Dependency Analysis for DAE to ODE Conversion and Model Reduction

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Abstract

A tool for the order reduction of differential algebraic equations (DAEs) is outlined in this report. Through the use of an equation dependency analysis and nonlinear function approximation, the algebraic equations can be divided into sets that require implicit or explicit solutions. If all of the algebraic variables can be solved or approximated explicitly, the DAE becomes a set of ordinary differential equations (ODEs). As a test case for the theory, a dynamic equilibrium binary distillation column model is analyzed with the generalized approach. The index 1 DAE model of 52 differential and 233 algebraic states is reduced to an ODE set of 26 differential states. Through simulations, the resulting ODE model solution is found to be in agreement with the original DAE model solution.

1. Introduction

DAEs consist of differential equations and algebraic equations. In the general form, the DAE problem is as follows:

$$\mathbf{f}(\dot{\mathbf{z}}, \mathbf{z}, t) = \mathbf{0}$$

where z is a vector of variables and t is a scalar. The DAE is nonlinear when the vector $\mathbf{f}$ is a nonlinear function of the derivative of $\mathbf{z}$, $\mathbf{z}$, or t. In order for the problem to be a DAE, at least one of the coefficients for the derivative of z must be zero. The DAE can be grouped into differential equations (f) and algebraic equations (g). The variables are also divided into differential variables (x) and algebraic variables (y).

$$\mathbf{f}(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{y}, t) = \mathbf{0}$$
$$\mathbf{g}(\mathbf{x}, \mathbf{y}, t) = \mathbf{0}$$

Large-scale nonlinear DAE models arise in object-oriented simulators, electrical circuit models, and many other models of physical processes. Reformulating the DAE model into an equivalent ODE model is desirable because of certain numerical advantages. These advantages include application of nonlinear model reduction techniques [5], no requirement for consistent initial conditions, and no numerical challenges associated with DAE systems of index greater than one [3].

One method of converting a DAE to an ODE is to solve the algebraic equations implicitly. Since the implicit solution of a large number of algebraic equations is computationally expensive, variables that can be solved explicitly are removed from the set y [6]. This partitioning and precedence ordering is performed by analyzing an incidence matrix $\mathbf{J}$ defined by

$$\mathbf{J}_{ij} = \begin{cases} 1 & \text{if } y_j \text{ appears in } g_i \\ 0 & \text{otherwise} \end{cases}$$

The assignment of variables to equations is made by performing row operations that transform $\mathbf{J}$ into a matrix with entries on the diagonals. Obtaining a precedence order and partitioning can be done using a manual directed graph (digraph) as a graphical approach, using matrix methods to produce a block diagonal lower matrix [8], or through tearing [1]. These techniques attempt to maximize the number of algebraic variables that can be solved explicitly. However, this problem is NP complete, meaning that all possible combinations of variables must be attempted to find a maximum set of explicit equations [4]. Another technique for order reduction is through relaxation of the algebraic states [7]. Relaxing directly generates a Gaussian elimination scheme when the algebraic equations are linear or made linear.

2. Equation Dependency Analysis

The method proposed in this work differs from previous work by analyzing a dependency matrix $\mathbf{M}^{-1}$ instead of the incidence matrix $\mathbf{J}$. It will be shown that $\mathbf{M}^{-1}$ can reveal more information about variable dependencies.

The dependency matrix $\mathbf{M}^{-1}$ is derived by first linearizing the DAE.

$$\mathbf{A}\dot{\mathbf{x}}' + \mathbf{B}\mathbf{x}' + \mathbf{C}\mathbf{y}' + \alpha t' = 0$$
$$\mathbf{D}\mathbf{x}' + \mathbf{E}\mathbf{y}' + \beta t' = 0$$

The prime indicates deviation from reference values (i.e. $\mathbf{x}' = \mathbf{x} - \mathbf{x}_{\text{ref}}$). $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, $\mathbf{D}$, and $\mathbf{E}$ are coefficient matrices and α and β are coefficient vectors. The reference values are selected to give non-zero coefficients for the deviation variables. Since the selection of reference values is arbitrary, the coefficients can be arbitrarily selected to be 1 if the equation contains the variable and 0 otherwise. In this case the matrix $\mathbf{E}$ is equivalent to the incidence matrix $\mathbf{J}$. Rearranging and combining the linear differential and algebraic equations results in the following matrix form:

$$\begin{bmatrix} \mathbf{A} & \mathbf{C} \\ \mathbf{0} & \mathbf{E} \end{bmatrix} \begin{bmatrix} \dot{\mathbf{x}}' \\ \mathbf{y}' \end{bmatrix} = -\begin{bmatrix} \mathbf{B} & \alpha \\ \mathbf{D} & \beta \end{bmatrix} \begin{bmatrix} \mathbf{x}' \\ t' \end{bmatrix}$$

The dependency matrix $\mathbf{M}^{-1}$ reveals the solution dependencies among the linearized equations.

