

The Differentiation Index and Industrial Dynamic Simulation

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Presentation outline:

- The usual background
- The problem at hand
- Index analysis
- The heart of the matter
- Results



Cargill at a glance

Cargill Inc. is an international marketer, processor, and distributor of agricultural, food, financial, and industrial products.

- Founded in 1865
- 97,000 employees in 56 countries
- Still privately held

Products range from high volume products

- sweeteners
- refined vegetable oils

to high value ingredients

- natural vitamin E
- soy protein isolate

to industrial products

- PLA (plastic from corn)
- steel

The Process Solutions Technology Development Center

The *Process Solutions TDC* is part of the new research organization within Cargill.

- Process modeling and optimization
- Process development from lab through piloting
- Cost estimation and process engineering
- Financial modeling

My group within the PS-TDC provides process modeling services. Tools are based on the particulars of a project.

- Process models - ACM
- Custom analyses (pinch, costing) - VBA
- Statistical models - SAS, JMP, or S-PLUS
- CFD - Fluent (soon)

Our group is small - each of us must be able to master new tools and analyses quickly. A strong math background is essential for success.

A simplified vapor submodel

A full vapor flow model has $5n + 10$ equations and variables, where n is the number of compounds present in the vapor. Assuming a single component and constant physical properties, one obtains the following greatly simplified model, which fails to properly initialize.

$$\frac{\partial \rho}{\partial t} = -\frac{\partial v \rho}{\partial x}$$

$$\frac{\partial H}{\partial t} = -v \frac{\partial H}{\partial x}$$

$$\frac{\partial P}{\partial x} = K \frac{v^2}{\rho}$$

$$H = C_P (T - T_0)$$

$$P = \frac{\rho}{mw} RT$$

ρ Density

H Specific enthalpy

v Velocity

P Pressure

T Temperature

Index analysis for DAEs

Consider a general differential-algebraic system (DAE):

$$\mathbf{F}(\dot{\mathbf{u}}, \mathbf{u}, t) = \mathbf{0}$$

The *differentiation index* is the minimum number of times some or all of the equations must be differentiated in order to uniquely determine $\dot{\mathbf{u}}$ as a continuous function of \mathbf{u} and t (Brenan et al., 1996).

Example:

$$\begin{aligned}\dot{u}_1 - u_2 &= 0 \\ u_1 &= e^{-3t}\end{aligned}$$

One differentiation doesn't determine $\dot{\mathbf{u}}$:

$$\begin{aligned}\ddot{u}_1 - \dot{u}_2 &= 0 \\ \dot{u}_1 &= -3e^{-3t}\end{aligned}$$

A second differentiation does:

$$\ddot{u}_1 = 9e^{-3t}$$

The index is therefore 2.

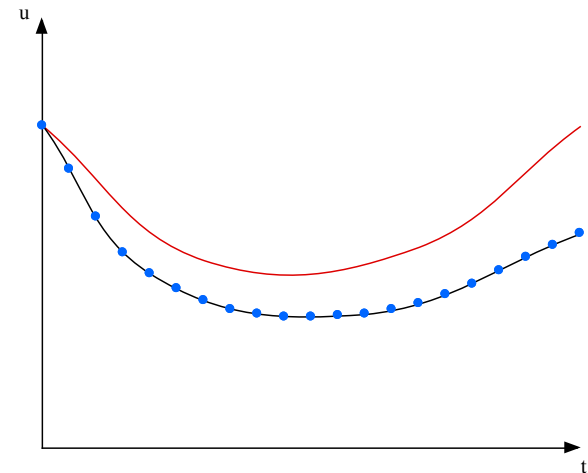
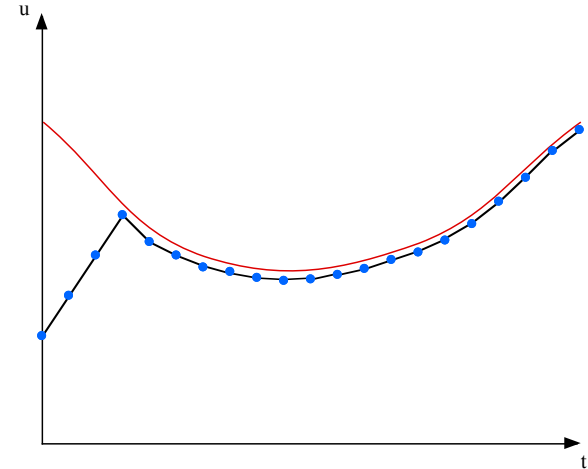
High index systems

A system is said to be *high index* if its index is at least 2.

High index systems contain *implicit constraints* between variables and their derivatives.

Implications:

- Some initial conditions may be inconsistent
- Numeric integration may fail or drift
- Degrees of freedom for initialization is less than number of differential variables



A necessary condition

Structural analysis investigates a necessary condition for low index - if there is no *output set assignment* for the highest occurring derivative of each variable, the system is high index.

$$\begin{array}{l} \dot{u}_1 - u_2 = 0 \\ u_1 - e^{-3t} = 0 \end{array} \begin{array}{|c|c|} \hline \dot{u}_1 & u_2 \\ \hline \times & \times \\ \hline & \\ \hline \end{array}$$

Our simple example system is structurally high index.

Dealing with high index systems

Given the set of differentiations performed during index analysis, an equivalent low index reformulation may be derived using the *method of dummy derivatives* (Mattsson and Söderlind, 1993).

Approach:

- Introduce one new algebraic variable (dummy derivative) for each differentiated equation
- Replace the corresponding derivative term with this new variable

From before: create three new *algebraic* variables u'_1 , u''_1 , and u'_2 . Append differentiated equations to the system and introduce these new variables.

$$u'_1 - u_2 = 0$$

$$u_1 = e^{-3t}$$

$$u''_1 - u'_2 = 0$$

$$u'_1 = -3e^{-3t}$$

$$u''_1 = 9e^{-3t}$$

Resulting system is low index, and solution in original variables is identical.

The differentiation index of a PDE

Consider a general PDE:

$$\mathbf{F}(\mathbf{u}_{x_i, i=1\dots m}, \mathbf{u}, \mathbf{x}) = 0$$

Definition: The *differentiation index with respect to x_j* is the number of times that some or all of the equations must be differentiated with respect to x_j in order to determine \mathbf{u}_{x_j} as a continuous function of \mathbf{u} and \mathbf{x} . (Martinson and Barton, 1998)

Example:

$$u_t + v_x = 0$$

$$u_x = \sin(4x)$$

The index w.r.t. t is 2.

The index w.r.t. x is 0.

Constraints on $\mathbf{u}_t(0, x)$, $\mathbf{u}(0, x)$ are given by interior differential equations on the hyperplane $t = 0$.

Other PDE index analyses

Define a *perturbation index* for a PDE together with its initial and boundary data and domain geometry (Campbell, 1997; Günther and Wagner, 1999) as the maximum order of derivatives of forcing functions and data that appear in the analytical solution.

Drawbacks:

- Defined only for certain classes of hyperbolic and parabolic systems
- Does not allow ready generalization of algorithms based on differentiation index of DAEs to PDEs
- Requires proper initial and boundary data, as well as analytical solution for analysis

Define an *algebraic index* (Campbell, 1997) for systems of the form

$$\mathbf{A}u_t + \mathbf{B}u_x + \mathbf{D}u_{xx} + \mathbf{C}u = \mathbf{0}$$

as the smallest value of $m + n$ such that

$$s^{-m}z^{-n} (s\mathbf{A} + z\mathbf{B} + z^2\mathbf{D} + \mathbf{C})^{-1}$$

is proper.

Advantages:

- Doesn't require analytical solution

Drawbacks:

- Defined only for linear systems
- Computation requires symbolic algebra

So, what's wrong with the vapor model?

Discretizations often preserve the index. Could the vapor sub-model be high index in t ? Let's try the simpler structural analysis first.

	$\dot{\rho}$	\dot{H}	v	P	T
$\dot{\rho} = -\frac{\partial v \rho}{\partial x}$	×		×		
$\dot{H} = -v \frac{\partial H}{\partial x}$		×	×		
$\frac{\partial P}{\partial x} = -K \frac{v^2}{\rho}$			×	×	
$H = C_P (T - T_0)$					×
$P = \frac{\rho}{mw} RT$				×	×

Structure does *not* indicate high index in t .

Full index analysis

Differentiating the last three equations once with respect to t produces

$$\dot{\rho} = -\frac{\partial v \rho}{\partial x}$$
$$\dot{H} = -v \frac{\partial H}{\partial x}$$

$$\dot{\rho} \frac{\partial P}{\partial x} + \rho \frac{\partial \dot{P}}{\partial x} - 2Kv\dot{v} = 0$$

$$\dot{H} - C_P \dot{T} = 0$$

$$\dot{P} - \frac{R}{mw} (\dot{\rho} T + \rho \dot{T}) = 0$$

This system gives all first order derivatives in t , so the system is not high index in t .

What about index in x ?

Even though the discretized system is a DAE in t , let's perform the shortcut analysis in x :

	$\dot{\rho}$	\dot{H}	\dot{v}	\dot{P}	T
$\frac{\partial \rho}{\partial t} = -\dot{v}\rho - v\dot{\rho}$	×		×		
$\frac{\partial H}{\partial t} = -v\dot{H}$		×			
$\dot{P} = -K\frac{v^2}{\rho}$				×	
$H = C_P (T - T_0)$					×
$P = \frac{\rho}{mw}RT$					×

Structural singularity means that the system is high index in x !

Who cares about index in x ?

How does a high index in x affect a problem to be solved as an evolution problem in t ?

In this case, high index in x produces a discretized problem with a high index in t *at a boundary node*.

There are only two degrees of freedom for boundary data, and the pressure boundary condition is mathematically unnecessary.

However, a typical finite difference spatial discretization will require the (mathematically unnecessary) boundary condition.

A closer look

Replacing the pressure drop equation with a Dirichlet condition on pressure produces the following system at the downstream end of the domain.

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= -\frac{\partial v \rho}{\partial x} \\ \frac{\partial H}{\partial t} &= -v \frac{\partial H}{\partial x} \\ P &= P_{\text{dome}} \\ H &= C_P (T - T_0) \\ P &= \frac{\rho}{mw} RT\end{aligned}$$

The problem understood

Recall the original output set assignment - in order to have a low index in t , the pressure drop equation must be solved for v .

	$\dot{\rho}$	\dot{H}	v	P	T
$\dot{\rho} = -\frac{\partial v \rho}{\partial x}$	×		×		
$\dot{H} = -v \frac{\partial H}{\partial x}$		×	×		
$\frac{\partial P}{\partial x} = -K \frac{v^2}{\rho}$			×	×	
$H = C_P (T - T_0)$					×
$P = \frac{\rho}{mw} RT$				×	×

When this equation is replaced by the boundary condition on pressure, the velocity must be assigned to another equation. In this case, the only choices are t -differential equations, and a high index system results.

The simple problem solved

At the exit node, perform a dummy reformulation.

$$\begin{aligned}\dot{\rho} &= -\frac{\partial v \rho}{\partial x} \\ H' &= -v \frac{\partial H}{\partial x} \\ P &= P_{TOP} \\ H &= C_P (T - T_0) \\ P &= \frac{\rho}{mw} RT \\ P' &= 0 \\ H' &= C_P T' \\ P' &= \dot{\rho} \frac{RT}{mw} + \frac{\rho R}{mw} T'\end{aligned}$$

Reformulating the original system is not so simple...

Wrapup

Lessons from this project:

- Understanding the differentiation index of a PDE system can be critical to successful modeling and simulation.
- Memo to simulation software vendors: Index analysis and dummy reformulation can and should be automated.

Dummy reformulation of the full model is still pending...

Selected Bibliography

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