Feedback Control of Nonlinear Differential-Algebraic-Equation Systems

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The output feedback control problem is addressed for a class of nonlinear multivariable high-index differential-algebraic-equation systems in semiexplicit form. Initially, an algorithmic procedure is developed and used to derive an equivalent state-space realization of the constrained system. An output feedback synthesis problem is then formulated on the basis of the derived state-space realization and solved through the combination of state feedback and appropriate state observers. The developed methodology is applied to a two-phase reactor, and its performance and robustness characteristics are evaluated through simulations.

Introduction

Chemical processes are inherently nonlinear and multivariable, and are typically modeled by coupled differential and algebraic equations (DAEs). The differential equations arise from dynamic conservation equations, while the algebraic equations commonly arise from thermodynamic equilibrium relations, empirical correlations, pseudo-steady-state assumptions, closure conditions, and so on. For many chemical processes, the algebraic equations are implicit and singular in nature, inhibiting a direct reduction of the process model to one consisting of pure differential equations.

Despite the above inherent complexities in the structure of chemical processes, traditional process control methods are based on linear ordinary differential equation (ODE) models, derived through approximate linearization of nonlinear ODE models. Application of such methods to processes with strong nonlinearities and algebraic constraints clearly limits the controller performance and the achievable control quality. These considerations indicate a need to develop control methodologies for nonlinear DAE systems.

Research on control of nonlinear ODE systems has advanced significantly to a stage where key system-theoretic concepts are well understood (Isidori, 1989; Nijmeijer and van der Schaft, 1990) and explicit controller synthesis results have been derived (for example, Kravaris and Kantor, 1990a,b; Kravaris and Arkun, 1991). On the other hand, research on DAE systems has focused mainly on their analysis and the development of efficient numerical simulation techniques. A key concept used to classify DAEs is that of the differential index (or simply index) (Gear and Petzold, 1984). Loosely speaking, the index of a DAE system is the minimum number of differentiations required to convert it to an equivalent ODE system. Clearly, ODE systems are DAE systems of index zero. DAE systems of index one also share similar properties with ODE systems. However, DAE systems with index greater than one (referred to as high-index systems) demonstrate significant differences compared to ODE systems (Petzold, 1982). The presence of underlying algebraic constraints in such systems makes the specification of consistent initial conditions a nontrivial problem (Leimkuhler et al., 1991; Pantelides, 1988), while the use of ODE methods for their numerical simulation may result in poor convergence properties (Petzold, 1982; Brenan, 1983). To overcome these difficulties, techniques involving combination of algebraic manipulations and differentiations have been proposed to reduce high-index DAEs to ODEs (Gear and Petzold, 1984; Gear, 1988) or index-one DAEs (Bachmann et al., 1990). These index reduction techniques have been used as the basis for the majority of proposed numerical simulation methods for high-index DAE systems (Gear and Petzold, 1984; Petzold, 1986; Chung and Westerberg, 1990; Secchi et al., 1993). Nonlinear constrained optimization techniques have also been proposed for this purpose (Renfro et al., 1987; Jarvis and Pantelides, 1992).

Few results are available on the control of DAE systems, with the exception of optimal control (Cuthrell and Biegler, 1987, 1989; Pantelides et al., 1992) using nonlinear optimization techniques. The problem of feedback controller synthesis has been addressed only for restricted classes of DAE systems that arise mainly in the context of mechanical systems. More specifically, state feedback stabilization and tracking results have been derived for a class of linear (Krishnan and McClamroch, 1990) and nonlinear (McClamroch, 1990; Krishnan and McClamroch, 1993; Yim and Singh, 1993) DAE systems. A related problem of control of constrained nonlinear ODE systems has also been studied (Chen and Shayman, 1992). Feedback regularization of a restricted class of singular nonlinear implicit differential equations has also been employed to overcome the singularity and use available ODE control methods (Christodoulou and Isik, 1990). A close look on the above research activity indicates the lack of a concrete methodological framework for studying feedback control problems for DAE systems that arise in chemical engineering. On the other hand, recent advances in modeling have established the fact that many chemical engineering processes are naturally modeled by high-index DAEs (Byrne and Ponzi, 1988; Hindmarsh and Johnson, 1988; Pantelides, 1988; Gani and Cameron, 1992).

Motivated by the above, the objective of this work is to develop a comprehensive framework for the analysis and feedback control of a broad class of nonlinear DAE systems. An explicit feedback controller synthesis methodology will be developed on the basis of an equivalent state-space realization for such systems. The application of the developed control methodology will be demonstrated on a two-phase reactor, modeled by an index-two DAE system.

DAE Systems: Preliminaries on Analysis and Control

We will consider nonlinear multi-input multi-output (MIMO) DAE systems with a description of the form:

$$\begin{aligned} \dot{x} &= f(x) + b(x)z + g(x)u \\ 0 &= k(x) + l(x)z \\ y_i &= h_i(x),\ i=1,\ \ldots,\ m \end{aligned} \tag{1}$$

where $x \in \mathbb{R}^n$ is the vector of differential variables (those for which we have explicit differential equations), $z \in \mathbb{R}^p$ is the vector of algebraic variables, $u \in \mathbb{R}^m$ is the vector of manipulated inputs, and y_i, $i=1, \ldots, m$ are the controlled outputs. In the above representation, $f(x)$ is an analytic vector field on $\mathbb{R}^n$, $k(x)$ is an analytic vector field on $\mathbb{R}^p$, $b(x)$, $g(x)$ and $l(x)$ are analytic matrices of dimensions $(n \times p)$, $(n \times m)$ and $(p \times p)$, respectively, whereas $h_i(x)$, $i=1, \ldots, m$ are analytic scalar fields. The above description of DAE systems (Eq. 1) is in the so-called semiexplicit form (Gear, 1988), with the algebraic variables z appearing linearly.

The consideration of semiexplicit DAE systems as compared to fully implicit ones is motivated by chemical process applications, where the differential equations are obtained explicitly from dynamic balances over mass and energy, and the algebraic equations typically arise from equilibrium relations, empirical correlations, and so on. Moreover, the linear occurrence of the algebraic variables z is also typical in chemical processes modeled by DAEs (such as, multiphase reaction and separation systems with phase equilibrium, where the algebraic variables include pressure and the interphase mass-transfer rates). Finally, the above representation of DAE systems (Eq. 1) includes ODE systems and DAE systems studied in the context of other engineering fields (McClamroch, 1990; Krishnan and McClamroch, 1993; Yim and Singh, 1993) as special cases. Although more general forms of DAE systems could be studied, Eq. 1 allows sufficient generality for a broad class of practical applications, and explicitness and analytical insight into the calculations.

For DAE systems of the form of Eq. 1, the index ν_d (Gear and Petzold, 1984) is defined as the minimum number of times the algebraic equations have to be differentiated to obtain a set of differential equations for the algebraic variables z. Clearly, if the matrix $l(x)$ is nonsingular, then the algebraic equations can be solved directly for the algebraic variables z. Differentiating the resulting expressions once, the differential equations for z can be obtained. Hence, such systems have index $\nu_d = 1$. On the other hand, if the matrix $l(x)$ is singular, then the algebraic equations are not directly solvable for z, and more differentiations are needed to obtain an equivalent ODE model. Hence, such systems have a high index ($\nu_d > 1$). Moreover, each differentiation of the algebraic equations introduces additional algebraic constraints, which give rise to nontrivial problems in the numerical simulation and control of such systems.

In this work, we will focus on high-index DAE systems. For index-one DAE systems (Eq. 1), the algebraic equations can be solved directly for the algebraic variables, to obtain:

$$z = -l(x)^{-1}k(x) \tag{2}$$

Substitution of the resulting expression for z (Eq. 2) in Eq. 1 yields the following state-space ODE model:

$$\begin{aligned} \dot{x} &= [f(x) - b(x)l(x)^{-1}k(x)] + g(x)u \\ y_i &= h_i(x),\ i=1,\ \ldots,\ m \end{aligned} \tag{3}$$

Thus, index-one DAE systems of the forms of Eq. 1 are similar to ODE systems, and analysis and control of such systems can be addressed directly on the basis of the equivalent ODE model (Eq. 3).

Methodological framework

The process description of Eq. 1 does not constitute a standard state-space model, owing to the presence of algebraic variables z. Moreover, for high-index DAE systems, the algebraic equations are not directly solvable for z and additional underlying constraints among the process variables are also present. As a result of these, system-theoretic issues like existence and uniqueness of solutions, stability, invertibility, and the formulation and solution of controller synthesis problems are rather obscure on the basis of this representation.

Motivated by these considerations, the following methodology will be used in this work:

- Initially, we will address the problem of deriving an explicit state-space realization of the constrained process, that is, a set of differential equations on x which describe the dynamics of the process consistent with the algebraic constraints:

$$k(x) + l(x)z = 0 \tag{4}$$

To this end, an algorithmic procedure will be developed which will allow to reconstruct z in terms of x and u and specify a set of algebraic constraints among the differential variables x, effectively yielding a state-space realization of the constrained process.

• The derived state-space realization will then be used as the basis for formulating and solving an output feedback controller synthesis problem.

Derivation of State-Space Realizations

Consider the description of the process dynamics:

$$\dot{x} = f(x) + b(x)z + g(x)u \tag{5}$$

and the algebraic constraints:

$$k(x) + l(x)z = 0 \tag{6}$$

The objective is to derive a state-space realization of the process, consistent with the imposition of the algebraic constraints. For the class of systems under consideration, this problem can be addressed efficiently using techniques and methodologies from nonlinear systems theory. More specifically, viewing the algebraic expressions $k(x)+l(x)z$ as a set of auxiliary outputs $\tilde{y}$ which are identically zero, and the algebraic variables z as auxiliary inputs, the problem becomes the one of specifying the zero dynamics of Eq. 5 with respect to $\tilde{y}$. Note the nonstandard form of the outputs $\tilde{y}$ that depend on the inputs z directly but in a singular way. The solution of the above problem entails the reconstruction of the algebraic variables z as functions of x, u in a way that ensures that Eq. 6 and any additional constraints generated by differentiating Eq. 6 are satisfied.

In what follows, an algorithmic procedure will be presented that solves the above problem. The procedure is based on Hirschorn's inversion algorithm (Hirschorn, 1979), which was introduced in the context of calculating the inverse of a MIMO nonlinear ODE system with a singular input/output map (in the sense of singularity of the characteristic matrix). The algorithm involves a sequence of elementary row operations that localize the singularity in specific outputs, followed by the differentiation of these outputs, until a nonsingular input/output relation is obtained that can be solved directly for the inputs.

Algorithmic procedure for reconstruction of algebraic variables

Iteration 1. Consider the algebraic equations in Eq. 6, where rank $l(x) = p_1 < p$.

Step 1. Calculate a $p \times p$ analytic nonsingular matrix $E^1(x)$, which:

(i) Rearranges the rows of the matrix $l(x)$ such that the first p_1 rows of $E^1(x)l(x)$ are linearly independent, and

(ii) Reduces the last $p-p_1$ rows of $E^1(x)l(x)$ to zero.

Pre-multiplying the algebraic equations in Eq. 6 by the matrix $E^1(x)$, the following relation is obtained:

$$0 = \begin{bmatrix} \bar{k}^1(x) \\ \hat{k}^1(x) \end{bmatrix} + \begin{bmatrix} \bar{l}^1(x) \\ 0 \end{bmatrix} z \tag{7}$$

where the matrix $\bar{l}^1(x)$ of dimension $p_1 \times p$ has full row rank and the vector fields $\bar{k}^1(x)$, $\hat{k}^1(x)$ are of dimensions p_1 and $(p-p_1)$, respectively.

Step 2. Differentiate the last $p-p_1$ equations of Eq. 7 once, to obtain the following set of algebraic equations:

$$0 = \begin{bmatrix} \bar{k}^1(x) \\ \tilde{k}^2(x) \end{bmatrix} + \begin{bmatrix} \bar{l}^1(x) \\ \tilde{l}^2(x) \end{bmatrix} z + \begin{bmatrix} 0 \\ \tilde{c}^2(x) \end{bmatrix} u \tag{8}$$

where

$$\tilde{k}^2(x) = [L_f\hat{k}^1_1(x) \; \cdots \; L_f\hat{k}^1_{p-p_1}(x)]^T$$

and

$$\tilde{l}^2(x) = \begin{bmatrix} L_{b_1}\hat{k}^1_1(x) & \cdots & L_{b_p}\hat{k}^1_1(x) \\ \vdots & & \vdots \\ L_{b_1}\hat{k}^1_{p-p_1}(x) & \cdots & L_{b_p}\hat{k}^1_{p-p_1}(x) \end{bmatrix},$$

$$\tilde{c}^2(x) = \begin{bmatrix} L_{g_1}\hat{k}^1_1(x) & \cdots & L_{g_m}\hat{k}^1_1(x) \\ \vdots & & \vdots \\ L_{g_1}\hat{k}^1_{p-p_1}(x) & \cdots & L_{g_m}\hat{k}^1_{p-p_1}(x) \end{bmatrix}$$

In the above relations, $\hat{k}^1_i(x)$ denotes the ith component of the vector field $\hat{k}^1(x)$ and $b_i(x)$, $g_i(x)$ denote the ith column vectors of the corresponding matrices.

