

Nonlinear Model Reduction of Differential Algebraic Equation (DAE) Systems

Chuli Sun and Juergen Hahn

Department of Chemical Engineering

Texas A&M University

College Station, TX 77843-3122

hahn@tamu.edu

**Prepared for presentation at the 2004 Annual Meeting, Austin, TX,
November 7-12**

Copyright © Chuli Sun and Juergen Hahn

November, 2004

Unpublished

AICHE shall not be responsible for statements or opinions contained in papers
or printed in its publications

Abstract

Most process models resulting from first principles consist of not only nonlinear differential equations but also contain nonlinear algebraic equations, resulting in nonlinear DAE systems. Since large-scale nonlinear DAE systems are too complex to be used for real-time optimization or control, model reduction of these types of models is a strategy that needs to be applied for online applications. However, in the past, model reduction techniques mainly focused on differential equations, and no general model reduction methods specifically geared towards reducing DAE systems have been proposed. Since in most cases, the number of algebraic equations by far exceeds the number of differential equations, it is insufficient to simply reduce the differential equations by conventional methods (POD, balancing, etc.) and leave the rest of the model intact.

This paper presents a novel technique for reducing nonlinear DAE systems. This method can reduce both the order of the model by eliminating some of the differential equations as well as the number and complexity of the algebraic equations. This is achieved by a 3-step approach: 1) performing order reduction of the differential equations and algebraic equations; 2) identifying correlation in the variables that connect the retaining differential equations to the algebraic ones; 3) reduction of the “input-output” behavior of the algebraic equations via system identification techniques.

This procedure has the advantages over other methods in that it addresses both reduction of the algebraic and the differential equations and that it results in a system where the algebraic equations can be represented by a feedforward neural network. This last property is important insofar as the reduced model does not require a DAE solver for its solution but can instead be computed by regular ODE solvers.

A more detailed description of the model reduction procedure is provided next: in a first step, the controllability and observability covariance matrices for the differential variables are computed. While a controllability covariance matrix can be computed for the algebraic as well as the differential variables, it is important to point out that the information contained in this matrix is only meaningful for the description of the input-to-state behavior of the differential equations. At the same time the covariance matrix can be used to determine the relationship between the algebraic variables. Since algebraic variables have no dynamics, the perturbation on the algebraic variables cannot introduce output responses which are not already reflected in the perturbation of the differential states. Therefore describing a state-to-output behavior for the algebraic variables is not meaningful. In a second step, balancing is applied to compute the state transformation matrix for the differential variables; and singular value decomposition is applied to determine the degree of correlation between the algebraic variables. The two transformation matrices obtained from these computations can then be applied to the system. The resulting model still has the same order and identical input-output behavior to the original system. However, it has the advantage that it can easily be determined how much a model can be reduced without losing the important parts for the input-output behavior of the system. The model reduction itself is performed by balanced truncation or residualization for the differential equations and by replacing the algebraic equations with an explicit expression obtained from system identification. Feedforward neural networks are used in this work for the reduction of the algebraic equations.

This technique is illustrated with a case study. The behavior of reduced-order models of a distillation column with 32 differential equations and 32 algebraic equations is compared.

1. Introduction

Most process models derived from first principles consist of differential as well as algebraic equations, resulting in differential-algebraic equation (DAE) systems [1, 2]. Models described by DAE systems are often of high order resulting in difficulties for online control due to the extensive computational effort. Reducing the size of the model while retaining important system properties for controller design is the main goal of control-relevant model reduction.

This paper presents a new technique for reducing nonlinear DAE systems for controller design. The method reduces both the order of the model by eliminating differential equations as well as the number and complexity of the algebraic equations. This technique addresses both reduction of the algebraic and the differential equations and results in a system where the algebraic equations can be represented by an explicit expression, e.g., a feedforward neural network. This last property is important insofar as the reduced model does not require a DAE solver for its solution but can instead be computed by regular ODE solvers.

