969</td>
<td>0.965</td>
<td>0.965</td>
</tr>
<tr>
<td>$z_f$</td>
<td>0.7811</td>
<td>0.7811</td>
<td>0.7811</td>
<td>0.7811</td>
</tr>
<tr>
<td>$T_f$ ($^\circ$C)</td>
<td>-179.9</td>
<td>-180.07</td>
<td>-179.9</td>
<td>-179.89</td>
</tr>
<tr>
<td>$y_{out}$</td>
<td>0.9990</td>
<td>0.9990</td>
<td>0.9956</td>
<td>0.9956</td>
</tr>
<tr>
<td>$P_{top}$ (kPa)</td>
<td>326.8</td>
<td>327.9</td>
<td>326.8</td>
<td>329.3</td>
</tr>
<tr>
<td>$H_s$ (%)</td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>$T_v$ ($^\circ$C)</td>
<td>-189.0</td>
<td>-189.16</td>
<td>-188.9</td>
<td>-189.15</td>
</tr>
<tr>
<td>$q_v$</td>
<td>0.09123</td>
<td>0.0923</td>
<td>0.09158</td>
<td>0.0933</td>
</tr>
<tr>
<td>$H_r$ (%)</td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>$P_r$ (kPa)</td>
<td>134.5</td>
<td>134.5</td>
<td>134.2</td>
<td>134.3</td>
</tr>
<tr>
<td>$T_r$ ($^\circ$C)</td>
<td>-185.8</td>
<td>-185.9</td>
<td>-185.8</td>
<td>-185.8</td>
</tr>
<tr>
<td>$x_r$</td>
<td>0.2558</td>
<td>0.4690</td>
<td>0.2496</td>
<td>0.4633</td>
</tr>
<tr>
<td>$y_r$</td>
<td>0.5672</td>
<td>0.6534</td>
<td>0.5602</td>
<td>0.6483</td>
</tr>
<tr>
<td>$H_c$ (%)</td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>50</td>
</tr>
</tbody>
</table>

The steady-state values generated from the HYSYS and wave models are compared in Table 3.1. The wave model predictions are in good agreement with the HYSYS steady states with the exception of the reboiler compositions ($x_r$ and $y_r$). This discrepancy is a direct result of the simplified condenser/reboiler model. However, the streams exiting the reboiler are not products nor do they significantly affect the column dynamics. Because this paper focuses on modeling of the column dynamics, the simple condenser/reboiler model is considered adequate.
3.4.2 Dynamic Simulation Results

A number of tests involving step changes in the feed air rate are simulated using the HYSYS model and the low-order wave model developed in MATLAB. Disturbances in other variables such as feed vapor fraction and nitrogen production rates produce similar dynamic responses; therefore these results are not included. Changes in feed composition generate different dynamic responses than do feed flow rate changes. However such disturbances are not very meaningful for a single column air separation plant.

First the feed air rate is decreased by 10 kmol/hr at $t = 1 \text{ hr}$. The model responses are shown in Figures 3.4 and 3.5. Figure 3.4 shows the top and bottom stage nitrogen vapor mole fractions in the column. Both the HYSYS model (solid line) and the low-order wave model (dashed line) predict a similar decrease in the overhead composition ($y_{out}$) since the reflux ratio decreases with lower reflux flow rate and constant product flow rates. However the transient responses produced by two models are noticeably different. In particular the wave model predicts faster $y_{out}$ dynamics than does the HYSYS model. Both models predict that the bottom composition $y(0)$ will decrease only slightly as the wave front moves upward in the column after the step change. Figure 3.5 shows that the composition profile is pinched in the lower part of the column and the value of $y(0)$ is bounded below by $y_{min}$. 

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Figure 3.4: $y_{out}$ and $y(0)$ responses for a -10 kmol/hr step change in the feed air flow rate (SSS2).

The composition profiles at $t = 1, 1.2$ and 5 hr shown in Figure 3.5 illustrate the profile sharpening behavior of the HYSYS model. As explained earlier this effect is due to the nonlinear equilibrium relationship which causes the propagation velocity to decrease with increasing nitrogen concentration. The top composition $y_{out}$ initially is very close to unity and travels slower in the HYSYS model than in the nonlinear wave model where only the inflection point of the wave front is tracked. In the HYSYS model $y_{out}$ decreases with an increasingly larger velocity until the wave approaches a new steady-state profile. By contrast the constant wave pattern assumed in the derivation of the wave model requires that all concentrations travel

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with the same velocity. Although the two models produce very similar $y_{out}$ values at the new steady state, the shapes of the composition profiles are significantly different.

To account for the distortion of the wave shape, Balasubramhanya and Doyle [10] propose the use of a Kalman filter to update the wave parameter $\gamma$ based on measurements of the overhead and bottom compositions. Rehm and Allgower [93] directly calculate on-line new values of $y_{min}$ and $y_{max}$ from the measured overhead and bottom compositions. To demonstrate the applicability of the wave model for on-line control applications, we show that at any instant in time $\gamma$ can be adjusted
such that the wave model produces a very similar concentration profile to that of the HYSYS model. Assuming the overhead composition is measured, the value of $\gamma$ at any time can be determined from the boundary condition $y(1) = y_{out}$ using the composition profile expression (3.8) when $y_{\text{min}}$ and $y_{\text{max}}$ remain constant. In Figure 3.6 the profiles generated from the updated $\gamma$ are compared to the HYSYS profiles in Figure 3.5 at $t = 1, 1.2$ and $5$ hr. The values calculated are $\gamma = 11.16$ at $t = 1$ hr, $\gamma = 14.37$ at $t = 1.2$ hr and $\gamma = 24.37$ at $t = 5$ hr. Clearly the use of a time-varying $\gamma$ allows much closer agreement with HYSYS results. Constant $\gamma$ is used in the subsequent simulations to illustrate the behavior of the non-adapted wave model.

Figure 3.7 shows the model responses obtained over a wide range of operating conditions when a series of smaller step changes (-5 kmol/hr at $t = 1, 4, 7$ hr and +5 kmol/hr at $t = 10, 13$ hr) in the feed air flow rate are introduced. For the first step change a similar discrepancy between the two models as in Figure 3.4 is observed. However the dynamic responses are in much closer agreement for the subsequent step changes. This occurs because the velocity difference between the inflection point tracked in the wave model and $y_{out}$ in the HYSYS model is reduced as the top composition moves away from the high purity region. This result supports the argument that the prediction error is caused primarily by the constant wave pattern assumption rather than the constant flow rate and holdup assumptions.
While the constant wave pattern assumption is required to achieve model order reduction, it does introduce modeling error since the actual plant exhibits more complex wave behavior. Now we show that the prediction accuracy of the nonlinear wave model depends strongly on the parameter values chosen for $\gamma$, $y_{\text{min}}$ and $y_{\text{max}}$. In Figures 3.8 and 3.9 the wave model derived from the SS1 profile is compared with the HYSYS model for a feed air flow rate change of -10 kmol/hr at $t = 1$ hr. The accuracy of the wave model is poor for both the overhead and bottom compositions. The $y(0)$ response is particularly poor as the effect of the air flow rate change is grossly exaggerated. The high purity operating conditions at SS1
Figure 3.7: $y_{out}$ response for multiple step change in the feed air flow rate (SS2).

yield an incorrect value for $y_{min}$, which in turn causes the dramatic differences in $y(0)$. As demonstrated in Figure 3.9, the estimated $y_{min}$ value of 0.7367 causes the bottom composition to drop below the actual low limit.

Figure 3.9 shows that the composition profile generated by the HYSYS model sharpens significantly as the wave travels up the column. The new steady-state value of the overhead composition is 0.963 while the wave model predicts a new steady-state value of 0.978. Note that the wave model predicts a smaller velocity for the overhead composition than does the HYSYS model. This is attributable to both the self-sharpening effect and the offsets in steady-state parameter estimation.
As shown in Figures 3.4 and 3.5, the prediction accuracy of the wave model is improved dramatically when a more representative wave profile is used to estimate the parameters.

Since overhead products of SS1 have very high purity, we are interested in modeling changes that lead to an ultra-high purity product. Figures 3.10 and 3.11 show the results obtained when the feed air flow rate is increased by 4 kmol/hr at \( t = 1 \) hr. As shown in Figure 3.10, both models predict an increase in the top composition. The HYSYS model reaches a steady-state composition of 0.9996 while the wave model predicts a steady-state composition of 0.99997. This difference

Figure 3.8: \( y_{out} \) and \( y(0) \) responses for a -10 kmol/hr step change in the feed air flow rate (SS1).
probably is caused by small errors in steady-state parameter estimation. A larger steady-state error is observed for the bottom composition. The initial and final steady-state composition profiles for the two models are shown in Figure 3.11. The wave model yields slightly larger compositions near the top of the column than does the HYSYS model. This discrepancy leads to the observed difference in the overhead composition transient responses. The difference between the bottom compositions are more significant due to the constant wave pattern assumption used in the wave model. As the wave travels down the column, the velocity at a fixed composition
Figure 3.10: $y_{out}$ and $y(0)$ responses for +4 kmol/hr step change in the feed air flow rate (SS2).

decreases due to the nonlinear equilibrium relationship. Therefore the HYSYS model bottom composition increases slower and converges to a smaller value.

When the plant is operated at ultra high purity, it is convenient to describe the top composition in terms of the oxygen in parts per million. In this case it is necessary to group the nitrogen and argon together and to formulate a wave model that describes the oxygen concentration profile. The formulation of the oxygen wave model is analogous to that presented earlier for nitrogen. Figure 3.12 shows the response of the overhead oxygen composition for a step change of +2.4 mol/hr in the feed air flow rate. Although a discrepancy in transient behavior is observed,
the new steady-state value is very close to that predicted by the HYSYS model. This occurs because the composition profile is very close to zero in the upper part of the column and a small distortion in the wave front does not significantly affect the overhead composition prediction. On the other hand, there is a more significant discrepancy in bottom oxygen compositions due to profile distortion (not shown). These conclusions are supported by the composition profiles shown in Figure 3.13.

### 3.5 Summary and Conclusions

The nonlinear wave modeling approach has achieved significant order reduction for the single nitrogen column studied in this paper. A nitrogen column is designed to
produce a high purity top product and has no purity requirement for the bottom stream. As a result, the wave profile parameters estimated from normal operating conditions are not suitable for model development. A small negative change in the air feed flow rate produces a more representative profile from which better parameter values can be obtained. Simulation results have shown that the low-order wave model is capable of producing acceptable prediction of composition responses for certain types of disturbances. However the constant wave pattern assumption used in the wave model development leads to prediction errors. We have shown that

Figure 3.12: Overhead oxygen composition responses for +2.4 kmol/hr step change in the feed air flow rate.
discrepancies between the nonlinear wave model and a first-principles HYSYS model can be made acceptably small by adjustment of the wave slope $\gamma$.

The nonlinear wave modeling approach can be applied to air separation plants containing three columns that produce purified nitrogen, oxygen and argon. Each column section will require a separate wave model. Additionally we will need to develop a nonlinear wave model for the ternary mixture in the upper column where all three components have significant concentrations. In a recent paper, Kienle [52] proposed linear superposition of nonlinear waves for multicomponent distillation columns. The primary motivation for derivation of the wave model is the dev-
opment of a model-based nonlinear control strategy for air separation plants. It is feasible to solve the single column model comprised of eight ordinary differential equations and fifteen algebraic equations in an optimization-based framework such as nonlinear model predictive control [70]. The control work will be pursued in parallel with the nonlinear wave modeling work.
Chapter 4

Model Predictive Control of Continuous Yeast Bioreactors Using Cell Population Balance Models

4.1 Introduction

*Saccharomyces cerevisiae* (Baker’s yeast) is an important microorganism in a number of industries including brewing, baking, food manufacturing and genetic engineering. Under routine operating conditions, continuous bioreactors producing *Saccharomyces cerevisiae* can exhibit autonomous and sustained oscillations [115]. The oscillations eventually disappear, presumably due to external disturbances or deficiencies in the medium. Similar oscillations have been observed in other continuous microbial cultures [67]. In most situations, oscillations adversely affect bioreactor operability and the objective is to eliminate the limit cycle behavior by stabilizing a chosen steady state. On the other hand, it may be desirable to induce and stabilize oscillations to increase the production of metabolites that are produced during a certain phase of the cell cycle [41]. To achieve these objectives, it is necessary to derive a dynamic model that describes the oscillatory behavior and to develop a control strategy that allows modification of the intrinsic reactor dynamics.

The mechanisms responsible for sustained oscillations in *Saccharomyces cerevisiae* cultures are controversial and a subject of current research. The oscillatory
behavior has been modeled by segregated structured models [20, 114], segregated unstructured models [43] and metabolic (cybernetic) models [50]. Unsegregated (also known as distributed) models are based on the assumption of a continuous and well-mixed biophase, while segregated models treat the biophase as a population of cells with different properties. Unstructured models have no chemical structure imposed on the biophase, while structured models are based on an assumed chemical structure. Segregated structured models are capable of representing a broad range of cell mechanisms. However, parameter identification and numerical solution of such models are very difficult due to the large number of variables involved. Moreover, Beuse et al. [15] show that the assumption of certain cell classes may lead to a structured segregated model [114] that cannot model experimentally observed changes of cell subpopulations over a range of dilution rates. A segregated unstructured model is proposed because this is perhaps the simplest model form that is able to predict periodic behavior of the cell population and its relation to cell cycle synchrony [43, 44].

Cybernetic models explain oscillations via metabolic events such as the competition between glucose oxidative and fermentative pathways [50]. Due to their unsegregated nature, this class of models cannot directly explain cell synchronization (i.e. the formation of distinct cell subpopulations) that accompanies the oscillations [21]. Instead, cell cycle synchrony is assumed to be a consequence of the metabolic oscillations. Our previous work [40] shows that induction synchrony can occur only
when the period of the metabolic forcing is equal to the period of the cell cycle. Consequently, metabolic models resort to a coincidental match of the metabolic and cell cycle periods to explain the observed cell cycle synchrony. As discussed in Section 4.2, we believe that segregated unstructured models based on population balance equations provide a more realistic description of the cell cycle events that lead to sustained oscillation in budding yeast cultures.

Although there exists a large number of papers on modeling of particulate systems, the literature on particulate system control is much more sparse. Controllability issues for population balance equation (PBE) models are studied by Semino and Ray [106]. The analysis results are used to design single-input, single-output control strategies that eliminates oscillatory behavior in an emulsion polymerization reactor [105]. Rawlings and so-workers design model-based controllers that allow regulation of the crystal size distribution in continuous crystalizers [26, 92]. Feedback linearizing control strategies based on moment models of continuous crystallizers are proposed by Chiu and Christofides [22].

In this chapter a linear model predictive control (LMPC) strategy based on a spatially discretized PBE model is proposed for the stabilization of oscillating yeast cultures. Cell mass is used as the internal cell coordinate to facilitate real-time measurement of the cell number distribution. The linear state-space model used for LMPC design is obtained by linearizing and temporally discretizing the nonlinear ordinary differential equations resulting from spatial discretization of the
PBE model. The LMPC strategy is designed to allow stabilization of steady-state and periodic solutions via direct control of the cell mass distribution.

The rest of the chapter is organized in four sections. In Section 4.2, our previous work on PBE modeling and control of oscillating microbial culture is reviewed and compared with the present contribution. The PBE model is presented in Section 4.3 along with the numerical solution procedure for the resulting set of partial differential/integral equations. In Section 4.4, the LMPC strategy is presented with special emphasis on the use of the discretized cell mass distribution as controlled outputs. Closed-loop simulation results for the attenuation and induction of oscillations also are shown in Section 4.4. Finally, a summary is given in Section 4.5.

4.2 Previous Work on Oscillating Microbial Cultures

Hjortso and Nielsen [43, 44] have developed models for oscillating microbial cultures involve coupling the population balance equation (PBE) for the cell age distribution to the substrate mass balance. The simplified cell cycle used in the derivation of the PBE model for budding yeast cultures is shown in Figure 4.1. The cell cycle has two control points: (i) the transition age \( a_t \) when a daughter cell becomes a mother cell capable of undergoing budding; and (ii) the division age \( a_d \) when the budding mother cell produces a daughter cell. The assumption of discrete control points is a simplification of the probabilistic division properties of real yeast cells. The control points are influenced by medium composition, especially the concentration of the
rate limiting substrate. The coupling of the PBE and the substrate balance equation establishes an internal feedback loop that can induce sustained oscillations. The basic mechanism can be explained as follows. A partially synchronized cell culture produces periodic changes in the medium, which in turn induces periodic changes in $a_t$ and $a_d$. This leads to further synchronization of the culture and ultimately results in sustained oscillations. A detailed description and analysis of this PBE model can be found in [43, 44].