Step 3. Evaluate the rank p_2 of the matrix:

$$\begin{bmatrix} \bar{l}^1(x) \\ \tilde{l}^2(x) \end{bmatrix} \tag{9}$$

If $p_2 = p$ then stop. If $p_2 < p$, then proceed to the next iteration, starting with the new set of algebraic equations (Eq. 8).

Iteration q. Consider the following set of algebraic equations obtained from iteration $q-1$:

$$0 = \begin{bmatrix} \bar{k}^1(x) \\ \bar{k}^2(x) \\ \vdots \\ \bar{k}^{q-1}(x) \\ \tilde{k}^q(x) \end{bmatrix} + \begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^{q-1}(x) \\ \tilde{l}^q(x) \end{bmatrix} z + \begin{bmatrix} 0 \\ \bar{c}^2(x) \\ \vdots \\ \bar{c}^{q-1}(x) \\ \tilde{c}^q(x) \end{bmatrix} u \tag{10}$$

with

$$\text{rank} \begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^{q-1}(x) \\ \tilde{l}^q(x) \end{bmatrix} = p_q < p$$

Then, there exists an analytic nonsingular $p \times p$ matrix $E^q(x)$ which:

(i) Rearranges the rows of $\tilde{l}^q(x)$ such that the first p_q rows of the matrix:

$$E^q(x) \begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^{q-1}(x) \\ \tilde{l}^q(x) \end{bmatrix}$$

are linearly independent, and

(ii) Reduces the last $p-p_q$ rows of the above matrix to zero. Furthermore, assuming that the augmented matrix:

$$\begin{bmatrix} \bar{l}^1(x) & 0 \\ \bar{l}^2(x) & \bar{c}^2(x) \\ \vdots & \vdots \\ \bar{l}^{q-1}(x) & \bar{c}^{q-1}(x) \\ \tilde{l}^q(x) & \tilde{c}^q(x) \end{bmatrix}$$

has rank p_q, the matrix $E^q(x)$ can be chosen so that the last $p-p_q$ rows of the matrix:

$$E^q(x)\begin{bmatrix} 0 \\ \bar{c}^2(x) \\ \vdots \\ \bar{c}^{q-1}(x) \\ \tilde{c}^q(x) \end{bmatrix}$$

are also identically equal to zero.

Step 1. Pre-multiply the algebraic equations (Eq. 10) by the matrix $E^q(x)$ to obtain:

$$0=\begin{bmatrix} \bar{k}^1(x) \\ \bar{k}^2(x) \\ \vdots \\ \bar{k}^q(x) \\ \hat{k}^q(x) \end{bmatrix}+\begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^q(x) \\ 0 \end{bmatrix}z+\begin{bmatrix} 0 \\ \bar{c}^2(x) \\ \vdots \\ \bar{c}^q(x) \\ 0 \end{bmatrix}u \qquad (11)$$

where the matrix:

$$\begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^q(x) \end{bmatrix}$$

of dimension $p_q \times p$ has full row rank, the matrix $\bar{c}^q(x)$ has dimension $(p_q-p_{q-1})\times m$ and the vector fields $\bar{k}^q(x)$, $\hat{k}^q(x)$ are of dimensions (p_q-p_{q-1}) and $(p-p_q)$, respectively.

Step 2. Differentiate the last $p-p_q$ equations of Eq. 11 once, to obtain the following set of algebraic equations:

$$0=\begin{bmatrix} \bar{k}^1(x) \\ \bar{k}^2(x) \\ \vdots \\ \bar{k}^q(x) \\ \tilde{k}^{q+1}(x) \end{bmatrix}+\begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^q(x) \\ \tilde{l}^{q+1}(x) \end{bmatrix}z+\begin{bmatrix} 0 \\ \bar{c}^2(x) \\ \vdots \\ \bar{c}^q(x) \\ \tilde{c}^{q+1}(x) \end{bmatrix}u \qquad (12)$$

Step 3. Evaluate the rank p_{q+1} of the matrix:

$$\begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^q(x) \\ \tilde{l}^{q+1}(x) \end{bmatrix}$$

If $p_{q+1}=p$ then stop, else repeat the above steps for the next iteration, starting with the new sets of algebraic equations (Eq. 12).

By construction, the algorithmic procedure generates a sequence of integers $p_1 \le p_2 \le \cdots \le p$. For a well-posed DAE system, the procedure converges after a finite number of iterations s, with the following final set of algebraic equations:

$$0=\begin{bmatrix} \bar{k}^1(x) \\ \bar{k}^2(x) \\ \vdots \\ \bar{k}^s(x) \\ \tilde{k}^{s+1}(x) \end{bmatrix}+\begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^s(x) \\ \tilde{l}^{s+1}(x) \end{bmatrix}z+\begin{bmatrix} 0 \\ \bar{c}^2(x) \\ \vdots \\ \bar{c}^s(x) \\ \tilde{c}^{s+1}(x) \end{bmatrix}u \qquad (13)$$

where the $p \times p$ matrix:

$$\begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^s(x) \\ \tilde{l}^{s+1}(x) \end{bmatrix}$$

has full rank, that is, $p_{s+1}=p$.

The final set of algebraic equations (Eq. 13) allows to reconstruct the algebraic variables z as a function of the differential variables x and the manipulated inputs u, as follows:

$$z=-\begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^s(x) \\ \tilde{l}^{s+1}(x) \end{bmatrix}^{-1}\left\{\begin{bmatrix} \bar{k}^1(x) \\ \bar{k}^2(x) \\ \vdots \\ \bar{k}^s(x) \\ \tilde{k}^{s+1}(x) \end{bmatrix}+\begin{bmatrix} 0 \\ \bar{c}^2(x) \\ \vdots \\ \bar{c}^s(x) \\ \tilde{c}^{s+1}(x) \end{bmatrix}u\right\} \qquad (14)$$

Moreover, the algorithmic procedure identifies a set of $\Sigma_{i=1}^{s}(p-p_i)$ algebraic constraints:

$$\begin{aligned} \hat{k}_1^1(x)&=0 \\ &\vdots \\ \hat{k}_{p-p_1}^1(x)&=0 \\ &\vdots \\ \hat{k}_1^s(x)&=0 \\ &\vdots \\ \hat{k}_{p-p_s}^s(x)&=0 \end{aligned} \qquad (15)$$

among the differential variables x, which must also hold. Proposition 1 that follows establishes the linear independence of the scalar fields in Eq. 15 (the proof is given in Appendix A).

Proposition 1. Consider the DAE system of Eq. 1 for which the proposed algorithmic procedure converges after s iterations. Then, the $\Sigma_{i=1}^{s}(p-p_i)$ scalar fields $\hat{k}_j^i(x)$, $i=1,\ldots,s$; $j=1,\ldots,(p-p_i)$ obtained during the algorithmic procedure are linearly independent.

Proposition 1 leads to the following observations for the DAE system of Eq. 1:

(1) Given $x \in \mathbb{R}^n$, the linear independence of the scalar fields implies that $\Sigma_{i=1}^{s}(p-p_i) \leq n$.

(2) The algebraic constraints of Eq. 15 allow a characterization of the state-space $\mathfrak{M} \subset \mathbb{R}^n$ where the differential variables x of the constrained DAE system (Eq. 1) must evolve. More specifically, $\mathfrak{M} = \{x \in \mathbb{R}^n : \hat{k}_j^i(x) = 0, i = 1, \ldots, s; j = 1, \ldots, (p-p_i)\}$, which, given the linear independence of the scalar fields $\hat{k}_j^i(x)$, is a smooth manifold of dimension $n - \Sigma_{i=1}^{s}(p-p_i)$.

(3) The linearly independent scalar fields $\hat{k}_j^i(x)$, $i = 1, \ldots, s$; $j = 1, \ldots, (p-p_i)$ can be used as a part of a nonlinear coordinate transformation to derive a state-space realization of the DAE system of Eq. 1. Details of the coordinate transformation and the resulting state-space realization are given in the next section.

Remark 1. Consider the DAE system (Eq. 1), for which the above algorithmic procedure has converged after s iterations, with the final set of algebraic equations (Eq. 13) solvable in z. Differentiating the obtained solution for z (Eq. 14) once more, a set of differential equations for z can be obtained. Hence, the index of the DAE system (Eq. 1) is exactly $s+1$. Moreover, according to Hirschorn (1979), the integer s represents the relative order of the auxiliary outputs $\tilde{y}$ with respect to the auxiliary inputs z for the system of Eq. 5. These observations establish a transparent relation between the concept of relative order and the concept of index.

Remark 2. The assumption on the rank of the augmented matrix made in iteration $q (q > 1)$ of the proposed algorithm is satisfied for all index-two (the most common among chemical processes) and many higher-index DAE systems of the form of Eq. 1. It essentially allows us to obtain $p - p_q$ algebraic equations involving only the differential variables x, in step 1 of iteration q. Thus, the algebraic equations obtained in step 2 of iteration q, which serve as the basis for iteration $q+1$, do not involve any derivatives of the inputs u. This facilitates the reconstruction of the algebraic variables z and the subsequent derivation of the state-space realization, independently of the feedback law used for the manipulated inputs u.

Remark 3. For the special classes of DAE systems considered in Krishnan and McClamroch (1990), McClamroch (1990), and Krishnan and McClamroch (1993) and under the assumptions made therein, the input/output map between the auxiliary outputs $\tilde{y}$ and the auxiliary inputs z is nonsingular and the above algorithmic procedure reduces to an explicit and direct reconstruction of z in terms of x and u.

State-space realizations of the DAE system

The derived relation for the algebraic variables z (Eq. 14) can be used to obtain a state-space realization of the DAE system of Eq. 1 by eliminating the algebraic variables from the modeling equations. The resulting state-space realization is given the following proposition (see Appendix A for the proof).

Proposition 2. Consider the DAE system of Eq. 1 for which the proposed algorithmic procedure converges after s iterations. Then the dynamic system:

$$\dot{x} = \left(f(x) - b(x) \begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^s(x) \\ \tilde{l}^{s+1}(x) \end{bmatrix}^{-1} \begin{bmatrix} \bar{k}^1(x) \\ \bar{k}^2(x) \\ \vdots \\ \bar{k}^s(x) \\ \tilde{k}^{s+1}(x) \end{bmatrix} \right) + \left(g(x) - b(x) \begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^s(x) \\ \tilde{l}^{s+1}(x) \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ \bar{c}^2(x) \\ \vdots \\ \bar{c}^s(x) \\ \tilde{c}^{s+1}(x) \end{bmatrix} \right) u$$

$$= \bar{f}(x) + \bar{g}(x) u \tag{16}$$

$$y_i = h_i(x), \; i = 1, \ldots, m$$

where $x \in \mathfrak{M} = \{x \in \mathbb{R}^n : \hat{k}_j^i(x) = 0; i = 1, \ldots, s; j = 1, \ldots, (p-p_i)\}$, is a state-space realization of the constrained process.

Remark 4. Consider the DAE system of Eq. 1 for which the proposed algorithmic procedure converges after s iterations, that is, its index is $s+1$ (see Remark 1). For the DAE system comprising of the original differential equations (Eq. 5) and the new set of algebraic equations obtained after the first iteration (Eq. 8), the proposed algorithm converges after $s-1$ iterations, that is, its index is s. Hence, it is clear that the proposed algorithmic procedure reduces the index of the DAE system in each iteration through a combination of algebraic manipulations and differentiations. This motivates a comparison of the proposed procedure with existing index reduction techniques developed in the framework of numerical simulation of high-index DAEs. The techniques of Gear and Petzold (1984) for linear implicit DAEs, and Gear (1988) for nonlinear implicit and semiexplicit DAEs, involve successive differentiation of all the (underlying) algebraic equations. The proposed procedure, on the other hand, exploits the specific form of Eq. 1 to explicitly identify the smallest subset of algebraic equations that need to be differentiated in each iteration. The numerical simulation algorithm of Chung and Westerberg (1990) for nonlinear implicit DAEs involves differentiation of a subset of the equations with a single Jacobian without any algebraic manipulations to identify the underlying algebraic constraints, thereby introducing higher-order derivatives of the original variables. Furthermore, the technique of Bachmann et al. (1990) for linear DAEs replaces a set of redundant differential equations with additional algebraic equations in each iteration to obtain an equivalent index-one DAE system; the proposed method, however, retains the differential equations and eliminates the algebraic variables instead, yielding an equivalent ODE system (Eq. 16).

