Nonlinear Model Reduction and Control for High-Purity Distillation Columns

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This article considers high-purity distillation columns with large recycle (and thus internal) flow rates. A singular perturbation analysis is employed to document a well-known observation for such columns, namely, the existence of fast and slow dynamics associated with internal and external flows, respectively. A nonlinear low-order model of the slow column dynamics, suitable for analysis and nonlinear feedback controller synthesis, is also derived. A two-tiered controller design procedure, which incorporates such a nonlinear controller, is finally proposed, and its performance and robustness characteristics are evaluated through simulations.

1. Introduction

High-purity distillation columns exhibit distinct static and dynamic characteristics that make them especially challenging to control (see, e.g., refs 1−3). The behavior of such columns is intrinsically nonlinear; as a result, linear control methods often become inadequate, necessitating either logarithmic variable transformations, which tend to "tame" the nonlinearity,[1,4,5] or inherently nonlinear control strategies.[6,7] Such columns also typically exhibit two distinctly different time constants:[8−11] (i) a large and dominant time constant with respect to external flow rates and a (ii) a small time constant with respect to internal flow rates. From a static perspective, they exhibit severe ill-conditioning in the form of different magnitudes of gains in different input directions.[12]

The above features have justifiably generated vigorous interest in control strategies for high-purity distillation columns based on low-order models that capture the essential control-relevant dynamics of the column. To this end, the approach in refs 5 and 10 involves the derivation of empirical one- or two-dimensional linear models of the dominant dynamics and their use within a robust linear controller design framework. Aiming at nonlinear controller designs, approaches based on the derivation of low-order nonlinear models have also been followed, either using compartmentalized modeling for different sections of the column[13] or using traveling-wave models.[14,15]

This paper focuses on high-purity distillation columns with large liquid/vapor recycle flow rates, generally considered as especially difficult to control.[3] Our objective is 3-fold:

1. To provide a rigorous justification of the two-time-scale behavior exhibited by such columns based on an analysis of a detailed tray-by-tray material balance model.

2. To develop an explicit nonlinear low-order model of the slow input/output column dynamics, suitable for analysis and controller design.

3. To illustrate how such a model can be used in a two-tiered controller design procedure that accounts rationally for the nonlinear two-time-scale dynamics of the column.

The focus throughout the paper is on a simple distillation column with three components, to highlight the inherent time-scale separation and the proposed model reduction and controller design method; the same approach can be used however in more complex columns. We begin with a brief description of the column considered and its detailed tray-by-tray material balance model. We subsequently describe a modeling framework based on singular perturbations, which allows documenting in a transparent way the time-scale separation present in the dynamics of such columns, where a fast dynamics corresponds to the individual stages in the column, while a slow dynamics corresponds to the overall column behavior. Within this singular perturbation framework, we outline a nonlinear model reduction procedure, which leads to a low-order nonlinear model of the overall column dynamics suitable for analysis and nonlinear feedback control. A simulation study is finally used to illustrate the efficacy of the proposed controller design framework.

2. Process Description and Model

Consider a distillation column with N trays (numbered from top to bottom), to which a saturated liquid feed containing a mixture of three components with mole fractions x_{1f}, x_{2f} of components 1 and 2, respectively, is fed at (molar) flow rate F on tray N_f. The heavy component 3 is the desired product and is removed at the bottom from the reboiler at flow rate B, while the lighter components 1 and 2 are removed at the top from the condenser at flow rate D. For simplicity, it is assumed that (i) the light components 1 and 2 have constant relative volatilities α_1 and α_2, respectively, with respect to the heavy component 3, (ii) the liquid and

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vapor streams leaving each tray are in equilibrium, (iii) vapor holdup on each tray is negligible, (iv) all components have the same density, heat capacity, and latent heats of vaporization, and (v) there is constant molar holdup and overflow on each tray. Thus, the vapor flow rate from each tray is equal to the vapor boilup V_B from the reboiler; the liquid flow rate from each tray in the enriching section is equal to the liquid recycle R from the condenser, while the liquid flow rate in the stripping section is equal to $R + F$.

Under the above assumptions a standard dynamic model of the column is easily obtained, given by the following ODE system:

$$\left.\begin{aligned} \dot{M}_C &= V_B - R - D \\ \dot{x}_{1,D} &= \frac{V_B}{M_C}(y_{1,1} - x_{1,D}) \\ \dot{x}_{2,D} &= \frac{V_B}{M_C}(y_{2,1} - x_{2,D}) \end{aligned}\right\}\text{condenser}$$

$$\left.\begin{aligned} \dot{x}_{1,i} &= \frac{1}{M_i}[V_B(y_{1,i+1} - y_{1,i}) + R(x_{1,i-1} - x_{1,i})] \\ \dot{x}_{2,i} &= \frac{1}{M_i}[V_B(y_{2,i+1} - y_{2,i}) + R(x_{2,i-1} - x_{2,i})] \end{aligned}\right\}\text{tray } i < N_f$$

$$\left.\begin{aligned} \dot{x}_{1,i} &= \frac{1}{M_i}[V_B(y_{1,i+1} - y_{1,i}) + R(x_{1,i-1} - x_{1,i}) + F(x_{1,i-1} - x_{1,i})] \\ \dot{x}_{2,i} &= \frac{1}{M_i}[V_B(y_{2,i+1} - y_{2,i}) + R(x_{2,i-1} - x_{2,i}) + F(x_{2,i-1} - x_{2,i})] \end{aligned}\right\}\text{tray } i \geq N_f$$

$$\left.\begin{aligned} \dot{M}_R &= R + F - V_B - B \\ \dot{x}_{1,B} &= \frac{1}{M_R}[R(x_{1,N} - x_{1,B}) - V_B(y_{1,B} - x_{1,B}) + F(x_{1,N} - x_{1,B})] \\ \dot{x}_{2,B} &= \frac{1}{M_R}[R(x_{2,N} - x_{2,B}) - V_B(y_{2,B} - x_{2,B}) + F(x_{2,N} - x_{2,B})] \end{aligned}\right\}\text{reboiler} \quad (1)$$

In the above model, M_C, $x_{1,D}$, and $x_{2,D}$ are the molar liquid holdup and mole fractions of components 1 and 2 in the condenser, M_i, $x_{1,i}$, and $x_{2,i}$ are the liquid holdup and mole fractions of 1 and 2 in tray i, while M_R, $x_{1,B}$, and $x_{2,B}$ are the corresponding holdup and mole fractions in the reboiler. Moreover, in the equations for the feed tray, $i = N_f$, the terms $F(x_{1,i-1} - x_{1,i})$ and $F(x_{2,i-1} - x_{2,i})$ are replaced with $F(x_{1f} - x_{1,i})$ and $F(x_{2f} - x_{2,i})$, respectively. Under the constant relative volatility assumption, the phase equilibrium relationships are given by

$$\begin{aligned} y_{1,i} &= \frac{\alpha_1 x_{1,i}}{1 + (\alpha_1 - 1)x_{1,i} + (\alpha_2 - 1)x_{2,i}} \\ y_{2,i} &= \frac{\alpha_2 x_{2,i}}{1 + (\alpha_1 - 1)x_{1,i} + (\alpha_2 - 1)x_{2,i}} \end{aligned} \quad (2)$$

where $y_{1,i}$ and $y_{2,i}$ are the mole fractions of 1 and 2, respectively, in the vapor stream leaving tray i.