In an earlier paper on binary fission organisms [55], the PBE model has been enhanced by replacing the discrete division control point with a division intensity.
function $T(a, S')$, where $a$ is the cell age and $S'$ is the "effective" substrate concentration. The function $T(a, S')$ represents the specific rate of cell division at age $a$ and approaches infinity as the cell age approaches some critical value $a_c(S')$. The effective substrate concentration ($S'$) is introduced to describe the delayed response of cell metabolism to changes in environmental conditions and is modeled as a filtered value of actual substrate concentration. These enhancements provide a more realistic description of cell cycle behavior than the conceptual models in [43, 44]. The resulting PBE model has been used as the basis for the development of a feedback linearizing control strategy. Rather than directly control the cell number distribution as in the present work, the nonlinear controller design is based on a simplified moment representation of the PBE model. Additional details can be found in [55].

Although it is natural to use cell age as the internal coordinate for PBE modeling of microbial cultures, there are complications associated with age domain models with respect to model-based controller design. In particular, the cell age distribution cannot be measured directly and it is difficult to develop an useful mapping between the age distribution and the cell size distribution. With recent developments in particle measurement technology [37, 90, 118], the particle size distribution now can be measured on-line. However, cell size is not a convenient internal coordinate for microbial cultures due to the difficulties associated with deriving cell size models. It is possible to establish a mapping between the cell mass distribution and the cell size distribution. Such mappings can be developed for certain microbial cultures with
the knowledge of the cell density, dry-matter content and cell geometry [9]. By using flow cytometry to analyze forward light scatter intensity that varies with bacteria dry mass, a method for determining biomass distribution in mixed bacterial population is reported in [99]. We use cell mass as the internal coordinate for deriving the PBE model and assume the cell mass distribution is measured.

4.3 PBE Model Development and Numerical Solution of the PBE Model

4.3.1 Model Development

The PBE model employed here contains several enhancements of the models used in our previous works [43, 55]. First, the binary fission culture studied in [55] is replaced by a budding yeast culture with the more complex cell cycle depicted in Figure 4.1. Second, cell mass is used as the internal coordinate rather than cell age as in [43, 55]. Third, the generation of newborn cells is modeled by a Gaussian-like probability function rather than by discrete control points as in [43]. Fourth, cell division and transition are affected by a filtered substrate concentration rather than a purely delayed substrate concentration as in [43].

The PBE is written as:

\[
\frac{\partial W(m, t)}{\partial t} + \frac{\partial [k(S')W(m, t)]}{\partial m} = \int_0^{m'} 2p(m, m')\Gamma (m', S') W(m', t) dm' - [D + \Gamma (m)] W(m, t)
\]
where: $W(m,t)$ is the number density of cells with mass $m$ at time $t$; $k(S')$ is the single cell growth rate; $S'$ is the effective substrate concentration; $p(m,m')$ is the probability that a newborn cell of mass $m$ is produced from a mother cell dividing at mass $m'$; $\Gamma(m,S')$ is the division intensity function; and $D$ is the dilution rate. The initial condition of the cell mass distribution is denoted as $W(m,0)$.

The division intensity function $\Gamma(m,S')$ models the tendency of budding cells to divide as they approach a certain critical mass. The function is assumed to have the form:

$$
\Gamma(m,S') = \begin{cases} 
0 & m \leq m_t^* + m_o \\
\gamma \exp[-\epsilon(m - m_d^*)^2] & m_t^* + m_o < m < m_d^* \\
\gamma & m \geq m_d^*
\end{cases}
$$

(4.2)

where $m_t^*$ is the transition mass, $m_o$ is the additional mass that mother cells must gain before division is possible, $\epsilon$ and $\gamma$ are constant parameters and $m_d^*$ is the mass at which the division intensity reaches its maximum value $\gamma$. The transition and division masses are functions of $S'$ as discussed later in this section. The parameter $\epsilon$ determines how rapidly the division rate increases as the cell mass approaches $m_d^*$. The division intensity function is plotted in Figure 4.2a for the parameter values listed in Table 4.1. It is important to note that the parameter values have been chosen to provide reasonable reactor operating conditions. As part of our future work, we intend to investigate the estimation of model parameters from experimental data generated in our laboratory.
The newborn cell probability function $p(m, m')$ describes the mass distribution of newborn cells resulting from cell division. This function is modeled as:

$$ p(m, m') = \begin{cases} 
A \left[ e^{-\beta(m-m_i^2)} + e^{-\beta(m-m'_i+m_i^2)} \right] & m' > m \text{ and } m' > m_i^* + m_o \\
0 & m' \leq m \text{ or } m' \leq m_i^* + m_o 
\end{cases} \quad (4.3) $$

where $m$ is the mass of the newborn cell, $m'$ is the mass of the budding mother cell, and $A$ and $\beta$ are constant parameters. The function $p(m, m')$ is set to zero for $m' \leq m_i^* + m_o$ (when no division can occur) or $m' \leq m$ (which is not physically
meaningful). The probability function \( p(m,m') \) obviously must satisfy:

\[
\int_0^{m'} p(m,m') \, dm = 1
\]  

(4.4)

The function (4.3) yields two identical Gaussian-like peaks in the mass domain, one centered at the substrate dependent transition mass \( m_1^* \) (corresponding to newborn mother cells) and one centered at \( m' - m_1^* \) (corresponding to newborn daughter cells). The function \( p(m,m') \) is plotted in Figure 4.2b for the parameter values in the Table 4.1.

Table 4.1: Continuous bioreactor nominal operating conditions.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \gamma )</td>
<td>200</td>
<td>( \epsilon )</td>
<td>5</td>
</tr>
<tr>
<td>( A )</td>
<td>( \sqrt{25/\pi} )</td>
<td>( \beta )</td>
<td>100</td>
</tr>
<tr>
<td>( S_l )</td>
<td>0.1 g/l</td>
<td>( S_h )</td>
<td>2 g/l</td>
</tr>
<tr>
<td>( K_t )</td>
<td>0.01</td>
<td>( K_d )</td>
<td>2</td>
</tr>
<tr>
<td>( m_{to} )</td>
<td>( 6 \times 10^{-13} ) g</td>
<td>( m_{do} )</td>
<td>( 11 \times 10^{-13} ) g</td>
</tr>
<tr>
<td>( m_{max} )</td>
<td>( 12 \times 10^{-13} ) g</td>
<td>( m_o )</td>
<td>( 1 \times 10^{-13} ) g</td>
</tr>
<tr>
<td>( Y )</td>
<td>0.4</td>
<td>( \mu_m )</td>
<td>( 5 \times 10^{-12} ) g/hr</td>
</tr>
<tr>
<td>( K_m )</td>
<td>25 g/l</td>
<td>( \alpha )</td>
<td>20</td>
</tr>
<tr>
<td>( D )</td>
<td>0.4 hr(^{-1} )</td>
<td>( S_f )</td>
<td>25 g/l</td>
</tr>
</tbody>
</table>

By incorporating the division intensity function (4.2) and the newborn cell probability function (4.3), the PBE model becomes more biologically plausible than conceptual models based on discrete control points [43]. However, sustained oscillations are more difficult to generate with the proposed PBE model because \( \Gamma(m,S') \) and \( p(m,m') \) introduce dispersive effects that tend to counteract the effects of cell synchrony. We have found that the functions used to model the substrate dependence...
of the transition mass \( (m_t^*) \) and the division mass \( (m_d^*) \) play important roles in the ability of the model to exhibit stable periodic solutions.

The following saturation functions are proposed for the transition and division masses:

\[
m_t^*(S') = \begin{cases} 
m_{t0} + K_t(S_t - S_h) & S' < S_t \\
m_{t0} + K_t(S' - S_h) & S' \in [S_t, S_h] \\
m_{t0} & S' > S_h \end{cases}
\]

\[
m_d^*(S') = \begin{cases} 
m_{d0} + K_d(S_t - S_h) & S' < S_t \\
m_{d0} + K_d(S' - S_h) & S' \in [S_t, S_h] \\
m_{d0} & S' > S_h \end{cases}
\]

where \( S_t, S_h, m_{t0}, m_{d0}, K_t \) and \( K_d \) are constant parameters. Note that both \( m_t^* \) and \( m_d^* \) are increasing functions of the effective substrate concentration \( S' \). Figure 4.3 shows \( m_t^*(S') \) and \( m_d^*(S') \) for the parameter values in Table 4.1. These functionalities are in general agreement with experimental data [6, 65] that the transition mass \( (m_t) \) and the division mass \( (m_d) \) are positive functions of nutritional conditions and that \( m_d \) is much more strongly affected than is \( m_t \). The ratio of the division and transition masses is reported to be 1.6–1.7 at good nutritional conditions and 1.15–1.2 at poor nutritional conditions [6, 65]. For the parameters in Table 4.1, the ratio of \( m_d^* \) and \( m_t^* \) is 1.8 for \( S' \geq 2 \) g/l and 1.5 for \( S' \leq 0.01 \) g/l. Since the division mass \( (m_d) \)
Figure 4.3: The division mass \( m_d^*(S') \) (——) and the transition mass \( m_t^*(S') \) (-----).

is less than the critical division mass \( m_d^* \), these ratios appear to be in reasonable agreement with published data.

The substrate balance is written as:

\[
\frac{dS}{dt} = D(S_f - S) - \int_0^\infty \frac{k(S')}{Y} W(m, t) dm \tag{4.7}
\]

where \( S \) is the actual substrate concentration, \( S' \) is the effective substrate concentrations, \( S_f \) is the feed substrate concentration and \( Y \) is a constant yield coefficient.
The single cell growth rate is assumed to follow simple Monod kinetics:

\[ k(S') = \frac{\mu_m S'}{K_m + S'} \]  

where \( \mu_m \) and \( K_m \) are constant parameters. The filtered substrate concentration is calculated as:

\[ \frac{dS'}{dt} = \alpha (S - S') \]  

where the constant parameter \( \alpha \) determines how rapidly cells respond to environmental changes [113].

As compared to conceptual models with discrete control points [43], the dynamic behavior of the proposed PBE model is more complex due to the incorporation of the filtered substrate concentration \( S' \) and the functions \( \Gamma(m, S') \) and \( p(m, m') \). These functions tend to create dispersive effects that counteract cell synchronization that leads to sustained oscillations. As shown below, the proposed model is capable of generating stable periodic solutions via the internal feedback mechanism described in [43]. A partially synchronized cell population induces periodic changes in the substrate concentration, which then leads to periodic changes in the transition and division masses. These two variables determine the mass of dividing mother cells and newborn daughter cells and therefore impose upper and lower bounds on the cell state space. Periodic changes in these boundaries create a stable attractor that overcomes the dispersive effects.
4.3.2 Numerical Solution

The PBE model is comprised of a coupled set of nonlinear algebraic, ordinary differential and integro-partial differential equations. Analytical solution of such models is possible only under very restrictive assumptions [43, 44]. Consequently, numerical solution is required when the PBE model is used in open-loop and closed-loop simulations. In our previous work on binary fission organisms [55], the PBE model is solved using a finite difference method. This method is simple to implement, but it is computationally inefficient and less accurate than alternative techniques based on weighted residuals [27].

We have found that orthogonal collocation on finite elements [27] provides efficient and robust solution of the PBE model. A finite cell mass domain, $0 \leq m \leq m_{\text{max}}$, is chosen such that the number of cells with mass $m > m_{\text{max}}$ is negligible. The PBE is approximated by a coupled set of nonlinear ordinary differential equations (ODEs) that are obtained by discretizing the mass domain. Integral expressions in the population and substrate balance equations are approximated using Gaussian quadrature [27]. The resulting set of nonlinear ODEs has the form:

$$\frac{dW_j}{dt} = -\frac{1}{h} k(S') \sum_{i=1}^{n} A_{j,i} W_i + h \sum_{i=1}^{n} 2w_i p_{j,i} \Gamma_i W_i$$  \hspace{1cm} (4.10)

$$-(D + \Gamma_j)W_j \quad j = 1, 2, \ldots, n$$

$$\frac{dS}{dt} = D(S_f - S) - \frac{k(S')}{Y} h \sum_{i=1}^{n} w_i W_i$$  \hspace{1cm} (4.11)

$$\frac{dS'}{dt} = \alpha(S - S')$$  \hspace{1cm} (4.12)
where: $W_j$ denotes the cell number density at collocation point $j$; $n$ is the total number of collocation points; $A$ is the collocation matrix [27]; $h$ scales the size of each finite element to unity; $w$ is a vector of quadrature weights [27]; $P_{j,i} = p(m_j, m_i)$ is the $(i,j)$ element of the matrix $P \in \mathbb{R}^{n \times n}$; and $\Gamma_i = \Gamma(m_i)$ is $i$-th element of the vector $\Gamma \in \mathbb{R}^n$. Both $P$ and $\Gamma$ are time varying because they are dependent on $S'$. Unless stated otherwise we use twelve equally spaced finite elements, each with eight internal collocation points that are determined as the roots of the appropriate Jacobi polynomial [96]. The total number of collocation points $n = 109$. The state vector of the resulting ODE model consists of the cell number density at each collocation point ($W_j$), as well as the substrate and filtered substrate concentrations ($S, S'$).

The accuracy of the proposed numerical solution procedure is evaluated by: (i) using a simplified model to compare the numerical solution to an analytical solution; (ii) and testing convergence of the numerical solution using different number of collocation points. An analytical solution of the PBE model can be obtained via the method of characteristics [42] under the following assumptions:

1. Constant single cell growth rate.

2. Constant division and transition masses.

3. Infinite division intensity at the division mass.

The assumption of constant cell growth decouples the PBE from the substrate balance equation. The assumption of discrete division and transition masses leads to
distinct mother (M) and daughter (D) cell populations. The PBE model is written for the two subpopulations as follows:

\[
\frac{\partial W_M(m,t)}{\partial t} + k \frac{\partial W_M(m,t)}{\partial m} = -DW_M(m,t) \tag{4.13}
\]

\[
\frac{\partial W_D(m,t)}{\partial t} + k \frac{\partial W_D(m,t)}{\partial m} = -DW_D(m,t) \tag{4.14}
\]

where: \(W_M\) and \(W_D\) are the cell number concentrations of mother and daughter cells respectively; and \(k\) is the constant single cell growth rate. Due to the infinite division intensity assumption, cell division is incorporated into the boundary conditions:

\[
W_M(m_t, t) = W_M(m_d, t) + W_D(m_t, t) \tag{4.15}
\]

\[
W_D(m_0, t) = W_M(m_d, t) \tag{4.16}
\]

where \(m_d\) is the constant division mass, \(m_t\) is the constant transition mass and \(m_0\) is the constant minimum cell mass.

Using the method of characteristics, the PBEs for the mother and daughter cell populations are solved in subdomains defined by characteristic curves with slopes of the growth rate \(k\). Figure 4.4 shows a comparison of the numerical and analytical solutions for the cell number distributions. The dilution rate is 0.25 hr\(^{-1}\), and the single cell growth rate is \(k = 4 \times 10^{-13}\) g/hr. The minimum cell mass, transition mass and division mass are \(m_0 = 4 \times 10^{-13}\) g, \(m_t = 8 \times 10^{-13}\) g, \(m_d = 12 \times 10^{-13}\) g,
respectively. The following initial distributions are used:

\[
W_M(m, 0) = 0 \\
W_D(m, 0) = 10^{13}e^{-(m-6\times10^{-13})^2}
\]  

(4.17)  
(4.18)

For this simple model, eight finite elements and five internal collocation points are found to be sufficient for numerical solution. The difference between the analytical and numerical solutions is obtained by interpolating the analytical solution to match the mass-time grid used for numerical solution. The results in Figure 4.4 demonstrate that the numerical solution provides a very close approximation of the analytical solution. Note that only the first three subdomains for the daughter and mother cells are solved analytically due to the increasingly complex expressions obtained for higher subdomain solutions [42].

