10.34: Numerical Methods Applied to Chemical Engineering

Lecture 19:
Differential Algebraic Equations

Recap

- Differential algebraic equations
  - Semi-explicit
  - Fully implicit
- Simulation via backward difference formulas

Recap

- How suitable are such approaches?
- Consider stirred tank example 1:

$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) - c_2(t)\right)$$

$$c_1(t) = \gamma(t)$$

Apply backward Euler method:

$$\left.\frac{dx}{dt}\right|_{t_k} = \frac{x(t_k) - x(t_{k-1})}{t_k - t_{k-1}} + O(t_k - t_{k-1})$$

$$c_1(t_k) = \gamma(t_k)$$

$$c_2(t_k) = \frac{1}{1 + \frac{Q}{V}(t_k - t_{k-1})}\left(c_2(t_{k-1}) + \frac{Q}{V}(t_k - t_{k-1})c_1(t_k)\right) + O((t_k - t_{k-1})^2)$$

Recap

- How suitable are such approaches?
- Consider stirred tank example 2:

$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) \quad c_2(t)\right)$$

$$c_2(t) = \gamma(t)$$

Apply backward Euler method:

$$c_2(t_k) = \gamma(t_k)$$

$$c_1(t_k) = c_2(t_k) + \frac{V}{Q}\left(\frac{c_2(t_k) - c_2(t_{k-1})}{t_k - t_{k-1}}\right) + O(t_k - t_{k-1})$$

Recap

- How suitable are such approaches?
- Consider the system of DAEs:

$$\dot{c}_2 = c_1(t)$$
$$\dot{c}_3 = c_2(t)$$
$$0 = c_3(t) - \gamma(t)$$

Apply backward Euler method:

$$c_3(t_k) = \gamma(t_k)$$

$$c_2(t_k) = \frac{c_3(t_k) - c_3(t_{k-1})}{t_k - t_{k-1}} + O(t_k - t_{k-1})$$

$$c_1(t_k) = \frac{c_2(t_k) - c_2(t_{k-1})}{t_k - t_{k-1}} + O(1)\,!$$

Recap

- Solution via backward Euler:
  - Stirred-tank example 1:
    - local truncation error: $O(\Delta t^2)$
  - Stirred-tank example 2:
    - local truncation error: $O(\Delta t)$
  - DAE example 3:
    - local truncation error: $O(1)$

Recap

- How suitable are such approaches?
- Consider the system of DAEs:

$$
\begin{aligned}
\dot{c}_1 &= c_1(t) + c_2(t) + c_3(t) \\
\dot{c}_2 &= -c_1(t) - c_2(t) + c_3(t) \\
0 &= c_1(t) + c_2(t)
\end{aligned}
$$

Apply backward Euler method:

Differential Index

- Consider stirred tank example 1:

$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) - c_2(t)\right) \quad (1)$$

$$c_1(t) = \gamma(t) \quad (2)$$

- How many time derivatives are needed to convert to a system of independent ODEs having differentials of all the unknowns?

derivative of (2)

$$\frac{dc_1}{dt} = \dot{\gamma}(t) \quad (3)$$

Called an index-1 DAE.

Differential Index

- Consider stirred tank example 2:

$$\frac{dc_2}{dt} = \frac{Q}{V}(c_1(t) - c_2(t)) \quad \textbf{(1)}$$

$$c_2(t) = \gamma(t) \quad \textbf{(2)}$$

- How many time derivatives are needed to convert to a system of ODEs?

substitute (1)

$$\frac{dc_2}{dt} = \dot{\gamma} \quad \rightarrow c_1(t) = c_2(t) + \frac{V}{Q}\dot{\gamma} \quad \textbf{(3)}$$

derivative of (2)

derivative of (3)

$$\frac{dc_1}{dt} - \frac{dc_2}{dt} = \frac{V}{Q}\ddot{\gamma}$$

substitute (1)

$$\frac{dc_1}{dt} = \frac{V}{Q}\ddot{\gamma} + \frac{Q}{V}(c_1(t) - c_2(t)) \quad \textbf{(4)}$$

Called an index-2 DAE.

