10.34 Numerical Methods Applied to Chemical Engineering Fall 2015

Homework #5: Differential Algebraic Equations (DAEs)

Problem 1. (35 points) We wish to simulate the concentrations of species A, B, and C in a constant-volume batch chemical reactor with isomerization kinetics

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

where all reactions are elementary, the tank initially contains pure A of concentration $C_A(0) = 1$ mol/liter, at 300 K, the first reaction has the rate constant $k_1 = 1000\ \mathrm{s}^{-1}$, and the second reaction has the rate constant $k_2 = 1\ \mathrm{s}^{-1}$ for the forward reaction and $k_3 = 1\ \mathrm{s}^{-1}$ for the backward reaction. Assume the reactor is isothermal at 300 K. The system of ODEs that you should simulate are

$$\frac{dC_A}{dt} = -k_1 C_A \tag{1}$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B + k_3 C_C \tag{2}$$

$$\frac{dC_C}{dt} = k_2 C_B - k_3 C_C. \tag{3}$$

1. Before proceeding to study this problem computationally, derive and analytical solution that can be used for checking the global truncation error of different computational approaches.

2. Since the total concentration of species is constant, the differential equation for the concentration of C can be re-written as an algebraic equation, so an equivalent DAE model for the process is

$$\frac{dC_A}{dt} = -k_1 C_A \tag{4}$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B + k_3 C_C \tag{5}$$

$$C_A + C_B + C_C = C_A(0) + C_B(0) + C_C(0). \tag{6}$$

   What are the differential variables, algebraic variables, and parameters associated with this system? Calculate the differential index of this DAE system. Write the DAE system in semi-explicit form,

$$\frac{d}{dt}\mathbf{y} = \mathbf{f}(\mathbf{y}, \mathbf{z}, t) \tag{7}$$

$$\mathbf{0} = \mathbf{g}(\mathbf{y}, \mathbf{z}, t). \tag{8}$$

3. Create a MATLABÈ function to numerically solve index-1 DAE systems in semi-explicit form using the backward Euler discretization. You may use any built-in MATLAB functions or code from your past homeworks to solve linear or nonlinear algebraic equations. However, you must code the algorithms for the numerical solution of the index-1 DAE system yourself.

4. Apply your MATLAB function to simulate the DAE system to obtain the concentrations of species A, B, and C in the constant-volume batch chemical reactor with isomerization. Report state trajectories for the three concentrations from $t = 0$ to $t = 10$ for $\Delta t = 0.0001$, 0.001, 0.01, 0.1, 1, and 10.

5. Use the analytical solutions to compute the absolute and relative error in each of your numerical solutions in Part 4 at time $t = \Delta t$ and $t = 10$ for each value of Δt. Plot the local truncation errors v.s. the value of time step size Δt on a loglog plot to determine the observed order of accuracy. Comment on whether your order of accuracy agrees with the theoretical derivation for the implicit Euler algorithm for index-1 DAEs. Do a similar plot for the global truncation error and comment whether its slope on a loglog plot is consistent with theoretical analysis.

6. For the simulation results in Part 4, plot the total computation time of the simulation algorithm vs. Δt. What is the minimum value for Δt that gives good results? Explain whether this value makes sense in terms of the time scales for this system. Is there any advantage to simulating this system as a DAE instead of an ODE? Propose an alternative numerical simulation approach that only requires the solution of two differential equations.

7. Consider the goal of simulating the system under adiabatic conditions rather than isothermal. The reaction rates have an Arrhenius dependence on temperature with energies of activation $E_{A,1} = 1.25 \times 10^4$ J/mol, $E_{A,2} = 1.53 \times 10^4$ J/mol, $E_{A,3} = 1.53 \times 10^4$ J/mol, and the pre-exponential factors can be computed from the values of k_1, k_2, and k_3 given in the problem statement for the temperature $T = 300$ K. The heat capacities for the three species (in J/mol·K) are:

$$C_{p,A} = 26.63 + 0.183\,T - 45.86 \times 10^{-6}\,T^2$$
$$C_{p,B} = 25.04 + 0.098\,T - 30.95 \times 10^{-6}\,T^2$$
$$C_{p,C} = 20.47 + 0.154\,T - 41.85 \times 10^{-6}\,T^2$$

The heats of reaction for the two forward reactions are $\Delta H_{r,1} = -570$ J/mol, $\Delta H_{r,2} = -170$ J/mol. The heat loss to the surroundings is negligible. Write the energy balance for the new adiabatic system as an algebraic equation and write the new system of equations in semi-explicit form. Simulate this system in MATLAB, using an initial temperature of $T = 300$ K, using a value for Δt that gives a global truncation error of less than 1% at the final time. What is the differential index of this new DAE system?

Problem 2. (15 points)

Consider the case of liquid level control for the tank in Figure 1. The tank has one input flow q_1 and one output flow q_2 (volumetric flow rates). The level of the liquid is h and the tank has a cross sectional area A. The dynamics of the system is represented by the conservation law,

$$A\frac{dh}{dt} = q_1 - q_2. \tag{9}$$

Consider h and q_2 as the unknowns of the system. q_1 is known but may not be a constant.

1. Assume the output flow q_2 is proportional to the square root of h by a constant R,

$$q_2 = R\sqrt{h}. \tag{10}$$

Equations 9 and 10 give a DAE system. Derive the index of the DAE system. If the initial liquid level $h(0)$ is known, what initial conditions should you use to satisfy the consistency requirement?

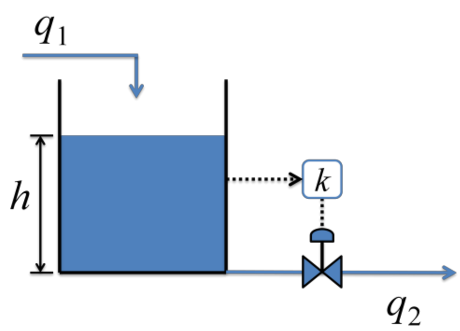

Figure 1: A tank with level control.

2. Assume we have a desired profile of liquid level in the tank,

$$h = \gamma(t) \tag{11}$$

Derive the index of the DAE system of equations 9 and 11. What initial conditions are needed to satisfy the consistency requirement?

3. Assume the input has a periodic profile as,

$$q_1(t) = 0.1 \sin^2(0.02\pi t) \text{ m}^3/\text{s}. \tag{12}$$

Solve the DAE system in part 1 with an initial condition of your choice. You may use MATLAB solvers. The values of the parameters are given as $A = 1 \text{ m}^2$, and $R = 0.1 \text{ m}^{5/2}\text{s}^{-1}$. State the initial conditions you used. Plot (i) the tank level and (ii) the output flow rate. What do you observe in the system characteristics?

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