From a conceptual standpoint, an advantage of the simplified model is that the cell cycle can be easily visualized. Figure 4.5 shows the numerical solution of the simplified model for the same test as in Figure 4.4 but with a longer time duration of eight hours. Note that discontinuities are observed due to the assumption of discrete control points. Budding mother cells divide into daughter cells and new mother cells when the mass \(m = m_d = 12 \times 10^{-13}\) g. At the cell transition mass \(m_t = 8 \times 10^{-13}\) g, the new mother cell density \(W_M(m_t, t)\) is the sum of the daughter cell density \(W_D(m_t, t)\), and the density of dividing mother cells \(W_M(m_d, t)\) as in (4.15). Similarly, the density of daughter cells with mass \(m_o\) equals the density of
cells divided as in (4.16). Because discrete control points are used and cell growth is independent of the medium, the shape of the cell distribution is invariant with respect to time within the same cell cycle and the total number of cells decreases.
Analytical solution of the detailed PBE model in (4.1)–(4.9) is not possible. In the remainder of the chapter, the model is solved numerically using twelve finite elements and eight internal collocation points. An appropriate number of internal collocation points \( n_c \) is chosen by performing a series of open-loop simulation tests with \( n_c = 6, 8 \) and 9 to check convergence of the numerical solution. The results for the initial cell number distribution (4.17)–(4.18) and two sets of operating conditions are shown in Figure 4.6. An oscillatory response is obtained for \( D = 0.25 \text{ hr}^{-1} \) and \( S_J = 20 \text{ g/l} \). This result indicates that \( n_c = 8 \) is sufficient to obtain an accurate solution. A steady-state solution is obtained with a larger dilution rate \( D = 0.4 \text{ hr}^{-1} \).
Figure 4.6: Open-loop simulation: steady-state solution with $n_c = 8$ (---) and oscillatory solutions with $n_c = 6$ (· · ·), $n_c = 8$ (−−−), and $n_c = 9$ (−−−).

and a larger feed substrate concentration $S_f = 25$ g/l. The corresponding substrate concentration dynamics also are shown in Figure 4.6. These results are consistent with experimental data [119].

4.4 Model Predictive Controller Design

The budding yeast PBE model is difficult to use directly for model-based controller design. A reasonable alternative is to use the PBE model to derive simpler ODE models that are more amenable to existing controller design techniques. Moment models have been developed for particulate systems such as continuous crystallizers.
[22] and emulsion polymerization reactors [51]. The moments of the distribution can be used as controlled outputs. For the aforementioned particulate processes, closed-form representation of the moment equations is possible because new particle generation depends only on lumped variables (e.g. initiator and monomer concentrations in emulsion polymerization). In [55] it is shown that binary fission organisms do not allow closure of the first and higher order moments because the birth rate of new cells always depends on the cell distribution. A similar problem occurs for the budding yeast PBE model.

In our previous work on binary fission organisms [55], a zeroth-order moment model is used to derive a feedback linearizing controller. A shortcoming of this approach is that the controller design model does not account for the segregated nature of the culture despite the fact that sustained oscillations are intimately connected to cell synchrony. Below we propose a model predictive control strategy for the budding yeast cultures based on a linear design model that preserves the segregated description of the PBE model.

### 4.4.1 Controller Formulation and Design

The controller design model is generated directly from the spatially discretized PBE model (4.10)–(4.12). The model equations are linearized about the steady-state operating point in Table 4.1 and then temporally discretized with sampling time \( \Delta t = 0.1 \text{ hr} \). The sampling time is chosen to be an order of magnitude less than the period of the oscillating culture (2 hours). The resulting state-space model has
the form of (1.1). State vector \( x \in \mathbb{R}^{111} \) is comprised of the cell number density at each collocation point \( (W_j) \) and the substrate and filtered substrate concentrations \( (S, S') \); the input vector \( u \in \mathbb{R}^{2} \) is comprised of \( D \) and \( S_f \); and the output vector \( y \in \mathbb{R}^{m} \) is defined below. As discussed in Section 4.2, we assume that the cell mass distribution can be measured or reconstructed from on-line measurements of the particle size distribution.

The controllability matrix for the pair \( (A, B) \) in (??) has rank four. This is not a surprising result given the large state dimension and the strong colinear behavior of the state variables. This indicates that the cell distribution cannot be modified arbitrarily with the two inputs available. Semino and Ray [106] propose an approximate controllability test for PBE models that can be placed in hereditary form via semi-analytical solution. Controllability is defined as the property that the state vector can be derived from a subspace \( \Gamma_1 \) to a subspace \( \Gamma_2 \) in a finite amount of time by appropriate choice of the inputs. The controllability test is successfully applied to emulsion polymerization reactors and continuous crystallizers. Unfortunately, the test does not appear to be applicable to microbial PBE models because they do not allow the required hereditary system representation. Therefore we investigate the ability of the MPC controller to stabilize steady-state and periodic solutions. While we consider partial control of the cell distribution, it is unnecessary to precisely establish a given cell distribution to achieve the control objectives (see below).
The controller design model is completed by defining the controlled output vector. The most straightforward approach is to choose the cell number density $W_j$ at each collocation point as a controlled output. This may be problematic because: (i) the resulting control problem is highly non-square (2 inputs, 109 outputs); (ii) cell number densities at nearby collocation points are strongly colinear because the basic shape of the distribution cannot be changed significantly by manipulating $D$ and $S_f$; and (iii) the substrate concentration also needs to be controlled to avoid washout. The third problem can be handled by defining the output vector as:

$$y = \begin{bmatrix} W_1 & W_2 & \cdots & W_N & S \end{bmatrix}^T$$  \hspace{1cm} (4.19)

We have found that good closed-loop performance can be obtained by controlling a subset of the cell number densities and the substrate concentration:

$$y = \begin{bmatrix} W_{j_1} & W_{j_2} & \cdots & W_{j_p} & S \end{bmatrix}^T$$  \hspace{1cm} (4.20)

where the indices $\{j_1, \ldots, j_p\}$ define the collocation points where the associated cell number density is used as a controlled output. In the subsequent simulation study, $\{j_1, \ldots, j_p\}$ are chosen as boundary points of the finite elements. While this approach is admittedly heuristic, problems may be encountered if the number of output variables is reduced further. Fewer output variables may not be able to represent the time-varying cell distribution which shifts position as the substrate concentration changes. While it may be possible to systematically determine the
controlled outputs using multivariate statistical methods [23], this was deemed to be beyond the scope of the current study. Below we compare the performance of MPC controllers which use the output vectors (4.19) and (4.20).

The major control objectives are: (i) stabilization of steady-state solutions to eliminate oscillations that adversely affect bioreactor stability and productivity; and (ii) stabilization of periodic attractors that may lead to increased production of metabolites synthesized only during part of the cell cycle [41]. Both objectives can be achieved by controlling the discretized cell number distribution because oscillatory behavior is closely linked to synchronization of the cell population.

The MPC controller is formulated as an infinite-horizon open-loop optimal control problem (1.3). The target vectors $u_s$ and $y_s$ can be constant or adjusted on-line using a disturbance model. The disturbance model is formulated as (1.6). The output disturbance estimate $\hat{d}$ is generated by a deadbeat observer [79]. As discussed above, there are insufficient degrees of freedom to drive the entire cell distribution to a specified target distribution. Therefore, target vectors $x_s$ and $u_s$ that minimize the steady state offset are found by solving the quadratic programming problem (1.9). Below we investigate MPC controller designs with and without the disturbance model.

4.4.2 Simulation Study

The proposed MPC strategy is evaluated using the discretized PBE model (4.10)–(4.12) as a surrogate for the continuous yeast bioreactor. Two controller formula-
tions are investigated using the alternative output vectors discussed above. The first controller uses the full-order output vector (4.19). This leads to a highly non-square control problem (2 inputs, 110 outputs) due to the large number of collocation points employed. The quadratic weighting matrices in the objective function (1.3) are chosen by trial-and-error as:

\[
Q = \begin{bmatrix}
0.01I_{109 \times 109} & 0 \\
0 & 10
\end{bmatrix}, \quad R = \begin{bmatrix}
10^5 & 0 \\
0 & 100
\end{bmatrix}, \quad S = 2R \tag{4.21}
\]

A control horizon \( N = 5 \) provides a reasonable compromise between closed-loop performance and computation time. The second controller uses the reduced-order output vector (4.20). This yields a lower dimensional problem with 14 output variables. The control horizon is chosen as \( N = 5 \) and the weighting matrices are chosen by trial-and-error as:

\[
Q = \begin{bmatrix}
0.1I_{13 \times 13} & 0 \\
0 & 8
\end{bmatrix}, \quad R = \begin{bmatrix}
2 \times 10^5 & 0 \\
0 & 500
\end{bmatrix}, \quad S = 4R \tag{4.22}
\]

Each controller is evaluated with and without disturbance models.

Figure 4.7 shows the ability of the MPC controller based on the full-order output vector to stabilize an initially oscillating culture at a desired steady-state operating point. The initial cell number distribution \( W(m, 0) \) is a highly synchronized distribution corresponding to the stable periodic solution in Figure 4.6, while the discretized cell distribution setpoint vector represents the steady-state solution in Figure 4.6.
The zeroth-order moment of the cell number distribution, \( w_0 = \int_0^\infty W(m, t) \, dm \), and the substrate concentration are shown as representative output variables. The MPC response with disturbance model is shown by the dashed line, while the solid line represents the response without disturbance model. The MPC controller is able to stabilize the reactor under initial conditions that lead to open-loop oscillations shown by the dotted line. The input and output responses of the MPC controller with disturbance model are more oscillatory than those obtained without the disturbance model. Although the performance may be improved by further fine tuning, the behavior is directly attributable to the additional dynamics introduced by the linear observer used to estimate the disturbances.

Figure 4.8 shows the results obtained for the MPC controller with reduced-order output vector for the same test as in Figure 4.7. The solid line is the MPC response, while the dashed line is the open-loop response obtained with the synchronized initial cell distribution. While the output responses are only slightly better than those in Figure 4.7, the MPC controller with reduced-order output vector provides much smoother input moves. We believe this behavior is a direct result of reducing the controlled output vector dimension and making the control problem less non-square. The associated time evolution of the cell number distribution is shown in Figure 4.9. The initial distribution is a highly synchronized with distinct subpopulations that lead to sustained oscillations. The controller attenuates the oscillations by counteracting cell synchrony via dispersion of the subpopulations.
The distribution approaches the desired steady-state distribution by the end of the 12 hour simulation.

We further evaluate the effect of the disturbance model on closed-loop performance when a modeling error is present. The modeling error is introduced by changing the cell growth rate parameter $K_m$ from 25 g/l to 20 g/l in the simulated plant, while the linear controller design model remains unchanged. Figure 4.10 shows the results obtained for the same oscillation attenuation test as in Figures 4.7 and 4.8. The response of the MPC controller with reduced-order output vector and disturbance model is shown by the solid line, while the dashed line is the response of
Figure 4.8: Oscillation attenuation: reduced-order output vector without disturbance model (——) and open-loop response (---).

the same MPC controller without disturbance model. Both controllers are able to attenuate the oscillations and drive the cell distribution to steady state. A notable difference is that input responses for the controller without disturbance model are much smoother. Another difference is that the controllers achieve two very different steady states. The distributions at $t = 24$ hr shown in Figure 4.11 show a potential advantage of the disturbance model. While the steady-state distribution obtained without the disturbance model (dashed line) is shifted from the setpoints (+), the distribution obtained with the disturbance model (solid line) matches the setpoints almost exactly. The disturbance model is useful only if precise control of the cell
Figure 4.9: Oscillation attenuation: cell number distribution corresponding to Figure 4.8 at four time instances.

number distribution is required. This may be beneficial, for example, if desired metabolites are preferentially produced by cells of a certain mass.

Figure 4.12 shows the ability of the MPC controller with reduced-order output vector to stabilize a desired periodic solution. A disturbance model is not used for this test. The initial cell number distribution corresponds to a steady-state solution, while distributions corresponding to the periodic solution in Figure 4.6 are defined as a time-varying setpoint trajectory. For this test, the weighting matrices are chosen
Figure 4.10: Oscillation attenuation with modeling error: reduced-order output vector with (——) and without (---) disturbance model.

by trial-and-error as:

\[
Q = \begin{bmatrix}
0.01I_{13 \times 13} & 0 \\
0 & 10
\end{bmatrix}, \quad R = \begin{bmatrix}
10^5 & 0 \\
0 & 100
\end{bmatrix}, \quad S = 2R
\]

(4.23)

Note that the controller stabilizes the desired periodic solution by generating oscillatory input moves. Although not shown, it is interesting to note that the observed oscillations are maintained with the same period when the controller is switched off and the system runs under open-loop conditions. The evolution of the cell number distribution is shown in Figure 4.13. Clearly the oscillating dynamics of the cell cul-
Figure 4.11: Oscillation attenuation with modeling error: distribution setpoint (+), reduced-order output vector with (---) and without (----) disturbance model corresponding to Figure 4.10.

ture is accompanied by marked synchronization of the cell population. Two distinct subpopulations can be identified after 24 hours of operation.

4.5 Summary and Conclusions

The dynamic model for the continuous yeast bioreactor is formulated by coupling the population balance equations (PBE) for the cell mass distribution to the substrate mass balance. We have shown that empirical functions used to describe the dependence of cell transition and division on the medium can be chosen such that the PBE model exhibits stable periodic solutions under reasonable operating conditions.
The model is solved numerically by spatially discretizing the PBE using orthogonal collocation on finite elements. The resulting nonlinear ordinary differential equation model is linearized and discretized in time to yield a linear state-space model suitable for MPC synthesis. The MPC controller is designed to stabilize steady-state and periodic solutions by regulating the discretized cell number distribution and the substrate concentration. Several MPC formulations have been evaluated via simulation. The best results are obtained when a subset of the discretized cell number distribution is used as the controlled outputs. The proposed methodology is the
Figure 4.13: Oscillation induction: synchronization of the cell distribution corresponding to Figure 4.12.

initial step in the development of an implementable control strategy for oscillating yeast cultures.
Chapter 5
A Hybrid Model Predictive Control Strategy for Plant-wide Control – Part I

5.1 Introduction

Linear model predictive control (LMPC) has been successfully applied to plant-wide control problems with hundreds of input and output variables [86]. LMPC can be expected to provide satisfactory performance if the controlled process is approximately linear over the typical range of operation. The industrial success of commercial techniques such as Dynamic Matrix Control demonstrates that LMPC can tolerate some degree of process nonlinearity. The standard approach for handling strong nonlinearities in the LMPC framework is to sacrifice performance by detuning the controller. However, some plants are sufficiently nonlinear to hinder the successful application of LMPC.

Nonlinear model predictive control (NMPC) has been proposed as an alternative to LMPC for plants with highly nonlinear behavior [70]. NMPC offers the same capabilities for interaction compensation and constraint handling as its linear counterpart. The key difference is that NMPC utilizes a nonlinear model to predict and optimize process performance. The use of NMPC for plant-wide control is problematic due to complications associated with dynamic modeling, state estimation...
and on-line optimization [39]. A nonlinear dynamic model of the entire plant is required for controller design. Such large-scale nonlinear models are extremely difficult to obtain using fundamental modeling and available techniques for empirical nonlinear modeling [83]. Another complication is that unmeasured state variables must be estimated from available on-line measurements. This requires the design of a nonlinear observer, which is a difficult task despite recent advances [78]. Even if a suitable nonlinear model is available, a nonlinear programming problem must be solved at each sampling period to generate the control moves. For large-scale systems the optimization problem may be computationally intractable due to the large number of decision variables and the complexity of the constraints resulting from the nonlinear model equations. While it must be argued that cheaper and faster computers soon will be available to solve plant-wide nonlinear optimization problems in real-time, a simple calculation in [121] has shown that a NMPC problem with 20 inputs and 20 outputs will not be able to be solved on-line until well into the next century given expected advances in computer technology. As a result, the judicious use of modeling assumptions [98] and simplified controller formulations [121] are required even for problems of moderate size and complexity.

In this chapter, we propose a plant-wide control strategy based on integrating LMPC and NMPC. The motivation for this approach is that most operating units in a typical chemical plant can be adequately described by linear dynamic models, while a small number of operating units account for the observed highly nonlinear
behavior. Unlike plant-wide control methods that employ time-scale decompositions [19, 60], the proposed approach is based on decomposing the plant according to the degree of nonlinearity. A model predictive control system for the decomposed plant is constructed by applying LMPC to the linear subsystems and NMPC to the nonlinear subsystems. We present a simple controller coordination strategy for plants that can be decomposed into a single linear subsystem and a single nonlinear subsystem. A simple reaction/separation process is used to compare the hybrid method to conventional LMPC and NMPC techniques in terms of closed-loop performance and on-line computation. The hybrid LMPC-NMPC method is developed further in Chapter 6.