Differential Index

- Consider DAE example 3:

$$\dot{c}_2 = c_1(t) \qquad (1)$$

$$\dot{c}_3 = c_2(t) \qquad (2)$$

$$0 = c_3(t) - \gamma(t) \qquad (3)$$

- How many time derivatives are needed to convert to a system of ODEs?

derivative of (3) $\dot{c}_3 = \dot{\gamma}$ → substitute (2) $c_2(t) = \dot{\gamma}$ (4)

↓

derivative of (4) $\dot{c}_2 = \ddot{\gamma}$ → substitute (1) $c_1(t) = \ddot{\gamma}$ (5)

↓

derivative of (5) $\dot{c}_1 = \dddot{\gamma}$ (6)

Called an index-3 DAE.

Differential Index

- The differential index of a semi-expicit DAE system is defined as the minimum number of differentiations required to convert the DAE to a system of independent ODEs.

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{y}, t)$$
$$0 = \mathbf{g}(\mathbf{x}, \mathbf{y}, t)$$

$$0 = \frac{d\mathbf{g}}{dt} = \mathbf{g}^{(1)}(\mathbf{x}, \mathbf{y}, \dot{\mathbf{y}}, t)$$
$$0 = \frac{d^2\mathbf{g}}{dt^2} = \mathbf{g}^{(2)}(\mathbf{x}, \mathbf{y}, \dot{\mathbf{y}}, t)$$
$$\vdots$$

solve for:

$$\frac{d\mathbf{y}}{dt} = \mathbf{s}(\mathbf{x}, \mathbf{y}, t)$$

Differential Index

- Consider another example:

$$\dot{c}_1 = c_1(t) + c_2(t) + c_3(t)$$
$$\dot{c}_2 = -c_1(t) - c_2(t) + c_3(t)$$
$$0 = c_1(t) + c_2(t)$$

  - How many time derivatives are needed to convert to a system of ODEs?

Differential Index

- The differential index of a semi-expicit DAE system is defined as the minimum number of differentiations required to convert the DAE to a system of ODEs.

- Index-1 example: $$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{y}, t) \quad (1)$$ $$0 = \mathbf{g}(\mathbf{x}, \mathbf{y}, t) \quad (2)$$

derivative of (2) — rearrange and substitute (1)