Remark 5. The algebraic constraints of Eq. 15, which are specified by the algorithmic procedure, provide an explicit means for the choice of consistent initial conditions for the differential variables x. Thus, numerical simulation techniques for explicit ODEs can be used for the solution of DAEs in the form of Eq. 1, on the basis of the state-space realization of Eq. 16.

In view of the fact that the differential variables x are constrained to evolve on the manifold $\mathfrak{M}$, of dimension $n - \Sigma_{i=1}^{s}(p-p_i)$, the state-space realization of Eq. 16 is not of minimal order. Such a realization can only be obtained in appropriate transformed coordinates. More specifically, given the linearly independent scalar fields $\hat{k}_j^i(x)$, $i=1, \ldots, s$, $j=1, \ldots, (p-p_i)$, one can always find $\kappa = n - \Sigma_{i=1}^s (p-p_i)$ scalar fields $\phi_1(x), \ldots \phi_\kappa(x)$ to complete a set of n linearly independent scalar fields that qualify for a nonlinear coordinate transformation. Under such a coordinate transformation:

$$\zeta = \begin{bmatrix} \zeta_1^{(0)} \\ \vdots \\ \zeta_\kappa^{(0)} \\ \zeta^{(1)} \\ \vdots \\ \zeta^{(s)} \end{bmatrix} = T(x) = \begin{bmatrix} \phi_1(x) \\ \vdots \\ \phi_\kappa(x) \\ \hat{k}^1(x) \\ \vdots \\ \hat{k}^s(x) \end{bmatrix} \quad (17)$$

the state-space realization of Eq. 16 takes the following form:

$$\dot{\zeta} = \begin{bmatrix} \dot{\zeta}_1^{(0)} \\ \vdots \\ \dot{\zeta}_\kappa^{(0)} \\ \dot{\zeta}^{(1)} \\ \vdots \\ \dot{\zeta}^{(s)} \end{bmatrix} = \begin{bmatrix} L_{\bar{f}}\phi_1(x) \\ \vdots \\ L_{\bar{f}}\phi_\kappa(x) \\ L_{\bar{f}}\hat{k}^1(x) \\ \vdots \\ L_{\bar{f}}\hat{k}^s(x) \end{bmatrix}_{x=T^{-1}(\zeta)} + \begin{bmatrix} L_{\bar{g}}\phi_1(x) \\ \vdots \\ L_{\bar{g}}\phi_\kappa(x) \\ L_{\bar{g}}\hat{k}^1(x) \\ \vdots \\ L_{\bar{g}}\hat{k}^s(x) \end{bmatrix}_{x=T^{-1}(\zeta)} u \quad (18)$$

$$y_i = h_i(x)\,|_{x=T^{-1}(\zeta)}, \; i=1, \ldots, m$$

where

$$L_{\bar{g}}\phi_i(x) = [L_{\bar{g}_1}\phi_i(x) \cdots L_{\bar{g}_m}\phi_i(x)]$$

$$L_{\bar{f}}\hat{k}^i(x) = \begin{bmatrix} L_{\bar{f}}\hat{k}_1^i(x) \\ \vdots \\ L_{\bar{f}}\hat{k}_{(p-p_i)}^i(x) \end{bmatrix},$$

$$L_{\bar{g}}\hat{k}^i(x) = \begin{bmatrix} L_{\bar{g}_1}\hat{k}_1^i(x) & \cdots & L_{\bar{g}_m}\hat{k}_1^i(x) \\ \vdots & & \vdots \\ L_{\bar{g}_1}\hat{k}_{(p-p_i)}^i(x) & \cdots & L_{\bar{g}_m}\hat{k}_{(p-p_i)}^i(x) \end{bmatrix}$$

and $\bar{g}_i(x)$ denotes the ith column of matrix $\bar{g}(x)$. Proposition 3 that follows gives a reduced-order state-space realization for the DAE system of Eq. 1 in these transformed coordinates (see Appendix A for a proof of the proposition).

Proposition 3. Consider the DAE system of Eq. 1 for which the proposed algorithmic procedure converges after s iterations. Then the dynamic system:

$$\dot{\zeta}^{(0)} = f^{(0)}(\zeta^{(0)}) + g^{(0)}(\zeta^{(0)})u$$

$$y_i = h_i(x)\,|_{x=T^{-1}(\zeta^{(0)},0,\ldots,0)}, \; i=1, \ldots, m \quad (19)$$

where

$$f^{(0)}(\zeta^{(0)}) = \begin{bmatrix} L_{\bar{f}}\phi_1(x) \\ \vdots \\ L_{\bar{f}}\phi_\kappa(x) \end{bmatrix}_{x=T^{-1}(\zeta^{(0)},0,\ldots,0)}$$

$$g^{(0)}(\zeta^{(0)}) = \begin{bmatrix} L_{\bar{g}}\phi_1(x) \\ \vdots \\ L_{\bar{g}}\phi_\kappa(x) \end{bmatrix}_{x=T^{-1}(\zeta^{(0)},0,\ldots,0)} \quad (20)$$

is a state-space realization of the constrained process, of dimension $(n - \Sigma_{i=1}^s (p-p_i))$.

In the following section, we will formulate and solve an output feedback controller synthesis problem for nonlinear DAE systems of the form of Eq. 1.

Feedback Controller Synthesis

Preliminaries

For a DAE system of Eq. 1, various system-theoretic issues (such as existence and uniqueness of solutions, equilibrium points and their stability, zero dynamics and characterization of minimum-phase behavior, and so on) can be addressed directly on the basis of the equivalent state-space realizations (Eq. 16 or Eq. 19) using existing results for ODE systems. These state-space realizations can also be the basis for the formulation and solution of an output feedback controller synthesis problem for DAE systems of the form of Eq. 1. In what follows, we will introduce some basic concepts that are relevant to analysis and controller synthesis purposes, on the basis of the state-space realization of Eq. 16.

For a DAE system of the form of Eq. 1, we define the relative order r_i of the output y_i with respect to the manipulated input vector u, as the minimum integer such that:

$$[L_{\bar{g}_1}L_{\bar{f}}^{r_i-1}h_i(x) \;\cdots\; L_{\bar{g}_m}L_{\bar{f}}^{r_i-1}h_i(x)] \not\equiv [0 \;\cdots\; 0]$$

for $x \in X \subset \mathfrak{M}$, where X is an open set containing the equilibrium point of interest. If no such integer exists, then $r_i = \infty$. It will be assumed that there is a finite relative order r_i for each output y_i to ensure output controllability. Then, the matrix:

$$C(x) = \begin{bmatrix} L_{\bar{g}_1}L_{\bar{f}}^{r_1-1}h_1(x) & \cdots & L_{\bar{g}_m}L_{\bar{f}}^{r_1-1}h_1(x) \\ \vdots & & \vdots \\ L_{\bar{g}_1}L_{\bar{f}}^{r_m-1}h_m(x) & \cdots & L_{\bar{g}_m}L_{\bar{f}}^{r_m-1}h_m(x) \end{bmatrix} \quad (21)$$

is known as the characteristic matrix (Claude, 1986) for the system of Eq. 16. A nonsingular characteristic matrix implies a nonsingular input/output map between the manipulated inputs u and the controlled outputs y, thereby allowing the use of combination of static state feedback laws and state observers to enforce a desired closed-loop input/output behavior (Daoutidis and Kravaris, 1994). For simplicity, it will be assumed that the characteristic matrix $C(x)$ (Eq. 21) is nonsingular on X. Moreover, it will also be assumed that the unforced zero dynamics for the system of Eq. 16 (or equivalently Eq. 19) is locally asymptotically stable, that is, the DAE system of Eq. 1 is minimum-phase.

Remark 6. In the case where the characteristic matrix $C(x)$ (Eq. 21) is singular, an output feedback controller can be derived through the combination of a *dynamic* state feedback law with state observers (Daoutidis and Kumar, 1994).

Problem formulation

Consider a minimum-phase DAE system of the form of Eq. 1 with the equivalent state-space realization (Eq. 16) and a nonsingular characteristic matrix $C(x)$. It is desired to derive a dynamic output feedback controller that uses the measurements of the outputs to enforce the following closed-loop objectives:

(1) Induce a closed-loop input/output response of the form:

$$y+\sum_{i=1}^{m}\sum_{j=1}^{r_i}\gamma_{ij}\frac{d^j y_i}{dt^j}=y_{sp} \tag{22}$$

where $y=[y_1\ \cdots\ y_m]^T$, $y_{sp}=[y_{sp1}\ \cdots\ y_{spm}]^T$ are the output and set point vectors, and $\gamma_{ij}=[\gamma_{ij}^1\ \cdots\ \gamma_{ij}^m]^T$ are vectors of adjustable parameters.

(2) Reject unmeasured disturbances and modeling errors.

(3) Ensure closed-loop input/output and internal stability, subject to the constraints imposed by the algebraic equations.

Controller synthesis

The output feedback controller synthesis problem for the DAE system of Eq. 1 will be addressed through a combination of state feedback with a suitable state observer. Following this approach, first, we will address the synthesis of a state feedback controller that induces the following input/output behavior:

$$\sum_{i=1}^{m}\sum_{j=0}^{r_i}\beta_{ij}\frac{d^j y_i}{dt^j}=v \tag{23}$$

where $v=[v_1\ \cdots\ v_m]^T$ is a vector of external reference inputs, $\beta_{ij}=[\beta_{ij}^1\ \cdots\ \beta_{ij}^m]^T$ are vectors of adjustable parameters, and provides input/output and internal stability in the closed-loop system, subject to the underlying constraints of Eq. 15. The main result is given in Theorem 1 that follows (for a proof see Appendix A).

Theorem 1. Consider a DAE system of the form of Eq. 1 with an equivalent state-space realization of the form of Eq. 16 for which $\det C(x)\neq 0$, $\forall x\epsilon X$. Then the static state feedback law:

$$u=\{[\beta_{1r_1}\ \cdots\ \beta_{mr_m}]C(x)\}^{-1}\left(v-\sum_{i=1}^{m}\sum_{j=0}^{r_i}\beta_{ij}L_f^j h_i(x)\right) \tag{24}$$

induces the input/output behavior:

$$\sum_{i=1}^{m}\sum_{j=0}^{r_i}\beta_{ij}\frac{d^j y_i}{dt^j}=v$$

subject to the underlying constraints imposed by the algebraic equations.

The bounded-input bounded-output (BIBO) stability of the closed-loop system can be ensured by a proper choice of the adjustable parameters β_{ij}^k. Besides BIBO stability of the closed-loop system, it is necessary to ensure the internal stability of the closed-loop system, that is, the local asymptotic stability of the unforced ($v=0$) closed-loop system. It can be verified that the unforced closed-loop system is locally asymptotically stable if the following two conditions hold:

(1) The parameters β_{ij}^k are chosen properly to ensure BIBO stability of the system with the input/output behavior of Eq. 23.

(2) The unforced zero dynamics of the process is locally asymptotically stable, that is, the process is minimum-phase.

Given the state feedback controller of Eq. 24 which induces the linear input/output behavior of Eq. 23, a linear error feedback controller with integral action can then be incorporated around the linear $v-y$ system to enforce the requested closed-loop input/output behavior of Eq. 22 and guarantee rejection of disturbances and modeling errors. For example, one such error feedback controller realization has the form (Daoutidis and Kravaris, 1994):

$$\begin{aligned}
\dot{\xi}_1^{(1)}&=\xi_2^{(1)}\\
&\ \vdots\\
\dot{\xi}_{r_1-1}^{(1)}&=\xi_{r_1}^{(1)}\\
\dot{\xi}_{r_1}^{(1)}&=([\gamma_{1r_1}\ \cdots\ \gamma_{mr_m}]^{-1})_1\left[(y_{sp}-y)-\sum_{i=1}^{m}\sum_{j=1}^{r_i-1}\gamma_{ij}\xi_{j+1}^{(i)}\right]\\
&\ \vdots\\
\dot{\xi}_1^{(m)}&=\xi_2^{(m)}\\
&\ \vdots\\
\dot{\xi}_{r_m-1}^{(m)}&=\xi_{r_m}^{(m)}\\
\dot{\xi}_{r_m}^{(m)}&=([\gamma_{1r_1}\ \cdots\ \gamma_{mr_m}]^{-1})_m\left[(y_{sp}-y)-\sum_{i=1}^{m}\sum_{j=1}^{r_i-1}\gamma_{ij}\xi_{j+1}^{(i)}\right]\\
v&=\sum_{i=1}^{m}\sum_{j=0}^{r_i-1}\beta_{ij}\xi_{j+1}^{(i)}+[\beta_{1r_1}\ \cdots\ \beta_{mr_m}][\gamma_{1r_1}\ \cdots\ \gamma_{mr_m}]^{-1}\\
&\quad\times\left[(y_{sp}-y)-\sum_{i=1}^{m}\sum_{j=1}^{r_i-1}\gamma_{ij}\xi_{j+1}^{(i)}\right]
\end{aligned} \tag{25}$$

where the symbol $(\ )_i$ denotes ith row of a matrix.