5.2 Illustrative Example

Consider a reaction/separation process which is designed to produce a product $B$ by irreversible reaction of a reactant $A$. The effluent from a continuous stirred tank reactor is introduced to a distillation column where separation of the reactant and product occurs. The overhead stream enriched in $A$ is recycled to the reactor assuming that inerts and light byproducts are not present in the system. Otherwise, an overhead vent stream would be required to avoid accumulation of these materials. The bottom stream enriched in $B$ is recovered as the product. The basic reactor model obtained from [117] is well studied. The model is derived by assuming a first-order reaction, constant volume operation, and that combined recycle and fresh feed stream temperature is maintained at a constant temperature by a fast regulatory
controller. The resulting reactor model is comprised of state equations for the reactor concentration \( C_A \) and the reactor temperature \( T \). The parameter values are same as those used in [117], except that the pre-exponential factor \( k_0 \) is reduced from \( 7.2 \times 10^{10} \text{ min}^{-1} \) to \( 5.14 \times 10^{10} \text{ min}^{-1} \). The control objective is to regulate the reactor temperature by manipulating the coolant temperature \( T_c \) assuming the coolant jacket dynamics are negligible. This scheme allows the reactor to be operated safely and effectively.

The distillation column consists of seven trays, a total condenser, and a reboiler. The effluent from the reactor is introduced as feed to the fourth tray. The assumptions used to derive the distillation column are discussed in [76]. In particular, the equimolal overflow assumption eliminates the need for energy balances. Tray-by-tray component balances [76] yield state equations for the liquid mole fraction of component \( A \) on each equilibrium stage \( (X_{An}) \), where \( n = 1 \) represents the condenser and \( n = 9 \) represents the reboiler. The control objective is to regulate the recycle mole fraction \( (X_{A1}) \) and the product mole fraction \( (X_{A9}) \) by manipulating the vapor rate \( (V) \) and the reflux rate \( (L) \). Overhead composition control is desirable to maximize the amount of reactant recycled to the reactor, while control of the bottom composition is required to meet product purity requirements. In practice, \( V \) and \( L \) may be manipulated by adjusting the reboiler heat duty and the reflux valve position. The complete reaction/separation model is included in Appendix C. The column model parameters are shown in Table 5.1.
Table 5.1: Nominal operating conditions for the reaction/separation system.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Variable</th>
<th>Value</th>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F$</td>
<td>45.022 L/min</td>
<td>$I$</td>
<td>$5.14 \times 10^{10}$ L/min</td>
<td>$X_{A1}$</td>
<td>0.95</td>
</tr>
<tr>
<td>$F_R$</td>
<td>54.978 L/min</td>
<td>$k_0$</td>
<td>8750 K</td>
<td>$X_{A2}$</td>
<td>0.826</td>
</tr>
<tr>
<td>$C_{Af}$</td>
<td>1 mol/L</td>
<td>$U_A$</td>
<td>$5 \times 10^{4}$ J/min $\cdot$ K</td>
<td>$X_{A3}$</td>
<td>0.709</td>
</tr>
<tr>
<td>$T_f$</td>
<td>350 K</td>
<td>$T_c$</td>
<td>309.480 K</td>
<td>$X_{A4}$</td>
<td>0.619</td>
</tr>
<tr>
<td>$V_r$</td>
<td>100 L</td>
<td>$C_A$</td>
<td>0.567 mol/L</td>
<td>$X_{A5}$</td>
<td>0.559</td>
</tr>
<tr>
<td>$\rho$</td>
<td>1000 g/L</td>
<td>$T$</td>
<td>350 K</td>
<td>$X_{A6}$</td>
<td>0.506</td>
</tr>
<tr>
<td>$C_p$</td>
<td>0.239 J/g-K</td>
<td>$M_1, M_9$</td>
<td>200 mol</td>
<td>$X_{A7}$</td>
<td>0.394</td>
</tr>
<tr>
<td>$(\Delta H)$</td>
<td>$5 \times 10^{4}$ J/mol</td>
<td>$M_2, ..., M_8$</td>
<td>50 mol</td>
<td>$X_{A8}$</td>
<td>0.235</td>
</tr>
<tr>
<td>$\rho_m$</td>
<td>1 mol/L</td>
<td>$L$</td>
<td>29.2 mol/min</td>
<td>$X_{A9}$</td>
<td>0.1</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>4</td>
<td>$V$</td>
<td>84.2 mol/min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 5.1 shows the open-loop responses of the outputs ($T, X_{A1},$ and $X_{A9}$) to step changes in the inputs ($T_c, V$). The solid line represents the response to a $-3$ K change in $T_c$ at $t = 5$ min followed by a $+10$ mol/min change in $V$ at $t = 50$ min. The dashed line represents the response to a $+3$ K change in $T_c$ at $t = 5$ min. The initial operating point corresponds to an unstable steady state for the reactor. It is obvious that the reactor dynamics are highly nonlinear and much faster than the column dynamics.

The linear model for LMPC design is obtained by linearizing the nonlinear model equations about the nominal operating point and discretizing with a sampling interval $\Delta T = 10$ s. The resulting model has the standard state-space form $(1.1)$. The state, input and output vectors are summarized as follows:

$$x = \begin{bmatrix} T & C_A & X_{A1} & X_{A2} & X_{A3} & X_{A4} & X_{A5} & X_{A6} & X_{A7} & X_{A8} & X_{A9} \end{bmatrix}^T$$

$$u = \begin{bmatrix} T_c & L & V \end{bmatrix}^T$$

$$y = \begin{bmatrix} T & X_{A1} & X_{A9} \end{bmatrix}^T$$
Figure 5.1: Open-loop simulation for step changes in cooling jacket temperature and boil-up rate.

The LMPC controller is formulated to minimize the following infinite horizon objective function (1.3). The control horizon $N = 15$. The tuning matrices $Q$, $R$, and
$S$ are chosen as follows:

$$Q = \begin{bmatrix} 100 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 50 \end{bmatrix}, \quad R = \begin{bmatrix} 0.001 & 0 & 0 \\ 0 & 0.001 & 0 \\ 0 & 0 & 0.001 \end{bmatrix}, \quad S = \begin{bmatrix} 0.001 & 0 & 0 \\ 0 & 100 & 0 \\ 0 & 0 & 100 \end{bmatrix}$$

The problem is solved subject to the input constraints:

$$\begin{bmatrix} 280 \text{ K} \\ 0 \text{ mol/min} \\ 0 \text{ mol/min} \end{bmatrix} \leq \begin{bmatrix} T_c \\ L \\ V \end{bmatrix} \leq \begin{bmatrix} 350 \text{ K} \\ 250 \text{ mol/min} \\ 250 \text{ mol/min} \end{bmatrix}$$

Output constraints are not considered in this example.

We assume the reactor temperature, recycle mole fraction, and product mole fraction can be measured on-line. The remaining state variables must be estimated from the available on-line measurements. Simultaneous state and disturbance estimation is performed by augmenting the process model with an output disturbance model (1.6). A Luenberger observer is used since the nominal operating point of the reactor is unstable. The estimated state variables are used to initialize the optimization problem at each time step, while the estimated disturbances are used to shift the target values $x_s$ and $u_s$ solved from (1.8).
Figure 5.2: LMPC for a setpoint change in the column mole fractions.

Figure 5.2 shows the closed-loop response obtained for setpoint changes of +0.02 and -0.05 in the column overhead and column bottom mole fractions, respectively.

LMPC provides good performance because the reactor remains near the nominal
point where the linear model was derived. The closed-loop response obtained for a
+5 K change in the reactor temperature setpoint is shown in Figure 5.3. Due to

Figure 5.3: LMPC for a setpoint change in the reactor temperature.
the strong reactor nonlinearities, the temperature tracking performance is very poor and the bottom mole fraction deviates significantly from its setpoint.

5.3 Integration of LMPC and NMPC

Setpoint changes in the recycle and product mole fractions are handled easily by LMPC because the column does not exhibit strong nonlinearities at moderate purities. However, LMPC yields unacceptably poor responses for reactor temperature setpoint changes due to the highly nonlinear reaction kinetics. As shown subsequently, this problem can be solved by applying NMPC to the entire plant. However, a more computationally efficient approach is to utilize nonlinear control only where necessary; i.e. apply NMPC to the reactor and apply LMPC to the column. This motivates the development of a new class of plant-wide control methods based on integrating LMPC and NMPC.

The proposed hybrid LMPC-NMPC control strategy consists of four steps:

1. Analysis of process nonlinearities.
2. Decomposition of the plant into linear and nonlinear subsystems.
3. Application of LMPC to the linear subsystems and NMPC to the nonlinear subsystems.
4. Coordination of the linear and nonlinear MPC controllers.

This chapter focuses on the final two problems for plants that can be decomposed into a single linear subsystem and a single nonlinear subsystem. The re-
action/separation system described above is an example of such a process. The next chapter will focus on the last three problems for more complicated processes.

The state-space model equations for the two subsystems can be written as:

\[ x_L(k+1) = A_L x_L(k) + A_N x_N(k) + B_L u_L(k) + B_N u_N(k) \]  \hspace{1cm} (5.1)

\[ y_L(k) = C_L x_L(k) + C_N x_N(k) \]  \hspace{1cm} (5.2)

\[ x_N(k+1) = f[x_L(k), x_N(k), u_L(k), u_N(k)] \]  \hspace{1cm} (5.3)

\[ y_N(k) = h[x_L(k), x_N(k)] \]  \hspace{1cm} (5.4)

where: the subscripts \( L \) and \( N \) denote the linear subsystem and the nonlinear subsystem variables, respectively; \( x_L, x_N \) are the state vectors; \( u_L \) and \( u_N \) are the input vectors; \( y_L \) and \( y_N \) are the output vectors; \( A_L, A_N, B_L, B_N, C_L \) and \( C_N \) are the linear state-space matrices; and \( f \) and \( h \) are nonlinear functions for the nonlinear subsystem. In each subsystem model, variables from the other subsystem can be viewed as measured disturbances. For the reaction/separation process, the column is the linear subsystem and the reactor is the nonlinear subsystem. As compared to conventional NMPC, an immediate advantage of the proposed approach is that a nonlinear model is required only for the nonlinear subsystem. This eliminates the need for a full nonlinear plant model, which rarely is available or economically feasible to develop.

Solutions to the LMPC and NMPC problems must be computed sequentially to achieve a substantial reduction in computational effort as compared to standard
NMPC. Sequential solution may be problematic because the linear and nonlinear subsystems are coupled via mass and energy flows. There are three different configurations for two-subsystem problem. While more details can be found in Chapter 6, the remainder of this Chapter focuses on developing a controller coordination strategy for fully coupled systems such as the reaction/separation process. The first step is to compute a solution of the LMPC problem using linear model of the entire plant rather than just the linear subsystem. The motivation for this approach is discussed below. The LMPC solution is used to compute the NMPC solution for the nonlinear subsystem.

To motivate the proposed controller coordination strategy, consider an alternative method in which the LMPC design is based on the linear subsystem model. The following information is required from the nonlinear subsystem to generate predictions over the LMPC control horizon $N_L$:

**State variables:** $x_N(k|k), \ldots, x_N(k + N_L - 1|k)$

**Input variables:** $u_N(k|k), \ldots, u_N(k + N_L - 1|k)$

The current value of the state vector $x_N(k|k)$ is available from on-line measurements and/or nonlinear state estimation. Future values of the state variables are not available until the NMPC problem is solved at the current time step, and the NMPC problem cannot be solved until the LMPC problem is solved. A possible solution to
this problem is to generate the unavailable future values from the NMPC solution obtained at the previous time step which will be discussed in details in Chapter 6.

The information exchange problem between controllers can be partially mitigated if the LMPC design is based on a linear model of the entire plant. The advantage of this approach is that the dependence of the LMPC problem on the NMPC solution is completely eliminated. As a result, the LMPC problem can be solved independently. It is important to emphasize that only the LMPC solution for the linear subsystem actually is utilized; the manipulated input moves for the nonlinear subsystem are not implemented. The LMPC solution is used to compute the NMPC solution for the nonlinear subsystem. The disadvantages of this approach are that a linear approximation of the nonlinear subsystem is introduced and a larger LMPC problem must be solved.

The LMPC problem is formulated as described previously. The LMPC solution yields all the input and state information required to solve the NMPC problem:

State variables: $x_L(k|k), \ldots, x_L(k + P_N - 1|k)$

Input variables: $u_L(k|k), \ldots, u_L(k + P_N - 1|k)$

where $P_N$ is the prediction horizon of the NMPC controller. The NMPC problem is formulated as (1.11). The decision variables are current and future values of the manipulated inputs in the nonlinear subsystem. NMPC control horizon is $N_N$. The
problem is solved subject to input constraints and equality constraints derived from the nonlinear model.

For the present example, we assume the reactor concentration must be estimated from reactor temperature measurements. An important advantage of the hybrid approach is that a nonlinear observer can be designed for the reactor subsystem rather than the entire plant. Simultaneous state and disturbance estimation is performed using an augmented reactor subsystem model. In this case, an input disturbance model is employed to handle the reactor instabilities. Nonlinear observer design is facilitated by representing the reactor subsystem in the continuous-time form,

\[
\dot{x}_N = \beta(y_N)x_N + \gamma(u_N + d_N) + \delta(x_L) \tag{5.5}
\]

\[
\dot{d}_N = 0
\]

\[
y_N = Cx_N
\]

where \(d_N \in \mathbb{R}\) is a vector of input disturbance variables. Nonlinear matrix functions \(\beta\) and \(\delta\) and constant vector \(\gamma\) are shown as follows.

\[
\beta(y_N) = \begin{bmatrix}
-\frac{F + F_R}{V_r} - k_0 \exp\left(\frac{-E}{RT}\right) & 0 \\
\frac{-\Delta H}{\rho C_p} k_0 \exp\left(\frac{-E}{RT}\right) & -\frac{F + F_R}{V_r} - \frac{U_A}{V_r \rho C_p}
\end{bmatrix},
\]

\[
\gamma = \begin{bmatrix}
0 \\
\frac{U_A}{V_r \rho C_p}
\end{bmatrix}, \quad \delta(x_L) = \begin{bmatrix}
\frac{F C_{AL}}{V_r} + \frac{\rho m R X A_1}{V_r} \\
\frac{F + F_R}{V_r} T_f
\end{bmatrix}
\]
Note that the model is linear in the unmeasured concentration $C_A$. The state affine model form allows the design of a simple nonlinear closed-loop observer [54]. The estimated state variables $\hat{x}_N(k)$ are used to initialize the NMPC problem at each time step, while the estimated disturbances $\hat{d}_N(k)$ are used to shift the input and output target values [70].

5.4 Simulation Study

We compare the hybrid LMPC-NMPC method to standard LMPC and NMPC using the reaction/separation process described previously. The NMPC controller is formulated as in (1.11) with the nonlinear model of the entire plant. The continuous-time nonlinear model is discretized using orthogonal collocation on finite elements [70] with a sampling period $\Delta t = 10\, s$. Due to the number of state variables in the column model, the resulting NMPC problem is much larger than that encountered in the hybrid approach where NMPC is applied only to the reactor. The standard NMPC problem is simplified by assuming full-state feedback and that the plant is not affected by unmeasured disturbances. This eliminates the need for a plant-wide nonlinear observer that generates estimates of the unmeasured state and disturbance variables. As a result, the simulation results for NMPC represent the best case scenario in terms of setpoint tracking performance and on-line computation. The NMPC controller is tuned with $N_N = 1, P_N = 2$ and:
$Q = \begin{bmatrix} 0.1 & 0 & 0 \\ 0 & 100 & 0 \\ 0 & 0 & 100 \end{bmatrix}, \quad R = \begin{bmatrix} 0.001 & 0 & 0 \\ 0 & 0.001 & 0 \\ 0 & 0 & 0.001 \end{bmatrix}, \quad S = \begin{bmatrix} 0.001 & 0 & 0 \\ 0 & 100 & 0 \\ 0 & 0 & 100 \end{bmatrix}$

Longer control and prediction horizons increase the computation time dramatically, but they have very little effect on closed-loop performance. The hybrid LMPC-NMPC controller is formulated as described in the previous section. The LMPC controller is tuned with $N_L = 15$ and:

$Q = \begin{bmatrix} 0.1 & 0 & 0 \\ 0 & 5 \times 10^4 & 0 \\ 0 & 0 & 5 \times 10^4 \end{bmatrix}, \quad R = \begin{bmatrix} 0.01 & 0 & 0 \\ 0 & 0.01 & 0 \\ 0 & 0 & 0.01 \end{bmatrix}, \quad S = \begin{bmatrix} 50 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

The NMPC controller is tuned with $N_N = 1$, $P_N = 4$, $Q = 2$, $R = 0.001$ and $S = 0.001$.