We consider the case where large vapor boilup V_B and liquid recycle R are used compared to the feed, distillate, and bottom product flow rates, to attain a high purity of the desired component 3 in the bottom product. High reflux flow rates are often used for high-purity separation of close-boiling mixtures. For the column, the key output to be controlled is the bottom product purity, that is, $x_{3,B} = 1 - x_{1,B} - x_{2,B}$, besides the two holdups M_C and M_R in the condenser and the reboiler, which behave as integrators. There are four flow rates, D, B, V_B, and R, that can be manipulated to control the process, in the presence of disturbances in the feed flow rate F and composition x_{1f} and x_{2f}.

3. Singular Perturbation Modeling

In this section we outline a modeling framework, based on singular perturbations, which allows documentation of the time-scale separation induced by the large recycle flow rates in the column. To this end, note that a large liquid recycle R implies an equally large vapor boilup V_B at the nominal steady state. On the other hand, the feed flow rate F, the distillate flow rate D, and the bottom product flow rate B are of the same order of magnitude. Thus, defining the small parameter $\epsilon = (D_{nom}/R_{nom})$ and $\kappa_1 = (V_{Bnom}/R_{nom}) = O(1)$, where the subscript “nom” refers to nominal steady-state values and $O(\cdot)$ is the standard order of magnitude notation, the terms involving the large parameter $(1/\epsilon)$ can be isolated in the model

$$\left.\begin{aligned} \dot{M}_C &= \frac{D_{nom}}{\epsilon}(\kappa_1\bar{V} - \bar{R}) - D \\ \dot{x}_{1,D} &= \frac{D_{nom}\kappa_1\bar{V}}{\epsilon M_C}(y_{1,1} - x_{1,D}) \\ \dot{x}_{2,D} &= \frac{D_{nom}\kappa_1\bar{V}}{\epsilon M_C}(y_{2,1} - x_{2,D}) \end{aligned}\right\}\text{condenser}$$

$$\left.\begin{aligned} \dot{x}_{1,i} &= \frac{D_{nom}}{\epsilon M_i}[\kappa_1\bar{V}(y_{1,i+1} - y_{1,i}) + \bar{R}(x_{1,i-1} - x_{1,i})] \\ \dot{x}_{2,i} &= \frac{D_{nom}}{\epsilon M_i}[\kappa_1\bar{V}(y_{2,i+1} - y_{2,i}) + \bar{R}(x_{2,i-1} - x_{2,i})] \end{aligned}\right\}\text{tray } i < N_f$$

$$\left.\begin{aligned} \dot{x}_{1,i} &= \frac{D_{nom}}{\epsilon M_i}[\kappa_1\bar{V}(y_{1,i+1} - y_{1,i}) + \bar{R}(x_{1,i-1} - x_{1,i})] + \frac{F}{M_i}(x_{1,i-1} - x_{1,i}) \\ \dot{x}_{2,i} &= \frac{D_{nom}}{\epsilon M_i}[\kappa_1\bar{V}(y_{2,i+1} - y_{2,i}) + \bar{R}(x_{2,i-1} - x_{2,i})] + \frac{F}{M_i}(x_{2,i-1} - x_{2,i}) \end{aligned}\right\}\text{tray } i \geq N_f$$

$$\left.\begin{aligned} \dot{M}_R &= \frac{D_{nom}}{\epsilon}(\bar{R} - \kappa_1\bar{V}) - B + F \\ \dot{x}_{1,B} &= \frac{D_{nom}}{\epsilon M_R}[\bar{R}(x_{1,N} - x_{1,B}) - \kappa_1\bar{V}(y_{1,B} - x_{1,B})] + \frac{F}{M_R}(x_{1,N} - x_{1,B}) \\ \dot{x}_{2,B} &= \frac{D_{nom}}{\epsilon M_R}\Big[\bar{R}(x_{2,N} - x_{2,B}) - \kappa_1\bar{V}(y_{2,B} - x_{2,B}) + \frac{F}{M_R}(x_{2,N} - x_{2,B}) \end{aligned}\right\}\text{reboiler} \quad (3)$$

In the above representation of the process model, $\bar{R}$ and $\bar{V}$ denote scaled manipulated input variables:

$$\bar{R} = \frac{R}{R_{nom}}, \qquad \bar{V} = \frac{V_B}{V_{Bnom}} \quad (4)$$

Thus, the process model has the general form

$$\dot{x} = f(x) + g^s(x)u^s + \frac{1}{\epsilon}g^l(x)u^l \quad (5)$$

where

$$x = [M_C \quad x_{1,D} \quad x_{2,D} \quad \cdots \quad x_{1,i} \quad x_{2,i} \quad \cdots \quad M_R \quad x_{1,B} \quad x_{2,B}]^T \in R^n$$

is the vector of state variables, $u^s = [D\ B]^T$ is the vector of manipulated inputs corresponding to small flow rates, and $u^l = [\bar{R}\ \bar{V}]^T$ is the vector of manipulated inputs corresponding to large flow rates, while $f(x)$ is a smooth vector field and $g^s(x)$ and $g^l(x)$ are smooth matrices with the following description:

$$f(x) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ \frac{F}{M_{N_f}}(x_{1f} - x_{1,N_f}) \\ \frac{F}{M_{N_f}}(x_{2f} - x_{2,N_f}) \\ \vdots \\ \frac{F}{M_i}(x_{1,i-1} - x_{1,i}) \\ \frac{F}{M_i}(x_{2,i-1} - x_{2,i}) \\ \vdots \\ F \\ \frac{F}{M_R}(x_{1,N} - x_{1,B}) \\ \frac{F}{M_R}(x_{2,N} - x_{2,B}) \end{bmatrix}$$

$$g^s(x) = \begin{bmatrix} -1 & 0 \\ 0 & 0 \\ 0 & 0 \\ \vdots & \\ 0 & 0 \\ 0 & 0 \\ \vdots & \\ 0 & 0 \\ 0 & 0 \\ \vdots & \\ 0 & -1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$g^l(x) = D_{nom} \begin{bmatrix} -1 & \kappa_1 \\ 0 & \frac{\kappa_1(y_{1,1} - x_{1,D})}{M_C} \\ 0 & \frac{\kappa_1(y_{2,1} - x_{2,D})}{M_C} \\ \vdots & \\ \frac{(x_{1,N_f-1} - x_{1,N_f})}{M_{N_f}} & \frac{\kappa_1(y_{1,N_f+1} - y_{1,N_f})}{M_{N_f}} \\ \frac{(x_{2,N_f-1} - x_{2,N_f})}{M_{N_f}} & \frac{\kappa_1(y_{2,N_f+1} - y_{2,N_f})}{M_{N_f}} \\ \vdots & \\ \frac{(x_{1,i-1} - x_{1,i})}{M_i} & \frac{\kappa_1(y_{1,i+1} - y_{1,i})}{M_i} \\ \frac{(x_{2,i-1} - x_{2,i})}{M_i} & \frac{\kappa_1(y_{2,i+1} - y_{2,i})}{M_i} \\ \vdots & \\ 1 & -\kappa_1 \\ \frac{(x_{1,N} - x_{1,B})}{M_R} & -\frac{\kappa_1(y_{1,B} - x_{1,B})}{M_i} \\ \frac{(x_{2,N} - x_{2,B})}{M_R} & -\frac{\kappa_1(y_{2,B} - x_{2,B})}{M_i} \end{bmatrix}$$

Note that the above model exhibits stiffness owing to the presence of the small parameter ϵ (or equivalently the large parameter $1/\epsilon$). This can also be seen by considering the limit as the recycle flow rate becomes infinitely large, that is, $\epsilon \to 0$, in which case we observe a discontinuous or *singular* perturbation in the model. This is indicative of the fact that the large recycle flow rate induces a time scale separation between the dynamics of the individual trays (fast, owing to the large "internal" flow rates) and the dynamics of the overall column (slow, owing to the small feed and product flow rates).

