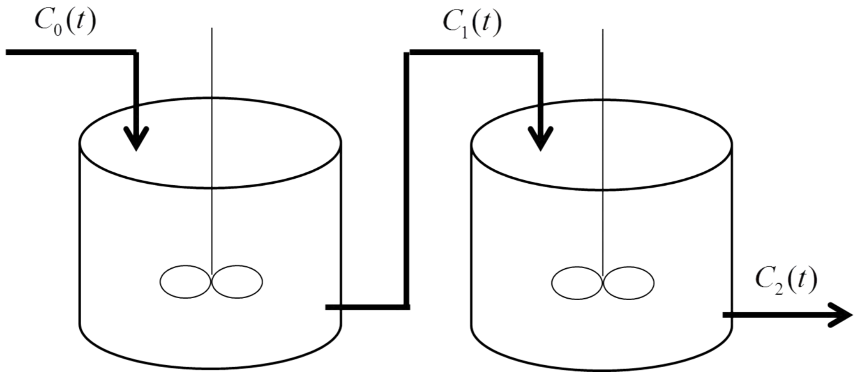
10.34 Numerical Methods Applied to Chemical Engineering

Quiz 2

- This quiz consists of three problems worth 35, 35, and 30 points respectively.
- There are 4 pages in this quiz (including this cover page). Before you begin, please make sure that you have all 4 pages.
- You have 2 hours to complete this quiz.
- You are free to use a calculator or any notes you brought with you.
- The points associated with each part of each problem are included in the problem statement. Please prioritize your time appropriately.

Problem 1. (35 points)

Consider two continuously stirred tank reactors (CSTRs) in series as shown in the figure below.



When $C_2(t)$ is controlled to be some known forcing function $g(t)$ and the reaction kinetics are first order, the dynamics of the system are modeled by

$$\frac{dC_1(t)}{dt} = \frac{C_0(t) - C_1(t)}{\tau} - k_1 C_1(t) \tag{1}$$

$$\frac{dC_2(t)}{dt} = \frac{C_1(t) - C_2(t)}{\tau} - k_2 C_2(t) \tag{2}$$

$$C_2(t) = g(t) \tag{3}$$

where τ denotes the residence time (equal for both reactors), k_1 and k_2 are first-order rate constants, and the states to be simulated are C_0, C_1, and C_2.

1. (12 points) Derive the index of the DAE system (1)–(3), assuming that $g(t)$ is known and infinitely differentiable.

2. (10 points) Determine a consistent initialization for the original variables in the system. If there are additional degrees of freedom, state the initial conditions that can be specified.

3. (6 points) Given $g(t) = t^2$, explicitly compute a consistent initialization at $t_0 = 0$ in terms of any specified variables from part 2 and the parameters τ, k_1, and k_2.

4. (7 points) Using the method of auxiliary (dummy) variables, derive an equivalent index-1 DAE system.

Problem 2. (35 points)

Consider the reaction, convection, and diffusion of an impurity I in a tubular reactor operating at steady state, where an undesired autocatalytic reaction

$$A + I \longrightarrow 2I$$

takes place. Assuming A is in excess, the impurity can be modeled by the second-order differential equation

$$v\frac{dC}{dx} = D\frac{d^2C}{dx^2} + kC_{A0}C \tag{1}$$

where $C(x)$ denotes the concentration of the impurity, $x \in [0, L]$ is the distance from the reactor entrance, v denotes the velocity, D denotes the diffusion coefficient, k denotes the rate constant, and C_{A0} denotes the excess concentration of A. The boundary conditions for this system are:

$$vC(0) - D\left.\frac{dC}{dx}\right|_{x=0} = 0 \tag{2}$$

$$C(L) = C_L \tag{3}$$

where C_L denotes the maximum level of impurity that can be handled in the product.

1. (5 points) Derive an equivalent set of first-order ordinary differential equations (ODEs) for the boundary value problem (1), with the vector of unknown (dependent) variables denoted by $\mathbf{u}(x)$.

2. (3 points) Define a two-point boundary condition function for the converted system of the form

   $$\mathbf{g}(\mathbf{u}(0), \mathbf{u}(L)) = \mathbf{B}_0\mathbf{u}(0) + \mathbf{B}_L\mathbf{u}(L) + \mathbf{b} = \mathbf{0}$$

   Give expressions for $\mathbf{B}_0$, $\mathbf{B}_L$, and $\mathbf{b}$.

3. (7 points) Describe the application of the shooting method on the set of ODEs derived in part 1 to solve the original BVP from $x = 0$ to $x = L$.

4. (8 points) Let D, v, k, $C_{A0} > 0$. Show that a forward Euler integration of the set of ODEs derived in part 1 will be unstable for any choice of step size Δx.

5. (12 points) A colleague suggests shooting backwards from $x = L$ to $x = 0$. Using that approach, can a spatial discretization (i.e., Δx) be chosen so that forward Euler integration is stable? If so, provide an expression for Δx that stabilizes the integration. Are there any advantages to making the change from forward shooting to backward shooting from a numerical point of view? Why, or why not?

Problem 3. (30 points)

Consider a version of the unsteady reaction-convection-diffusion equation applied to electrons in a semiconductor device (i.e., the drift-diffusion equations)

$$\frac{\partial n}{\partial t} = D_n \frac{\partial^2 n}{\partial x^2} + v_d \frac{\partial n}{\partial x} - Bn - Kn^2 \tag{1}$$

where $n(x,t)$ denotes the concentration of electrons, $x \in [0, L]$ defines the spatial variable, D_n denotes the electron diffusion coefficient, v_d denotes the effective drift velocity, and B and K denote band-to-band and Auger recombination rate constants, respectively. The initial and boundary conditions for this system are

$$n(x, 0) = 0 \tag{2}$$

$$n(0, t) = \phi_0 \tag{3}$$

$$n(L, t) = \phi_L \tag{4}$$

where ϕ_0 and ϕ_L are constants.

1. (12 points) Derive method-of-lines equations (using finite differencing) for the PDE (1) that are second-order accurate in space. Grid the spatial domain from $i = 0, 1, \ldots, N+1$. What is the space between nodes, Δx? Define an equation at every node in the interior of the domain and give the initialization for the method-of-lines equations.

2. (12 points) Derive the finite difference equations for the PDE (1) that are second-order accurate in space and first-order accurate in time. Again, grid the spatial domain from $i = 0, 1, \ldots, N+1$ and define an equation at every node in the interior of the domain. Is your method explicit or implicit?

3. (6 points) Estimate the concentration of electrons at the midpoint $x = L/2$ and at time $t = 1$ using the derived finite difference equations from part 2 with a spatial discretization of $\Delta x = L/2$ and temporal discretization of $\Delta t = 1$. Write your answer in terms of parameters and any provided initial and boundary conditions in equations (2)–(4).