Figure 5.4 provides a comparison of the hybrid LMPC-NMPC and NMPC controllers for a $+10$ K change in the reactor temperature setpoint. Both controllers clearly outperform the standard LMPC controller (Figure 5.2). The NMPC controller provides a faster temperature response due to the nonlinear formulation of the entire system and the shorter control and prediction horizons used ($N_N = 1$, $P_N = 2$). On the other hand, the hybrid controller yields much smaller deviations in the column mole fractions due to the longer control and prediction horizons ($N_L = 15$, $P_L = \infty$) used in the LMPC controller. The sluggish NMPC performance for the column is due to the short control and prediction horizon lengths (10 and 20 sec.
respectively). As shown in Figure 5.1, the dominant time constant of the column is about 15–20 minutes. Significant performance improvement is expected if the horizon lengths are dramatically increased. However, reasonable increases in the horizon lengths yield little improvement in performance but significantly increase the computational load.

A simultaneous setpoint change in the reactor temperature (+20 K), the recycle mole fraction (+0.02) and the product mole fraction (−0.05) is shown in Figure 5.5. As before, the temperature response of the NMPC controller is significantly faster than that of the hybrid controller. The two controllers provide similar performance for the recycle mole fraction setpoint change, while the hybrid controller yields superior tracking of the product mole fraction setpoint change.

Even with the availability of increasingly powerful computers, the rigorous solutions of most plant-wide NMPC problems remains intractable. The major advantage of the hybrid method as compared to NMPC is computation time. For a typical 30 minute MATLAB simulation on a DEC 433 workstation, the hybrid controller requires approximately 3 minutes of CPU time while the NMPC controller requires about 40 minutes. It is important to note that NMPC execution times would be increased further by the introduction of a nonlinear state/disturbance estimator. These results demonstrate that the hybrid method can provide a suitable compromise between closed-loop performance and on-line computation for the class of nonlinear processes considered.
Figure 5.4: Hybrid LMPC-NMPC (——) and NMPC (----) for a setpoint change in the reactor temperature.

5.5 Summary and Conclusions

This chapter represents a first step in developing a comprehensive methodology for plant-wide control via integration of LMPC and NMPC. The proposed method in-
Figure 5.5: Hybrid LMPC-NMPC (—) and NMPC (— —) for setpoint changes in the reactor temperature and column mole fractions.

Involves decomposing the plant into linear and nonlinear subsystems and applying the appropriate MPC technology to each subsystem. A simple method for coordinating...
the LMPC and NMPC controllers for plants that can be decomposed into a single linear subsystem and a single nonlinear subsystem was presented. The proposed approach was compared to LMPC and NMPC using a prototypical reactor/separator process with recycle. The next chapter will focus on the plant decomposition, MPC solution sequence and controller coordination methods, and stability analysis.
Chapter 6

A Hybrid Model Predictive Control Strategy for Plant-wide Control — Part II

6.1 Introduction

The synthesis of plant-wide control systems is considered to be one of the most important design problems in process control [112]. The plant-wide control problem includes: selection of controlled variables, manipulated variables and measured variables; formulation of the control structure connecting the variables; and specification of the controller type [73, 108]. The problem originally was studied by Buckley [19]. Because of the inherent complexity, considerable research has been focused on decomposition of the plant-wide problem into simpler problems based on time-scale differences and functional groups. In a series of paper by Stephanopoulos and co-workers [8, 73, 74, 75], the selection of plant-wide control structures is formulated as an optimization problem. This problem then is decomposed vertically based on disturbance dynamics and horizontally based on functional groups to yield modular feedback optimizing control problems. The same authors address the synthesis of regulatory loops, selection of secondary measurements, state estimation and synthesis of control structures for two representative chemical processes.
A tiered framework for solution of the plant-wide control problem proposed by Price and Georgakis [85] is based on grouping the control loops in multiple tiers based on the relative importance of the associated control objectives. Zheng and co-workers [122] propose a hierarchical procedure for formulating control structures based on minimizing economic penalties first using a steady-state model and then using a dynamic model. Ng and Stephanopoulos [81] develop a hierarchical procedure that successively increases the resolution of flowsheet control structure. Based on the optimizing feedback approach [73], Skogestad [108] develops a procedure for identifying controlled variables which lead to near optimal operation when the variables are maintained at constant setpoints. Luyben et al. [60] propose a heuristic design procedure for generating a decentralized control structure. Most existing plant-wide control techniques are based on the use of decentralized control loops. An exception is the modular multivariable controllers [68] used in [81].

In principle model predictive controllers can be applied to entire plant-wide control problem. The predictive controller usually is placed on top of regulatory control loops designed to handle fast dynamics and maintain inventories. The predictive controller is executed less frequently to regulate the product quality variables and to ensure the satisfaction of equipment and process constraints. An additional steady-state feedback optimization problem can be included to solve for the optimal state and input targets based on measured disturbances and/or unknown disturbances estimated from observers [80]. This strategy is used in the multilayer approach in...
and the tiered framework in [85]. Therefore the procedures discussed above can be used to select controlled outputs for regulatory control, predictive control and on-line optimization.

The multivariable and constraint handling ability of model predictive control (MPC) make it an attractive alternative to decentralized control. However there still are challenges associated with the application of MPC to plant-wide control problems including [81]: i) nonlinear process dynamics; ii) poor model uncertainty characterization; and iii) large-scale on-line optimization. Linear model predictive control (LMPC) has been applied successfully to industrial processes with hundreds of input and output variables [86]. However process nonlinearities may preclude the successful application of LMPC and nonlinear model predictive control (NMPC) may be required. Because a nonlinear dynamic model is used for prediction and a nonlinear programming problem for is required to calculate the optimal input moves, NMPC yields complications associated with dynamic modeling, state estimation and on-line solution of the optimization problem [39]. Despite these difficulties, a NMPC controller has been developed for the Tennessee Eastman Challenge Process by the judicious use of modeling and controller simplifications [97].

Motivated by the fact that highly nonlinear dynamic behavior typically is associated with a small number of unit operations, we proposed a hybrid model predictive control strategy for plant-wide control in Chapter 5. This approach has the advantage of utilizing NMPC only where necessary while exploiting the computational
efficiency of LMPC. The design procedure is illustrated using a representative process example: a reaction/separation system with recycle. First the plant is decomposed into a large linear subsystem (the distillation column) and a small nonlinear subsystem (the reactor) based on the nonlinearity of the unit operations. LMPC is applied to the column and NMPC is applied to the reactor. Two controller coordination strategies are proposed to account for the interconnections between the two subsystems due to the column recycle stream. Simulation results have shown that the performance of the hybrid MPC controller is comparable to that of a NMPC controller and superior to that of a LMPC controller. On the other hand, the computational cost of the hybrid controller is only eight percent of that of the NMPC controller.

Although the hybrid LMPC-NMPC strategy is promising for plant-wide applications, there remain several unresolved difficulties. Since there exist numerous possibilities for decomposition of a complicated plant, a systematic decomposition procedure is needed. To achieve significant computational cost reduction, the subsystem MPC controllers need to be solved sequentially. Typically approximations are required because solution of a particular MPC problem requires information available only after the other MPC problems are solved. A sequential design procedure is needed to minimize the amount of unavailable information. When subsystem couplings preclude exact solution of the MPC problems, it is necessary to develop controller coordination strategies to handle the information exchange prob-
lem. Characterization of the class of plants for which the hybrid MPC strategy is stabilizing needs to be developed. Finally exploitation of individual subsystem time-scale properties offers the possibility of further reductions in on-line computation. All these issues are studied in this chapter.

The remainder of the chapter is organized as follows. In Section 6.2, a plant decomposition algorithm is presented and applied to a large-scale styrene plant flowsheet. Hybrid MPC strategies for both two-subsystem and multi-subsystem problems are presented in Section 6.3. This section includes solution of the sequential design problem and its application to the styrene plant, the development of controller coordination methods and stability analysis for a specific class of nonlinear systems. In Section 6.4 the controller coordination methods and a multi-time scale extension are applied to reactor/separator system considered in Chapter 5. Finally a summary and conclusion are given in Section 6.5.

6.2 Plant Decomposition

The plant is decomposed based on the nonlinearity properties of the unit operations. In this paper the relative nonlinearity of the unit operations is determined \textit{a priori}. While rigorous nonlinearity measures have been proposed [33, 111], the requirement of a complete nonlinear plant model makes these techniques difficult to apply to complex flowsheets. The objective of the decomposition procedure is to partition the plant into interconnected linear and nonlinear subsystems, each consisting of multiple unit operations. The decomposition algorithm presented in Section 6.2.1
is designed to produce the smallest number of subsystems. In Section 6.2.2 the algorithm is applied to a styrene plant flowsheet.

### 6.2.1 Plant Decomposition Algorithm

The required information for the plant decomposition (partitioning) algorithm is a vector containing the nonlinearity properties of all unit operations and a matrix describing the unit connections:

- **unit operation nonlinearity vector** $n$: $n_i = 1$ if $u_i$ is nonlinear; $n_i = 0$ if $u_i$ is linear.

- **unit operation connection matrix** $C$: $C_{ij} = 1$ if $u_i$ affects $u_j$; $C_{ij} = 0$ otherwise.

where $u_i$ denotes the $i$-th unit operation. If there is a total number of $N$ unit operations in the plant-wide system, $n$ is a $N \times 1$ vector and $C$ is a $N \times N$ matrix.

The solution of the decomposition problem can be represented by: 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 of each subsystem; and iii) a subsystem connection matrix $\Gamma$ that provides the subsystem connection information. These quantities are defined formally below:

- **decomposition matrix** $X$: $X_{i,j} = 1$ if $u_i$ is contained in $g_j$; $X_{i,j} = 0$ otherwise.

- **subsystem nonlinearity vector** $Y$: $Y_i = 1$ if $g_i$ is nonlinear; $Y_i = 0$ otherwise.
subsystem connection matrix $\Gamma$: $\Gamma_{i,j} = 1$ if $g_i$ affect $g_j$; $\Gamma_{i,j} = 0$ otherwise.

where $g_j$ denotes the $j$-th subsystem. The partition has to satisfy the following constraints:

1. Every unit operation belongs to one and only one subsystem.

2. All unit operations in a given subsystem 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 an objective function representing the number of subsystems is minimized. In Appendix D.1 the optimization problem is formulated as a binary polynomial programming problem. This problem can be transformed into a binary linear programming (LP) problem [88] with $Z$ decision variables and $3N$ constraints where:

$$Z = \sum_{M=0}^{N} \binom{N}{M}$$

$$\binom{N}{M} = \frac{N}{M(N-M)!}$$

For the styrene plant considered in the next section, $N = 16$ which leads to 1048576 decision variables and 48 constraints. While the optimization approach provides a
Figure 6.1: Schematic representation of the plant partitioning algorithm.

rigorous solution of the decomposition problem, the following iterative algorithm is simpler and more efficient for the type of plant-wide control problems typically encountered.
A schematic representation of the partitioning algorithm is shown in Figure 6.1 where \( k \) is the index for the subsystem and \( b_i \) is an element of a \( N \times 1 \) flag vector which is set to unity after unit \( i \) and all its connected units with the same nonlinearity property are assigned to the same subsystem. The partitioning algorithm is designed to find the \( N \times M \) decomposition matrix \( X \) where the total number of subsystems \( M \) is minimized. The algorithm is comprised of three loops. The inner loop assigns all units \( j \) with same nonlinearity property that directly connect to a given unit \( i \) to the same subsystem \( k \). The second loop repeats the first loop until no additional units can be added to the current subsystem. The outer loop creates additional subsystems if there are remaining units unassigned. After obtaining the decomposition matrix \( X \), the subsystem connection matrix \( \Gamma \) is found from \( X \) and the unit connection matrix \( C \) as follows:

\[
\Gamma_{ij} = \begin{cases} 
1 & \text{if } X_i^T C X_j \geq 1 \\
0 & \text{otherwise}
\end{cases}
\] 

where \( X_i \) denotes the \( i \)th column of \( X \) corresponding to the \( i \)-th subsystem. The scalar \( X_i^T C X_j \) is a positive integer if any units in subsystem \( i \) affect any units in subsystem \( j \).

6.2.2 Application to a Styrene Plant Flowsheet

A styrene plant example is used to illustrate the decomposition algorithm because it contains a large number of unit operations and several recycle streams. A flowsheet
of the styrene plant is shown in Figure 6.2 where: the feed consists of ethylene and benzene; ethylbenzene (EB) is formed in the first reactor; the first reactor effluent 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 second reactor products are fed to a series of columns to produce high purity styrene and EB for recycle back to the styrene reactor. More details on the EB/styrene process can be found elsewhere [45, 116].

Among the sixteen unit operations the exothermic EB reactor, the high purity EB column (overhead EB purity 99.6%) and the EB/styrene splitter (overhead styrene purity 99.9%) are considered nonlinear; the rest of the unit operations are considered linear. Note that the styrene reactor is endothermic and therefore it is treated as a linear unit. The nonzero elements of the connection matrix for the styrene plant 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}, C_{14,16}\}. The nonzero elements of the unit operation nonlinearity vector are \{n_4, n_6, n_{13}\}.

From this information the decomposition algorithm generates the connection matrix $X$, subsystem nonlinearity property vector $Y$ and subsystem connection
Figure 6.2: Styrene plant flowsheet.

matrix $\Gamma$:

$$X^T = \begin{bmatrix} 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$
The decomposed styrene plant flowsheet is shown in Figure 6.3. Subsystem 1 is a large group of linear unit operations including all the EB production units except the EB reactor and EB column. The EB reactor and EB column are the components of the 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. Since the styrene column is connected only to the EB/styrene column, it forms a single unit linear subsystem 6. The subsystem connection summarized by the matrix $\Gamma$ is illustrated in Figure 6.3. Both subsystems 2 and 3 are fully coupled with subsystem 1. Subsystem 3 is connected to subsystem 4 because the purified EB is fed to the styrene reactor. Subsystem 4 is fully coupled with subsystem 5 via the dehydrogenation products and the recycle EB rich stream. Subsystem 6 is affected only by subsystem 5.

\[
Y = \begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix} \quad \Gamma = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}
\]
Figure 6.3: Decomposed styrene plant flowsheet.

6.3 Model Predictive Control Strategy

Given the plant decomposition into linear and nonlinear subsystems, it is natural to apply linear model predictive control (LMPC) to the linear subsystems and to apply nonlinear model predictive control (NMPC) to the nonlinear subsystems. Little reduction in computation time can be realized if the on-line optimization problem is formulated for the entire process based on linear and nonlinear models for the corresponding subsystems. Therefore it is necessary to pursue sequential solution of
the individual MPC subsystem problems. Sequential solution of the MPC problems is not straightforward since the subsystems are coupled by mass and energy flows. For example information from a subsystem downstream is required when a recycle stream is present. Therefore controller coordination methods are needed to address the information exchange problem between subsystem MPC controllers. Determination of an appropriate MPC solution sequence also is an important problem because certain solution sequences may require less unknown information than other sequences. For some plants the subsystems resulting from nonlinearity decomposition have significant differences in time scales. For example the reaction/separation process considered in Section 6.4 the reactor dynamics are generally much faster than the column dynamics. This offers the possibility of solving the subsystem MPC problems at different sampling rates. In Section 6.3.1 the two subsystem problem is used to illustrate the MPC coordination methods and their properties. A general sequential MPC solution algorithm for complex plants is proposed in Section 6.3.2. Finally the multi-rate MPC problem is discussed in Section 6.3.3.

