Dependency Analysis for DAE to ODE Conversion and Model Reduction

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Motivations

- Order reduction
- Nonlinear balancing doesn't work with algebraic equations
- Avoid DAE challenges
  - Consistent initial conditions
  - High index (>1) DAEs

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

$$\longrightarrow \quad \mathbf{f}(\dot{\mathbf{x}}, \mathbf{x}, t) = \mathbf{0}$$

$\mathbf{y} = \text{algebraic}$

$\mathbf{x} = \text{differential}$

Previous Work-Methods to Eliminate y

$$\mathbf{J}_{\mathbf{ij}} = \begin{cases} 1 & \text{if } \mathbf{y}_{\mathrm{j}} \text{ appears in } \mathbf{g}_{\mathbf{i}} \\ 0 & \text{otherwise} \end{cases}$$

Convert to lower triangular block diagonal form (Tarjan's algorithm)

Diagonal blocks can be solved independently

Linearize DAE (x' = deviation from normal conditions)

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

$$\mathbf{D}\mathbf{x}' + \mathbf{E}\mathbf{y}' + \boldsymbol{\beta} t' = \mathbf{0}$$

Matrix Form

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

α and β are typically 0

Dependency Matrix (**M**)

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

The solution to $\mathbf{z}_\mathbf{i}$ is independent of $\mathbf{b}_\mathbf{j}$ (and equation j) if $\mathbf{M}^{-1}{}_{\mathbf{ij}} = 0$ for all $j \neq i$. This allows one to identify variables that can be removed.

$$\mathbf{z}_\mathbf{i} = \sum_\mathbf{j} \mathbf{M}^{-1}{}_{\mathbf{ij}} \mathbf{b}_\mathbf{j}$$

- Lower triangular block diagonalization of $\mathbf{M}^{-1}$
- Diagonal blocks can be solved independently starting with the top block

$$\mathbf{M}^{-1} = \begin{bmatrix} Block & 0 & 0 \\ X & Block & 0 \\ X & X & Block \end{bmatrix}$$

- Advantages of analyzing $\mathbf{M}^{-1}$ over $\mathbf{J}$
  - Variable dependencies are easily identified
  - Extra algebraic equations can be identified and eliminated

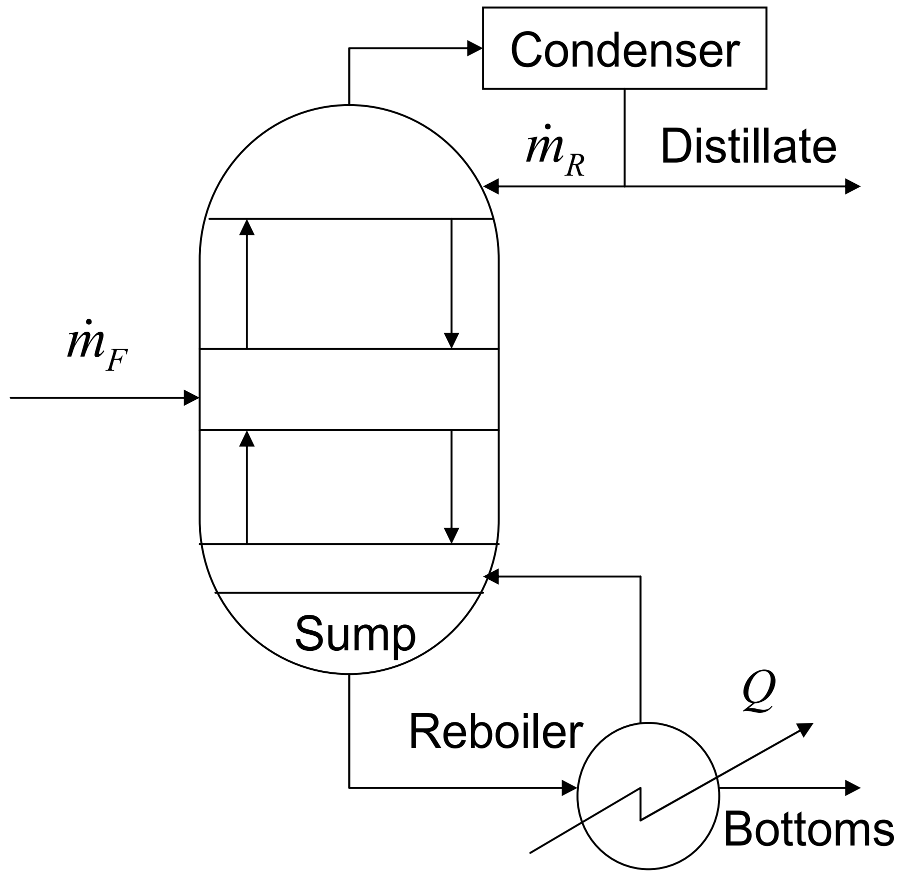
Binary Distillation Model

Model Size

52 differential

\+ <u>233 algebraic</u>

285 total states



Incidence Matrix (*X* denotes non-zero submatrix)