2. Model reduction of DAE systems

The work presented in this paper focuses on DAE systems of the following form

$$\begin{aligned}\dot{x} &= f(x, z, u) \\ 0 &= g(x, z) \\ y &= h(x)\end{aligned}\tag{1}$$

The reduction is performed by first determining state transformations that transform the system into a form appropriate for model reduction which is then followed by a truncation/system identification procedure.

2.1. Computation of transformations

For ordinary differential equation (ODE) systems, the procedure of computing the transformation matrix via balancing of controllability and observability covariance matrices was presented in Hahn and Edgar [3]. However, since algebraic equations do not represent dynamic behavior, it is not meaningful to compute the controllability and observability covariance matrices for the entire systems (differential states and algebraic variables). Therefore, a modified version of the balancing procedure is presented for application to DAE systems: (1) the system is originally at steady state and is then excited by changes in the inputs along the lines of the computation procedure for the controllability covariance matrix; data are collected along the trajectories generated by these excitations and a covariance matrix

$$W = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}, \quad \begin{aligned} W_{11} &\in \mathfrak{R}^{d \times d}, & W_{12} &\in \mathfrak{R}^{d \times (n-d)}, \\ W_{21} &\in \mathfrak{R}^{(n-d) \times d}, & W_{22} &\in \mathfrak{R}^{(n-d) \times (n-d)}. \end{aligned}\tag{2}$$

is computed, where W_{11} is equal to W_C , the controllability covariance matrix of the differential states and W_{22} is the covariance matrix of the algebraic variables; (2) the observability covariance matrix, W_O , is computed for states described by the differential equations; (3) the transformation T_1 for the states, x , is computed from balancing W_C and W_O ; (4) a singular value decomposition of W_{22}

$$W_{22} = U_2 \Sigma_2 V_2^*\tag{3}$$

is used to compute the transformation T_2 for the algebraic variables, z , where $T_2 = U_2$.

2.2. Transformed system

Transformations T_1 and T_2

$$\begin{aligned} \bar{x} = T_1 x \Rightarrow x = T_1^{-1} \bar{x} & \quad \bar{z} = T_2 z \Rightarrow z = T_2^{-1} \bar{z} \\ x, \bar{x} \in \mathfrak{R}^d & \quad z, \bar{z} \in \mathfrak{R}^{n-d} \end{aligned} \quad (4)$$

can be applied to the original model (equation (1)) resulting in the transformed system

$$\begin{aligned} \dot{\bar{x}} &= T_1 f(T_1^{-1} \bar{x}, T_2^{-1} \bar{z}, u) = \bar{f}(\bar{x}, \bar{z}, u) \\ 0 &= g(T_1^{-1} \bar{x}, T_2^{-1} \bar{z}) = \bar{g}(\bar{x}, \bar{z}) \\ y &= h(T_1^{-1} \bar{x}) = \bar{h}(\bar{x}) \end{aligned} \quad (5)$$

where \bar{f} , \bar{g} , \bar{h} represent nonlinear functions of the transformed system. This transformed system has the same number of differential and algebraic equations as the original system and identical input-output behavior. However, the differential states as well as the algebraic variables are ordered in descending order with their importance to the control-relevant behavior of the model. Essentially, the system (5) is in a set of coordinates suitable for reducing the size of the model.

2.3. Order reduction of differential and algebraic equations

Once the system is transformed into a form suitable for model reduction, the number of differential equations and algebraic equations are reduced by truncation, resulting in

$$\begin{aligned} \dot{\bar{x}}_1 &= P_1 \bar{f}(\bar{x}, \bar{z}, u) \\ \bar{x}_2 &= \bar{x}_{2,ss} \\ 0 &= P_2 \bar{g}(\bar{x}, \bar{z}) \\ \bar{z}_2 &= \bar{z}_{2,ss} \\ y &= \bar{h}(\bar{x}) \end{aligned} \quad , \quad \bar{x} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix}, \quad P_1 = [I_{k \times k} \quad 0] \\ \bar{z} = \begin{bmatrix} \bar{z}_1 \\ \bar{z}_2 \end{bmatrix}, \quad P_2 = [I_{m \times m} \quad 0] \end{aligned} \quad (6)$$

where \bar{x}_1 contains the states of the reduced system, \bar{x}_2 represents the states that are reduced and k is the number of differential equations in the reduced-order model.

2.4. Further reduction of algebraic equations via system identification

So far, the number of differential and algebraic equations has been reduced separately by the described technique. It is possible to obtain a more suitable system of even smaller size and lesser complexity. Consider equation (7), which is part of the DAE system (6)

$$0 = P_2 \bar{g}(\bar{x}, \bar{z}) \quad (7)$$

where $\bar{x} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix}$ and $\bar{z} = \begin{bmatrix} \bar{z}_1 \\ \bar{z}_2 \end{bmatrix}$, which allows to rewrite equation (8) as

$$0 = \hat{g}(\bar{x}_1, \bar{z}_1) \quad (8)$$

where \hat{g} represents a new nonlinear function containing variables \bar{x}_1 and \bar{z}_1 only. The relationship between \bar{x}_1 and \bar{z}_1 needs to be retained in the reduced model to achieve a good approximation of the behavior of the original system. Since the inputs and the outputs of the

algebraic equations are dependent in a static manner, it is sufficient to identify this static relationship between \bar{x}_1 and \bar{z}_1 as shown in equation (9)

$$\bar{z}_1 = \tilde{g}(\bar{x}_1) \quad (9)$$

resulting in the following system:

$$\begin{aligned} \dot{\bar{x}}_1 &= P_1 \bar{f}(\bar{x}, \bar{z}, u) = \hat{f}(\bar{x}_1, \bar{z}_1, u) \\ \bar{x}_2 &= \bar{x}_{2,ss} \\ \bar{z}_1 &= \tilde{g}(\bar{x}_1) \\ \bar{z}_2 &= \bar{z}_{2,ss} \\ y &= \bar{h}(\bar{x}) = \hat{h}(\bar{x}_1) \end{aligned} \quad (10)$$

It has to be taken into account for the identification procedure that the relationship between \bar{x}_1 and \bar{z}_1 is usually nonlinear. One type of model that is able to take this property into account is artificial neural network (ANN). The resulting reduced system is given by

$$\begin{aligned} \dot{\bar{x}}_1 &= \hat{f}(\bar{x}_1, \bar{z}_1, u) \\ \bar{z}_1 &= \tilde{g}(\bar{x}_1), \quad (\text{here : } \bar{z}_1 = \text{ANN}(\bar{x}_1)) \\ y &= \hat{h}(\bar{x}_1) \end{aligned} \quad (11)$$

3. Case study

3.1. Model description

Consider a distillation column with 30 trays for separation of a binary mixture. The column has 32 differential states (concentrations of component A). The Wilson equation is used for computation of the vapor-liquid equilibrium, resulting in a model with 32 differential equations and 32 algebraic equations. The reflux ratio is set to 3.0 and serves as the manipulated variable while the concentration of the distillate is the output of the system.

3.2. Order reduction of differential and algebraic equations

When balancing is applied for the reduction of the differential equations, the main criterion to determine the number of states to be retained is based on the magnitude of the Hankel singular values of the balanced covariance matrices. Sorted by the magnitude from large to small, the first 15 Hankel singular values are shown in Fig. 1 and Table 1 lists the values of the first 6. For this example, truncated systems that contain 2, 3 and 5 states were investigated. The singular values in the matrix Σ_2 (Equations 2) indicate that a system with 3 algebraic variables is sufficient for models reduced by balancing.

It can also be concluded that systems with more states will more closely approximate the original system. However, there is always a tradeoff between the performance, i.e., the quality of the approximation, and efficiency, i.e., the required computational effort, as is illustrated in Table 2. Based on Fig. 2 and Table 2, it can be concluded that the reduced system with 3 differential equations results in a very good approximation to the original system with a relatively small computational burden.

3.3. Further reduction of algebraic equations via neural network

The neural net contains 1 hidden layer and 1 output layer, with 5 nodes in the hidden layer and 3 nodes in the output layer. Hyperbolic tangent functions were used in the hidden layer and linear functions in the output layer. The network was trained using the Levenberg-Marquardt algorithm [4, 5]. After order reduction has been performed, the remaining differential states serve as the inputs to the neural network while the outputs are given by the remaining algebraic variables.

Three cases are compared to illustrate the performance of the presented method for model reduction of DAE system: (1) a linearized system with 32 differential equations and 32 algebraic variables; (2) only the differential equations are reduced by balanced truncation while the algebraic equations remain unchanged, resulting in a reduced system with 3 differential equations and 32 algebraic variables; (3) the system is reduced by the presented procedure, i.e., differential equations as well as algebraic equations are reduced by truncation and the effect that the states have on the remaining algebraic variables is identified by a neural network. This last reduced system contains 3 differential equations and a neural network with three inputs and three outputs. Fig. 3 shows a comparison of the performance of these three reduced-order systems for step changes in the input of -10% and +10%. Several observations can be made based upon Fig. 3: (1) the upper and the lower trajectories are not symmetric, which illustrates the nonlinearity of the original system; (2) the performance of the linearized system is not as good as the ones using a nonlinear reduced model; (3) the reduced model including a neural network provides a good approximation to the full-order system. Although the reduced DAE system is a fairly small model, it exhibits better performance than case 1 and performance comparable to model 2 and to the original system.

4. Conclusions

This paper presents a new approach for the reduction of nonlinear DAE systems. The investigated technique performs order-reduction of the differential equations and reduces the size and complexity of the model. One of the strong points of this approach is that reduction of the differential and the algebraic equations is not performed independently from one another, but the interplay between the states and the algebraic variables is taken into account.

The procedure has been illustrated by applying it to a model of a distillation column. The algebraic equations were reduced by identifying a feedforward neural network resulting in a model of significantly smaller size that is also easier to simulate since the algebraic variables can be computed via an explicit expression.

References

- [1] K. E. Brenan, S. L. Campbell, L. R. Petzold, Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations, North-Holland, 1989
- [2] G.D. Byrne, P.R. Ponzi, Differential-algebraic systems, their application and solutions, Computer and Chemical Engineering 12 (5) (1988), 377-382
- [3] J. Hahn, T.F. Edgar, Balanced approach to minimal realization and model reduction of stable nonlinear systems, Ind. Eng. Chem. Res. 41 (2002), 2204-2212
- [4] K. Levenberg, A method for the solution of certain problems in least squares, Quart. Appl. Math., 2 (1944), 164-168
- [5] D. Marquardt, An algorithm for least-squares estimation of nonlinear parameters, SIAM J. Appl. Math., 11 (1963), 431-441

Table 1: Hankel singular values for states

State	1	2	3	4	5	6
Singular Value	0.048	0.0023	0.0002	0.00006	0.000009	0.000006
% of sum	94.9%	4.5%	0.4%	0.12%	0.0178%	0.0119%

Table 2: Comparison of computation times for reduced-order models

States	2	3	5	32
Time (Seconds)	0.06	0.07	0.14	0.4

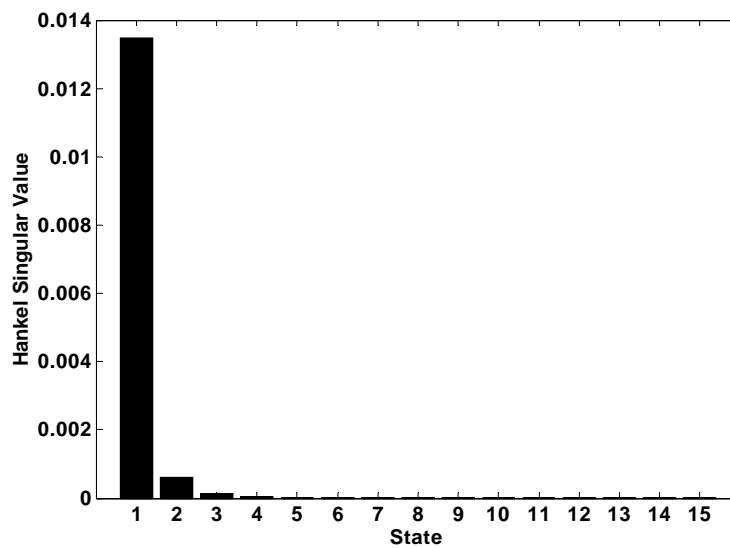


Fig. 1. Hankel singular values of the distillation column model

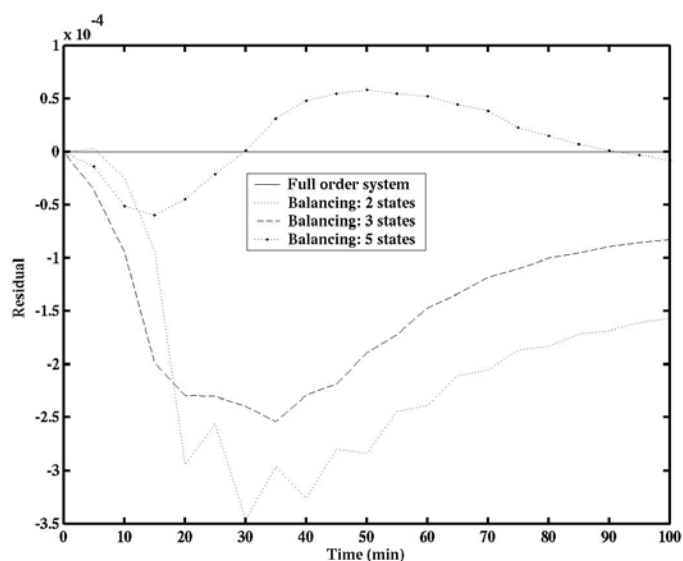


Fig. 2. Comparison of reduced systems with different number of remaining differential equations

Note: the curves represent the offsets between the values of each case and the corresponding values of the full-order system.

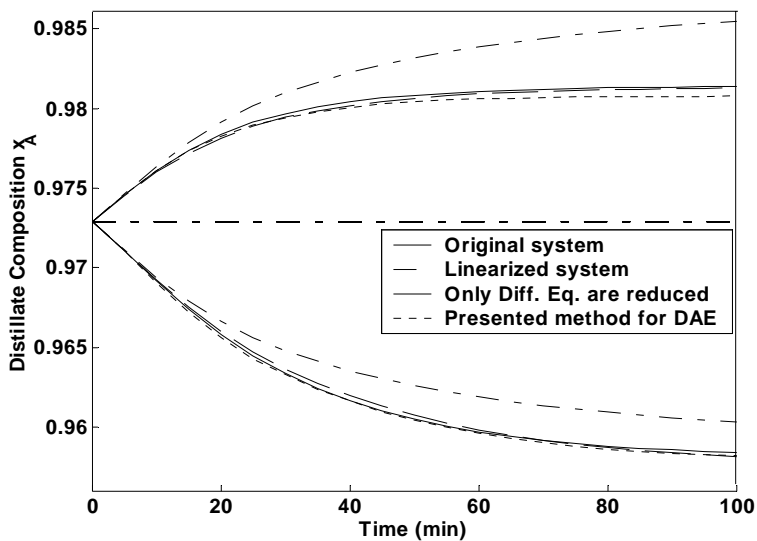


Fig. 3. Performance of presented method for DAE model reduction