6.3.1 Two Subsystem Problems

For the simplest case of two subsystems, there are three possible plant configurations shown in Figure 6.4:

1. The linear subsystem affects the nonlinear subsystem.

2. The nonlinear subsystem affects the linear subsystem.
3. The linear and nonlinear subsystem are fully coupled.

The state-space model equations for the two subsystems can be written as (5.1)–(5.4), which represents a fully coupled plant. If the nonlinear subsystem does not affect the linear subsystem, then $A_N$, $B_N$ and $C_N$ become zero matrices. If the linear subsystem does not affect the nonlinear subsystem, then $f$ and $h$ are independent of $x_L$ and $u_L$. Clearly different MPC solution sequences are appropriate for each plant configuration in Figure 6.4.
For 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 using information from the first MPC controller. The necessary information from the first MPC controller is available even if the control horizon \((N)\) of the first controller is shorter than that of the second controller because the first subsystem can be iterated in open-loop fashion with constant input \(u^*(k)\) to yield the future state variables. The third configuration in Figure 6.4 is more challenging since the two subsystems are fully coupled. An example of such a fully coupled system is considered in Section 6.4 where the effluent from a nonlinear reactor is processed by distillation column and the recovered reactant is recycled to the reactor. For such systems at a given time step \(k\) the solution of each MPC problem requires information from the other MPC solution. Clearly some type of approximation is required to obtain an implementable sequential solution procedure.

Two sequential solution approaches for fully coupled two subsystems plants are discussed in Chapter 5, but only one approach was evaluated via simulation for the reaction/separation process. In this method a LMPC controller designed for the entire plant is solved first and then the NMPC controller for the nonlinear subsystem is solved using the LMPC solution only for the linear subsystem. Here this is called the global coordination method. It can be viewed as a transformation from the third configuration to the first configuration in Figure 6.4 since the entire plant is unidirectionally connected to the nonlinear subsystem. This approach is appropriate
for the reaction/separation process because the reactor model is low dimensional. Therefore the plant-wide LMPC problem is not much larger than the column LMPC problem. In Chapter 5 the performance of the hybrid LMPC-NMPC controller is shown to be comparable to that of a NMPC controller applied to the entire system and superior to that of a LMPC controller. Here the global controller coordination approach is discussed in more detail than in Chapter 5. Besides the size increase of the LMPC problem, another drawback of this approach is that the reactor is approximated by a linear model in the LMPC problem. If the complexity of the two subsystems are comparable then the global coordination method obviously is less desirable.

The other controller coordination method briefly discussed in Chapter 5 uses the solution of the MPC problems at the previous time step to solve the MPC problems at the current time step. This eliminates the information exchange problem and allows the LMPC and NMPC problems to be formulated separately for the respective subsystems. A simplified version of this approach is based on the simplifying assumption that the current state and input variables from the first subsystem remains constant in the future. When the LMPC problem is solved first the nonlinear state and input variables are treated as constant disturbances in the LMPC steady-state target calculation:

$$\begin{align*}
\min_{x_L^*(k),u_L^*(k)} &= [u_{L_{ref}} - u_L^*(k)]^T R_x [u_{L_{ref}} - u_L^*(k)] \\
&= \text{(6.3)}
\end{align*}$$

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subject to:

\[ x^s_L(k) = A_L x^s_L(k) + B_L u^s_L(k) + A_N x_N(k|k) + B_N u_N(k|k-1) \]

\[ y^ref_L = C_L x^s_L(k) + C_N x_N(k|k) + \hat{d}_L(k) \]

\[ u_{L,\text{min}} \leq u^s_L(k) \leq u_{L,\text{max}} \]

where: \( x^s_L(k) \) and \( u^s_L(k) \) are the steady-state state and input targets, respectively, at time step \( k \); and \( \hat{d}_L(k) \) is an estimated step output disturbance. The targets are calculated by minimizing the difference between the input target and the input setpoint \( u^ref_L \) subject to steady-state equality and inequality constraints. The steady-state targets for the NMPC problem are calculated similarly using \( x_L(k|k) \) and \( u_L(k|k) \) obtained from the LMPC problem. This is the simplest approach to account for the coupling between subsystems because only one time step ahead predictions are used. This is called the local steady-state coordination method since future state and input variables are assumed to remain constant in the future.

A more sophisticated sequential solution approach for handling information exchange between the subsystems that does not require the steady-state assumption is outlined below. In this method the evolution of future state and input variables is included in the subsystem MPC problems. Assume the LMPC is solved first. At time step \( k \), an estimate of the future nonlinear state and input variables is available.
from the NMPC solution at time $k - 1$:

$$X_N(k - 1) = \begin{bmatrix} x_N^T(k|k - 1) & \cdots & x_N^T(k + P_N - 1|k - 1) & \cdots & x_N^T(k + N_L - 1|k - 1) \end{bmatrix}^T$$

$$U_N(k - 1) = \begin{bmatrix} u_N^T(k|k - 1) & \cdots & u_N^T(k + N_N - 2|k - 1) & \cdots & u_N^T(k + N_L - 1|k - 1) \end{bmatrix}^T$$

where: $X_N(k - 1)$ and $U_N(k - 1)$ denote vectors of future nonlinear state and input variables calculated at time step $k - 1$; $P_N$ and $N_N$ are the prediction and control horizons for the NMPC problem; and $N_L$ is the control horizon for the LMPC problem. Note that $N_L$ generally is greater than $P_N$ and $N_N$. In this case the last $N_L - P_N$ elements of $X_N(k - 1)$ are obtained by open-loop simulation of the nonlinear subsystem equations with constant input: $u_N(k + j|k - 1) = u_N(k + N_N - 2|k - 1) \forall j \geq N_N - 1$. A simpler approach is to assume that $x_N(k + j|k - 1) = x_N(k + P_N - 1|k - 1) \forall j \geq P_N$. The QP formulation of the LMPC problem is modified from that given in [80] to incorporate $X_N(k - 1)$ and $U_N(k - 1)$. The modified QP matrices are presented in Appendix D.2. The steady-state target calculation (6.3) is modified by using $x_N(k + N_L - 1|k - 1)$ and $u_N(k + N_L - 1|k - 1)$ in place of $x_N(k)$ and $u_N(k|k - 1)$, respectively.
After obtaining the LMPC solution, the following information is available to the NMPC problem:

\[
X_L(k) = \begin{bmatrix} x_L^T(k|k) & x_L^T(k + 1|k) & \cdots & x_L^T(k + N_L|k) \end{bmatrix}^T
\]
\[
U_L(k) = \begin{bmatrix} u_L^T(k|k) & u_L^T(k + 1|k) & \cdots & u_L^T(k + N_L - 1|k) \end{bmatrix}^T
\]

where: \(X_L\) and \(U_L\) denote vectors of future linear state and input variables, respectively, calculated at the current time step \(k\). These values are incorporated directly in the equality constraints representing the discretized nonlinear model equations. This approach is called the local dynamic coordination method. It is an enhancement of the local steady-state coordination method because dynamic information from each subsystems is used in the MPC calculations. The local coordination methods offer a computational advantage over the global coordination method discussed earlier if the nonlinear subsystem is sufficiently high order.

\subsection*{6.3.2 Multiple Subsystem Problems}

Although not presented here for the sake of brevity, the controller coordination methods discussed above can be extended in a straightforward fashion to multiple subsystem problems. However for complex processes such as the styrene plant that yield multiple subsystems, the determination of an appropriate solution sequence is much more difficult than that for two subsystem problems. One class of decomposed
plants for which the solution sequence problem is solved trivially has the form:

\[
x_1(k+1) = f_1[x_1(k), u_1(k)] \]
\[
x_2(k+1) = f_1[x_1(k), x_2(k), u_1(k), u_2(k)]
\]
\[
\vdots
\]
\[
x_{M-1}(k+1) = f_{M-1}[x_1(k), \ldots, x_{M-1}(k), u_1(k), \ldots, u_{M-1}(k)]
\]
\[
x_M(k+1) = f_{M-1}[x_1(k), \ldots, x_M(k), u_1(k), \ldots, u_M(k)]
\]

where: \( M \) is the number of subsystems; \( x_i(k) \) and \( u_i(k) \) are the state and input vectors, respectively, of the \( i \)-th subsystem; and \( f_i(\cdot) \) are (possibly) nonlinear functions. If a particular subsystem is linear the associated state-space equation can be written analogously to (5.1). This is called a triangular decomposition since the \( i \)-th subsystem depends only on the input and state variables of first \( i \) subsystems. For such systems it is obvious that the appropriate MPC solution sequence is \( g_1, g_2, \ldots, g_{n-1}, g_n \) where \( g_i \) is the \( i \)-th subsystem. This allows each MPC problem to be solved exactly without any approximations.

Triangular systems of the form (6.4) are precisely the class of nonlinear systems for which we are able to prove closed-loop stability of the hybrid LMPC-NMPC method. The proof of the following result, which is based on the theorems in [103] will be presented in a future paper and is omitted here for the sake of brevity. Assume that the MPC problems are feasible and the resulting feedback control laws
are represented as:

\[ u_i(k + j|k) = h_j^i [x_1(k), \ldots, x_i(k)] \quad j \in [0, N_i - 1], \ i \in [1, M] \tag{6.5} \]

where \( N_i \) is the control horizon of the \( i \)-th MPC controller and \( h_j^i(\cdot) \) are nonlinear functions. If the following assumptions hold:

1. \( f_i(x_1, \ldots, x_i, u_1, \ldots, u_i) \) is Lipschitz in its arguments \( \forall i \in [1, M] \).

2. \( h_j^i(x_1, \ldots, x_i) \) is Lipschitz in its arguments \( \forall j \in [0, N_i - 1], \forall i \in [1, M] \).

then \( x(k) = \begin{bmatrix} x_1^T(k) & \ldots & x_M^T(k) \end{bmatrix}^T = 0 \) is a locally asymptotically stable fixed point of the closed-loop system:

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

Note that if the \( i \)-th subsystem is linear then the function \( f_i(\cdot) \) and \( h_j^i(\cdot) \) are guaranteed to be Lipschitz [77].

When recycle streams exist in a complex system such as the styrene plant (see Figure 6.2), the resulting decomposed plant (see Figure 6.3) usually is highly interconnected. In this case it is difficult to determine an appropriate solution sequence or to prove closed-loop stability. Clearly the amount of unknown information required by each MPC controller depends on the solution sequence. The optimization problem presented in Appendix D.3 is formulated to obtain a solution sequence with the least amount of information required from the unsolved subsystems. While it
may be possible to develop a rigorous solution of this optimization problem using methods developed for the traveling salesman problem [58], the computational complexity motivated us to investigate alternative approaches. For the styrene plant problem it is possible to enumerate and evaluate all 6! solution sequences. For more complex systems this may not be tractable.

Below we present an iterative algorithm for determining the solution sequence based on the subsystem connection matrix $\Gamma$ and subsystem nonlinearity property vector $Y$. The algorithm produces a solution sequence represented by the $M \times M$ matrix $\Psi$, where the element $\Psi_{i,j} = 1$ if the $j$th subsystem is the $i$-th subsystem solved. The algorithm shown schematically in Figure 6.5 consists of two loops. The outer loop simply increments the solution sequence index, while the inner loop determines the next subsystem to be solved. Three vectors are introduced and re-evaluated every iteration of the outer loop based on the updated matrix $\Psi$. 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 the previous iterations. The criteria for determining which subsystem to select are ranked below according to their priorities:

1. The subsystem is affected by the least number of other subsystems not yet selected.

2. The subsystem affects the most number of other subsystems not yet selected.
3. The subsystem is linear.

4. The subsystem has the lowest number in the flowsheet.

Now the iterative algorithm for MPC sequence selection is applied to the de­
composed styrene plant flowsheet in Figure 6.3. The resulting sequence is shown
in Figure 6.6. Both the EB column 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 upstream of the EB/styrene column. The EB/styrene 
column is selected second because it affects two other subsystems. 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 upstream of the styrene col­
umn. The styrene column is solved fourth. The EB plant units (subsystem 1) are 
chosen before the EB reactor because subsystem 1 is linear. The iterative approach 
generates a unique solution, but there may exist alternative sequences that require 
the same amount of unknown information. For example the solution of subsystems 
1 and 2 before subsystems 4 and 6 is identical to the sequence in Figure 6.6 with 
regard to unknown information. Therefore engineering judgment may be necessary 
to determine the final solution sequence.

6.3.3 Multi-Rate Problems

Decomposition according to nonlinearity properties may result in subsystems that 
have significant time-scale differences. In the reaction/separation example consid­
ered in the next section the reactor has much faster dynamics than does the distilla­
tion column. Computational efficiency can be further enhanced by solving the MPC 
controller for the slower subsystem at a lower frequency. This approach is particu-
Figure 6.6: MPC sequential solution for styrene plant.

larly desirable if the nonlinear subsystems have slower dynamics because this allows less frequent solution of the NMPC controllers.

Below we consider the alternative case where the linear subsystem dynamics are slower because this is the case for the reaction/separation example. For simplicity the development is restricted to two subsystem problems and the local dynamic coordination method discussed earlier. Assume the sampling rate of the NMPC controller is $\Delta t_N$ and that of LMPC problem is $\Delta t_L$ 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 $k_L$, $t = k_L \Delta t_L$ and 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 $k_N = nk_L$:

$$X_N(k_N - 1) = \left[ x_N^T(k_L|k_N - 1) \cdots x_N^T(k_L + P_N|k_N - 1) \cdots x_N^T(k_L + N_L - 1|k_N - 1) \right]^T$$

$$U_N(k_N - 1) = \left[ u_N^T(k_L|k_N - 1) \cdots u_N^T(k_L + N_L|k_N - 1) \cdots u_N^T(k_L + N_L - 1|k_N - 1) \right]^T$$

Here $P_N$ and $N_N$ are the NMPC prediction and control horizons, respectively, expressed as integer multiples of the linear sampling time $\Delta t_L$: $\bar{P}_N = \text{int} \left( \frac{P}{n} \right)$ and $\bar{N}_N = \text{int} \left( \frac{N}{n} \right)$. As before $x_N$ beyond the NMPC prediction horizon can be obtained via open-loop simulation 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. The NMPC solutions are based on the linear state and input variable predictions available at time $k_L$:

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

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

where $j \in [0, n - 1]$. The NMPC results are implemented every $\Delta t_N$ time units.
6.4 Simulation Example

The reaction/separation process studied in Chapter 5 is used to illustrate the MPC controller coordination methods presented in Section 6.3. For this example the linear subsystem (column) and the nonlinear subsystem (reactor) are easily determined. The combined model can be represented as in (5.1)–(5.4) with state, input and output vectors defined as follows:

\begin{align*}
    x_L &= \begin{bmatrix} X_{A1} & X_{A2} & X_{A3} & X_{A4} & X_{A5} & X_{A6} & X_{A7} & X_{A8} & X_{A9} \end{bmatrix}^T \\
    u_L &= \begin{bmatrix} L & V \end{bmatrix}^T, \quad y_L = \begin{bmatrix} X_{A1} & X_{A9} \end{bmatrix}^T \\
    x_N &= \begin{bmatrix} T & C_A \end{bmatrix}^T, \quad u_N = T_c, \quad y_N = T
\end{align*}

The model parameters are given in Table 5.1.

In Chapter 5 only the global controller coordination method is investigated via simulation and compared to standard plant-wide LMPC and NMPC. The hybrid LMPC-NMPC approach is shown to offer tremendous performance improvements over LMPC especially for operation at an unstable operating point of the reactor. While the hybrid controller offers comparable performance to the NMPC controller, the computation time for a 30 min simulation is reduced from 40 minutes to 3 minutes. Below all three controller coordination methods and the multi-rate controller formulation discussed in Section 6.3 are evaluated. The controller tuning parame-
ters for each coordination method are listed below. The sampling period is \( \Delta t = 10 \) seconds.

1. Global coordination approach:

LMPC: \( N_L = 15, \ P_L = \infty, \)

\[
Q = \begin{bmatrix}
0.1 & 0 & 0 \\
0 & 5 \times 10^4 & 0 \\
0 & 0 & 5 \times 10^4
\end{bmatrix}, \quad R = \begin{bmatrix}
0.01 & 0 & 0 \\
0 & 0.01 & 0 \\
0 & 0 & 0.01
\end{bmatrix}, \quad S = \begin{bmatrix}
50 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

NMPC: \( N_N = 1, \ P_N = 4, \ Q = 2, \ R = 0.001, \ S = 0.001 \)

2. Local steady-state coordination approach:

LMPC: \( N_L = 15, \ P_L = \infty, \)

\[
Q = \begin{bmatrix}
5 \times 10^4 & 0 \\
0 & 5 \times 10^4
\end{bmatrix}, \quad R = \begin{bmatrix}
0.01 & 0 \\
0 & 0.01
\end{bmatrix}, \quad S = \begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix}
\]

NMPC: \( N_N = 1, \ P_N = 5, \ Q = 2, \ R = 0.001, \ S = 0.001 \)

3. Local dynamic coordination approach: all tuning parameters are identical to those of local steady-state coordination approach.
Figure 6.7: LMPC-NMPC: +10 K change in reactor temperature setpoint.

In Figure 6.7 the three controller coordination approaches are compared for a +10 K change in the reactor temperature setpoint. All three methods rapidly bring the reactor temperature to the new setpoint while rejecting the disturbance that prop-
agates through the distillation column. The closed-loop dynamics of the reactor is
slightly improved for the second and third approaches due to the longer prediction
horizons used. Note that the input moves for the nonlinear subsystem are virtually
identical for all three approaches. More significant differences are observed in column
performance as the global and local dynamic approaches perform much better than
the local steady-state approach. This is attributable to the steady-state approxi­
mation 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 is attributable to differences in the coordination
methods. The global method uses a linear approximation of the reactor in the global
LMPC solution, while the local dynamic method uses the previous NMPC solution
to generate the current LMPC solution and is based on the assumption that the
nonlinear variables are constant beyond the relatively short NMPC horizons. The
input moves for the linear subsystem are least aggressive for the local steady-state
method, while the input moves for first and third methods are comparable.

In Figure 6.8 the three methods are compared for an unmeasured +5 K dis­
turbance in the reactor feed temperature. The global approach produces the least
amount of overshoot in the reactor temperature. The local dynamic approach of­
ers very similar performance, while the local steady-state approach yields relatively
poor column performance.
Figure 6.8: LMPC-NMPC: +5 K disturbance in reactor feed temperature.

In Figure 6.9 the multi-rate approach discussed in Section 6.3 is compared to the single rate approach where the local dynamic controller coordination method is used in both cases. Since the column dynamics are significantly slower than the
reactor dynamics, the LMPC controller is executed at a frequency of 60 seconds while the NMPC controller is executed every 10 seconds (i.e. \( n = 6 \)). As expected
the two methods yield very similar performance for the reactor. The column performance obtained with the multi-rate controller is slightly degraded, which is largely attributable to less aggressive input moves. Note that \( \tilde{P}_N \) and \( \tilde{N}_N \) are zeros because both \( P_N \) and \( N_N \) are less than \( n = 6 \). Therefore the multi-rate controller is effectively equivalent to a local steady-state controller except that the LMPC controller is solved at a lower frequency with a longer control horizon due to the larger sampling period. It is interesting to note that the multi-rate method outperforms the single-rate local steady-state method (compare Figures 6.7 and 6.9). This may be attributable to the longer control horizon used for the multi-rate LMPC controller. The simulation time for the multi-rate controller is approximately two minutes which represents a modest improvement over the single-rate controllers. More significant reductions in computation time are expected when the NMPC controllers can be executed less frequently than the LMPC controllers.

6.5 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 developed. The plant is decomposed into a number of linear and nonlinear subsystems based on the nonlinearity properties and interconnections of the unit operations. An iterative decomposition algorithm has been developed and applied to a complex styrene plant flowsheet. Linear and nonlinear MPC is applied to the decomposed subsystems according to their nonlinearity properties. An iterative se-
quential solution algorithm that attempts to minimize the unavailable information from other subsystems have been developed and applied to the decomposed styrene flowsheet. The hybrid LMPC-NMPC approach is stabilizing for a class of triangular systems for which the MPC solution sequence problem is trivially solved. Three alternative controller coordination strategies have been developed to deal with plants with more complex interconnections. An extension for multi-rate control has been presented for plants which can be decomposed into subsystems with different timescale properties. A reaction/separation example is used to compare the different controller coordination methods. The global and local dynamic controller coordination approaches are shown to provide the best closed-loop performance.
Chapter 7

Conclusion and Recommendations

In previous chapters model predictive control (MPC) strategies have been developed for a gas pipeline network described by nonlinear ordinary differential equations and a bioreactor described by population balance equations; a reduced-order model is constructed for a cryogenic distillation column that facilitates the development of a nonlinear model predictive control (NMPC) strategy; finally a novel plant-wide control approach is formulated based on the integration of linear and nonlinear MPC. In this chapter, the most important results are summarized and suggestions for future work are outlined.

7.1 Model Predictive Control of Gas Pipeline Networks

In Chapter 2, a linear model predictive control (LMPC) strategy is developed for a representative gas pipeline network. The full-order nonlinear model is derived from mass balance equations and the Virial equation of state to describe pressures at discrete node points along the network. These node points represent the locations of production plants, customer plants and pipeline joints. The resulting model is high dimensional. Due to physical dimensions of the pipelines, the full-order model exhibits multiple time scales and is poorly conditioned. Based on time-scale
properties of the state variables, reduced-order models are obtained by combining node points with fast dynamics. The reduced models offers dramatic improvements in simulation efficiency and numerical conditioning with minimal loss of prediction accuracy. A LMPC controller based on the reduced-order model is designed. The LMPC controller provides excellent closed-loop performance for a wide variety of setpoint changes and disturbances. However infeasibility of the LMPC quadratic program may occur due to output constraints. Three alternative output constraint handling techniques are incorporated to resolve infeasibilities in the LMPC quadratic program and their relative performance is evaluated. The simulation results indicate that the proposed LMPC strategy can significantly improve the operability of large-scale pipeline networks with complex configurations.

A possible enhancement to the pipeline work is a more general model reduction approach based on singular perturbation theory [53]. The singular perturbation approach offers a more rigorous standard for model reduction. However physical interpretation of the reduced model may be more difficult. This approach has been applied to complicated electrical power networks [53]. Praxair currently is implementing a MPC control strategy derived from this work on their gas pipeline networks.
7.2 Order Reduction of Cryogenic Distillation Column Models

A nonlinear wave model is developed for cryogenic distillation columns in Chapter 3. Significant order reduction is achieved for a single nitrogen column. The low-order model is compared to a rigorous HYSYS model which is based on first principles. Simulation results have shown that the low-order wave model is capable of producing acceptable prediction of composition responses for disturbances in the feed flow rate if the wave model parameters are estimated from judiciously chosen steady-state composition profiles. Simulation results have also illustrated that the constant wave pattern assumption used in the wave model development is responsible for significant prediction error because the actual composition profiles are self-sharpening. We have shown that discrepancies between the nonlinear wave model and a first-principles HYSYS model can be reduced to an acceptable level by adjustment of $\gamma$.

Since Chapter 3 only represents the initial step in the development of a nonlinear model-based approach for cryogenic column control, there is considerable work remaining in both process modeling and controller design. The first step should be the development of an on-line parameter adaptation algorithm to accurately estimate $\gamma$. The overhead and bottom compositions can be chosen as measured variables. The parameter $\gamma$ can be estimated by a nonlinear observer [10] or calculated based on boundary conditions for the measured variables [93]. Next the nonlinear wave modeling approach should be applied to air separation plants containing multiple
columns that produce purified nitrogen, oxygen and argon. Each column section will require a separate wave model. In the multi-column case, the parameter $y_{\text{min}}$ will change when the feed composition varies. It is recommended to estimate $y_{\text{min}}$ based on a boundary condition on the feed composition. Additionally it will be necessary to develop a nonlinear wave model for the ternary mixture in the upper column where all three components have significant concentrations. In a recent paper, Kienle [52] proposed linear superposition of nonlinear waves for multicomponent distillation columns.

The primary motivation for derivation of the wave model is the development of a model-based nonlinear control strategy for air separation plants. Optimization-based strategies such as nonlinear model predictive control [70] that are based on the wave model may be implemented on the detailed HYSYS model. Before controller implementation the model equations describing the sump and reboiler dynamics may be further simplified by assuming perfect perform of the low level regulatory controllers.

### 7.3 Oscillating Yeast Cultures

In Chapter 4, a dynamic model for continuous yeast bioreactors is formulated by coupling the population balance equation (PBE) for the cell mass distribution to the substrate mass balance. The empirical functions used to describe the dependence of cell transition and division on the medium are chosen such that the PBE model exhibits stable periodic solutions under reasonable operating conditions. The model
is solved numerically by spatially discretizing the PBE using orthogonal collocation on finite elements. The resulting nonlinear ordinary differential equation model is linearized and discretized in time to yield a linear state-space model suitable for LMPC synthesis. The MPC controller is designed to stabilize steady-state and periodic solutions by regulating the discretized cell number distribution and the substrate concentration. The closed-loop results have shown that the oscillatory behavior of the cell culture is closely related to synchronization of the cell cycle.

Chapter 4 is part of a continuing investigation on the dynamics and control of oscillatory yeast bioreactors. Using the mass domain model described in Chapter 4, Zhang et al. [120] have performed a rigorous bifurcation analysis of the model and developed a feedback linearization controllers for attenuating sustained oscillations. Mhaskar [72] has modified the mass domain model to include chemical structure of the medium. A critical goal is the estimation of unknown parameters in the empirical model functions from experimental data. The ultimate goal should be experimental testing of the controllers developed.

7.4 Hybrid LMPC-NMPC for Plant-wide Control

In Chapters 5 and 6, a systematic methodology has been developed for plant-wide control applications by integrating LMPC and NMPC. An outline of the method is presented in Chapter 5 along with some encouraging initial simulation results. In Chapter 6, the hybrid method is studied more systematically. First the plant is
decomposed into a number of linear and nonlinear subsystems based on the nonlinearity properties and interconnections of the unit operations. An iterative decomposition algorithm is developed and applied to a complex styrene plant flowsheet. Based on the decomposition results, LMPC and NMPC controllers are applied to the decomposed subsystems according to their nonlinearity properties. An iterative sequential solution algorithm is developed to minimize the unavailable information in MPC calculations. It has been applied to the decomposed styrene flowsheet. The hybrid LMPC-NMPC approach is shown to be stabilizing for a class of triangular systems. Finally three alternative controller coordination strategies have been developed to deal with plants with more complex interconnections. An extension for multi-rate control has been presented for plants which can be decomposed into subsystems with different time-scale properties. A reaction/separation example is used to compare the different controller coordination methods. The global and local dynamic controller coordination approaches are shown to provide the best closed-loop performance.

Currently the nonlinearity properties of the unit operations are assumed to be known from the model equations (reaction/separation example) or from qualitative information in the literature (styrene example). It is desirable to develop techniques to measure unit nonlinearity directly from plant data. Such a statistical approach was proposed by Billings and Voon [17] and implemented on a high-purity distillation column by Pearson and Ogunnaike [83]. Efficient solution techniques
for the plant decomposition and solution optimization should be developed from the combinatorial optimization literature [58]. It also is important to extend the controller coordination methods to a multi-subsystem problems and to apply the hybrid LMPC-NMPC method to a larger plant-wide problem such as the Tennessee Eastman Problem [25] and the styrene plant example. Additionally stability results should be developed for a more general class of interconnected systems.
Bibliography


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Appendix A

Supplement to Chapter 2

A.1 Nomenclature for Chapter 2

$B_i$: second Virial coefficient at node i (ft$^3$)

$C_v$: valve characteristic constant

$d_p$: pipe diameter (in)

$E_f$: pipe efficiency factor

$e_f$: pressure control loop filtered error

$F_{i,1}$: withdraw rate (kcfh) at node i, i = 1, 4, 6, 9, 11, 12, 14, 16, 17, 19, 22, 25, 26, 28, 30

$F_{10,j}$: production rate (kcfh) of plant 10-j, j = 1, 2, 3

$F_{24,j}$: production rate (kcfh) of plant 24-j, j = 1, 2

$F_{29,j}$: production rate (kcfh) of plant 29-1

$f_r$: friction factor

$Frq_{10,j}$: production setpoint (kcfh) of plant 10-j, j = 2, 3

$Frq_{24,j}$: production setpoint (kcfh) of plant 24-j, j = 1, 2

$Frq_{29,j}$: production setpoint (kcfh) of plant 29-1

$K_c$: let down station controller gain (%/psig)

$L$: pipe length (mile)
\( l \): percent valve opening

\( N_i \): molar holdup (lb-mole) at node \( i \)

\( P_i \): pressure (psig) at node \( i \)

\( P_{sp} \): setpoint (psig) for let-down pressure controller

\( R \): gas constant (psia—ft\(^3\)/lb mol—R)

\( S_g \): oxygen specific gravity

\( T \): pipeline temperature (R)

\( t_d \): dead time of closed-loop plants (min)

\( V_i \): node volume \( i \) (ft\(^3\))

\( Z_m \): mean compressibility

**Greek Letters:**

\( \eta \): pressure control loop accumulated error

\( \eta_f \): filtered accumulated error

\( \Gamma \): plant constraint vector

\( \Gamma_x \): subset of plant constraint variables used as state variables

\( \rho_{sc} \): molar density (lb mol/ft\(^3\)) of \( O_2 \) at 1 atm and 60 °F

\( \tau_{10,j} \): time constant of closed-loop cryogenic plant 10-\( j \), \( j = 2, 3 \)

\( \tau_{24,j} \): time constant of closed-loop cryogenic plant 24-\( j \), \( j = 1, 2 \)

\( \tau_{29,1} \): time constant of closed-loop cryogenic plant 29-1

\( \tau_f \): PI controller error filter time constant
\( \tau_i \): PI controller integral time

\( \theta \): pipe leg parameters

Superscripts:

ss: steady-state value

### A.2 Full-Order Pipeline Network Model

\[
\dot{P}_1(t) = \rho_{sc} f_2(P_1)[f_1(P_1, P_2) + F_{i,1}] 
\]  
(A.1)

\[
\dot{P}_2(t) = \rho_{sc} f_2(P_2)[f_1(P_2, P_1) + f_1(P_2, P_3) + f_1(P_2, P_4)] 
\]  
(A.2)

\[
\dot{P}_3(t) = \rho_{sc} f_2(P_3)[f_1(P_3, P_2) + f_1(P_3, P_5)] 
\]  
(A.3)

\[
\dot{P}_4(t) = \rho_{sc} f_2(P_4)[f_1(P_4, P_2) + F_{4,1}] 
\]  
(A.4)

\[
\dot{P}_5(t) = \rho_{sc} f_2(P_5)[f_1(P_5, P_3) + f_1(P_5, P_6) + f_1(P_5, P_7)] 
\]  
(A.5)

\[
\dot{P}_6(t) = \rho_{sc} f_2(P_6)[f_1(P_6, P_5) + F_{6,1}] 
\]  
(A.6)

\[
\dot{P}_7(t) = \rho_{sc} f_2(P_7)[f_1(P_7, P_6) + f_1(P_7, P_8)] 
\]  
(A.7)

\[
\dot{P}_8(t) = \rho_{sc} f_2(P_8)[f_1(P_8, P_7) + f_1(P_8, P_9) + f_1(P_8, P_{10})] 
\]  
(A.8)

\[
\dot{P}_9(t) = \rho_{sc} f_2(P_9)[f_1(P_9, P_8) + F_{9,1}] 
\]  
(A.9)

\[
\dot{P}_{10}(t) = \rho_{sc} f_2(P_{10})[f_1(P_{10}, P_9) + f_1(P_{10}, P_{11}) + f_1(P_{10}, P_{13}) + F_{10,1} + F_{10,2} + F_{10,3}] 
\]  
(A.10)

\[
\dot{P}_{11}(t) = \rho_{sc} f_2(P_{11})[f_1(P_{11}, P_{10}) + f_1(P_{11}, P_{12}) + F_{11,1}] 
\]  
(A.11)