Stiff models such as the one above are not particularly suitable for the synthesis of model-based controllers. For example, standard inversion-type or optimization-type controllers designed on the basis of such stiff models are inherently ill-conditioned: they contain the large parameters of the model, which act as "high gains" and amplify the effect of even small modeling or measurement errors, with detrimental consequences on stability and performance (see, e.g., refs 16−18). The rational paradigm for addressing the control of such two-time-scale systems involves (i) the derivation of separate (nonstiff) systems that describe the dynamics in the fast and slow time scale and (ii) the design of separate fast and slow controllers on the basis of these systems, to stabilize the fast dynamics, if they are unstable, and to achieve desired closed-loop performance objectives in the slow time scale (see, for example, ref 18). However, a complication for the system of eq 5 arises from the fact that the small parameter ϵ appears in all of the state equations. This implies that although there exist two time scales in the dynamics of such systems, there is no explicit separation between fast and slow state variables; all the state variables exhibit fast transients followed by slower dynamics. This should be contrasted with standard singularly perturbed systems of the form

$$\begin{aligned} \dot{\zeta} &= F(\zeta,\eta,u,\epsilon) \\ \epsilon\dot{\eta} &= G(\zeta,\eta,u,\epsilon) \end{aligned} \qquad (6)$$

with a nonsingular $(\partial G(\zeta,\eta,u,0)/\partial\eta)$, for which the states η are the fast ones and the states ζ are the slow ones. The next section addresses the model reduction and controller design problems for the system of eq 5. The procedure followed is conceptually similar to the one used for standard singularly perturbed systems, albeit technically more complicated.

4. Nonlinear Model Reduction and Control

We begin with the derivation of a description of the fast dynamics of the process. To this end, let us define the fast time scale $\tau = (t/\epsilon)$, which is in the order of magnitude of the residence time in the individual stages of the column with the large internal flow rates. In this time scale the system of eq 5 takes the form

$$\frac{dx}{d\tau} = \epsilon f(x) + \epsilon g^s(x)u^s + g^l(x)u^l \qquad (7)$$

Considering the limit $\epsilon \to 0$, we obtain the following description of the fast dynamics of the system:

$$\frac{dx}{d\tau} = g^l(x)u^l \tag{8}$$

Note that the inputs u^s have no effect on the fast dynamics; only the inputs u^l corresponding to the large flow rates have an effect and can be used for control in this fast time scale. A natural control objective in this time scale is the stabilization of the liquid holdups in the condenser and the reboiler which behave like integrators. This is easily achieved by using simple proportional controllers for the inputs $u^l = [\bar{R}\ \bar{V}]^T$:

$$\begin{aligned} \bar{R} &= 1 - \bar{K}_{c1}(M_{Cnom} - M_C) \\ \bar{V} &= 1 - \bar{K}_{c2}(M_{Rnom} - M_R) \end{aligned} \tag{9}$$

The above relations are equivalent to standard proportional control laws

$$R = R_{nom} - K_{c1}(M_{Cnom} - M_C)$$

$$V_B = V_{Bnom} - K_{c2}(M_{Rnom} - M_R)$$

with the proportional gains $K_{c1} = R_{nom}\bar{K}_{c1}$ and $K_{c2} = V_{Bnom}\bar{K}_{c2}$.

We turn now to the slow time scale t to obtain a description of the slow dynamics. In particular, multiplying eq 5 by ϵ and considering the limit $\epsilon \to 0$, it is evident that the following algebraic constraints have to be satisfied in the slow dynamics:

$$g^l(x)u^l = \begin{bmatrix} \kappa_1\bar{V} - \bar{R} \\ \kappa^1\bar{V}(y_{1,1} - x_{1,D}) \\ \kappa_1\bar{V}(y_{2,1} - x_{2,D}) \\ \vdots \\ \kappa_1\bar{V}(y_{1,i+1} - y_{1,i}) + \bar{R}(x_{1,i-1} - x_{1,i}) \\ \kappa_1\bar{V}(y_{2,i+1} - y_{2,i}) + \bar{R}(x_{2,i-1} - x_{2,i}) \\ \vdots \\ \bar{R} - \kappa_1\bar{V} \\ \bar{R}(x_{1,N} - x_{1,B}) - \kappa_1\bar{V}(y_{1,B} - x_{1,B}) \\ \bar{R}(x_{2,N} - x_{2,B}) - \kappa_1\bar{V}(y_{2,B} - x_{2,B}) \end{bmatrix} = 0 \tag{10}$$

The above constraints essentially denote the (quasi) steady-state condition for the fast dynamics described in eq 8. With the above observation, referring back to the system description in eq 5 and considering the limit $\epsilon \to 0$ in the slow time scale t, it follows that the term $(g^l(x)u^l)/\epsilon$ is indeterminate. Defining this finite but unknown term as the additional variables $z = \lim_{\epsilon\to 0} (g^l(x)u^l)/\epsilon$, we obtain the following description of the slow dynamics of the system of eq 5:

$$\begin{aligned} \dot{x} &= f(x) + g^s(x)u^s + b(x)z \\ 0 &= g^l(x)u^l \end{aligned} \tag{11}$$

where $b(x)$ is a diagonal matrix given by

$$b(x) = \text{diag}\begin{bmatrix} D_{nom} \\ \dfrac{D_{nom}}{M_C} \\ \dfrac{D_{nom}}{M_C} \\ \vdots \\ \dfrac{D_{nom}}{M_i} \\ \dfrac{D_{nom}}{M_i} \\ \vdots \\ D_{nom} \\ \dfrac{D_{nom}}{M_R} \\ \dfrac{D_{nom}}{M_R} \end{bmatrix}$$

Equation 11 is a differential algebraic equation (DAE) system with nontrivial index,[16] due to the fact that the algebraic equations $0 = g^l(x)u^l$ in eq 11 are singular with respect to the “algebraic” variables z.