A combination of the static state feedback law of Eq. 24 with the linear error feedback controller of Eq. 25 provides a mixed error and state feedback controller that induces the desired closed-loop objectives. A dynamic output feedback controller that enforces these closed-loop objectives can then be derived by combining the state feedback controller (Eq. 24) and the linear error feedback controller (Eq. 25) with an appropriate state observer. Following the procedure of Daoutidis and Kravaris (1994) for stable processes, the equivalent state-space realization of Eq. 16 itself can be used as an open-loop observer to estimate the states x; while for open-loop unstable minimum-phase processes, the stable modes of the zero dynamics can be used instead for the state reconstruction. A more detailed exposition along the above lines is omitted for brevity.

Application of the Control Methodology to a Two-Phase Reactor

A broad class of chemical processes modeled by high index DAE systems consists of multiphase systems where the individual phases are in thermodynamic equilibrium. Typical examples of such systems include distillation columns, multiphase

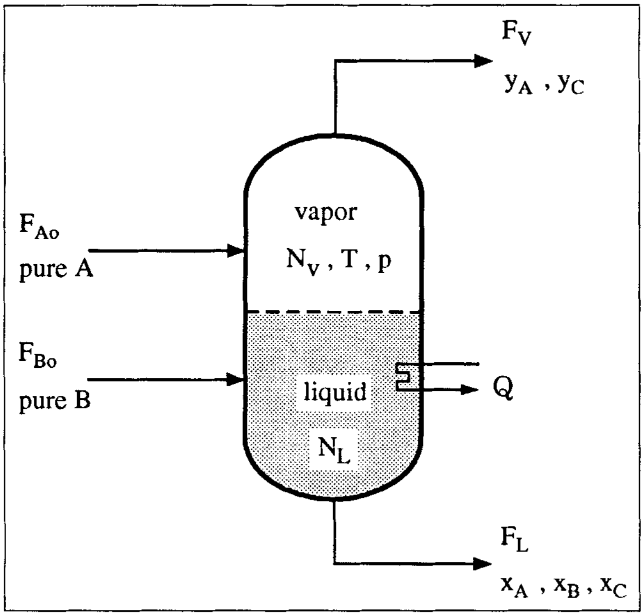

Figure 1. Two-phase reactor.

reactors, multiphase separation units, and so on. In what follows we will consider a vapor-liquid reaction system in a CSTR, with the two phases in physical equilibrium. Several fluid-fluid reaction systems that fall in the framework of the example can be found in Doraiswamy and Sharma (1984).

Process description

Consider the two-phase (liquid- and vapor-phase) reactor shown in Figure 1. Reactants A and B are fed to the CSTR as pure vapor and liquid streams, respectively, at molar flow rates F_{Ao} and F_{Bo}, while the two outlet streams from the liquid and vapor phases have molar flow rates F_L and F_V, respectively. It is assumed that the individual phases are well-mixed and they are in physical equilibrium at pressure p and temperature T, that is, the chemical reaction is slow compared to the mass transfer across the interface. The molar specific heat capacity c_p, density ρ, and latent heat of vaporization ΔH^u are also assumed to be constant and equal for all the species. Reactant A diffuses into the liquid phase, where a reaction of the form:

$$A + B \rightarrow C$$

takes place. The rate of formation of the product C is given by:

$$R_C = k_o \exp(-E_a/RT) C_A C_B V_L$$

$$= k_o \exp(-E_a/RT) N_L \rho x_A x_B$$

where k_o and E_a are the pre-exponential factor and activation energy, respectively, N_L is the liquid-phase molar holdup, C_A, C_B and x_A, x_B are the molar concentrations and mole fractions of the reactants A and B in the liquid phase, and V_L is the liquid holdup volume, given by:

$$V_L = \frac{N_L}{\rho}$$

Product C then diffuses out into the vapor phase (product phase). Reactant B is assumed to be nonvolatile, that is, only the reactant A and the product C are present in the vapor phase while all the three species are present in the liquid phase.

The dynamic conservation equations for this process consist of the total mole balances in the liquid and vapor phases, the mole balance for the species A in the vapor phase, the mole balances for species A, B in the liquid phase, and the total enthalpy balance. The total enthalpy in the two phases is given by:

$$H = N_L H_l + N_V H_v$$

where H_l, H_v are the molar enthalpies in the liquid and vapor phases respectively, given by:

$$H_l = c_p T$$

$$H_v = H_l + \Delta H^v$$

$$= c_p T + \Delta H^v$$

In addition to these differential equations, the model consists of algebraic relations which include phase-equilibrium relations for the species A and C present in both phases, and the ideal gas law for the vapor phase. For simplicity, Raoult's law is assumed for the phase-equilibrium relations:

$$p y_A = P_A^s x_A$$

$$p y_C = P_C^s x_C$$

where y_A, $y_C = (1 - y_A)$ are the mole fractions of A and C in the vapor phase, and P_A^s, P_C^s are the saturation vapor pressures for A and C, given by the following Antoine relation:

$$P_A^s = \exp\left(30.5 - \frac{3{,}919.7}{T - 34.1}\right)$$

$$P_C^s = \exp\left(30.0 - \frac{5{,}000}{T + 70}\right)$$

Under the above assumptions, the process description takes the form:

$$\frac{dN_V}{dt} = F_{Ao} - N_A + N_C - F_V$$

$$\frac{dy_A}{dt} = \frac{F_{Ao}(1 - y_A)}{N_V} - \left(\frac{1 - y_A}{N_V}\right) N_A - \left(\frac{y_A}{N_V}\right) N_C$$

$$\frac{dN_L}{dt} = F_{Bo} - F_L - R_C + N_A - N_C$$

$$\frac{dx_A}{dt} = -\left(\frac{F_{Bo} x_A + R_C(1 - x_A)}{N_L}\right) + \left(\frac{1 - x_A}{N_L}\right) N_A + \left(\frac{x_A}{N_L}\right) N_C$$

$$\frac{dx_B}{dt} = \left(\frac{F_{Bo}(1 - x_B) - R_C(1 - x_B)}{N_L}\right) - \left(\frac{x_B}{N_L}\right) N_A + \left(\frac{x_B}{N_L}\right) N_C$$

$$\frac{dT}{dt} = \frac{F_{Ao}}{(N_L + N_V)} (T_{Ao} - T) + \frac{F_{Bo}}{(N_L + N_V)} (T_{Bo} - T)$$

Table 1. Reactor Parameters and Variables and their Nominal Values

Variable	Description	Nominal Value
c_p	Molar heat capacity (J/mol·K)	80
E_a	Activation energy (kJ/mol)	110
F_{Ao}	Inlet vapor stream molar flow rate (mol/s)	171.25
F_{Bo}	Inlet liquid stream molar flow rate (mol/s)	300
F_L	Outlet liquid stream molar flow rate (mol/s)	375
F_V	Outlet vapor stream molar flow rate (mol/s)	50
k_o	Preexponential factor (m³/mol·s)	1.0e+11
N_L	Liquid-phase molar holdup (kmol)	12.807
N_V	Vapor-phase molar holdup (kmol)	12.839
Q	Heat input (kW)	100
R	Universal gas constant (J/mol·K)	8.314
T	Reactor temperature (K)	341.51
T_{Ao}	Inlet vapor stream temperature (K)	310
T_{Bo}	Inlet liquid stream temperature (K)	298
V_T	Reactor volume (m³)	3.0
x_A	Mole fraction of species A in liquid phase	0.238
x_B	Mole fraction of species B in liquid phase	0.677
y_A	Mole fraction of species A in vapor phase	0.716
ΔH_R	Heat of reaction (kJ/mol)	50
ΔH^v	Latent heat of vaporization (kJ/mol)	20
ρ	Liquid-phase molar density (kmol/m³)	15

$$+\frac{R_c}{(N_L+N_V)}\left(T-\frac{\Delta H_R}{c_p}\right)+\frac{\Delta H^v}{(N_L+N_V)c_p}(N_A-N_C)+\frac{1}{(N_L+N_v)c_p}Q$$

$$0=-x_AP_A^s+py_A$$

$$0=-(1-x_A-x_B)P_C^s+p(1-y_A)$$

$$0=-N_VRT+p\frac{(V_T\rho-N_L)}{\rho} \tag{26}$$

In the above equations, N_A is the molar rate of transfer of reactant A from the vapor of the liquid phase, N_C is the molar rate of transfer of product C from the liquid to the vapor phase, Q is the heat input to the reactor and V_T is the reactor volume. A detailed description of the process parameters and variables is given in Table 1 along with their nominal steady-state values. For this process, it is desired to control the composition of the vapor phase y_A and the temperature T, using the vapor stream outlet flow rate F_v and the heat input Q as the manipulated inputs.

Defining the differential variables:

$$x_1=N_V,\ x_2=y_A,\ x_3=N_L,\ x_4=x_A,\ x_5=x_B,\ x_6=T$$

the algebraic variables:

$$z_1=N_A,\ z_2=N_C,\ z_3=p$$

the controlled outputs:

$$y_1=y_A,\ y_2=T$$

and the manipulated inputs:

$$u_1=F_V,\ u_2=Q$$

the above process description takes the form of Eq. 1 with:

$$f(x)=\begin{bmatrix} F_{Ao} \\ \dfrac{F_{Ao}(1-x_2)}{x_1} \\ F_{Bo}-F_L-R_C \\ -\left(\dfrac{F_{Bo}x_4+R_C(1-x_4)}{x_3}\right) \\ \left(\dfrac{(F_{Bo}-R_C)(1-x_5)}{x_3}\right) \\ \left(\dfrac{1}{x_1+x_3}\right)\left[F_{Ao}(T_{Ao}-x_6)+F_{Bo}(T_{Bo}-x_6)+R_C\left(x_6-\dfrac{\Delta H_R}{c_p}\right)\right] \end{bmatrix}$$

$$b(x)=\begin{bmatrix} -1 & 1 \\ -\left(\dfrac{1-x_2}{x_1}\right) & -\left(\dfrac{x_2}{x_1}\right) \\ 1 & -1 \\ \left(\dfrac{1-x_4}{x_3}\right) & \left(\dfrac{x_4}{x_3}\right) \\ -\left(\dfrac{x_5}{x_3}\right) & \left(\dfrac{x_5}{x_3}\right) \\ \left(\dfrac{\Delta H^v}{(x_1+x_3)c_p}\right) & -\left(\dfrac{\Delta H^v}{(x_1+x_3)c_p}\right) \end{bmatrix},$$

$$g(x)=\begin{bmatrix} -1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & \left(\dfrac{1}{(x_1+x_3)c_p}\right) \end{bmatrix}$$

$$k(x)=\begin{bmatrix} -x_4P_A^s \\ -(1-x_4-x_5)P_C^s \\ -Rx_1x_6 \end{bmatrix},\quad l(x)=\begin{bmatrix} 0 & 0 & x_2 \\ 0 & 0 & (1-x_2) \\ 0 & 0 & \dfrac{(V_T\rho-x_3)}{\rho} \end{bmatrix}$$

$$h_1(x)=x_2$$

$$h_2(x)=x_6 \tag{27}$$

Clearly, the matrix $l(x)$ is singular indicating a high index for the DAE system.

A common approach to avoid modeling this process by a high-index DAE system is to assume negligible vapor holdup compared to the liquid holdup, thus eliminating the need to model the vapor dynamics. The modeling equations under this simplifying assumption consist solely of differential equations obtained from the total mole balance, the mole balances for species A, B, and the total enthalpy balance where the total enthalpy is given by:

$$H = N_L H_l = N_l c_p T$$

Based on this simplifying assumption, the following ODE model can be easily derived:

$$\frac{dN_L}{dt} = F_{Ao} + F_{Bo} - F_L - F_V - R_C$$

$$\frac{dx_A}{dt} = \frac{1}{N_L}\{F_{Ao}(1-x_A) - F_{Bo}x_A - F_V(y_A - x_A) - R_C(1-x_A)\}$$

$$\frac{dx_B}{dt} = \frac{1}{N_L}\{-F_{Ao}x_B + F_{Bo}(1-x_B) + F_V x_B - R_C(1-x_B)\}$$

$$\frac{dT}{dt} = \frac{1}{N_L c_p}\{F_{Ao}(c_p(T_{Ao}-T) + \Delta H^v) + F_{Bo}c_p(T_{Bo}-T) - F_V \Delta H^v + R_C(c_p T - \Delta H_R) + Q\} \quad (28)$$

where y_A can be directly eliminated from the above ODE model using the following equilibrium relation:

$$y_A = \frac{P_A^s x_A}{P_A^s x_A + P_C^s(1 - x_A - x_B)}$$

Clearly, the accuracy of this model depends on the validity of the assumption that the vapor holdup N_V is negligible compared to the liquid holdup N_L. This assumption will not hold at high pressures when the vapor holdup becomes comparable to the liquid holdup. In the final section, the performance of the nonlinear output feedback controller based on the DAE model (Eq. 26) will be compared with that of a nonlinear output feedback controller based on the simplified ODE model (Eq. 28) to demonstrate the superiority of the former over the latter.

The next section discusses the derivation of the equivalent state-space realization for the DAE model (Eq. 26) following the proposed algorithmic procedure and the resulting output feedback controller.

State-space realization

Iteration 1. Consider the original algebraic equations:

$$0 = k(x) + l(x)z$$

where $k(x)$, $l(x)$ are given in Eq. 27 and

$$\text{rank } l(x) = p_1 = 1$$

Step 1. The following matrix:

$$E^1(x) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & -\left(\frac{x_2\rho}{V_T\rho - x_3}\right) \\ 0 & 1 & -\left(\frac{(1-x_2)\rho}{V_T\rho - x_3}\right) \end{bmatrix}$$

was used to pre-multiply the algebraic equations to obtain:

$$0 = -\begin{bmatrix} Rx_1x_6 \\ P_A^s x_4 - \left(\frac{\rho R x_1 x_2 x_6}{V_T\rho - x_3}\right) \\ P_C^s(1 - x_4 - x_5) - \left(\frac{\rho R x_1(1-x_2)x_6}{V_T\rho - x_3}\right) \end{bmatrix} + \begin{bmatrix} 0 & 0 & \left(\frac{V_T\rho - x_3}{\rho}\right) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} \quad (29)$$

Thus, identifying two constraints:

$$0 = \begin{bmatrix} \bar{k}_1^1(x) \\ \bar{k}_2^1(x) \end{bmatrix} = \begin{bmatrix} \exp\left(30.5 - \frac{3{,}919.7}{x_6 - 34.1}\right)x_4 - \left(\frac{\rho R x_1 x_2 x_6}{V_T\rho - x_3}\right) \\ \exp\left(30.0 - \frac{5{,}000}{x_6 + 70}\right)(1 - x_4 - x_5) - \left(\frac{\rho R x_1(1-x_2)x_6}{V_T\rho - x_3}\right) \end{bmatrix} \quad (30)$$

among the differential variables x.

Step 2. The last 2 equations of Eq. 29 were differentiated once, to obtain the following set of algebraic equations:

$$0 = \begin{bmatrix} Rx_1x_6 \\ \bar{k}_1^2(x) \\ \bar{k}_2^2(x) \end{bmatrix} + \begin{bmatrix} 0 & 0 & \left(\frac{V_T\rho - x_3}{\rho}\right) \\ \bar{l}_{11}^2(x) & \bar{l}_{12}^2(x) & 0 \\ \bar{l}_{21}^2(x) & \bar{l}_{22}^2(x) & 0 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ \bar{c}_{11}^2(x) & \bar{c}_{12}^2(x) \\ \bar{c}_{21}^2(x) & \bar{c}_{22}^2(x) \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \quad (31)$$

A detailed description of the individual terms in Eq. 31 is included in Appendix B and is omitted here for the sake of brevity.

Step 3. The rank of the matrix:

$$\begin{bmatrix} 0 & 0 & \left(\dfrac{V_T\rho - x_3}{\rho}\right) \\ \bar{l}^2_{11}(x) & \bar{l}^2_{12}(x) & 0 \\ \bar{l}^2_{21}(x) & \bar{l}^2_{22}(x) & 0 \end{bmatrix}$$

was evaluated to be $p_2 = 3 = p$. Thus, the algorithmic procedure converged after $s = 1$ iteration implying that the DAE system of Eq. 26 has index $\nu_d = 2$.

From Eq. 31, it follows that the algebraic variables $z_1 = N_A$, $z_2 = N_C$ are given by:

$$\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = -\left(\frac{1}{\det(\bar{l}^2(x))}\right)\begin{bmatrix} \bar{l}^2_{22}(x) & -\bar{l}^2_{12}(x) \\ -\bar{l}^2_{21}(x) & \bar{l}^2_{11}(x) \end{bmatrix} \times \left\{\begin{bmatrix} \bar{k}^2_1(x) \\ \bar{k}^2_2(x) \end{bmatrix} + \begin{bmatrix} \bar{c}^2_{11}(x) & \bar{c}^2_{12}(x) \\ \bar{c}^2_{21}(x) & \bar{c}^2_{22}(x) \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}\right\} \quad (32)$$

where:

$$\det(\bar{l}^2(x)) = \bar{l}^2_{11}(x)\bar{l}^2_{22}(x) - \bar{l}^2_{12}(x)\bar{l}^2_{21}(x)$$

Substitution of Eq. 32 into the differential equations of the DAE system (Eq. 26) gives the corresponding state-space realization in the form of Eq. 16:

$$\frac{dx_1}{dt} = \left\{f_1(x) - \frac{\bar{l}^2_{11}\bar{k}^2_2 - \bar{l}^2_{21}\bar{k}^2_1 - \bar{l}^2_{22}\bar{k}^2_1 + \bar{l}^2_{12}\bar{k}^2_2}{\det(\bar{l}^2)}\right\} - \{1 + t_1(x)\}u_1 + t_2(x)u_2$$

$$\frac{dx_2}{dt} = \left\{f_2(x) + \frac{(\bar{l}^2_{22}\bar{k}^2_1 - \bar{l}^2_{12}\bar{k}^2_2)(1-x_2) + (\bar{l}^2_{11}\bar{k}^2_2 - \bar{l}^2_{21}\bar{k}^2_1)x_2}{\det(\bar{l}^2)x_1}\right\} - t_3(x)u_1 - t_4(x)u_2$$

$$\frac{dx_3}{dt} = \left\{f_3(x) - \frac{\bar{l}^2_{22}\bar{k}^2_1 - \bar{l}^2_{12}\bar{k}^2_2 - \bar{l}^2_{11}\bar{k}^2_2 + \bar{l}^2_{21}\bar{k}^2_1}{\det(\bar{l}^2)}\right\} + t_1(x)u_1 - t_2(x)u_2$$

$$\frac{dx_4}{dt} = \left\{f_4(x) - \frac{(\bar{l}^2_{22}\bar{k}^2_1 - \bar{l}^2_{12}\bar{k}^2_2)(1-x_4) + (\bar{l}^2_{11}\bar{k}^2_2 - \bar{l}^2_{21}\bar{k}^2_1)x_4}{\det(\bar{l}^2)x_3}\right\} + t_5(x)u_1 + t_6(x)u_2$$

$$\frac{dx_5}{dt} = \left\{f_5(x) - \left(\frac{x_5}{\det(\bar{l}^2)x_3}\right)(\bar{l}^2_{11}\bar{k}^2_2 - \bar{l}^2_{21}\bar{k}^2_1 - \bar{l}^2_{22}\bar{k}^2_1 + \bar{l}^2_{12}\bar{k}^2_2)\right\} - \left(\frac{x_5}{x_3}\right)t_1(x)u_1 + \left(\frac{x_5}{x_3}\right)t_2(x)u_2$$

$$\frac{dx_6}{dt} = \left\{f_6(x) - \left(\frac{\Delta H^v}{(x_1+x_3)c_p\det(\bar{l}^2)}\right)(\bar{l}^2_{22}\bar{k}^2_1 - \bar{l}^2_{12}\bar{k}^2_2 - \bar{l}^2_{11}\bar{k}^2_2 + \bar{l}^2_{21}\bar{k}^2_1)\right\} + t_7(x)u_1 + \left\{\frac{1}{(x_1+x_3)c_p} + t_8(x)\right\}u_2 \quad (33)$$

where $x \in \mathfrak{M} = \{x \in \mathbb{R}^6 : \bar{k}^1_1(x) = 0,\ \bar{k}^1_2(x) = 0\}$ ($\bar{k}^1_1(x)$, $\bar{k}^1_2(x)$ are given in Eq. 30) and $t_i(x)$, $i = 1, \ldots, 8$ are nonlinear functions of the differential variables x whose specific forms are included in Appendix B.

Controller synthesis

Referring to the model of Eq. 33, it is straightforward to verify that the relative orders of the controlled outputs $y_1 = x_2$, $y_2 = x_6$ with respect to the manipulated input vector $u = [u_1\ \ u_2]^T$ are as follows:

$$r_1 = 1; \quad r_2 = 1 \quad (34)$$

and the characteristic matrix:

$$C(x) = \begin{bmatrix} -t_3(x) & -t_4(x) \\ t_7(x) & \left\{\dfrac{1}{(x_1+x_3)c_p} + t_8(x)\right\} \end{bmatrix}$$

is nonsingular. Thus, a closed-loop input/output decoupled response of the following form was requested:

$$y_1 + \gamma^1_{11}\frac{dy_1}{dt} = y_{sp1}$$
$$y_2 + \gamma^2_{21}\frac{dy_2}{dt} = y_{sp2} \quad (35)$$

According to Theorem 1, the static state feedback controller:

$$u = \left\{\begin{bmatrix} \beta^1_{11} & 0 \\ 0 & \gamma^2_{21} \end{bmatrix} C(x)\right\}^{-1} \times \begin{bmatrix} v_1 - \beta^1_{10}x_2 - \beta^1_{11}\left\{f_2(x) - \dfrac{(\bar{l}^2_{22}\bar{k}^2_1 - \bar{l}^2_{12}\bar{k}^2_2)(1-x_2) + (\bar{l}^2_{11}\bar{k}^2_2 - \bar{l}^2_{21}\bar{k}^2_1)x_2}{\det(\bar{l}^2)x_1}\right\} \\ v_2 - \beta^2_{20}x_6 - \beta^2_{21}\left\{f_6(x) + \left(\dfrac{\Delta H^v}{(x_1+x_3)c_p\det(\bar{l}^2)}\right)(\bar{l}^2_{22}\bar{k}^2_1 - \bar{l}^2_{12}\bar{k}^2_2 - \bar{l}^2_{11}\bar{k}^2_2 + \bar{l}^2_{21}\bar{k}^2_1)\right\} \end{bmatrix} \quad (36)$$

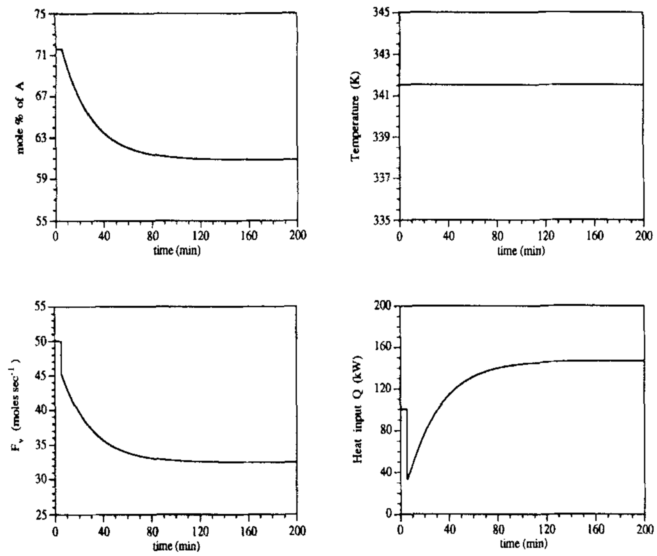

Figure 2. Closed-loop profiles of controlled outputs and manipulated inputs for a 15% decrease in the set point for mole fraction of species *A* in vapor phase.

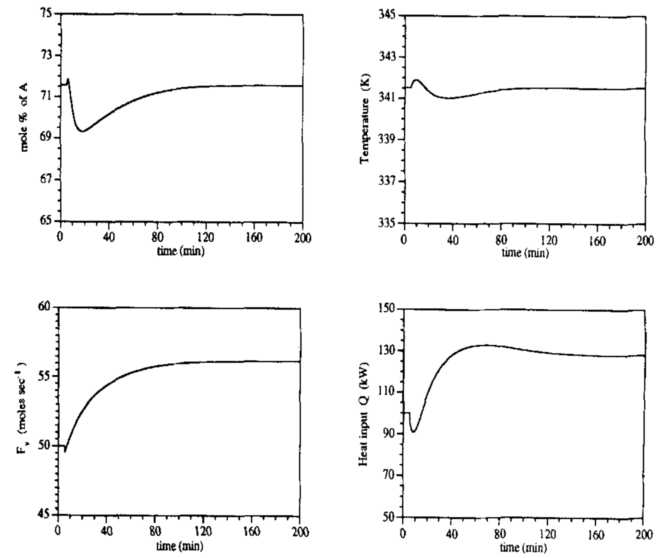

Figure 4. Closed-loop profiles of controlled outputs and manipulated inputs under a 5% increase in the inlet flow rate F_{Ao}.

induces the following linear input/output behavior:

$$\beta_{10}^1 y_1 + \beta_{11}^1 \frac{dy_1}{dt} = v_1$$

$$\beta_{20}^2 y_2 + \beta_{21}^2 \frac{dy_2}{dt} = v_2 \tag{37}$$

between the inputs $v = [v_1 \ v_2]^T$ and the outputs y.

The output feedback controller that induces the requested response of Eq. 35 subject to integral action, was derived by combining the state feedback controller of Eq. 36 with a linear error feedback controller of the form of Eq. 25 and a state observer. Following the approach of Daoutidis and Kravaris (1994), the process model (Eq. 33) was used for the purpose of state observation, given the open-loop stability of the process at the nominal equilibrium point (see Table 1). The controller was tuned by choosing the following set of parameters:

$$\beta_{10}^1 = 1.0, \quad \beta_{11}^1 = 1{,}500 \text{ s}$$

$$\beta_{10}^2 = 1.0, \quad \beta_{21}^2 = 800 \text{ s}$$

$$\gamma_{11}^1 = 1{,}500 \text{ s}, \quad \gamma_{21}^2 = 800 \text{ s}$$

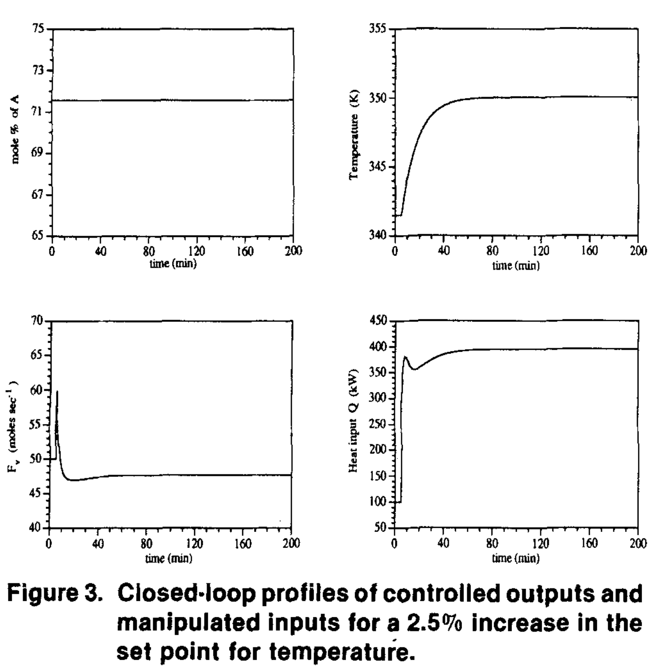

Figure 3. Closed-loop profiles of controlled outputs and manipulated inputs for a 2.5% increase in the set point for temperature.

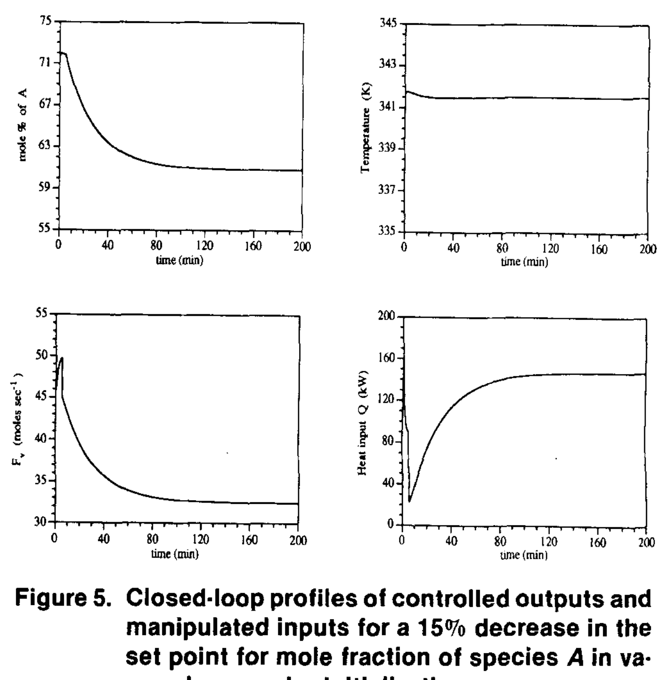

Figure 5. Closed-loop profiles of controlled outputs and manipulated inputs for a 15% decrease in the set point for mole fraction of species *A* in vapor phase under initialization error.

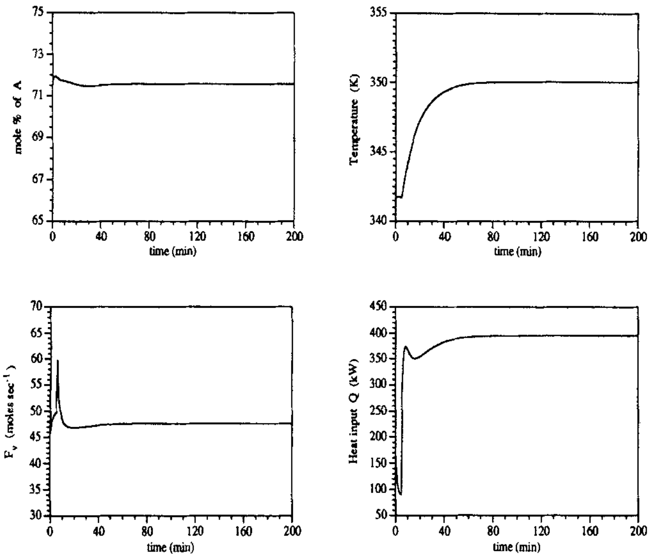

Figure 6. Closed-loop profiles of controlled outputs and manipulated inputs for a 2.5% increase in the set point for temperature under initialization error.

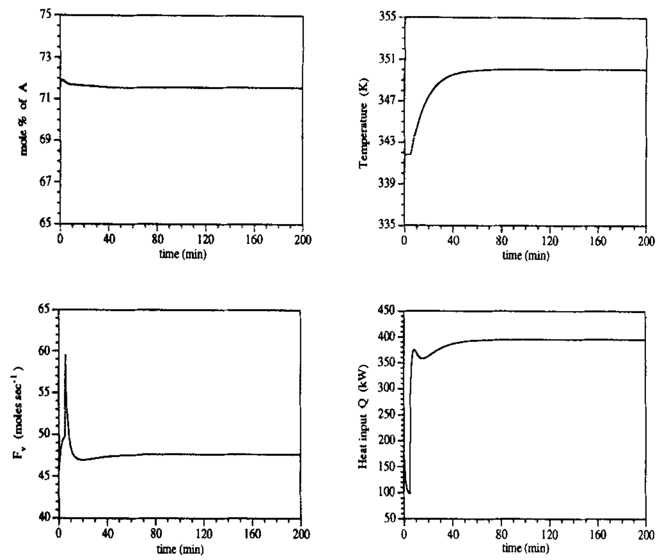

Figure 8. Closed-loop profiles of controlled outputs and manipulated inputs for a 2.5% increase in the set point for temperature under parametric uncertainties.

Discussion of controller performance

The set point tracking and disturbance rejection capabilities of the controller were evaluated through simulations.

The first two simulation runs addressed the set point tracking capabilities of the controller. In the first run, the process, which initially was at its nominal steady state, was subjected to a 15% decrease in y_{sp1}, or equivalently, an increase in the desired mole fraction of the product C in the vapor phase, at time $t=5$ min. The corresponding closed-loop profiles are shown in Figure 2. Clearly, the controller enforced the requested first-order response for y_1, while maintaining y_2 at its nominal value.

In the second run, the process was subjected to a 2.5% increase in y_{sp2}, that is, an increase in the desired reactor temperature T, at time $t=5$ min. Again, the controller induced the requested first-order response for y_2, while maintaining y_1 at its nominal value. The output and manipulated input profiles are shown in Figure 3.

The third run addressed the disturbance rejection capabilities of the controller. The process at its nominal steady state was subjected to an unmeasured 5% increase in the vapor stream inlet flow rate F_{Ao} at time $t=5$ min. It can be seen from the

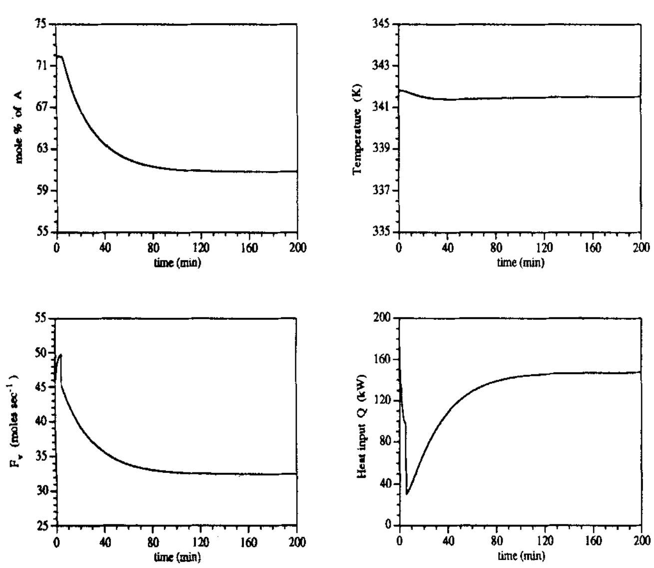

Figure 7. Closed-loop profiles of controlled outputs and manipulated inputs for a 15% decrease in the set point for mole fraction of species *A* in vapor phase under parametric uncertainties.

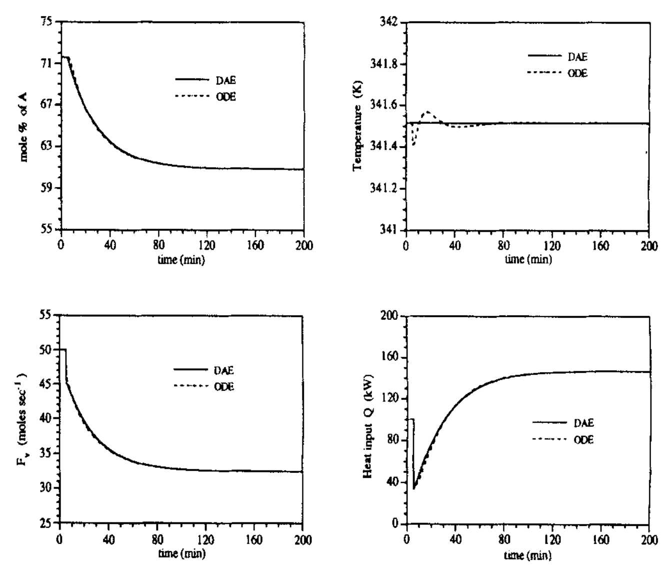

Figure 9. Comparison of closed-loop profiles of outputs and inputs for a 15% decrease in the set point for mole fraction of *A* in vapor phase under DAE- and ODE-based controllers.

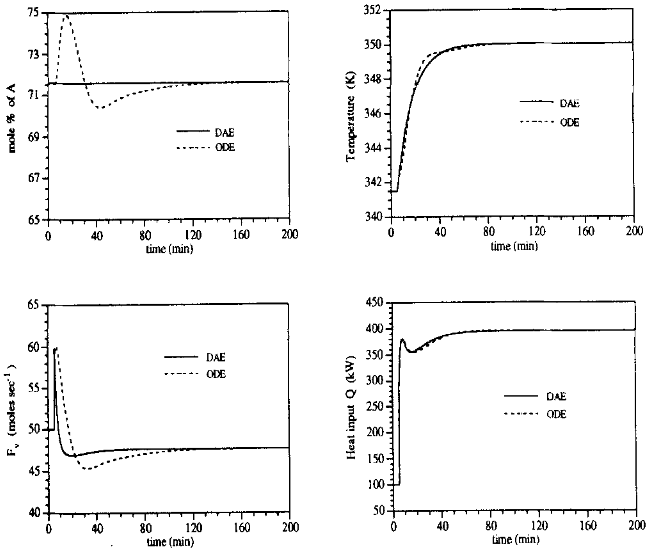

Figure 10. Comparison of closed-loop profiles of outputs and inputs for a 2.5% increase in the set point for temperature under DAE- and ODE-based controllers.

closed-loop profiles in Figure 4 that the two outputs return smoothly to their respective set points, after initial deviations.

In the next two runs, the set point tracking capability of the controller in the presence of initialization errors was studied. The observer state corresponding to the liquid holdup N_L was subjected to a 5% initialization error, and a 15% decrease in y_{sp1} was imposed at time $t=5$ min. Figure 5 includes the corresponding closed-loop profiles. Figure 6 shows the closed-loop profiles when a 2.5% increase in y_{sp2} was imposed at $t=5$ min, under the same initialization error. As expected, the profiles depict a slight initial deterioration of the controller performance with the overall performance being very satisfactory.

The performance of the controller under modeling errors was also studied. Figure 7 shows the closed-loop profiles when a 15% decrease in y_{sp1} was imposed at $t=5$ min under 5% errors in the values of molar heat capacity c_p and molar density ρ in the liquid phase. Figure 8 shows the closed-loop profiles for the same parametric uncertainties, when a 2.5% increase in y_{sp2} was imposed at $t=5$ min. Despite these parametric uncertainties, the controller provided very good closed-loop responses.

The subsequent runs compare the performance of the nonlinear output feedback controller based on the DAE model (Eq. 26) with that of a nonlinear output feedback controller based on the simplified ODE model of Eq. 28. Figure 9 shows the respective plots for the two controllers when the process was subjected to a 15% decrease in y_{sp1} at time $t=5$ min. The ODE-based controller provides a good response for y_1, but it does not provide the decoupled response as requested. In Figure 10, the closed-loop profiles for both controllers are shown for a 2.5% increase in y_{sp2}. Clearly, the performance of the ODE-based controller has deteriorated significantly compared to the DAE-based controller. While, the DAE-based controller provides the smooth, decoupled responses as requested, the closed-loop output profiles for the ODE-based controller show significant deviations in y_1 and oscillations in y_2, thus demonstrating the superiority of the DAE-based controller over the ODE-based one.

Conclusions

In this article, we presented a systematic feedback controller synthesis framework for a broad class of nonlinear MIMO DAE systems in semiexplicit form. The coupled differential and algebraic equations in such systems do not constitute a standard state-space description, suitable for analysis and controller synthesis. For this reason, an algorithmic procedure was initially developed for the derivation of equivalent state-space realizations for such systems. The procedure entails the reconstruction of the algebraic variables and the specification of algebraic constraints among the differential variables imposed by the algebraic equations. An output feedback control methodology that achieves desired closed-loop characteristics was then developed, through combination of state feedback and state observers. The developed control methodology was applied to a two-phase reactor modeled by an index-two DAE system with excellent servo and regulatory performance.

Acknowledgment

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Notation

b, g, l = matrices in the DAE model
E^i = $p \times p$ nonsingular matrices
f, k = vector fields in the DAE model
$\bar{f}$ = vector field in state-space realization of dimension n
$\bar{g}$ = matrix in state-space realization of dimension n
$\bar{k}^i, \hat{k}^i, \tilde{k}^i$ = vector fields in the algorithm
$\bar{l}^i, \tilde{l}^i, \bar{c}^i, \tilde{c}^i$ = matrices in the algorithm
h_i = scalar fields in the DAE model
m = number of manipulated inputs and controlled outputs
$\mathfrak{M}$ = constrained manifold where differential variables evolve
n = number of differential variables
p = number of algebraic variables
p_i = ranks of matrices in the algorithm
s = number of iterations for convergence of algorithm
y_{sp} = vector of output set points

Greek letters

β_{ij}, γ_{ij} = vectors of adjustable parameters
ζ = vector of state variables in transformed coordinates
ξ = vector of states of linear error feedback controller
ϕ_i = scalar fields for coordinate transformation

Math symbols

$\mathbb{R}$ = real line
$\mathbb{R}^i$ = i-dimensional Euclidean space
T = transpose
$L_f k$ = Lie derivative of a scalar field k with respect to vector field f

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Appendix A

Proof of proposition 1

Consider a DAE system (Eq. 1) for which the algorithm converges after s iterations, that is, $p_{s+1}=p$. The aim is to prove that the $\Sigma_{i=1}^{s}(p-p_i)$ scalar fields $\hat{k}_j^i(x)$, $i=1,\ldots,s$; $j=1,\ldots,(p-p_i)$ are linearly independent. The scalar fields $\hat{k}_j^i(x)$ are said to be linearly independent if the corresponding gradient vector fields:

$$d\hat{k}_j^i(x)=\left[\frac{\partial \hat{k}_j^i(x)}{\partial x_1}\cdots\frac{\partial \hat{k}_j^i(x)}{\partial x_n}\right]$$

are linearly independent (Kravaris and Kantor, 1990a). Similarly, a scalar field $\lambda_0(x)$ will be said to be linearly dependent on scalar fields $\lambda_1(x),\ldots,\lambda_s(x)$ if the vector field $d\lambda_0(x)$ is linearly dependent on the vector fields $d\lambda_1(x),\ldots,d\lambda_s(x)$.

A proof will be given following an inductive procedure similar to that of Silverman (1969). The key idea of the proof is to show that if, for any iteration q, a scalar field $\hat{k}_r^q(x)$ is linearly dependent on the scalar fields $\hat{k}_1^1(x),\ldots,\hat{k}_{p-p_1}^1(x)$, $\ldots,\hat{k}_1^q(x),\ldots,\hat{k}_{r-1}^q(x),\hat{k}_{r+1}^q(x),\ldots,\hat{k}_{p-p_q}^q(x)$, then:

(*i*) $p_{q+1}<p$; and

(*ii*) There exists a scalar field $\hat{k}_r^{q+1}(x)$ in iteration $q+1$, which is linearly dependent on the scalar fields $\hat{k}_1^1(x),\ldots,\hat{k}_{p-p_1}^1(x),\ldots,\hat{k}_1^{q+1}(x),\ldots,\hat{k}_{r-1}^{q+1}(x),\hat{k}_{r+1}^{q+1}(x),\ldots,\hat{k}_{p-p_{q+1}}^{q+1}(x)$, thereby implying by induction that $p_{s+1}<p$, which clearly is a contradiction.

Let iteration q be the first iteration when a scalar field $\hat{k}_r^q(x)\in\{\hat{k}_1^q(x),\ldots,\hat{k}_{p-p_q}^q(x)\}$ is linearly dependent on the remaining scalar fields in the set:

$$\mathcal{K}^q(x)=\left\{\begin{matrix}\hat{k}_1^1(x),\ldots,\hat{k}_{p-p_1}^1(x),\\ \hat{k}_1^2(x),\ldots,\hat{k}_{p-p_2}^2(x),\\ \vdots\\ \hat{k}_1^q(x),\ldots,\hat{k}_{r-1}^q(x),\hat{k}_{r+1}^q(x),\ldots,\hat{k}_{p-p_q}^q(x)\end{matrix}\right\}$$

Define the following two disjoint subsets of scalar fields:

$$\mathfrak{K}^{q,I}(x) = \{\hat{k}_j^i(x) \in \mathfrak{K}^q(x) : d\hat{k}_j^i(x)b(x) \text{ is a row of the matrix } L^q(x)\}$$

$$\mathfrak{K}^{q,II}(x) = \{\hat{k}_j^i(x) \in \mathfrak{K}^q(x) : d\hat{k}_j^i(x)b(x) \text{ is a linear combination of the rows of } L^q(x)\}$$

where:

$$L^q(x) = \begin{bmatrix} \bar{l}^1(x) \\ \vdots \\ \bar{l}^{q+1}(x) \end{bmatrix}$$

Furthermore, define the vector fields $\hat{K}^{q,I}(x)$, $\hat{K}^{q,II}(x)$ comprising of the scalar fields in the sets $\mathfrak{K}^{q,I}(x)$, and $\mathfrak{K}^{q,II}(x)$, respectively, such that:

$$L^q(x) = \begin{bmatrix} \bar{l}^1(x) \\ d\hat{K}^{q,I}(x)b(x) \end{bmatrix}$$

Then, owing to the linear dependence of the scalar field $\hat{k}_r^q(x)$ on the scalar fields in the set $\mathfrak{K}^q(x)$, there exist row vectors $R_1(x)$ and $R_2(x)$ such that:

$$d\hat{k}_r^q(x) = R_1(x)d\hat{K}^{q,I}(x) + R_2(x)d\hat{K}^{q,II}(x) \tag{38}$$

Moreover, by the definition of the two subsets $\mathfrak{K}^{q,I}(x)$, $\mathfrak{K}^{q,II}(x)$ and the assumption on the rank of the augmented matrix in the algorithm, there exists a matrix $S_1(x)$ such that:

$$d\hat{K}^{q,II}(x)b(x) = S_1(x)\begin{bmatrix} \bar{l}^1(x) \\ d\hat{K}^{q,I}(x)b(x) \end{bmatrix} = S_1(x)L^q(x)$$

$$d\hat{K}^{q,II}(x)g(x) = S_1(x)\begin{bmatrix} 0 \\ d\hat{K}^{q,I}(x)g(x) \end{bmatrix} \tag{39}$$

From Eq. 38 and Eq. 39, it follows that:

$$\bar{l}_r^{q+1}(x) = d\hat{k}_r^q(x)b(x) = R_1(x)d\hat{K}^{q,I}(x)b(x) + R_2(x)S_1(x)L^q(x) \tag{40}$$

proving that the row vector $\bar{l}_r^{q+1}(x)$ is linearly dependent on the rows of the matrix $L^q(x)$, that is, $p_{q+1}<p$.

The relation in Eq. 40 implies that in step 1 of iteration $q+1$, the row vector $\bar{l}_r^{q+1}(x)$ and the row vector $\bar{c}_r^{q+1}(x) = d\hat{k}_r^q(x)g(x)$ can be reduced to zero through elementary row operations. Under the requisite row operation, the corresponding algebraic constraint:

$$0 = \hat{k}_r^{q+1}(x) = \{d\hat{k}_r^q(x)f(x) - R_1(x)d\hat{K}^{q,I}(x)f(x)\} - R_2(x)S_1(x)\begin{bmatrix} \bar{k}^1(x) \\ d\hat{K}^{q,I}(x)f(x) \end{bmatrix}$$

$$= R_2(x)d\hat{K}^{q,II}(x)f(x) - R_2(x)S_1(x)\begin{bmatrix} \bar{k}^1(x) \\ d\hat{K}^{q,I}(x)f(x) \end{bmatrix} \tag{41}$$

is obtained. Also, by definition, the $p_{q+1}\times p$ matrix $L^q(x)$ has full row rank, which implies that there exists a matrix:

$$L^{q^\dagger}(x) = L^{q^T}(x)[L^q(x)L^{q^T}(x)]^{-1}$$

such that $L^q(x)L^{q\dagger}(x) = I_{p_{q+1}}$. Thus, from Eq. 39 it follows that:

$$R_2(x)S_1(x) = R_2(x)d\hat{K}^{q,II}(x)b(x)L^{q^\dagger}(x)$$

Substituting the above relations for $R_2(x)S_1(x)$ in Eq. 41 the following relation is obtained:

$$\hat{k}_r^{q+1}(x) = R_2(x)d\hat{K}^{q,II}(x) \times \left\{ f(x) - b(x)L^{q^\dagger}(x)\begin{bmatrix} \bar{k}^1(x) \\ d\hat{K}^{q,I}(x)f(x) \end{bmatrix} \right\} \tag{42}$$

Furthermore, consider the matrix:

$$d\hat{k}^{q,II}(x)b(x) = \begin{bmatrix} d\hat{k}_1^{q,II}(x)b(x) \\ \vdots \\ d\hat{k}_{r-1}^{q,II}(x)b(x) \\ d\hat{k}_{r+1}^{q,II}(x)b(x) \\ \vdots \\ d\hat{k}_{p-p_{q+1}}^{q,II}(x)b(x) \end{bmatrix}$$

with its rows linearly dependent on the rows of $L^q(x)$, by the definition of the set $\mathfrak{K}^q(x)$. Then, there exists a matrix $\gamma^q(x)$ such that:

$$d\hat{k}^{q,II}(x)b(x) = \gamma^q(x)L^q(x)$$

Clearly,

$$\gamma^q(x) = d\hat{k}^{q,II}(x)b(x)L^{q\dagger}(x)$$

Thus, the rows of $d\hat{k}^{q,II}(x)b(x)$ (and correspondingly the rows of $d\hat{k}^{q,II}(x)g(x)$) can be reduced to zero through row operations in step 1 of iteration $q+1$, yielding the remaining $p-p_{q+1}-1$ algebraic constraints (besides the constraint in Eq. 41):

$$0 = \begin{bmatrix} \hat{k}_1^{q+1}(x) \\ \vdots \\ \hat{k}_{r-1}^{q+1}(x) \\ \hat{k}_{r+1}^{q+1}(x) \\ \vdots \\ \hat{k}_{p-p_{q+1}}^{q+1}(x) \end{bmatrix} = d\hat{k}^{q,II}(x)f(x) - \gamma^q(x)\begin{bmatrix} \bar{k}^1(x) \\ d\hat{K}^{q,I}(x)f(x) \end{bmatrix}$$

$$= d\hat{k}^{q,II}(x)\left\{ f(x) - b(x)L^{q^\dagger}(x)\begin{bmatrix} \bar{k}^1(x) \\ d\hat{K}^{q,I}(x)f(x) \end{bmatrix} \right\} \tag{43}$$

From the relations in Eq. 42 and Eq. 43, and the definition of $\hat{K}^{q,II}(x)$ it follows that:

$$\hat{k}_r^{q+1}(x) = R_2(x)\alpha^{q+1}(x) = \sum_{i=1}^{\kappa} R_{2,i}(x)\alpha_i^{q+1}(x) \tag{44}$$

where $\alpha^{q+1}(x) = [\alpha_1^{q+1}(x) \cdots \alpha_\kappa^{q+1}(x)]^T$ such that:

$$\alpha_i^{q+1}(x) \in \hat{\mathcal{K}}^{q+1}(x)$$

and $R_{2,i}(x)$ is the ith component of the row vector $R_2(x)$.