\[
\dot{P}_{12}(t) = \rho_{sc} f_2(P_{12})[f_1(P_{12}, P_{11}) + F_{12,1}] 
\]  
(A.12)
\begin{align*}
\dot{P}_{13}(t) &= \rho_{sc}f_2(P_{13})[f_1(P_{13}, P_{10}) + f_1(P_{13}, P_{14}) + f_1(P_{13}, P_{15})] \quad (A.13) \\
\dot{P}_{14}(t) &= \rho_{sc}f_2(P_{14})[f_1(P_{14}, P_{13}) + F_{14,1}] \quad (A.14) \\
\dot{P}_{15}(t) &= \rho_{sc}f_2(P_{15})[f_1(P_{15}, P_{13}) + f_1(P_{15}, P_{16}) + f_1(P_{15}, P_{17}) + f_1(P_{15}, R_5)] \quad (A.15) \\
\dot{P}_{16}(t) &= \rho_{sc}f_2(P_{16})[f_1(P_{16}, P_{15}) + F_{16,1}] \quad (A.16) \\
\dot{P}_{17}(t) &= \rho_{sc}f_2(P_{17})[f_1(P_{17}, P_{15}) + F_{17,1}] \quad (A.17) \\
\dot{P}_{18}(t) &= \rho_{sc}f_2(P_{18})[f_1(P_{18}, P_{15}) + f_1(P_{18}, P_{19}) + f_1(P_{18}, P_{20})] \quad (A.18) \\
\dot{P}_{19}(t) &= \rho_{sc}f_2(P_{19})[f_1(P_{19}, P_{18}) + F_{19,1}] \quad (A.19) \\
\dot{P}_{20}(t) &= \rho_{sc}f_2(P_{20})[f_1(P_{20}, P_{18}) + f_1(P_{20}, P_{21}) + f_1(P_{20}, P_{22}, l)] \quad (A.20) \\
\dot{P}_{21}(t) &= \rho_{sc}f_2(P_{21})[f_1(P_{21}, P_{20}) + F_{21,1}] \quad (A.21) \\
\dot{P}_{22}(t) &= \rho_{sc}f_2(P_{22})[f_1(P_{22}, P_{23}) + f_1(P_{22}, P_{20}, l)] \quad (A.22) \\
\dot{P}_{23}(t) &= \rho_{sc}f_2(P_{23})[f_1(P_{23}, P_{22}) + f_1(P_{23}, P_{24}) + f_1(P_{23}, P_{25})] \quad (A.23) \\
\dot{P}_{24}(t) &= \rho_{sc}f_2(P_{24})[f_1(P_{24}, P_{23}) + F_{24,1} + F_{24,2}] \quad (A.24) \\
\dot{P}_{25}(t) &= \rho_{sc}f_2(P_{25})[f_1(P_{25}, P_{23}) + f_1(P_{25}, P_{26}) + f_1(P_{25}, P_{27}) + F_{25,1}] \quad (A.25) \\
\dot{P}_{26}(t) &= \rho_{sc}f_2(P_{26})[f_1(P_{26}, P_{25}) + F_{26,1}] \quad (A.26) \\
\dot{P}_{27}(t) &= \rho_{sc}f_2(P_{27})[f_1(P_{27}, P_{25}) + f_1(P_{27}, P_{28}) + f_1(P_{27}, P_{29})] \quad (A.27) \\
\dot{P}_{28}(t) &= \rho_{sc}f_2(P_{28})[f_1(P_{28}, P_{27}) + F_{28,1}] \quad (A.28) \\
\dot{P}_{29}(t) &= \rho_{sc}f_2(P_{29})[f_1(P_{29}, P_{27}) + f_1(P_{29}, P_{30}) + F_{29,1}] \quad (A.29) \\
\dot{P}_{30}(t) &= \rho_{sc}f_2(P_{30})[f_1(P_{30}, P_{29}) + F_{30,1}] \quad (A.30) \\
\dot{F}_{10,2}(t) &= \frac{1}{\tau_{10,2}}[F_{10,2}(t - t_d) - F_{10,2}(t)] \quad (A.31)
\end{align*}
\[ \dot{F}_{10,3}(t) = \frac{1}{\tau_{10,3}}[Frq_{10,3}(t - t_d) - F_{10,3}(t)] \]  
(A.32)

\[ \dot{F}_{24,1}(t) = \frac{1}{\tau_{24,1}}[Frq_{24,1}(t - t_d) - F_{24,1}(t)] \]  
(A.33)

\[ \dot{F}_{24,2}(t) = \frac{1}{\tau_{24,2}}[Frq_{24,2}(t - t_d) - F_{24,2}(t)] \]  
(A.34)

\[ \dot{F}_{29,1}(t) = \frac{1}{\tau_{29,1}}[Frq_{29,1}(t - t_d) - F_{29,1}(t)] \]  
(A.35)

\[ l = l_{ss} + K_c e_f + \frac{K_c}{\tau_f} \eta_f \]  
(A.36)

\[ \dot{\eta}(t) = P_{sp} - P_{20} \]  
(A.37)

\[ \dot{e}_f(t) = \frac{1}{\tau_f}(P_{sp} - P_{20} - e_f) \]  
(A.38)

\[ \dot{\eta}_f = \frac{1}{\tau_f}(\eta - \eta_f) \]  
(A.39)
Appendix B

Supplement to Chapter 3

B.1 Nomenclature for Chapter 3

$B$: dimensionless mass transfer coefficient

$F$: feed air flow rate (kmol/hr)

$F_{GN2}$: gas nitrogen production rate (kmol/hr)

$F_L$: returning liquid stream flow in reboiler (kmol/hr)

$F_{LN2}$: liquid nitrogen production rate (kmol/hr)

$F_{rl}$: liquid flow leaving reboiler (kmol/hr)

$F_{rv}$: vapor flow leaving reboiler (kmol/hr)

$F_s$: sump outlet flow (kmol/hr)

$F_V$: vaporizing stream flow in reboiler (kmol/hr)

$H_c$: condenser level (%)

$H_r$: reboiler level (%)

$H_s$: sump level (%)

$h_i^0$: reference enthalpy of pure component $i$ (kJ/kmol)

$h_l$: liquid enthalpy (kJ/kmol)

$h_v$: vapor enthalpy (kJ/kmol)

$L$: liquid molar flow rate in column (kmol/hr)
$M_i$: liquid molar holdup in reboiler (kmol)

$M_v$: vapor molar holdup in reboiler (kmol)

$N$: number of theoretical stages

$n_i$: stage liquid holdup (kmol)

$n_v$: stage vapor holdup (kmol)

$P_{N_2}^{sat}$: nitrogen vapor pressure (kPa)

$P_{O_2}^{sat}$: oxygen vapor pressure (kPa)

$P_f$: feed stage pressure (kPa)

$P_r$: reboiler pressure (kPa)

$Q$: heat transfer rate between the condenser and reboiler (kJ/hr)

$q$: feed air vapor fraction

$q_v$: expansion valve exit stream vapor fraction

$R$: gas constant (m$^3$kPa/kmolK)

$r$: priming ratio

$s$: wave front position

$T^o$: reference temperature (°C)

$T_c$: condenser temperature (°C)

$T_f$: feed stage temperature (°C)

$T_r$: reboiler temperature (°C)

$T_v$: expansion valve exit stream temperature (°C)

$V$: vapor molar flow rate in column kmol/hr

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$V_c$: condenser volume (m$^3$)

$V_r$: reboiler volume (m$^3$)

$V_s$: sump volume (m$^3$)

$w$: wave propagation velocity (hr$^{-1}$)

$x$: liquid composition

$x_{N_2}^w$: expansion valve exit stream liquid nitrogen composition

$x_{O_2}^w$: expansion valve exit stream liquid oxygen composition

$x_{N_2}^L$: reboiler returning liquid nitrogen composition

$x_{O_2}^L$: reboiler returning liquid oxygen composition

$x_c$: condenser liquid composition

$x_f$: feed stage liquid composition

$x_{in}$: column section entering liquid composition

$x_{out}$: column section exiting liquid composition

$x_r$: reboiler liquid phase composition

$y$: vapor composition

$y^*$: equilibrium vapor composition

$y_{N_2}^w$: expansion valve exit stream vapor nitrogen composition

$y_{O_2}^w$: expansion valve exit stream vapor oxygen composition

$y_{N_2}^V$: reboiler vaporizing stream nitrogen composition

$y_{O_2}^V$: reboiler vaporizing stream oxygen composition

$y_{in}$: column section entering vapor composition
$y_{out}$: column section exiting vapor composition

$y_{min}$: concentration limit as $z \to -\infty$

$y_{max}$: concentration limit as $z \to +\infty$

$y_r$: reboiler vapor phase composition

$z$: dimensionless spatial coordinate

$z_f$: feed air nitrogen composition

$\alpha$: relative volatility

$\gamma$: wave front slope

$\nu$: dimensionless wave velocity

$\tau$: dimensionless time coordinate

$\xi$: wave coordinate
Appendix C

Supplement to Chapter 5

C.1 Model Equations for the Reaction/Separation Example

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

\[ \dot{T} = \frac{(F + F_R)}{V_r} (T_f - T) + \frac{-\Delta H}{\rho C_p} k_0 \exp \left( -\frac{E}{RT} \right) C_A + \frac{U A}{V_r \rho C_p} (T_c - T) \quad (C.2) \]

\[ \dot{X}_{A1} = \frac{1}{M_1} (V Y_{A2} - L X_{A1} - \rho_m F_R X_{A1}) \quad (C.3) \]

\[ \dot{X}_{A2} = \frac{1}{M_2} [L (X_{A1} - X_{A2}) + V (Y_{A3} - Y_{A2})] \quad (C.4) \]

\[ \dot{X}_{A3} = \frac{1}{M_3} [L (X_{A2} - X_{A3}) + V (Y_{A4} - Y_{A3})] \quad (C.5) \]

\[ \dot{X}_{A4} = \frac{1}{M_4} [L (X_{A3} - X_{A4}) + V (Y_{A5} - Y_{A4})] \quad (C.6) \]

\[ \dot{X}_{A5} = \frac{1}{M_5} [(F + F_R) C_A + L X_{A4}] \quad (C.7) \]

\[ -\{L + \rho_m (F + F_R)\} X_{A5} + V (Y_{A6} - Y_{A5}) \]

\[ \dot{X}_{A6} = \frac{1}{M_6} \{ [L + \rho_m (F + F_R)] (X_{A5} - X_{A6}) + V (Y_{A7} - Y_{A6}) \} \quad (C.8) \]

\[ \dot{X}_{A7} = \frac{1}{M_7} \{ [L + \rho_m (F + F_R)] (X_{A6} - X_{A7}) + V (Y_{A8} - Y_{A7}) \} \quad (C.9) \]

\[ \dot{X}_{A8} = \frac{1}{M_8} \{ [L + \rho_m (F + F_R)] (X_{A7} - X_{A8}) + V (Y_{A9} - Y_{A8}) \} \quad (C.10) \]

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

\[ -(L + \rho_m (F + F_R) - V) X_{A9} \]  

(C.11)
where: $F$, $C_A$, and $T_f$ are the volumetric flowrate, concentration of $A$, and temperature, respectively, of the reactor feed stream; $F_R$, $X_A$, and $\rho_n$ are the volumetric flowrate, mole fraction of $A$, and molar density, respectively, of the recycle stream; $F + F_R$, $C_A$, and $T$ are the volumetric flowrate, 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 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:

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

where $\alpha$ is the relative volatility.
Appendix D
Supplement to Chapter 6

D.1 Optimization Formulation of the Plant Decomposition Problem

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

\[
\max_{X,Y} \sum_{k=1}^{N} \left[ \prod_{i=1}^{N} (1 - \tilde{X}_{i,k}) \right] + \sum_{k=1}^{N} (1 - \tilde{Y}_k) \tag{D.1}
\]

subject to:

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

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

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

Because the number of subsystems \(M\) is not known 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 \(\tilde{Y}\) have identical meanings to those for the matrix \(X\) and \(Y\), respectively, defined in Section 6.2 except that the number of subsystems is assumed to be \(N\).

There is a total of \((N + 1)N\) decision variables corresponding to the elements of \(\tilde{X}\) and \(\tilde{Y}\). The expression \(\prod_{i=1}^{N} (1 - \tilde{X}_{i,k})\) for a given column \(k\) is one only if every element of column \(k\) is zero; 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, the corresponding $\tilde{Y}_k$ 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. The third constraint guarantees that every unit operation in a subsystem is connected to at least one other unit operation in the same subsystem. The matrix $X$ and $Y$ are constructed from $\bar{X}$ and $\bar{Y}$, respectively, by eliminating the zero columns that correspond to empty subsystems.

**D.2 QP Formulation of LMPC for Local Dynamic Controller Coordination**

The linear model predictive control (LMPC) problem can be formulated as a quadratic programming (QP) problem [80] even though the coupled linear system (5.1) depends on the nonlinear subsystem state and input variables as well as the linear subsystem variables. The LMPC objective function (1.3) can be algebraically manipulated to yield the following quadratic program with decision variables $u_L(k)$:

$$\min_{U_L(k)} \begin{bmatrix} U_L(k) \end{bmatrix}^T H U_L(k) + 2 \begin{bmatrix} U_L(k) \end{bmatrix}^T \begin{bmatrix} G_1 \bar{X}_N(k) + G_2 \bar{U}_N(k) + G_3 x_L(k) - F u_L(k - 1) \end{bmatrix}$$

(D.2)
where $U_L(k)$, $X_N(k)$ and $U_N(k)$ are defined as:

\[
U_L(k) = \begin{bmatrix}
    u_L(k | k) & u_L(k + 1 | k) & \cdots & u_L(k + N_L - 1 | k)
\end{bmatrix}^T
\]

\[
X_N(k) = \begin{bmatrix}
    x_N(k | k) & x_N(k + 1 | k) & \cdots & x_N(k + P_N | k) & \cdots & x_N(k + N_L - 1 | k)
\end{bmatrix}^T
\]

\[
U_N(k) = \begin{bmatrix}
    u_N(k | k) & u_N(k + 1 | k) & \cdots & u_N(k + N_N - 1 | k) & \cdots & u_N(k + N_L - 1 | k)
\end{bmatrix}^T
\]

Generally the NMPC prediction horizon $(P_N)$ and control horizon $(N_N)$ are 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 model in an open-loop fashion with constant input vector $u_N(k + N_N - 1 | k)$ or by assuming the state vector remaining 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 (D.2) can be calculated from the system and tuning matrices:

\[
H = \begin{bmatrix}
    B_L^TQB_L + R + 2S & B_L^TA_L^TQB_L - S & \cdots & B_L^TA_L^{N_L-1}QB_L \\
    B_L^TQA_LB_L - S & B_L^TQB_L + R + 2S & \cdots & B_L^T(A_L)^{N_L-2}QB_L \\
    \vdots & \vdots & \ddots & \vdots \\
    B_L^T(A_L)^{N_L-1}B_L & B_L^T(A_L)^{N_L-2}B_L & \cdots & B_L^TQB_L + R + 2S
\end{bmatrix}
\]

\[
G_1 = \begin{bmatrix}
    B_L^TQA_N & B_L^TA_L^TQA_N & \cdots & B_L^TA_L^{N_L-1}QA_N \\
    B_L^TQA_LA_N & B_L^TQA_N & \cdots & B_L^TA_L^{N_L-2}QA_N \\
    \vdots & \vdots & \ddots & \vdots \\
    B_L^T(A_L)^{N_L-1}A_N & B_L^T(A_L)^{N_L-2}A_N & \cdots & B_L^TQA_N
\end{bmatrix}
\]
where $\overline{Q}$ is defined as follows for stable systems [80]:

$$
\overline{Q} = \sum_{i=0}^{\infty} [A_L^T]^i C_L^T Q C_L A_L^i
$$

(D.3)

For unstable systems the QP matrices can be obtained following [80] by introducing additional matrices that account for the nonlinear state and input variables.

### D.3 Optimization formulation of the MPC solution sequence problem

The subsystem connection matrix $\Gamma$ is required for solution of MPC sequence problem. Recall that $\Gamma_{i,j} = 1$ if subsystem $i$ affects subsystem $j$ and $\Gamma_{i,j} = 0$ otherwise.

Define the vector $d$ where $d_j = \sum_{i=1}^{M} \Gamma_{i,j}$ for $j = 1 \ldots M$ and $M$ is the total number of subsystems. The decision variables are the elements of the $M \times M$ matrix $\Psi$ where $\Psi_{k,j} = 1$ if and only if subsystem $j$ is the $k$th subsystem solved. The objective
function is:

\[
\min_{\Psi_{k,j}} \sum_{k=1}^{M} \sum_{j=1}^{M} \left[ d_j - \sum_{i=1}^{k-1} \sum_{i=1}^{M} \Psi_{i,i} \Gamma_{i,j} \right] \Psi_{k,j}
\]  

subject to:

\[
\begin{align*}
\sum_{k=1}^{M} \Psi_{k,j} &= 1 \\
\sum_{j=1}^{M} \Psi_{k,j} &= 1
\end{align*}
\]

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

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Dean of the Graduate School

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Date of Examination:

12 December 2000

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