How to simulate in Simulink: DAE, DAE-EKF, MPC & MHE

Tamal Das

PhD Candidate
IKP, NTNU

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Outline

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Differential algebraic equations (DAE)

Types of DAEs: Fully implicit and Semi-explicit

Notation

- $x:$ Differential variables
- $z:$ Algebraic variables
- $y = \left[x^T \; z^T\right]$

Fully implicit DAE

$$F\left(y, \frac{dy}{dt}\right) = 0$$
$$y\left(0\right) = y_0$$

Semi-explicit DAE

$$\frac{dx}{dt} = f\left(x, z\right)$$
$$0 = g\left(x, z\right)$$

DAEs in Chemical Engineering

In ChemEng, mathematical models consist of the following:

- Dynamic conservation laws [Differential equations]
  - Mass balance
  - Energy balance
- Static conservation laws [Algebraic equations]
- Constitutive equations [Algebraic equations]
  - Equation of state
  - Pressure drop equation
  - Heat transfer equation
- Physical and operating constraints [Algebraic equations]
  - Desired operation
  - Design constraints

Index of a DAE

- In ChemEng, commonly encountered DAEs are semi-explicit

$$\frac{dx}{dt} = f(x,z);\ 0 = g(x,z)$$

- Index of DAEs determines how hard it is to solve them

Index 1-DAE

$\frac{\partial g}{\partial z}$ is non-singular

- $det\left(\frac{\partial g}{\partial z}\right) \neq 0$
- $\frac{\partial g}{\partial z}$ is full rank matrix

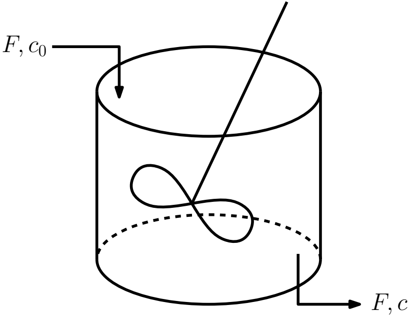
Higher index (2,3,...-) DAEs

$\frac{\partial g}{\partial z}$ is singular

- $det\left(\frac{\partial g}{\partial z}\right) = 0$
- $\frac{\partial g}{\partial z}$ is not full rank matrix

Examples of DAE indices

$$\frac{dc}{dt} = \frac{(c_0 - c)}{\tau}$$



CSTR with volume V
Residence time
$\tau = \frac{V}{F}$
Differential variable $(x): c$
Algebraic variable $(z): c_0$

Index 1-DAE

- $c_0 = \gamma(t)$ is specified;
  $\therefore \; g = c_0 - \gamma(t)$
- $\frac{\partial g}{\partial z} = \frac{\partial g}{\partial c_0} = 1$ (Full rank)

Higher index (2,3,...-) DAEs

- $c = \gamma(t)$ is specified;
  $\therefore \; g = c - \gamma(t)$
- $\frac{\partial g}{\partial z} = \frac{\partial g}{\partial c_0} = 0$ (not full rank)

How to determine DAE index?

Index $=$ Number of differentiations of $g(x, z)$ w.r.t time necessary to get a differential equation for each algebraic variable

Index 1-DAE

- $c_0 = \gamma(t)$ is specified
- Derivative 1: $\frac{dc_0}{dt} = \gamma'(t)$
- Index $= 1$

Higher index (2,3,...-) DAEs

- $c = \gamma(t)$ is specified
- Derivative 1: $\frac{dc}{dt} = \gamma'(t)$
- Rearrange: $\frac{c_0 - c}{\tau} = \gamma'(t)$
- Derivative 2: $\frac{dc_0}{dt} - \frac{dc}{dt} = \tau\gamma''$
- Rearrange: $\frac{dc_0}{dt} = \gamma' + \tau\gamma''$
- Index $= 2$

Why is Index of a DAE important?

- Index 1-DAEs are easy whereas higher index-DAEs are hard
- Higher index DAEs are hard due to initialization of variables (among others)
- In ChemEng, DAEs of both kinds are encountered

$$\frac{dx}{dt} = f(x, z);\ 0 = g(x, z)$$

$$det\left(\frac{\partial g}{\partial z}\right) \neq 0 \text{ (Index 1-DAE), or}$$

$$det\left(\frac{\partial g}{\partial z}\right) = 0 \text{ (Higher index DAE)}$$

- Where does one encounter higher index DAEs in ChemEng
  - Making simplifications in process models
  - Converting simulation problems into control problems

Initialization issues of DAEs

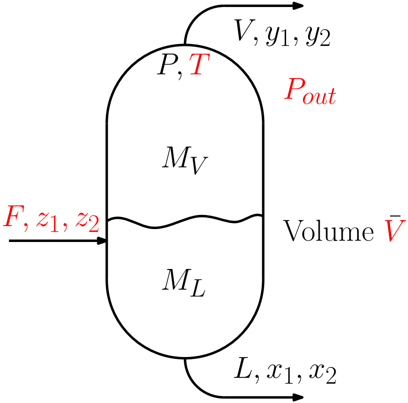
Index 1-DAE (Easy)

- Initialize differential variables $x(0)$
- Solve $g(x(0), z(0)) = 0$ for algebraic variables $z(0)$

Higher index DAEs (Hard)

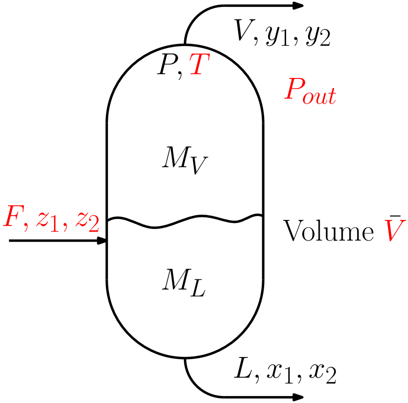
- $x(0)$ and $z(0)$ are interdependent
- $x(0)$ and $z(0)$ cannot be specified independently
- If specified independently, leads to inconsistent initial conditions
- DAE solver will crash

DAE example: Two component dynamic flash calculation



$$\left.\begin{aligned}
\dot{M}_T &= F - V - L \\
\dot{M}_1 &= Fz_1 - Vy_1 - Lx_1 \\
\dot{M}_2 &= Fz_2 - Vy_2 - Lx_2 \\
M_T &= M_L + M_V \\
M_1 &= M_L x_1 + M_V y_1 \\
M_2 &= M_L x_2 + M_V y_2 \\
x_1 + x_2 &= y_1 + y_2
\end{aligned}\right\} \text{7 Conservation equations}$$

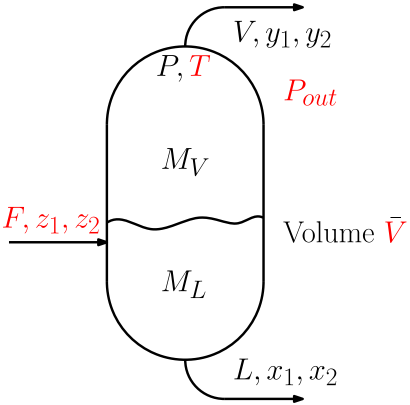
DAE example: Two component dynamic flash calculation



$$\left.\begin{aligned} y_1 &= K_1 x_1 \\ y_2 &= K_2 x_2 \\ K_1 &= f^{K_1}(T, P) \\ K_2 &= f^{K_2}(T, P) \\ \rho_L &= f^L(x_1) \\ \rho_V &= f^V(T, P) \\ L &= h^L(M_L, \rho_L) \\ V &= h^V(P - P_{out}) \end{aligned}\right\} \text{8 Constitutive equations}$$

$$\left.\bar{V} = \frac{M_L}{\rho_L} + \frac{M_V}{\rho_V}\right\} \text{Design}$$

DAE example: Two component dynamic flash calculation



- 3 differential equations
- 3 differential variables
- 13 algebraic equations
- 13 algebraic variables
- We can find an output set for all the algebraic and differential variables
- Index 1

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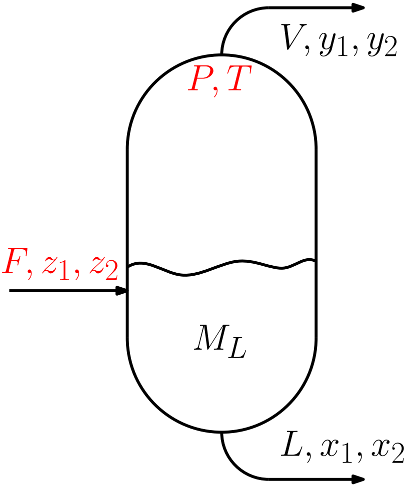
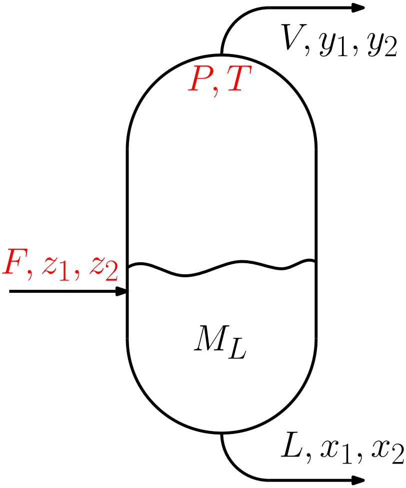
DAE example: Modified two component dynamic flash



$$\left.\begin{aligned}
\dot{M}_L &= F - V - L \\
\dot{M}_1 &= Fz_1 - Vy_1 - Lx_1 \\
\dot{M}_2 &= Fz_2 - Vy_2 - Lx_2 \\
M_1 &= M_L x_1 \\
M_2 &= M_L x_2 \\
x_1 + x_2 &= y_1 + y_2
\end{aligned}\right\} \text{6 Conservation equations}$$

DAE example: Modified two component dynamic flash



$$\left.\begin{aligned} y_1 &= K_1 x_1 \\ y_2 &= K_2 x_2 \\ K_1 &= f^{K_1}(T, P) \\ K_2 &= f^{K_2}(T, P) \\ L &= h^L(M_L, \rho_L) \\ \rho_L &= f^L(x_1) \end{aligned}\right\} \text{6 Constitutive equations}$$

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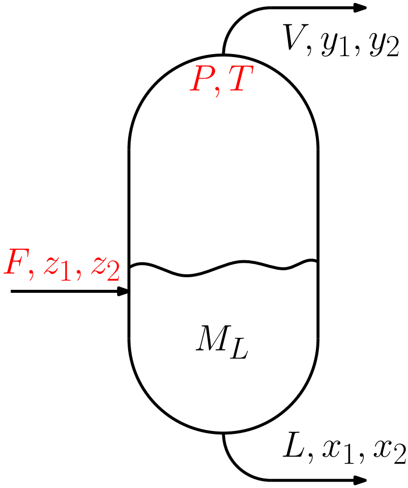
DAE example: Modified two component dynamic flash



- 3 differential equations
- 3 differential variables
- 9 algebraic equations
- 9 algebraic variables
- We cannot find an output set for algebraic variable V.
- We need to differentiate twice to get there
- Index 2

Solving higher index DAE problems

- Reduce index to 1 or 0
- Find consistent initial conditions for all the variables of the new system
- Solve the new system as a Index 1 DAE system or 0 index system (ODE system)
- The procedure[1] is explained on the MATLAB website with added support functions:
  - Index / order reduction ('reduceDAEIndex')
  - Finding consistent initial guesses ('decic')
  - DAE solvers: ode15i, ode15s, or ode23t

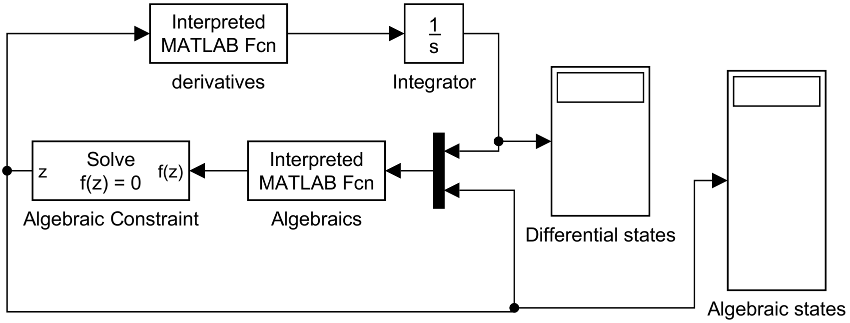
[1] https://se.mathworks.com/help/symbolic/solve-differential-algebraic-equations.html

Solving index 1-DAE: Robertson DAE in Simulink

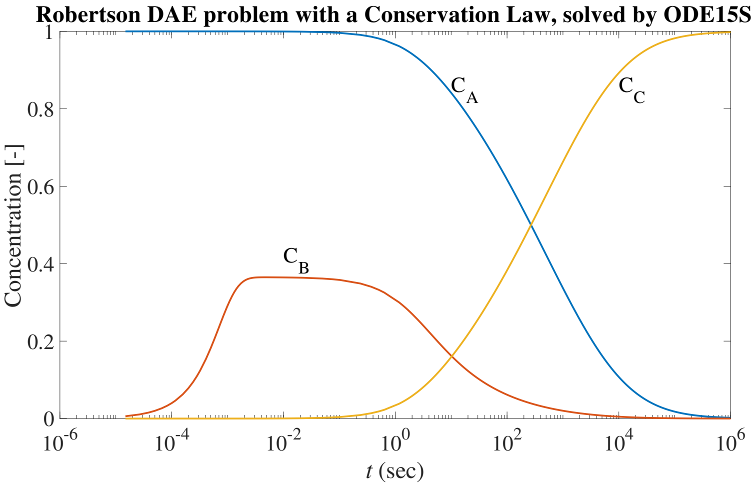
$$\mathrm{A} \rightleftharpoons \mathrm{B} + \mathrm{C}$$
$$\mathrm{B} \rightarrow \mathrm{C}$$

$$\frac{dC_A}{dt} = -0.04C_A + 10^4 C_B C_C$$
$$\frac{dC_B}{dt} = 0.04C_A - 10^4 C_B C_C - 3 \times 10^7 C_B^2$$
$$0 = 1 - (C_A + C_B + C_C)$$

Solving index 1-DAE problem in Simulink: Implementation



Solving index 1-DAE problem in Simulink: Result



Extended Kalman filter (EKF) for DAE

Continuous-discrete EKF algorithm for DAE

$$\frac{dx}{dt} = f(x,z) + w$$
$$0 = g(x,z)\,; \;\; y = h(x,z) + v$$

$$x^{aug} = \begin{bmatrix} x \\ z \end{bmatrix}; \;\; f^{aug} = \begin{bmatrix} f \\ g \end{bmatrix}$$

$$\frac{d\hat{x}}{dt} = f(\hat{x})\,; \;\; L = \begin{bmatrix} I \\ -\left(\frac{\partial g}{\partial z}\right)^{-1}\left(\frac{\partial g}{\partial x}\right) \end{bmatrix}$$

$$\frac{dP}{dt} = \left(\frac{\partial f^{aug}}{\partial x^{aug}}\right) P + P\left(\frac{\partial f^{aug}}{\partial x^{aug}}\right)^T + LQL^T$$

$$K_k = P_k^- \left(\frac{\partial h}{\partial x^{aug}}\right)^T \left(R_k + \left(\frac{\partial h}{\partial x^{aug}}\right) P_k^- \left(\frac{\partial h}{\partial x^{aug}}\right)^T\right)^{-1}$$

$$\hat{x}_k^{aug,+} = \hat{x}_k^{aug,-} + K_k\left(y_k - h_k\left(\hat{x}_k^{aug,-}\right)\right)$$

$$P_k^+ = \left(I - K_k\left(\frac{\partial h}{\partial x^{aug}}\right)\right) P_k^- \left(I - K_k\left(\frac{\partial h}{\partial x^{aug}}\right)\right)^T + K_k R_k K_k^T$$

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Moving horizon estimation (MHE)

- MHE is a dynamic optimization problem
- At each sample time, a set of past few measurements are used to provide a state estimate
- This problem is discretized to a nonlinear program (NLP) [for nonlinear estimation]
- NLP is solved using IPOPT solver in CasADi
- CasADi is interfaced with Simulink using system block to provide online state estimation

Conclusions

- DAE systems are hard: particularly higher index DAEs
- Two approaches:
  - simultaneous (Mass matrix solver)
  - sequential (Simulink with Algebraic constraint block)
- Estimation for DAE systems: CD-DAE-EKF in Simulink
- MPC in Simulink using system block and CasADi
- MHE in Simulink using system block and CasADi
- For simulation files and this presentation, follow[2]

Thank you for your attention

[2] folk.ntnu.no/tamald