$$
\mathbf{M}\begin{bmatrix} \dot{\mathbf{x}} \\ \mathbf{y} \end{bmatrix} \rightarrow \left[\begin{array}{cc|cccccccc}
X & 0 & X & 0 & 0 & X & 0 & 0 & 0 & 0 \\
0 & X & 0 & 0 & 0 & X & X & X & 0 & 0 \\
\hline
0 & 0 & X & 0 & 0 & 0 & 0 & 0 & X & 0 \\
0 & 0 & 0 & X & 0 & 0 & X & X & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & X & X \\
0 & 0 & 0 & X & 0 & X & 0 & 0 & 0 & 0 \\
0 & 0 & X & 0 & X & 0 & X & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & X & 0 & 0 & X & 0 & 0 \\
0 & 0 & 0 & 0 & X & 0 & 0 & 0 & X & 0 \\
0 & 0 & 0 & 0 & X & 0 & 0 & 0 & 0 & X
\end{array}\right]
\left[\begin{array}{c}
\dot{\mathbf{x}}_{\mathbf{A}} \\
\dot{\mathbf{h}} \\
\hline
\mathbf{y}_{\mathbf{A}} \\
\mathbf{x}_{\mathbf{L}} \\
\mathbf{T} \\
\dot{\mathbf{n}}_{\mathbf{V}} \text{ or } \dot{\mathbf{n}}_{\mathbf{L}} \\
\mathbf{h}_{\mathbf{V}} \\
\mathbf{h}_{\mathbf{L}} \\
\mathbf{P}_{\mathbf{A}}^{\mathbf{sat}} \\
\mathbf{P}_{\mathbf{B}}^{\mathbf{sat}}
\end{array}\right]
$$