Claim. The gradient vectors $dR_{2,i}(x)$ are linearly dependent on the row vectors of $d\hat{K}^{q+1,I}(x)$ and $d\hat{K}^{q+1,II}(x)$.

If the above claim is true, then it is straightforward to verify that the gradient vector $d\hat{k}_r^{q+1}(x)$ is linearly dependent on the row vectors of $d\hat{K}^{q+1,I}(x)$, $d\hat{K}^{q+1,II}(x)$, that is, the scalar field $\hat{k}_r^{q+1}(x)$ is linearly dependent on the scalar fields in the set $\hat{\mathcal{K}}^{q+1}(x)$. Thus, the whole argument can be repeated for iteration $(q+1)$ implying that $p_{q+2}<p$. By induction, it can then be shown that $p_{s+1}<p$, leading to a contradiction.

Proof of Claim. Consider the relation in Eq. 38. Without loss of generality, it is assumed that the scalar fields in the sets $\hat{\mathcal{K}}^{q,I}(x)$ and $\hat{\mathcal{K}}^{q,II}(x)$ are linearly independent. If there are some scalar fields in the set $\hat{\mathcal{K}}^{q,II}(x)$ that are linearly dependent on the others, then the corresponding component of $R_2(x)$ will be identically equal to zero. Let $\mu = \mu_1 + \mu_2$, where μ_1, μ_2 denote the number of scalar fields in the sets $\hat{\mathcal{K}}^{q,I}(x)$ and $\hat{\mathcal{K}}^{q,II}(x)$, respectively. Then it is always possible to find $n-\mu$ scalar fields $\psi_1(x), \ldots, \psi_{n-\mu}(x)$ which together with the scalar fields in the sets $\hat{\mathcal{K}}^{q,I}(x)$ and $\hat{\mathcal{K}}^{q,II}(x)$ comprise a set of n linearly independent scalar fields, thus, qualifying for a nonlinear coordinate transformation. Consider such a coordinate transformation:

$$\zeta = \begin{bmatrix} \zeta_1 \\ \vdots \\ \zeta_{\mu_1} \\ \zeta_{\mu_1+1} \\ \vdots \\ \zeta_\mu \\ \zeta_{\mu+1} \\ \vdots \\ \zeta_n \end{bmatrix} = \begin{bmatrix} \hat{k}_1^{q,I}(x) \\ \vdots \\ \hat{k}_{\mu_1}^{q,I} \\ \hat{k}_1^{q,II}(x) \\ \vdots \\ \hat{k}_{\mu_2}^{q,II}(x) \\ \psi_1(x) \\ \vdots \\ \psi_{n-\mu}(x) \end{bmatrix}$$

In the new coordinates ζ, the row vectors $d\hat{k}_i^{q,I}(\zeta)$ take the form $[0 \cdots 0\ 1\ 0 \cdots 0]$ with the nonzero entry 1 in the ith position, while the row vectors $d\hat{k}_i^{q,II}(\zeta)$ take the form $[0 \cdots 0\ 1\ 0 \cdots 0]$ with the nonzero entry 1 in the (μ_1+i)th position. Clearly, the row vector $d\hat{k}_r^q(\zeta)$ must have the form $[* \cdots *\ 0 \cdots 0]$, that is, only the first μ entries can be nonzero (denoted by $*$). Thus, it follows that $(\partial R_{2,j}(\zeta)/\partial \zeta_l) \equiv 0, j=1, \ldots, \mu_2; l=(\mu+1), \ldots, n$ which implies that the gradient vectors $dR_{2,j}(\zeta)$ must be linearly dependent on the row vectors of $d\hat{K}^{q,I}(\zeta)$ and $d\hat{K}^{q,II}(\zeta)$, completing the proof of the claim.

Proof of proposition 2

The algebraic constraints of Eq. 13 identified by the proposed algorithmic procedure directly imply that the algebraic variables z vary according to the relation of Eq. 14. It is then straightforward to show that for a set of initial conditions $x(0)$ such that $\hat{k}_j^i(x(0))=0$; $i=1, \ldots, s$; $j=1, \ldots, (p-p_i)$, and z satisfying Eq. 14, the algebraic constraints of Eq. 15 and Eq. 6 are satisfied and the differential variables x evolve on $\mathfrak{M}$. A direct substitution of Eq. 14 in the differential equations of Eq. 5 yields the state-space realization of the constrained system given by Eq. 16, completing the proof of the proposition.

Proof of proposition 3

Consider the state-scape realization of Eq. 18 of the constrained process where, $x(t) \in \mathfrak{M}$, that is, $\hat{k}_j^i(x(t))=0$; $i=1, \ldots, s$; $j=1, \ldots, (p-p_i)$. In the transformed coordinates ζ, the condition $x(t)\in\mathfrak{M}$ implies that the variables $\zeta_j^{(i)}$; $i=1, \ldots, s$; $j=1, \ldots, (p-p_i)$ are identically zero, which directly leads to the state-space realization of Eq. 19.

Proof of theorem 1

Consider the DAE system of Eq. 1 which, under the control law of Eq. 24, yields the following closed-loop DAE system:

$$\begin{aligned} \dot{x} &= f(x) + b(x)z + g(x)\{[\beta_{1r_1} \cdots \beta_{mr_m}]C(x)\}^{-1} \times \left(v - \sum_{i=1}^{m}\sum_{j=0}^{r_i} \beta_{ij}L_f^j h_i(x)\right) \\ 0 &= k(x) + l(x)z \\ y_i &= h_i(x);\ i=1, \ldots, m \end{aligned} \tag{45}$$

A state-space realization for the closed-loop DAE system of Eq. 45 can be obtained following the algorithmic procedure proposed earlier. It is straightforward to show that the algorithmic procedure converges after exactly s iterations, identifying the same algebraic constraints among x (Eq. 15) and yielding the following relation for z:

$$z = -\begin{bmatrix} \bar{l}^1(x) \\ \bar{l}^2(x) \\ \vdots \\ \bar{l}^2(x) \\ \bar{l}^{s+1}(x) \end{bmatrix}^{-1} \begin{bmatrix} \bar{k}^1(x) \\ \bar{k}^2(x) \\ \vdots \\ \bar{k}^s(x) \\ \bar{k}^{s+1}(x) \end{bmatrix} + \begin{bmatrix} 0 \\ \bar{c}^2(x) \\ \vdots \\ \bar{c}^2(x) \\ \bar{c}^{s+1}(x) \end{bmatrix} \times \{[\beta_{1r_1} \cdots \beta_{mr_m}]C(x)\}^{-1}\left(v - \sum_{i=1}^{m}\sum_{j=0}^{r_i}\beta_{ij}L_f^j h_i(x)\right)\Bigg\} \tag{46}$$

Thus, the state-space realization of the closed-loop dynamics takes the form:

$$\begin{aligned} \dot{x} &= \bar{f}(x) + \bar{g}(x)C^{-1}(x)[\beta_{1r_1} \cdots \beta_{mr_m}]^{-1} \times \left\{v - \sum_{i=1}^{m}\sum_{j=0}^{r_i}\beta_{ij}L_f^j h_i(x)\right\} \\ y_i &= h_i(x);\ i=1, \ldots, m \end{aligned} \tag{47}$$

where $x \in \mathfrak{M}$ and $\bar{f}(x)$, $\bar{g}(x)$ are defined in Eq. 16. Calculating the expressions for the derivatives of the outputs, that is, $d^j y_i / dt^j$, $i=1, \ldots, m$; $j=1, \ldots, r_i$, on the basis of Eq. 47 and substituting in Eq. 23, it is then straightforward to show that the input/output behavior of Eq. 23 is indeed enforced.

Appendix B

This section includes a detailed description of the terms involved in the state-space representation of the DAE system of Eq. 26 and the resulting feedback controller:

$$\tilde{k}_1^2 = -\beta_1[f_1(x) + \beta_2 f_3(x)] + P_A^s f_4(x) + \gamma_1(x_1+x_3) f_6(x)$$

$$\tilde{k}_2^2 = -\beta_1\beta_2\left(\frac{1-x_2}{x_2}\right) f_3(x) - P_C^s[f_4(x) + f_5(x)] + \gamma_2(x_1+x_3) f_6(x)$$

$$\tilde{l}_{11}^2 = \beta_1(1-\beta_2) + P_A^s\left(\frac{1-x_4}{x_3}\right) + \gamma_1\left(\frac{\Delta H^v}{c_p}\right)$$

$$\tilde{l}_{12}^2 = \beta_1\beta_2 + P_A^s\left(\frac{x_4}{x_3}\right) - \gamma_1\left(\frac{\Delta H^v}{c_p}\right)$$

$$\tilde{l}_{21}^2 = \gamma_2\left(\frac{\Delta H^v}{c_p}\right) - \beta_1\beta_2\left(\frac{1-x_2}{x_2}\right) - P_C^s\left(\frac{1-x_4-x_5}{x_3}\right)$$

$$\tilde{l}_{22}^2 = \beta_1\left[-1 + \left(\frac{\beta_2(1-x_2)}{x_2}\right)\right] - P_C^s\left(\frac{x_4+x_5}{x_3}\right) - \gamma_2\left(\frac{\Delta H^v}{c_p}\right)$$

$$\tilde{c}_{11}^2 = \beta_1 x_2$$

$$\tilde{c}_{12}^2 = \frac{\gamma_1}{c_p}$$

$$\tilde{c}_{21}^2 = \beta_1(1-x_2)$$

$$\tilde{c}_{22}^2 = \frac{\gamma_2}{c_p}$$

$$t_1(x) = -\left(\frac{\beta_1}{\det(\tilde{l}^2)}\right)[(\tilde{l}_{11}^2 + \tilde{l}_{12}^2 + \tilde{l}_{21}^2 + \tilde{l}_{22}^2)x_2 - \tilde{l}_{12}^2 - \tilde{l}_{11}^2]$$

$$t_2(x) = -\left(\frac{1}{c_p \det(\tilde{l}^2)}\right)[(\tilde{l}_{11}^2 + \tilde{l}_{12}^2)\gamma_2 - (\tilde{l}_{21}^2 + \tilde{l}_{22}^2)\gamma_1]$$

$$t_3(x) = -\left(\frac{\beta_1}{x_1 \det(\tilde{l}^2)}\right)[\{(\tilde{l}_{22}^2 + \tilde{l}_{12}^2)x_2 - \tilde{l}_{12}^2\}(1-x_2) + \{\tilde{l}_{11}^2 - (\tilde{l}_{21}^2 + \tilde{l}_{11}^2)x_2\}x_2]$$

$$t_4(x) = -\left(\frac{1}{x_1 c_p \det(\tilde{l}^2)}\right)[(\tilde{l}_{22}^2\gamma_1 - \tilde{l}_{12}^2\gamma_2)(1-x_2) + (\tilde{l}_{11}^2\gamma_2 - \tilde{l}_{21}^2\gamma_1)x_2]$$

$$t_5(x) = -\left(\frac{\beta_1}{x_3 \det(\tilde{l}^2)}\right)[\{(\tilde{l}_{22}^2 + \tilde{l}_{12}^2)x_2 - \tilde{l}_{12}^2\}(1-x_4) + \{\tilde{l}_{11}^2 - (\tilde{l}_{21}^2 + \tilde{l}_{11}^2)x_2\}x_4]$$

$$t_6(x) = -\left(\frac{1}{x_3 c_p \det(\tilde{l}^2)}\right)[(\tilde{l}_{22}^2\gamma_1 - \tilde{l}_{12}^2\gamma_2)(1-x_4) + (\tilde{l}_{11}^2\gamma_2 - \tilde{l}_{21}^2\gamma_1)x_4]$$

$$t_7(x) = t_1(x)\left(\frac{\Delta H^v}{(x_1+x_3)c_p}\right)$$

$$t_8(x) = -t_2(x)\left(\frac{\Delta H^v}{(x_1+x_3)c_p}\right)$$

where

$$\beta_1 = \frac{\rho R x_6}{V_T\rho - x_3}$$

$$\beta_2 = \frac{x_1 x_2}{V_T\rho - x_3}$$

$$\gamma_1 = \left(\frac{1}{x_1+x_3}\right)\left[\frac{3,919.7}{(x_6-34.1)^2} P_A^s x_4 - \rho R \beta_2\right]$$

$$\gamma_2 = \left(\frac{1}{x_1+x_3}\right)\left[\frac{5,000}{(x_6+70)^2} P_C^s(1-x_4-x_5) - \left(\frac{\beta_2(1-x_2)\rho R}{x_2}\right)\right]$$

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