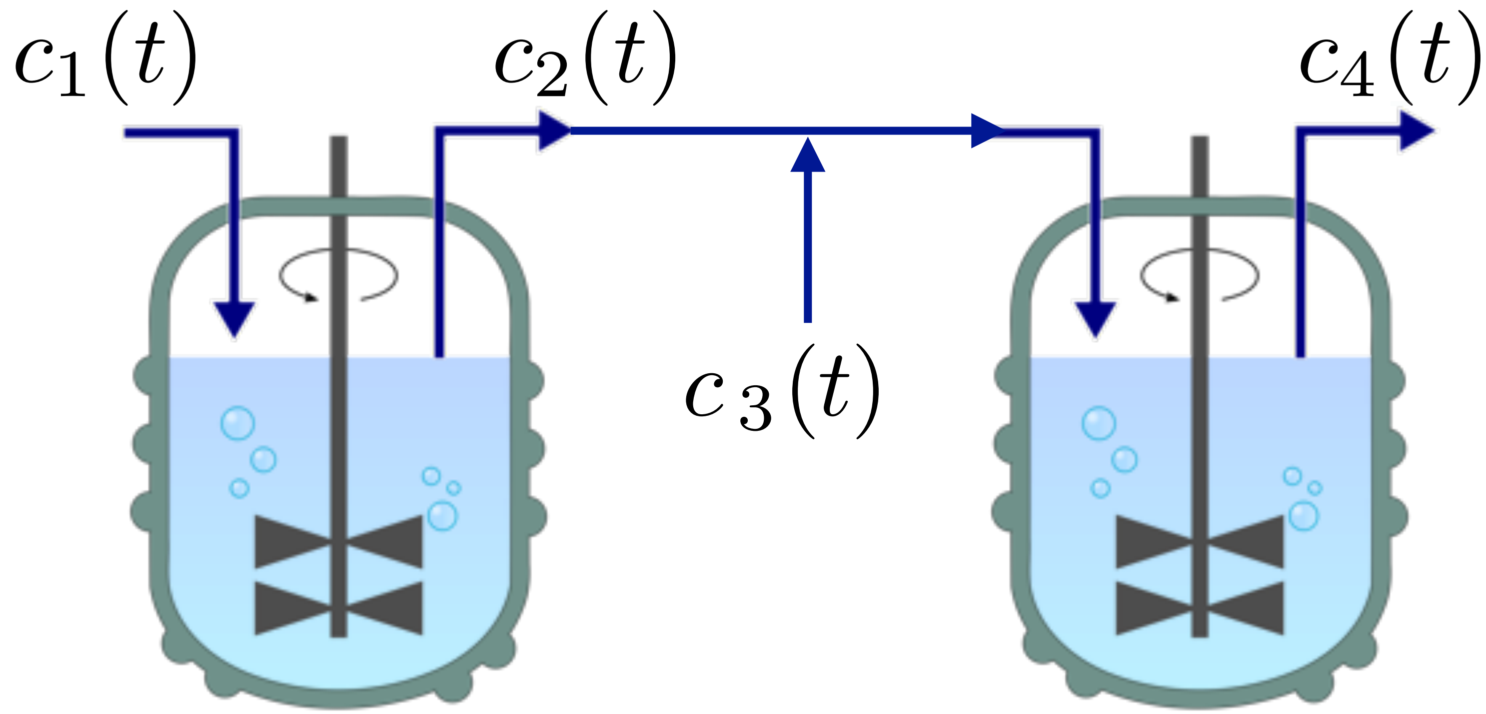
$$0 = \frac{d\mathbf{g}}{dt} = \frac{\partial \mathbf{g}}{\partial \mathbf{x}}\frac{d\mathbf{x}}{dt} + \frac{\partial \mathbf{g}}{\partial \mathbf{y}}\frac{d\mathbf{y}}{dt} + \frac{\partial \mathbf{g}}{\partial t} \rightarrow \frac{\partial \mathbf{g}}{\partial \mathbf{y}}\frac{d\mathbf{y}}{dt} = -\frac{\partial \mathbf{g}}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}, \mathbf{y}, t) - \frac{\partial \mathbf{g}}{\partial t}$$

If $\frac{\partial \mathbf{g}}{d\mathbf{y}}$ is full rank then the DAE is index-1:

$$\frac{d\mathbf{y}}{dt} = -\left(\frac{\partial \mathbf{g}}{d\mathbf{y}}\right)^{-1}\left(\frac{\partial \mathbf{g}}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}, \mathbf{y}, t) + \frac{\partial \mathbf{g}}{\partial t}\right)$$

Differential Index

- Example, determine the differential index:



$$\frac{dc_2}{dt} = \frac{Q_1}{V_1}(c_1(t) - c_2(t))$$

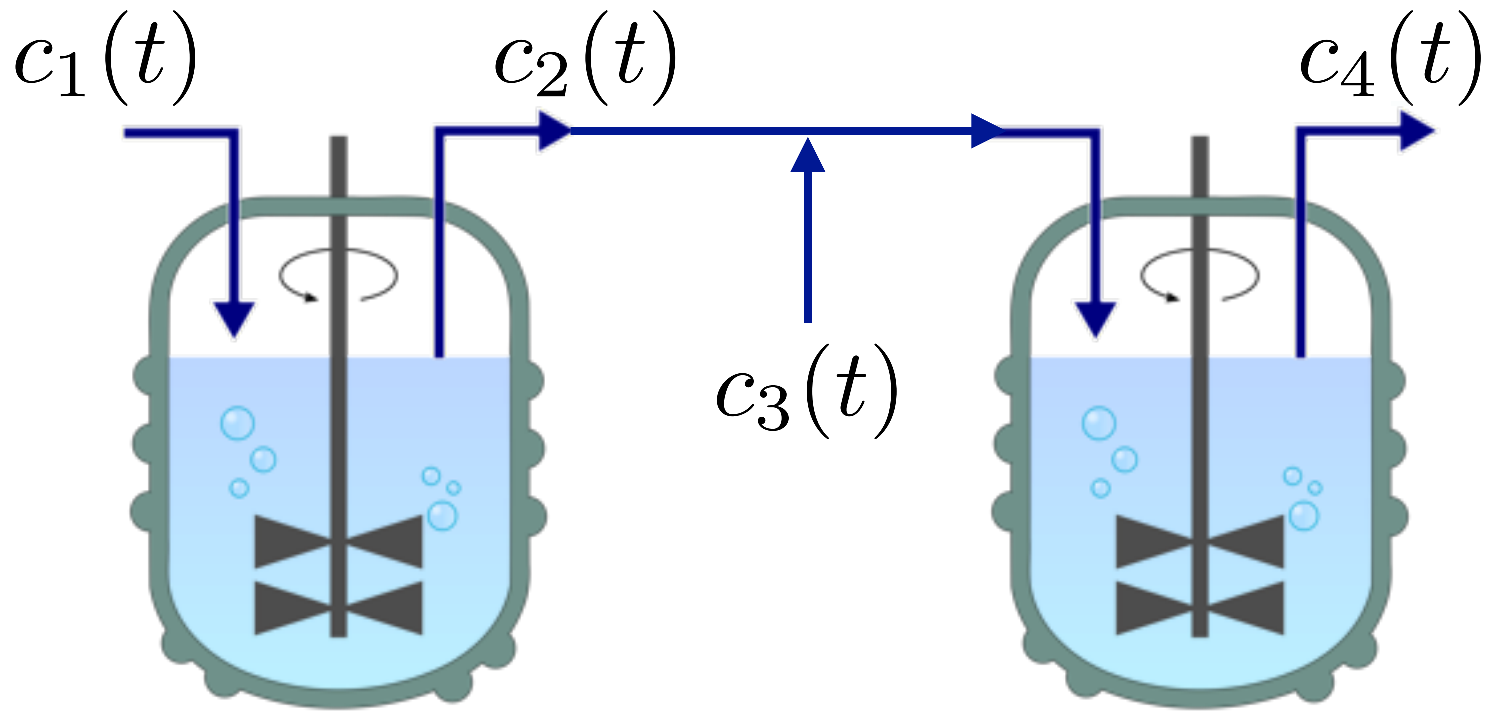
$$\frac{dc_4}{dt} = \frac{Q_1}{V_2}c_2(t) + \frac{Q_2}{V_2}c_3(t) - \frac{Q_1 + Q_2}{V_2}c_4(t)$$

$$c_1(t) = \gamma_1(t)$$

$$c_3(t) = \gamma_2(t)$$

Differential Index

- Example, determine the differential index:



$$\frac{dc_2}{dt} = \frac{Q_1}{V_1}(c_1(t) - c_2(t))$$

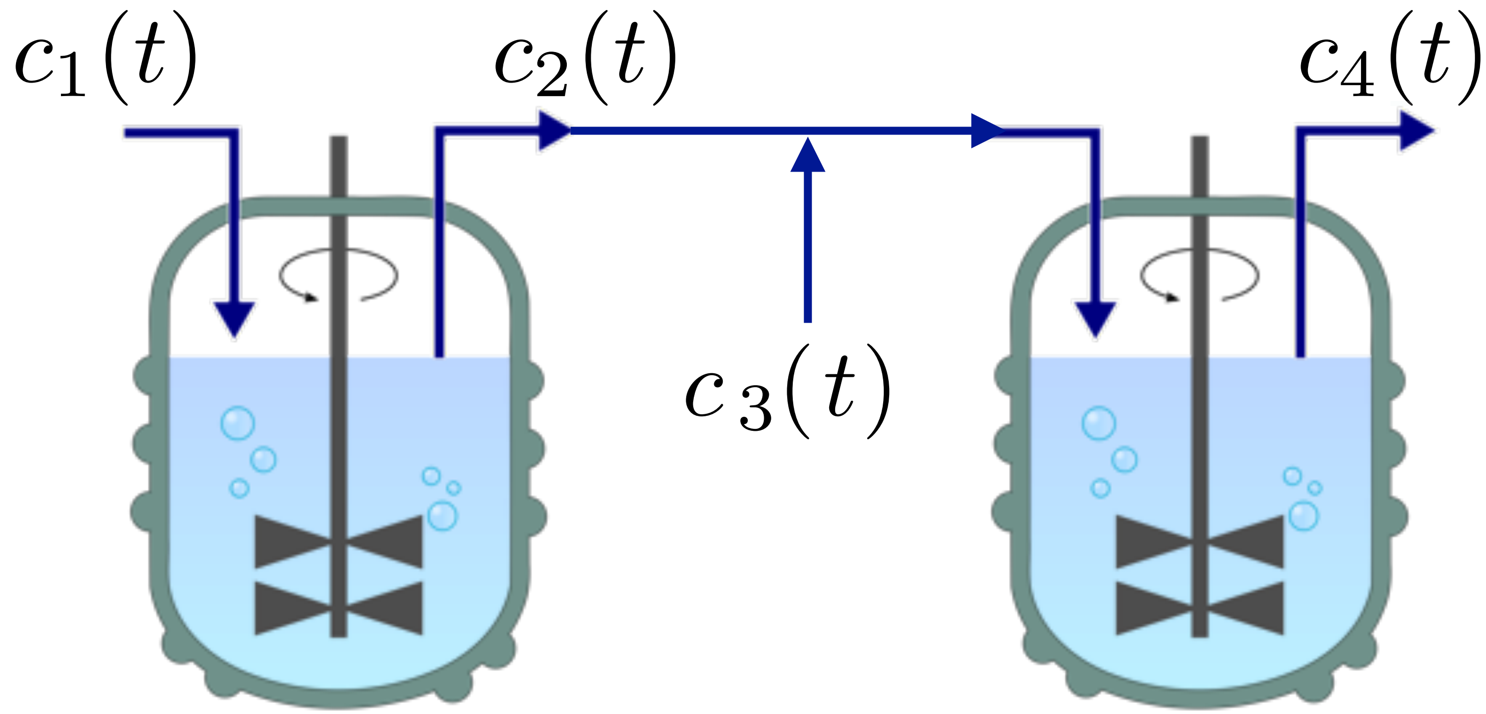
$$\frac{dc_4}{dt} = \frac{Q_1}{V_2}c_2(t) + \frac{Q_2}{V_2}c_3(t) - \frac{Q_1 + Q_2}{V_2}c_4(t)$$

$$c_3(t) = \gamma_1(t)$$

$$c_4(t) = \gamma_2(t)$$

Differential Index

- Example, determine the differential index:



$$\frac{dc_2}{dt} = \frac{Q_1}{V_1}(c_1(t) - c_2(t))$$

$$\frac{dc_4}{dt} = \frac{Q_1}{V_2}c_2(t) + \frac{Q_2}{V_2}c_3(t) - \frac{Q_1 + Q_2}{V_2}c_4(t)$$

$$c_1(t) = \gamma_1(t)$$

$$c_2(t) = \gamma_2(t)$$

Dynamics of DAE Systems

- Solution of stirred tank example 1:

index 1 $c_1(t) = \gamma(t)$

$$c_2(t) = c_2(0)e^{-(Q/V)t} + \frac{Q}{V}\int_0^t \gamma(t')e^{-(Q/V)(t-t')}dt'$$