M is a square 285 x 285 matrix

Incidence Matrix (J) – Block Diagonalized

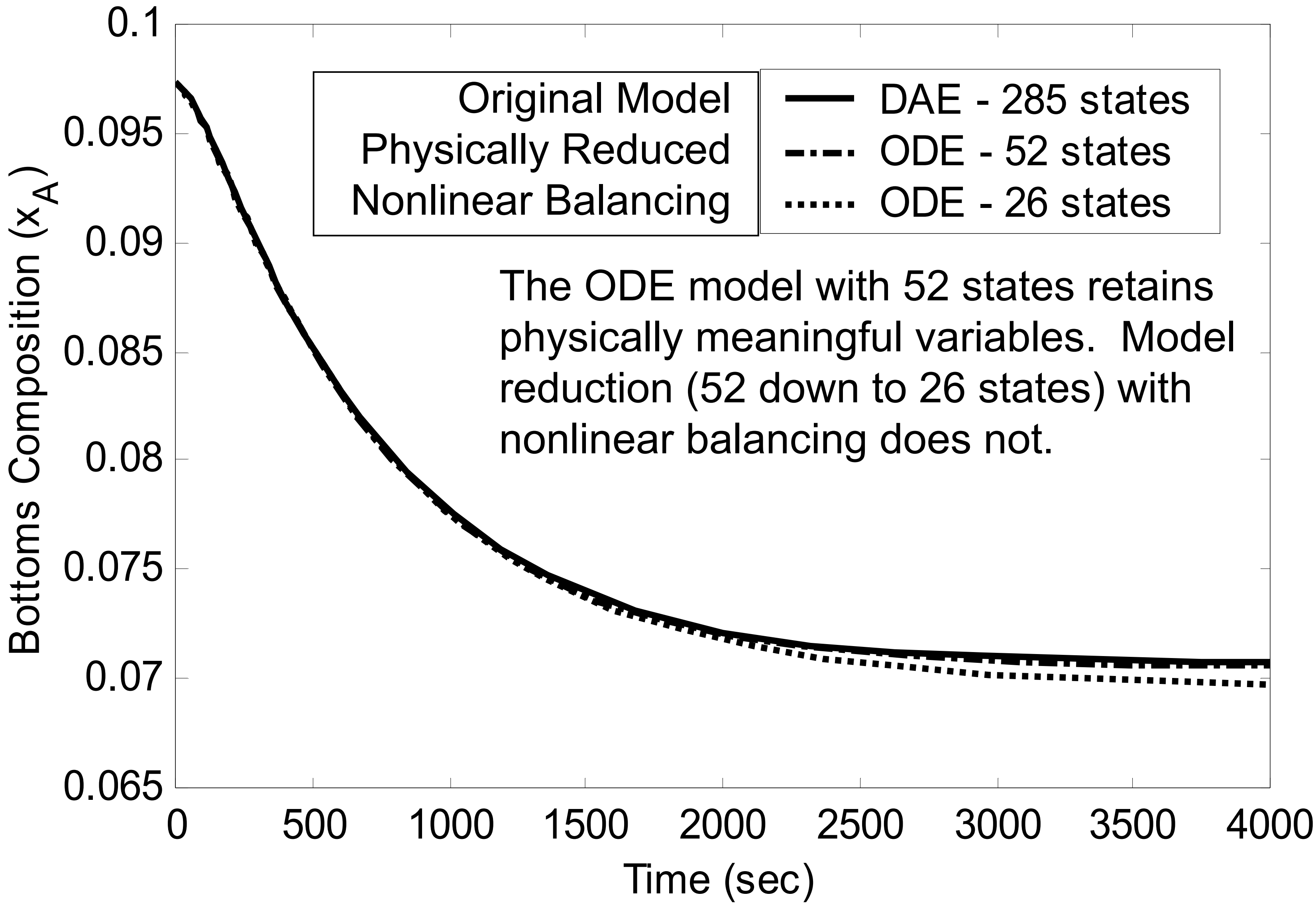
$$\mathbf{J} = \begin{bmatrix} X & 0 & X & 0 & 0 & 0 & 0 & 0 \\ X & X & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & X & X & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & X & \boxed{X} & 0 & 0 & 0 & 0 \\ 0 & X & 0 & X & \boxed{X} & 0 & 0 & 0 \\ 0 & X & 0 & 0 & 0 & \boxed{X} & 0 & 0 \\ 0 & 0 & 0 & 0 & X & X & \boxed{X} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & X & \boxed{X} \end{bmatrix} \qquad [\mathbf{y}] \rightarrow \begin{bmatrix} \mathbf{T} \\ \mathbf{P_A}^{\mathbf{sat}} \\ \mathbf{P_B}^{\mathbf{sat}} \\ \boxed{\mathbf{h_L}} \\ \boxed{\mathbf{y_A}} \\ \boxed{\mathbf{h_V}} \\ \boxed{\mathbf{x_L}} \\ \boxed{\dot{\mathbf{n}}_V \text{ or } \dot{\mathbf{n}}_L} \end{bmatrix}$$

Dependency Matrix ($\mathbf{M}^{-1}$)

$$
\mathbf{M}^{-1} = \left[\begin{array}{cccccccc|cc}
X & X & X & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
X & X & X & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
X & X & X & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
X & X & X & X & 0 & 0 & 0 & 0 & 0 & 0 \\
X & X & X & 0 & X & 0 & 0 & 0 & 0 & 0 \\
X & 0 & X & 0 & X & X & 0 & 0 & 0 & 0 \\
X & X & X & X & X & X & X & 0 & 0 & 0 \\
X & X & X & X & X & X & X & X & 0 & 0 \\
\hline
X & X & X & X & 0 & X & X & X & X & 0 \\
X & X & X & X & X & X & X & X & 0 & X
\end{array}\right]
\quad
\begin{bmatrix} \mathbf{y} \\ \dot{\mathbf{x}} \end{bmatrix} \rightarrow
\begin{bmatrix}
\mathbf{T} \\ \mathbf{P_A}^{\mathbf{sat}} \\ \mathbf{P_B}^{\mathbf{sat}} \\ \mathbf{h}_{\mathrm{L}} \\ \mathbf{y}_{\mathrm{A}} \\ \mathbf{h}_{\mathrm{V}} \\ \mathbf{x}_{\mathrm{L}} \\ \dot{\mathbf{n}}_{\mathrm{V}} \text{ or } \dot{\mathbf{n}}_{\mathrm{L}} \\ \dot{\mathbf{x}}_{\mathrm{A}} \\ \dot{\mathbf{h}}
\end{bmatrix}
$$

$\mathbf{M}^{-1}$ shows more dependency information than **J** and when ODE derivates can be solved explicitly.

5% step in reboiler duty



More Information:

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