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{A} & \mathbf{C} \\ \mathbf{0} & \mathbf{E} \end{bmatrix}^{-1}$$

The variable dependency information in $\mathbf{M}^{-1}$ can be illustrated by a linear system of $\mathbf{A}\mathbf{x} = \mathbf{b}$. When $\mathbf{A}$ is invertible, the solution to $\mathbf{x}$ is $\mathbf{A}^{-1}\mathbf{b}$. Each element of the vector $\mathbf{x}$ is computed from the corresponding row of $\mathbf{A}^{-1}_{ij}$ and the vector $\mathbf{b}$.

$$\mathbf{x}_i = \sum_j \mathbf{A}^{-1}_{ij} \mathbf{b}_j$$

However, the solution to $\mathbf{x}_i$ is independent of $\mathbf{b}_j$ if $\mathbf{A}^{-1}_{ij} = 0 \; \forall \; j{\neq}i$. If $\mathbf{x}_i$ is independent of $\mathbf{b}_j$ then it is also independent of equation j. The dependencies in the linear system also apply to the corresponding nonlinear system. Therefore, linearizing the DAE reveals the structure of the nonlinear system dependencies.

The matrix $\mathbf{M}^{-1}$ can be converted to lower triangular block diagonal form with Tarjan's algorithm [8]. Each block along the diagonal is a set of algebraic equations that require a simultaneous solution. Explicit approximations to implicit solutions can be attempted to further reduce the DAE order [2].

3. Case study with a binary distillation column model

A binary distillation column model, described in Appendix A, is employed to show a practical application of the DAE to ODE model conversion. The DAE model has 52 differential equations and 233 algebraic equations. The independent variables are:

$$\begin{bmatrix} \dot{\mathbf{x}} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \dot{\mathbf{x}}_A & \dot{\mathbf{h}} & | & \mathbf{y}_A & \mathbf{x}_L & \mathbf{T} & \dot{\mathbf{n}}_V \text{ or } \dot{\mathbf{n}}_L & \mathbf{h}_V & \mathbf{h}_L & \mathbf{P}_A^{sat} & \mathbf{P}_B^{sat} \end{bmatrix}^T$$

During the linearization step, the reference values are selected to give non-zero coefficients for the deviation variables. Since the reference values are arbitrary, the non-zero coefficients are shown by X if the equation contains the variable and 0 otherwise.

$$\mathbf{M}\begin{bmatrix} \dot{\mathbf{x}} \\ \mathbf{y} \end{bmatrix} \rightarrow \begin{bmatrix} X & 0 & X & 0 & 0 & X & 0 & 0 & 0 & 0 \\ 0 & X & 0 & 0 & 0 & X & X & X & 0 & 0 \\ 0 & 0 & X & 0 & 0 & 0 & 0 & 0 & X & 0 \\ 0 & 0 & 0 & X & 0 & 0 & X & X & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & X & X \\ 0 & 0 & 0 & X & 0 & X & 0 & 0 & 0 & 0 \\ 0 & 0 & X & 0 & X & 0 & X & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & X & 0 & 0 & X & 0 & 0 \\ 0 & 0 & 0 & 0 & X & 0 & 0 & 0 & X & 0 \\ 0 & 0 & 0 & 0 & X & 0 & 0 & 0 & 0 & X \end{bmatrix} \begin{bmatrix} \dot{\mathbf{x}}_A \\ \dot{\mathbf{h}} \\ \hline \mathbf{y}_A \\ \mathbf{x}_L \\ \mathbf{T} \\ \dot{\mathbf{n}}_V \text{ or } \dot{\mathbf{n}}_L \\ \mathbf{h}_V \\ \mathbf{h}_L \\ \mathbf{P}_A^{sat} \\ \mathbf{P}_B^{sat} \end{bmatrix}$$

The non-zero values of $\mathbf{M}^{-1}$ show the dependencies between the variables and equations. The non-zero values of $\mathbf{M}^{-1}$ in lower triangular block diagonal form are shown below with the corresponding variable order.

$$\mathbf{M}^{-1} = \left[\begin{array}{cccccccc|cc} X & X & X & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ X & X & X & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ X & X & X & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ X & X & X & X & 0 & 0 & 0 & 0 & 0 & 0 \\ X & X & X & 0 & X & 0 & 0 & 0 & 0 & 0 \\ X & X & X & 0 & X & X & 0 & 0 & 0 & 0 \\ X & X & X & X & X & X & X & 0 & 0 & 0 \\ X & X & X & X & X & X & X & X & 0 & 0 \\ \hline X & X & X & X & X & X & X & X & X & 0 \\ X & X & X & X & X & X & X & X & 0 & X \end{array}\right] \begin{bmatrix} \mathbf{y} \\ \dot{\mathbf{x}} \end{bmatrix} \rightarrow \begin{bmatrix} \mathbf{T} \\ \mathbf{P}_A{}^{sat} \\ \mathbf{P}_B{}^{sat} \\ \mathbf{h}_L \\ \mathbf{y}_A \\ \mathbf{h}_V \\ \mathbf{x}_L \\ \dot{\mathbf{n}}_V \text{ or } \dot{\mathbf{n}}_L \\ \dot{\mathbf{x}}_A \\ \dot{\mathbf{h}} \end{bmatrix}$$

Equations 1-3 indicate that T, $P_A{}^{sat}$, and $P_B{}^{sat}$ must be solved simultaneously since the corresponding equations form one block. The equations for $P_A{}^{sat}$, and $P_B{}^{sat}$ can be explicitly substituted into the bubble point temperature equation.

$$P = x_A P_A{}^{sat}(T) + (1 - x_A)P_B{}^{sat}(T)$$

For the cyclohexane / heptane binary mixtures, an explicit temperature solution is approximated by a second order polynomial in composition.

$$T = c_1 + c_2 x_A + c_3 x_A{}^2$$

The vector c was calculated with a least squares fit with data from the sets $x_A \in \begin{bmatrix} 0 & 1 \end{bmatrix}$ to be $c = \begin{bmatrix} 385.42 & -21.57 & 3.736 \end{bmatrix}^T$. The polynomial fit has a mean sample error of 0.012 K and a maximum sample error of 0.04 K.

The molar flow rates can form the last block along the diagonal. Since the molar flow rate equations are linear, they can be solved explicitly. After solving the flow rates the dependency matrix indicates that the differential equation variables can now be solved explicitly. If extraneous algebraic equations were present in the model, they could be identified at this point since the equations for $\dot{x}_A$ and $\dot{h}$ have no further dependencies. By explicitly solving all of the algebraic equations, the model is in an ODE form. In this form, nonlinear model reduction techniques can be applied to further reduce the number of differential states.

5. Nonlinear model reduction

As an ODE, the distillation column model is available for further model reduction through balanced covariance matrices or proper orthogonal decomposition (POD). POD was chosen for this example and the number of differential states was reduced to 26. Figure 1 shows the bottoms composition after a 5% increase in reboiler duty.
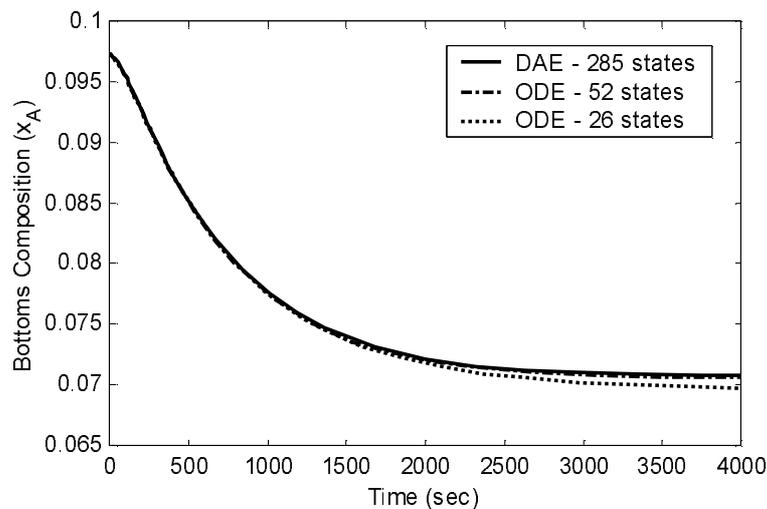
Figure 1 - 5% Step Change in Reboiler Duty

The ODE model with 52 states approximates the 285 state DAE very well. The ODE model with 26 states also approximates the DAE model well but with a larger offset in the steady-state value of composition. ODE models with fewer than 20 states performed poorly, indicating that there are at least 20 dynamic degrees of freedom in the binary distillation column model.

6. Summary

The order reduction of algebraic equations for DAEs is proposed through an equation dependency analysis. As a first step, the equation dependency on the variables is determined by linearizing the DAE and inverting the coefficient matrix corresponding to the differential derivatives and algebraic variables. After a transformation to lower triangular block diagonal form, the independent equations or systems of equations can be identified and solved.

1. Linearize the set of DAEs
2. Compute the dependency matrix, $\mathbf{M}^{-1}$
3. Transform $\mathbf{M}^{-1}$ to the lower triangular block diagonal form
4. Solve successive independent groups of variables given by successive blocks
5. Perform nonlinear model reduction techniques on the ODEs

As a test case for the theory, an index 1 DAE model of a distillation column was reduced to the ODE form and further reduced with POD. Simulations confirmed that the ODE model is a good approximation to the DAE counterpart.

7. References

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Appendix A

Description
Dynamic binary distillation column model with equilibrium stages

Diagram
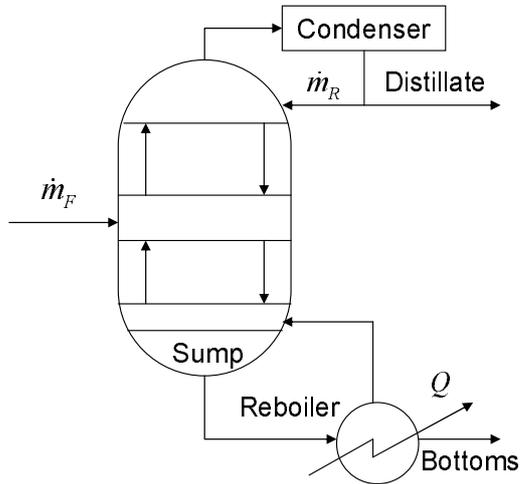
Manipulated Variables (3)

$\dot{m}_F$	Feed rate (gm/sec)
$\dot{m}_R$	Reflux rate (gm/sec)
Q	Reboiler heating rate (J/sec)

Differential States (52)

x_A	Liquid mole fraction
h	Specific enthalpy (J/mol)

Algebraic States (178)

y_A	Vapor mole fraction
x_L	Liquid mole fraction
T	Temperature (K)
$\dot{n}_V$	Vapor molar flow rate (mol/sec)
$\dot{n}_L$	Liquid molar flow rate (mol/sec)
h_V	Specific vapor enthalpy (J/mol)
h_L	Specific liquid enthalpy (J/mol)
P_i^{sat}	Saturation pressure of compound j (Pa)

Other

n_L	Liquid molar holdup (mol)
$MW_F(x_A)$	Molecular weight of feed stream (gm/mol)
$MW_R(x_A)$	Molecular weight of reflux stream (gm/mol)
P	Column pressure (Pa)
$h_{Vj}(T)$	Specific vapor enthalpy of compound j (J/mol)
$h_{Lj}(T)$	Specific liquid enthalpy of compound j (J/mol)

Differential Equations
Component A mole balance at each stage

$$\dot{x}_A = \frac{1}{n_L}\left(y_{A_{in}}\dot{n}_{V_{in}} + x_{A_{in}}\dot{n}_{L_{in}} - y_{A_{out}}\dot{n}_{V_{out}} - x_{A_{out}}\dot{n}_{L_{out}} + \left(x_{A_{feed}}\frac{\dot{m}_{feed}}{MW_{feed}(x_A)}\right)\right)$$

Energy balance at each stage

$$\dot{h} = \frac{1}{n_L}\left(h_{V_{in}}\dot{n}_{V_{in}} + h_{L_{in}}\dot{n}_{L_{in}} - h_{V_{out}}\dot{n}_{V_{out}} - h_{V_{out}}\dot{n}_{L_{out}} + \left(h_{L_{feed}}\frac{\dot{m}_{feed}}{MW_{feed}(x_A)}\right) + (Q)\right)$$

Algebraic Equations
Raoult's law for VLE

$$y_A = \frac{x_A P_A^{sat}}{P}$$

Liquid mole fraction equation

$$x_L = \frac{h - h_V}{h_L - h_V}$$

Bubble point temperature equation

$$P = x_A P_A^{sat} + (1 - x_A)P_B^{sat}$$

Vapor molar flow rate equation

$$\dot{n}_{V_{out}} = \left(\dot{n}_{V_{in}} + \dot{n}_{L_{in}}\right)(1 - x_L)$$

Liquid molar flow rate equation

$$\dot{n}_{L_{out}} = \left(\dot{n}_{V_{in}} + \dot{n}_{L_{in}}\right)x_L$$

Vapor enthalpy equation

$$h_V = y_A h_{VA}(T) + (1 - y_A)h_{VB}(T)$$

Liquid enthalpy equation

$$h_L = x_A h_{LA}(T) + (1 - x_A)h_{LB}(T)$$

Pure component j saturated vapor pressure equation (DIPPR database)

$$P_j^{sat} = \exp\left(A + \frac{B}{T} + C\ln(T) + DT^E\right)$$