- Solution of stirred tank example 2:

index 2 $c_1(t) = \gamma(t) + \frac{V}{Q}\dot{\gamma}$ $\quad c_2(t) = \gamma(t)$

- Solution of DAE example 3:

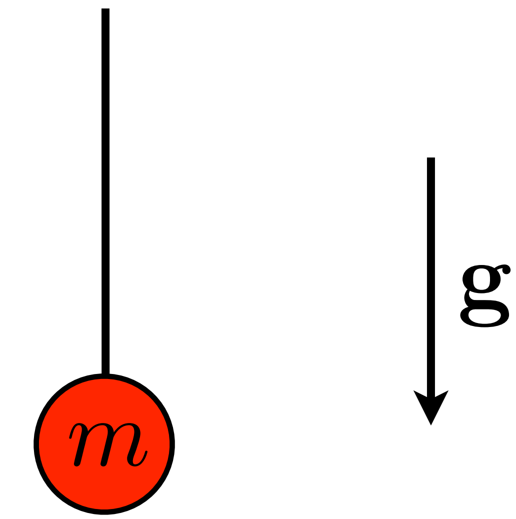
index 3 $c_1(t) = \ddot{\gamma}$ $\quad c_2(t) = \dot{\gamma}$ $\quad c_3(t) = \gamma$

- Higher index indicates greater sensitivity to changes in forcing function.

Dynamics of DAE Systems

- Physical example: pendulum

$$\dot{\mathbf{x}} = \mathbf{v}(t)$$
$$m\dot{\mathbf{v}} = -k(t)\mathbf{x}(t) + m\mathbf{g}$$
$$\|\mathbf{x}(t)\|_2^2 = L^2$$



- position, velocity, stiffness: $\mathbf{x}(t)\ \mathbf{v}(t)\ k(t)$
- Identify differential and algebraic variables.
  $\mathbf{x}(t)\ \mathbf{v}(t)$ $\qquad$ $k(t)$
- Identify index of the DAE system.

(1) $\frac{d}{dt}\|\mathbf{x}(t)\|_2^2 = 2\mathbf{v}(t)\cdot\mathbf{x}(t) = 0$

(2) $\frac{d}{dt}(\mathbf{v}(t)\cdot\mathbf{x}(t)) = \frac{1}{m}(-k(t)\mathbf{x}(t) + m\mathbf{g})\cdot\mathbf{x}(t) + \|\mathbf{v}(t)\|_2^2 = 0$

(3) $\frac{d}{dt}\left(\frac{1}{m}(-k(t)\mathbf{x}(t) + m\mathbf{g})\cdot\mathbf{x}(t) + \|\mathbf{v}(t)\|_2^2\right)$

$$= -\frac{1}{m}\frac{dk}{dt}\|\mathbf{x}(t)\|_2^2 - 2\frac{1}{m}k(t)\mathbf{v}(t)\cdot\mathbf{x}(t) + \mathbf{g}\cdot\mathbf{v} + \frac{2}{m}(-k(t)\mathbf{x}(t) + m\mathbf{g})\cdot\mathbf{v}(t) = 0$$

Simulation of DAE Systems

- Consider DAE example 3:

$$\dot{c}_2 = c_1(t) \qquad\qquad \dot{c}_1 = \dddot{\gamma}$$

$$\dot{c}_3 = c_2(t) \quad \rightarrow \quad \dot{c}_2 = \ddot{\gamma}$$

$$0 = c_3(t) - \gamma(t) \qquad \dot{c}_3 = \dot{\gamma}$$

  - Can't I just solve the set of ODEs found when determining that the DAE system is index-3?