Note that the number of constraints in eq 10 is the same as the dimension of the state (or “differential”) variables x. This would imply that there is no slow dynamics, or equivalently no time-scale multiplicity, in the column. However, the constraints in eq 10 are not linearly independent. In particular, one can obtain the last three components (corresponding to the reboiler) as linear combinations of the others. More specifically, labeling the components of the constraints in eq 10 as C0, C1, C2 (condenser), i1, i2 (tray i), and R0, R1, R2 (reboiler) for simplicity of notation, it can be easily verified that

$$\begin{aligned} \text{R0} &= -\text{C0} \\ \text{R1} &= (x_{1,B} - x_{1,D})\text{C0} - \text{C1} - \sum_{i=1}^{N} i1 \\ \text{R2} &= (x_{2,B} - x_{2,D})\text{C0} - \text{C2} - \sum_{i=1}^{N} i2 \end{aligned} \tag{12}$$

Thus, defining $\hat{g}^l(x)u^l$ as the vector field consisting of the first $n - 3$ components of $g^l(x)u^l$ that are linearly independent, and correspondingly $\hat{z}$ as the vector of algebraic variables consisting of the first $n - 3$ components of z, the slow dynamics are described by the DAE system:

$$\begin{aligned} \dot{x} &= f(x) + g^s(x)u^s + \hat{b}(x)\hat{z} \\ 0 &= \hat{g}^l(x)u^l \end{aligned} \tag{13}$$

with the differential variables $x \in R^n$ and the algebraic variables $\hat{z} \in R^p$ ($p = n - 3$), where $\hat{b}(x)$ is a sparse matrix of dimension $n \times p$ and has the form given Chart 1. For the DAE system in eq 13, the index is defined as the number of times the algebraic equations $0 = \hat{g}^l(x)u^l$ have to be differentiated to be able to obtain expressions for $\dot{z}$, that is, reduce the DAE into an equivalent ODE. However, note that the algebraic equations involve the manipulated inputs u^l and, thus, the index may depend

Chart 1

$$\hat{b}(x) = \begin{bmatrix} D_{\rm nom} & 0 & 0 & & & & & & \\ 0 & \frac{D_{\rm nom}}{M_{\rm C}} & 0 & & & & & & \\ 0 & 0 & \frac{D_{\rm nom}}{M_{\rm C}} & & & & & & \\ & & & \cdots & & & & & \\ & & & & \frac{D_{\rm nom}}{M_i} & 0 & & & \\ & & & & 0 & \frac{D_{\rm nom}}{M_i} & & & \\ & & & & & & \cdots & & \\ & & & & & & & \frac{D_{\rm nom}}{M_N} & 0 \\ & & & & & & & 0 & \frac{D_{\rm nom}}{M_N} \\ -D_{\rm nom} & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\ \frac{D_{\rm nom}(x_{1,\rm B} - x_{1,\rm D})}{M_{\rm R}} & -\frac{D_{\rm nom}}{M_{\rm R}} & 0 & \cdots & -\frac{D_{\rm nom}}{M_{\rm R}} & 0 & \cdots & -\frac{D_{\rm nom}}{M_{\rm R}} & 0 \\ \frac{D_{\rm nom}(x_{2,\rm B} - x_{2,\rm D})}{M_{\rm R}} & 0 & -\frac{D_{\rm nom}}{M_{\rm R}} & \cdots & 0 & -\frac{D_{\rm nom}}{M_{\rm R}} & \cdots & 0 & -\frac{D_{\rm nom}}{M_{\rm R}} \end{bmatrix}$$

on the control law for $u^{\rm l}$. More specifically, the first constraint, that is, $0 = \kappa_1\bar{V} - \bar{R}$, does not involve any of the differential variables x and hence the index of this DAE system is not well-defined since any differentiation of this constraint will not involve the algebraic variables z. A well-defined index of the above DAE system exists only if these inputs $u^{\rm l}$ vary according to a feedback control law $u^{\rm l} = u^{\rm l}(x)$. In particular, under the proportional feedback control in eq 9, one differentiation of the constraints $0 = \hat{g}^{\rm l}(x)u^{\rm l}(x)$ yields a set of algebraic equations that can be solved for $\hat{z}$ in terms of x and $u^{\rm s}$:

$$\hat{z} = \alpha(x) + \beta(x)u^{\rm s}$$

That is, the DAE system in eq 13 has an index $\nu_{\rm d} = 2$ (another differentiation would yield the expression for $\dot{z}$). Thus, $0 = \hat{g}^{\rm l}(x)u^{\rm l}(x)$ are the only constraints in the differential variables x and the slow dynamics in the column is consequently of order $n - p = 3$, while the fast dynamics is of dimension $n - 3$.

An explicit ODE description of order three of this slow column dynamics can be obtained in transformed coordinates by incorporating the constraints $\hat{g}^{\rm l}(x)u^{\rm l}(x)$ in these coordinates. More specifically, considering the nonlinear coordinate change,

$$\begin{bmatrix} \zeta \\ \eta \end{bmatrix} = T(x) = \begin{bmatrix} M_{\rm R} \\ x_{1,\rm B} \\ x_{2,\rm B} \\ \hat{g}^{\rm l}(x)u^{\rm l}(x) \end{bmatrix} \quad (14)$$

in the new coordinates ζ and η, the states $\eta = \hat{g}^{\rm l}(x)u^{\rm l}(x) \equiv 0$ and can be eliminated. The following nonlinear ODE model of order three is then obtained, in terms of the state variables $\zeta = [M_{\rm R}\ x_{1,\rm B}\ x_{2,\rm B}]^{\rm T}$,

$$\dot{\zeta} = (\bar{f}(x) + \bar{b}(x)\alpha(x))_{x=T^{-1}(\zeta,0)} + (\bar{g}^{\rm s}(x) + \bar{b}(x)\beta(x))_{x=T^{-1}(\zeta,0)} \quad (15)$$

where $\bar{f}(x)$ is a vector field consisting of the last three components of $f(x)$ and $\bar{b}(x)$ and $\bar{g}^{\rm s}(x)$ are matrices consisting of the last three rows of $\hat{b}(x)$ and $g^{\rm s}(x)$, respectively. This is precisely the model of the nonlinear slow dynamics induced by the large recycle flow rates in the column; this model can be used efficiently for analysis and controller design purposes.

Note that, in this slow time scale, only the inputs corresponding to the small flow rates $u^{\rm s} = [D\ B]^{\rm T}$ are available to control the slow dynamics. The two outputs to be controlled in this slow time scale are the bottom product purity, that is, $y_1 = (1 - x_{1,\rm B} - x_{2,\rm B})$ and $y_2 = M_{\rm R} + M_{\rm C}$; the latter output, that is, the total holdup in the reboiler and the condenser, must be stabilized in the slow time scale too, as it is not affected by the internal flow rates in the column and behaves as an integrator.

Remark 1. An important feature of the slow column dynamics is that its dimension (three) is constant, irrespective of the total number of trays in the column. In a more general column with c components, the dimension of the slow dynamics of the overall column will be c ($c + 1$, if energy balances are also included).

Remark 2. The proposed two-tiered controller design framework, with the natural separation of the different flow rates according to their magnitude, and their use as manipulated inputs in the appropriate time scale (small flow rates in the slow time scale, large flow rates in the fast time scale) leads to inherently well-conditioned controllers, avoiding excessive variations in the order of magnitude of the manipulated flow rates.

Remark 3. In the previous discussion, we addressed only the control of the product composition at the bottom. Often, it is desired to control product composition in both the distillate and the bottom product, leading to three outputs to be controlled in the slow time scale. However, there are only two manipulated inputs D and B that can be directly manipulated in the slow time scale. This can be overcome through a more general

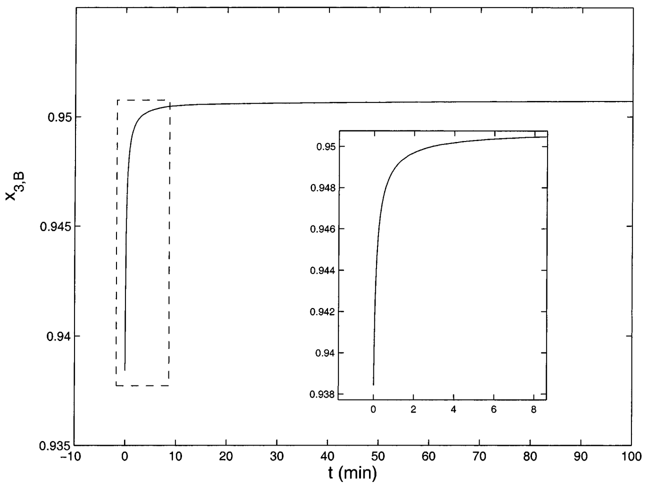

Figure 1. Profile for bottom product purity obtained starting from slightly perturbed initial conditions, depicting the two-time-scale behavior.

composite controller design approach. More specifically, the setpoints for the condenser/reboiler holdups used in the fast proportional control can be treated as additional manipulated input variables in the slow time

Table 1. Description of Column Variables and Their Nominal Values

variable	description	value
B	bottom product flow rate (mol/min)	50.0
D	distillate flow rate (mol/min)	50.0
F	feed flow rate (mol/min)	100.0
K_{c1}	proportional controller gain (min^{-1})	20.0
K_{c2}	proportional controller gain (min^{-1})	20.0
M_C	condenser liquid holdup (mol)	180.0
M_i	liquid holdup on tray i (mol)	175.0
M_R	reboiler liquid holdup (mol)	200.0
N	total no. of trays	15
N_f	feed tray	8
R	liquid recycle flow rate (mol/min)	1000.0
V_B	vapor boilup flow rate (mol/min)	1050.0
α_1	relative volatility of component 1	1.5
α_2	relative volatility of component 2	1.3

scale, leading to a cascaded control configuration where the slow control law decides the variation for these setpoints while the fast controllers track these slowly varying setpoints in the fast time scale using the liquid recycle and vapor boilup flow rates. However, in this case, the DAE system of eq 13 that describes the slow dynamics of the column is *nonregular*[19] since the algebraic constraints explicitly involve the setpoints for

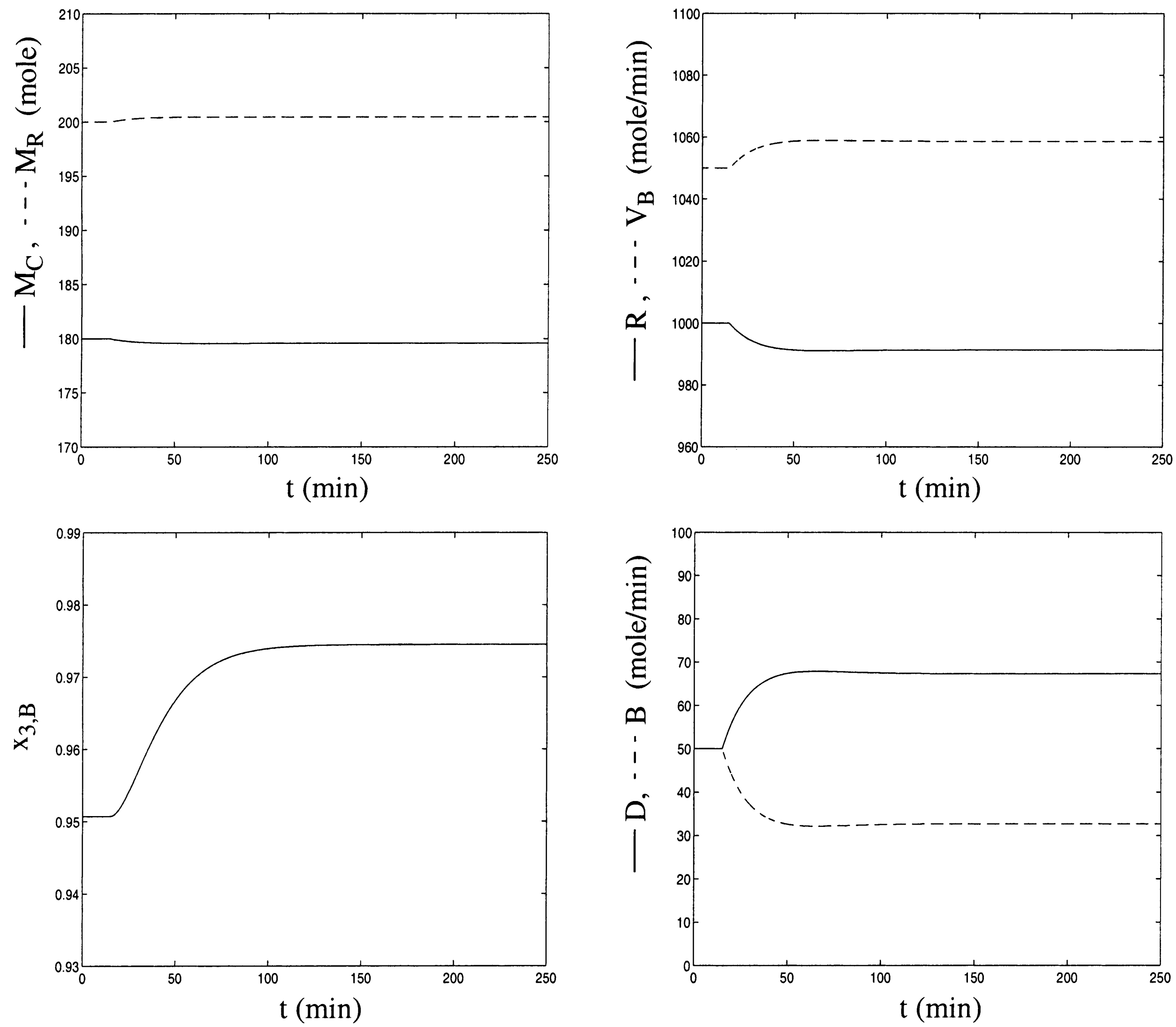

Figure 2. Closed-loop input−output profiles under controller designed on the basis of the detailed model, in the nominal case.

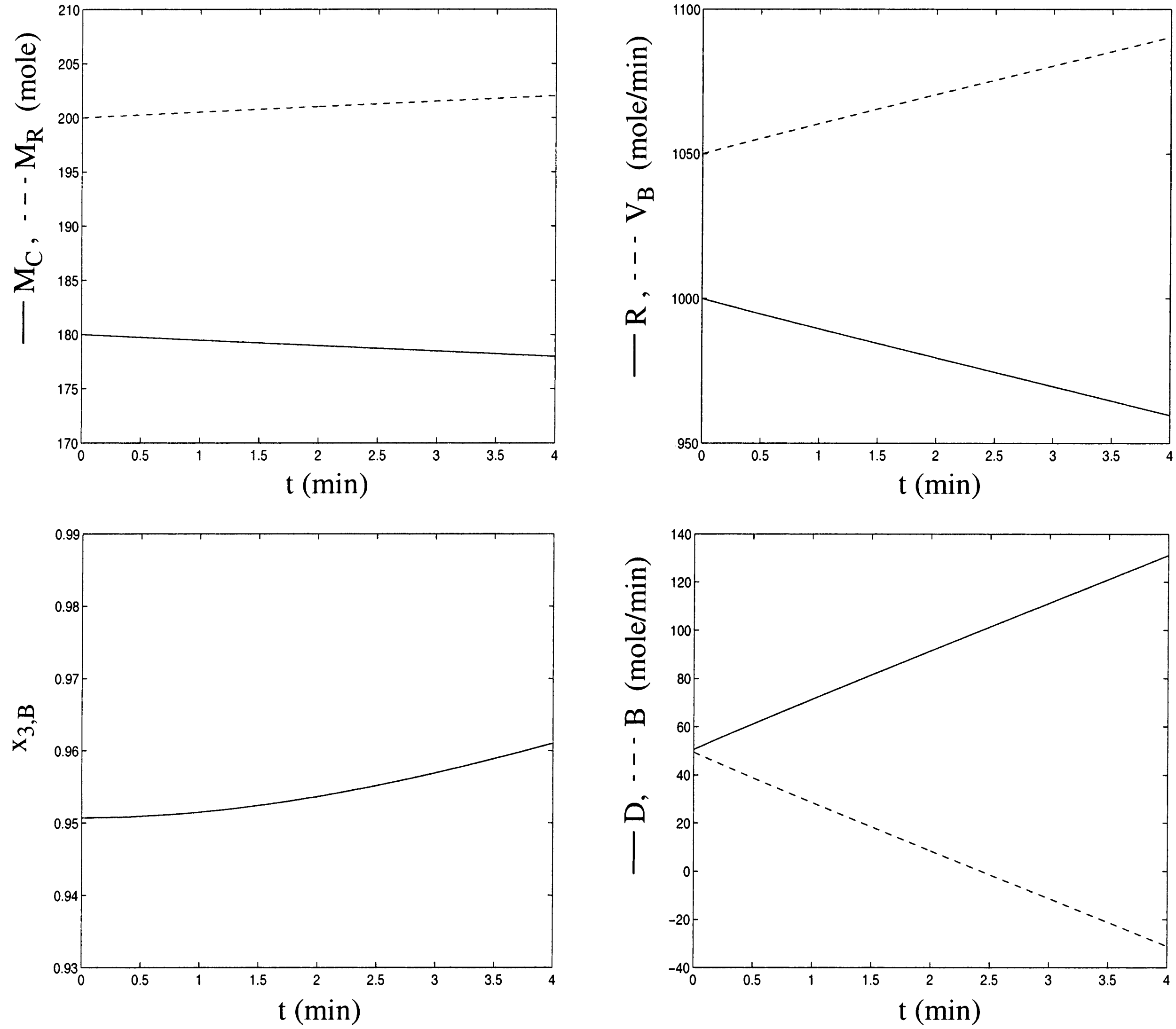

Figure 3. Closed-loop input−output profiles under controller designed on the basis of the detailed model, in the presence of 1% error in α_1.

the reboiler/condenser holdups, which are manipulated inputs. Thus, a feedback regularization is required for the derivation of state-space realizations and controller design (see ref 19).

5. Simulation Study

In this section we focus on a specific column with large internal flow rates, and we illustrate the application and efficacy of the proposed controller design framework. The nominal values of the process variables at steady state for the column considered, as well as the gains of the proportional level controllers employed, are given in Table 1.

Initially, we simulated the column model of eq 1 with the above parameters, starting from an initial condition slightly perturbed from the nominal steady state to illustrate the two-time-scale behavior. In these simulations we implemented the proportional controllers for the holdups M_R and M_C in the fast time scale, to ensure the stability of these holdups in the fast time scale, which is necessary for a meaningful simulation run. Figure 1 shows the profile for the bottom product purity $x_{3,B}$ from $t = 0$ to $t = 100$ min, and a zoom-in view of the first few minutes. Clearly, the plot shows a fast initial transient within the first few seconds followed by a slow transient to the final steady-state value over a longer time period, demonstrating thus the two-time-scale behavior of the column.

For this column with the two-time-scale dynamics, we applied the proposed nonlinear controller design framework and studied its performance and robustness through simulations of the detailed model of eq 1. In particular, for the slow time scale, a nonlinear input/output linearizing controller was designed on the basis of the state-space realization in eq 15 to control the two outputs y_1 and y_2 using the inputs u^s. The relative orders of the two outputs are $r_1 = 1$ and $r_2 = 1$. Thus, the controller was designed to enforce first-order decoupled responses of the form

$$y_i + \gamma_{i1}\frac{dy_i}{dt} = v_i, \qquad i = 1, 2 \tag{16}$$

The resulting input/output linearizing controller was coupled with an external linear controller with integral

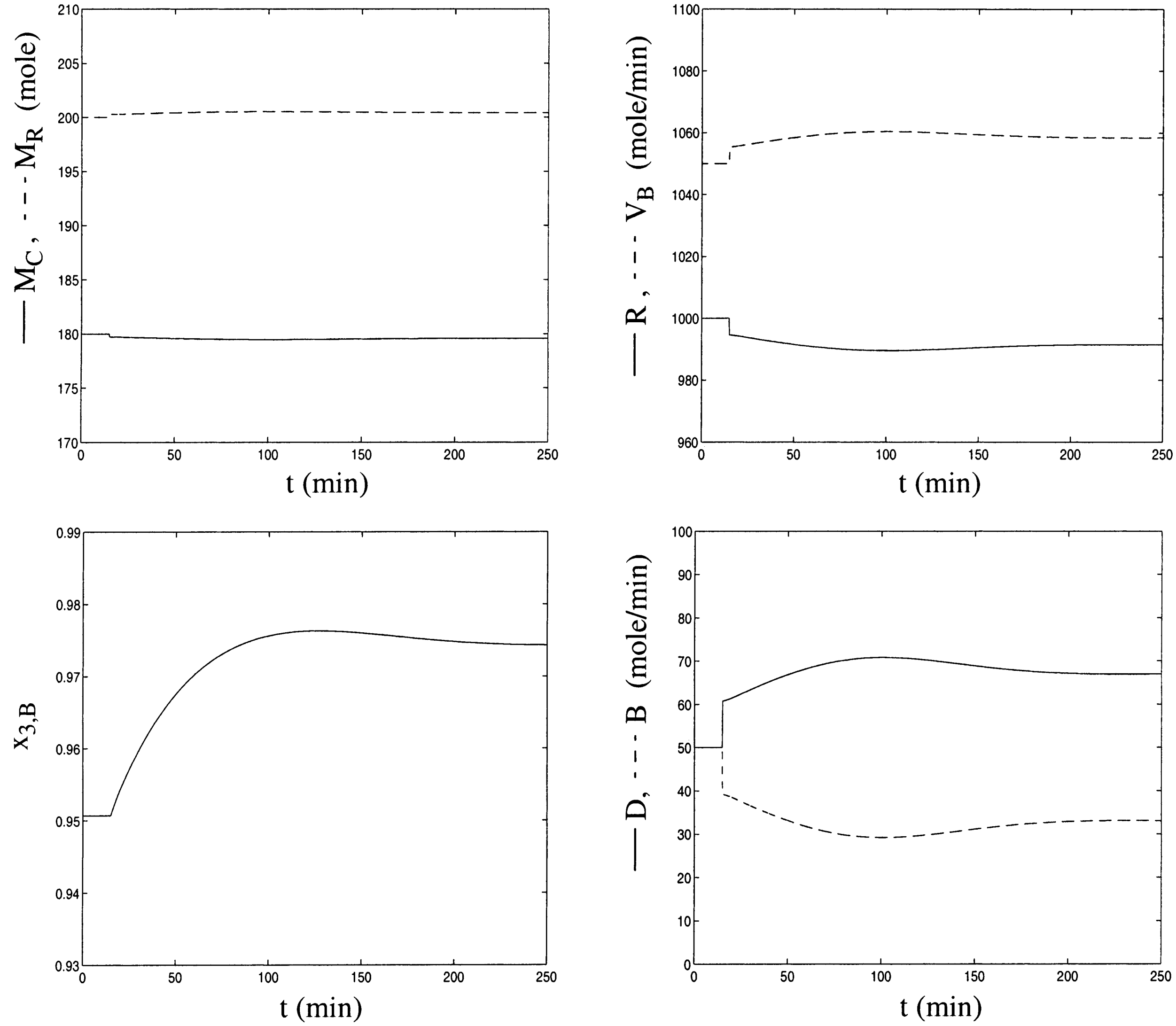

Figure 4. Closed-loop input–output profiles under controller designed on the basis of a reduced-order model for slow column dynamics, in the nominal case.

action to enforce the response:

$$y_i + \gamma_{i1}\frac{dy_i}{dt} = y_{isp}, \qquad i = 1, 2 \tag{17}$$

in the nominal closed-loop system and asymptotically reject the effects of (constant) errors in the process parameters and disturbances in the feed composition, that is, x_{1f}, x_{2f}; y_{1sp} and y_{2sp} denote the setpoints for the respective outputs. The controller was tuned with the parameters $\gamma_{11} = 20$ min and $\gamma_{21} = 20$ min.

The performance of the proposed controller was compared with that of an analogous input/output linearizing controller designed on the basis of the detailed stiff model in eq 1 under the same proportional control for u^l in eq 9 (such an approach does not account for the two-time-scale nature of the process). On the basis of the model in eq 1, the relative orders of the two outputs are $r_1 = 2$ and $r_2 = 1$. Thus, the controller was designed to enforce the closed-loop input/output responses:

$$y_1 + \beta_{11}\frac{dy_1}{dt} + \beta_{12}\frac{d^2y_1}{dt^2} = y_{1sp} \tag{18}$$

$$y_2 + \beta_{21}\frac{dy_2}{dt} = y_{2sp}$$

and tuned with the parameters $\beta_{11} = 30$ min, $\beta_{12} = 255$ min^2, and $\beta_{21} = 20$ min. In all simulation runs, the detailed model in eq 1 was used to simulate the process.

Figure 2 shows the closed-loop profiles for the inputs and the controlled outputs under the latter controller, designed without accounting for the time-scale multiplicity, for a 2.5% increase in the setpoint for bottom product purity at $t = 15$ min. In this nominal case, without any modeling errors, the controller yields the requested input/output responses. However, this controller is highly sensitive to small modeling errors since the feedback control law for D and B involve the large flow rates R and V_B, which magnify the effects of these small modeling errors. Figure 3 shows the closed-loop input/output profiles in the presence of a small, 1%, error in α_1, without any setpoint changes. Clearly, the effect of this small modeling error is highly magnified

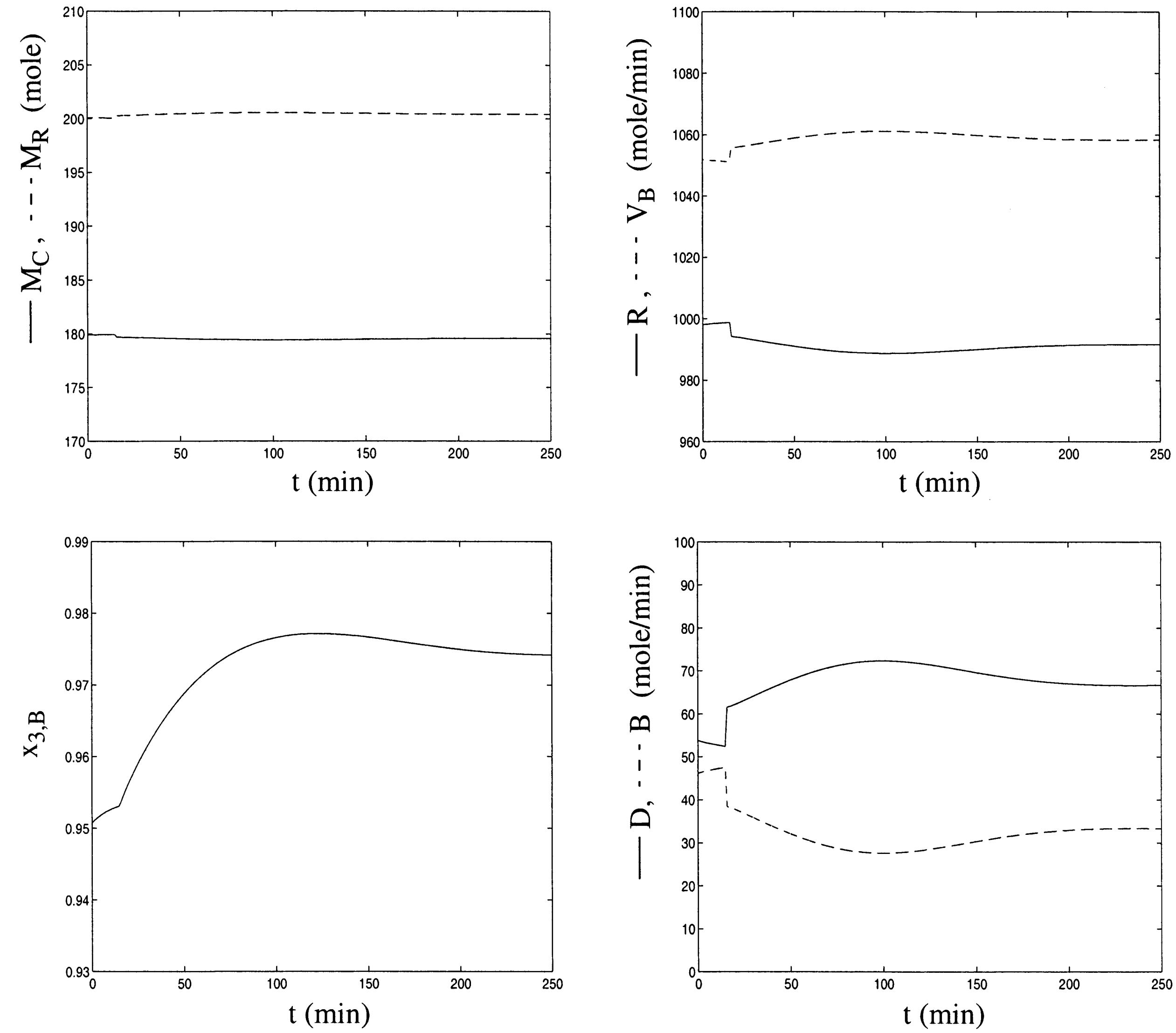

Figure 5. Closed-loop input−output profiles under controller designed on the basis of a reduced-order model for slow column dynamics, in the presence of modeling errors in α_1, α_2 and disturbances in x_{1f}, x_{2f}.

and the controller evaluates very large control action for D and B which consequently leads to closed-loop instability.

Figure 4 shows the performance of the proposed controller designed on the basis of the reduced-order model for the slow column dynamics, for a 2.5% increase in y_{1sp} at $t = 15$ min. Clearly, the controller yields excellent tracking in the nominal case. Figure 5 shows the performance of the controller for the same setpoint change, in the presence of 5% error in α_1, −5% and 10% unmeasured step disturbances in the feed composition x_{1f} and x_{2f}. Clearly, the controller is not very sensitive to these modeling errors and disturbances (the calculated control action is close to that in the nominal case) and yields excellent performance in tracking the setpoint change and rejecting the effects of these errors and disturbances. Figure 6 shows the closed-loop input−output profiles for the same setpoint change and errors/disturbances and a 10% (measured) increase in the feed flow rate F_o at $t = 15$ min. Again, the controller yields excellent performance. The simulation runs clearly demonstrate the excellent performance and robustness characteristics of the proposed input/output linearizing controller designed on the basis of the reduced model for the slow column dynamics, as opposed to the controller designed on the basis of the overall model, which is highly sensitive to small modeling errors that are always present.

6. Conclusions

In this article, we addressed the nonlinear model reduction and control for high-purity distillation columns with large recycle (and thus internal flow rates) compared to feed and product flow rates. The presence of large internal flow rates leads to a time-scale separation in the dynamics of such columns, where the individual stages have a fast dynamics in a time scale of the order of the residence times of these stages, while the overall column has a slow dynamics of very low order. A singular perturbation analysis of the detailed tray-by-tray model of the column led to a rigorous documentation of these well-known observations. This analysis also led to an explicit nonlinear low-order model for the slow input/output column dynamics and a natural separation of the manipulated inputs into the large liquid and vapor recycle flow rates which should be used to control the fast dynamics in the individual stages, and the small product flow rates which should be used to address control objectives for the overall

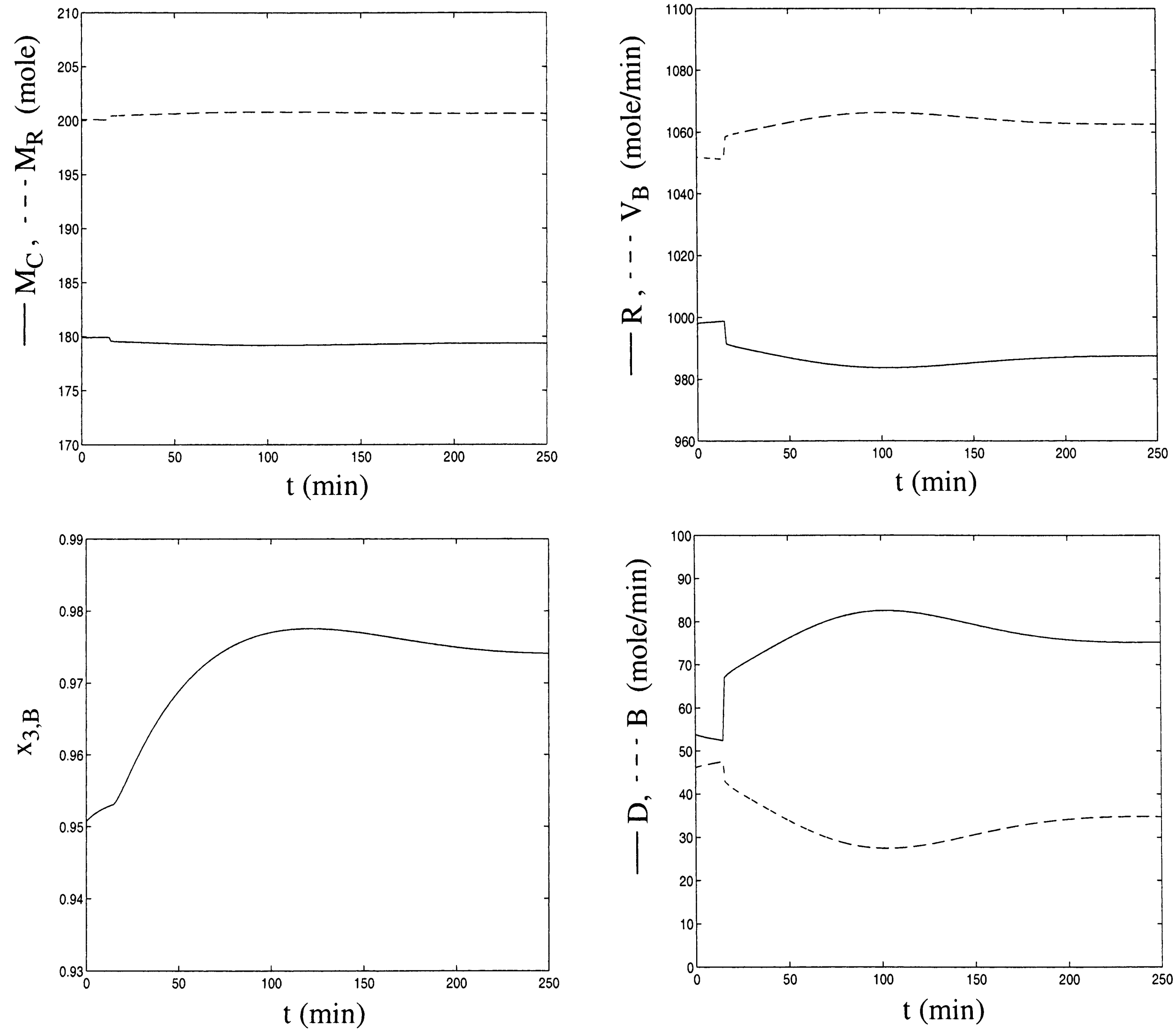

Figure 6. Closed-loop input–output profiles under controller designed on the basis of a reduced-order model for slow column dynamics, in the presence of modeling errors in α_1, α_2, disturbances in x_{1f}, x_{2f} and a step increase in F.

column in the slow time scale. This two-tiered controller design framework, with a nonlinear controller designed on the basis of the derived low-order model of the slow column dynamics, was shown through simulations to have excellent performance and robustness characteristics.

The proposed model reduction and controller design method was illustrated on a rather simplified high-purity distillation column with three components. However, the same time-scale separation arises in more complex high-purity columns with possibly nonideal liquid-/vapor-phase behavior and significant thermal effects. The proposed approach is applicable to such complex industrial columns as well. A similar time-scale separation will also arise in high-purity reactive distillation columns with large recycle and internal flow rates, where the interaction between the simultaneous reaction and distillation is known to lead to highly nonlinear behavior in the column. Finally, this time-scale separation is analogous to the one present in reaction-separation networks with large material recycle; a similar model reduction and control framework has been proposed for such systems too,[20] leading to a controller design framework which naturally reconciles "distributed" control in individual units in the fast time scale with "supervisory" control of the entire network in the slow time scale.

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