Simulation of DAE Systems

- In general, index-1 semi-explicit DAEs can be safely handled by certain stiff integrators in MATLAB (ode15s, ode23t)
- For generic DAEs, specific DAE solvers are usually needed (SUNDIALS, DAEPACK)
- Initial conditions for such equations must be prescribed consistently, or numerical errors can occur.
  - Consider the pendulum:
    - Can it's initial position be specified arbitrarily?
    - Can it's initial velocity be specified arbitrarily?
    - Can the initial stiffness be specified arbitrarily?

Simulation of DAE Systems

- Consistent initialization of initial value problems: $\{\dot{\mathbf{x}}(0), \mathbf{x}(0)\}$
  - index-0 DAE (ODE-IVP): $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t)$
    - 1. $\mathbf{x}(0) \rightarrow \dot{\mathbf{x}}(0) = \mathbf{f}(\mathbf{x}(0), 0)$
    - 2. $\dot{\mathbf{x}}(0)$ solve $\dot{\mathbf{x}}(0) = \mathbf{f}(\mathbf{x}(0), 0)$
    - 3. $\mathbf{c}(\mathbf{x}(0), \dot{\mathbf{x}}(0)) = 0$ solve with $\dot{\mathbf{x}}(0) = \mathbf{f}(\mathbf{x}(0), 0)$
  - fully implicit DAE: $\mathbf{f}(\mathbf{x}, \dot{\mathbf{x}}, t) = 0$
    - 2N unknowns for N equations
    - apparently N degrees of freedom to specify
    - hidden constraints reduce these degrees
  - with differential states $\mathbf{x}$ and algebraic states $\mathbf{y}$,
    $\mathbf{f}(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{y}, t) = 0 \qquad \{\dot{\mathbf{x}}(0), \mathbf{x}(0), \mathbf{y}(0)\}$

Simulation of DAE Systems

- Consistent initialization, example stirred tank 1:

$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) \quad c_2(t)\right) \quad (1)$$

$$c_1(t) = \quad (t) \quad (2)$$

Convert to system of ODEs

$$\frac{dc_1}{dt} = \, \dot{} \, (t)$$

$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) \quad c_2(t)\right) \quad (3)$$

Consistent initial conditions:

constrained by algebraic equation (2)	constrained by differential equation (3)	unconstrained
$c_1(0) = \gamma(0)$	$\dot{c}_2(0) = \frac{Q}{V}(c_1(0) - c_2(0))$	$c_2(0) = c_0$

Simulation of DAE Systems

- Consistent initialization, example stirred tank 2:

$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) - c_2(t)\right) \quad (1)$$

$$c_2(t) = \gamma(t) \quad (2)$$

Convert to system of ODEs

$$\frac{dc_2}{dt} = \dot{\gamma} \quad (3)$$

$$\frac{dc_1}{dt} = \frac{V}{Q}\ddot{\gamma} + \frac{Q}{V}(c_1(t) - c_2(t))$$

Consistent initial conditions:

constrained by algebraic equation (2)

$$c_2(0) = \gamma(0)$$

constrained by differential equation (1)

$$c_1(0) = c_2(0) + \frac{V}{Q}\dot{c}_2(0)$$

constrained by differential equation (3)

$$\dot{c}_2(0) = \dot{\gamma}(0)$$

Simulation of DAE Systems

- Consider another example:

$$\dot{c}_1 = c_1(t) + c_2(t) + c_3(t)$$
$$\dot{c}_2 = -c_1(t) - c_2(t) + c_3(t)$$
$$0 = c_1(t) + c_2(t)$$

  - Derive consistent initial conditions:

Simulation of DAE Systems

- Consider another example:

$$\dot{c}_1 = c_1(t) + c_2(t) + c_3(t)$$
$$\dot{c}_2 = -c_1(t) - c_2(t) + c_3(t)$$
$$0 = c_1(t) + c_2(t) + 2c_3(t)$$

  - Derive consistent initial conditions: