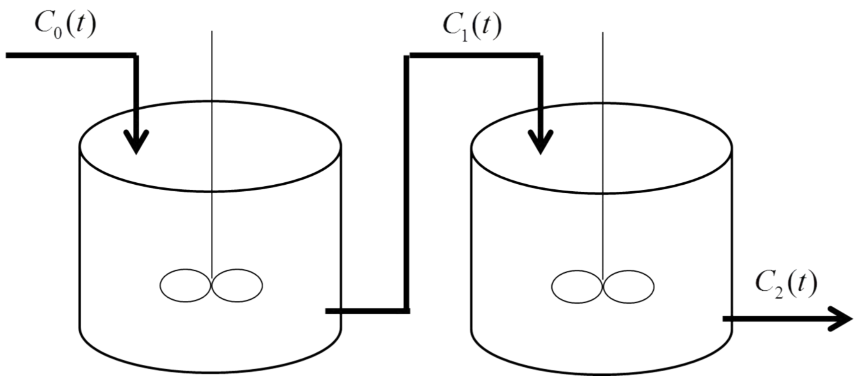
10.34 Numerical Methods Applied to Chemical Engineering

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.

   Solution: The first step is to identify the differential and algebraic variables in the system. The differential variables are $C_1(t)$ and $C_2(t)$, the algebraic variable is $C_0(t)$, and the parameters are τ, k_1, and k_2. To derive the index, we must take derivatives of (1)–(3) until we have a complete set of first-order ODEs for all states. Start with taking a derivative of the algebraic equation,

$$\dot{C}_2(t) = \dot{g}(t). \tag{3$'$}$$

   Substitute (3′) into (2),

$$\dot{g}(t) = \frac{1}{\tau}\Big(C_1(t) - C_2(t)\Big) - k_2 C_2(t). \tag{4$'$}$$

   Take a derivative of (4′),

$$\ddot{g}(t) = \frac{1}{\tau}\Big(\dot{C}_1(t) - \dot{C}_2(t)\Big) - k_2 \dot{C}_2(t). \tag{4$''$}$$

   Substitute (1) into (4″),

$$\ddot{g}(t) = \frac{1}{\tau}\left[\frac{1}{\tau}\Big(C_0(t) - C_1(t)\Big) - k_1 C_1(t) - \dot{C}_2(t)\right] - k_2 \dot{C}_2(t). \tag{5$''$}$$

Rearrange this for $C_0(t)$

$$C_0(t) = \ddot{g}(t)\tau^2 + \big(1 + k_1\tau\big)C_1(t) + \big(\tau + k_2\tau^2\big)\dot{C}_2(t) \tag{5''}$$

Substitute (3′) into this expression and take another derivative,

$$\dot{C}_0(t) = \dddot{g}(t)\tau^2 + \big(1 + k_1\tau\big)\dot{C}_1(t) + \big(\tau + k_2\tau^2\big)\ddot{g}(t) \tag{5'''}$$

We now have a complete set of first-order ODEs given by (1), (2), and (5‴). It took us three derivatives of the orginal ODEs to derive a complete set of ODEs such that the **index is three**.

Deduct 2 points for not specifying complete ODE set.

Deduct at most 10 points for incorrect index depending on exact error.

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.

   Solution: For a consistent initialization, we must specify the original variables in the DAE. We also know that the original equations (1)–(3) must be satisfied at the initial time such that the maximum number of degrees of freedom (DOFs) is given by

$$\begin{array}{rl} 5 & \text{variables } \{C_0(t_0),\ C_1(t_0),\ \dot{C}_1(t_0),\ C_2(t_0),\ \dot{C}_2(t_0)\} \\ \underline{-3} & \text{equations } \{(1),\ (2),\ \text{and } (3)\} \\ 2 & \text{maximum \# of DOFs} \end{array}$$

   However, as derived in part 1, we have an index three problem with implicit constraints that should also be satisfied during initialization. Implicit constraints constrain the values of the original variables in the system. Looking back through part 1, we notice that (3′) and (4″) constrain the values of $\dot{C}_1(t)$ and $\dot{C}_2(t)$, which appear in (1)–(3). Therefore, (3′) and (4″) represent implicit constraints for this system.

   These two additional implicit constraints reduce the degrees of freedom by two. As a result, we expect the system to be completely specified by the forcing function $g(t)$ (i.e., zero DOFs due to implicit constraints). A consistent initialization must satisfy

$$\dot{C}_1(t_0) = \frac{1}{\tau}\Big(C_0(t_0) - C_1(t_0)\Big) - k_1 C_1(t_0) \tag{4}$$

$$\dot{C}_2(t_0) = \frac{1}{\tau}\Big(C_1(t_0) - C_2(t_0)\Big) - k_2 C_2(t_0) \tag{5}$$

$$C_2(t_0) = g(t_0) \tag{6}$$

$$\dot{C}_2(t_0) = \dot{g}(t_0) \tag{7}$$

$$\ddot{g}(t_0) = \frac{1}{\tau}\Big(\dot{C}_1(t_0) - \dot{C}_2(t_0)\Big) - k_2\dot{C}_2(t_0) \tag{8}$$

   [We can determine $C_2(t_0)$ and $\dot{C}_2(t_0)$ from (6) and (7) directly, respectively. We can solve for $C_1(t_0)$ and $\dot{C}_1(t_0)$ by substituting these into (5) and (8), respectively. Lastly, we can use these results to solve for $C_0(t_0)$ using (4).]

   Deduct 5 points for missing implicit constraint (4″).

Deduct at most 3 points for not specifying the variables you need to solve for and what equations they should be determined from.

Deduct at most 2 points for missing the other implicit constraint $(3')$ and math errors.

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.

Solution: Based on our result from part 2, we know that our initialization is specified entirely by the forcing function $g(t_0)$ i.e., there are no additional variables that need to be specified. Let us first derive explicit equations for the consistent initialization entirely in terms of $g(t_0)$,

$$C_2(t_0) = g(t_0)$$

$$\dot{C}_2(t_0) = \dot{g}(t_0)$$

$$C_1(t_0) = \tau\dot{g}(t_0) + (1 + k_2\tau)g(t_0)$$

$$\dot{C}_1(t_0) = \tau\ddot{g}(t_0) + (1 + k_2\tau)\dot{g}(t_0)$$

$$C_0(t_0) = \tau^2\ddot{g}(t_0) + \Big[\tau(1 + k_1\tau) + \tau(1 + k_2\tau)\Big]\dot{g}(t_0) + (1 + k_1\tau)(1 + k_2\tau)g(t_0)$$

Now we must simply insert the value of the function $g(t)$ and its derivatives at $t = 0$. We can easily derive $g(t) = t^2$, $\dot{g}(t) = 2t$, and $\ddot{g}(t) = 2$ such that $g(0) = 0$, $\dot{g}(0) = 0$, and $\ddot{g}(0) = 2$. Substituting these into the above expressions gives a consistent initialization for the original DAE for $g(t) = t^2$ i.e.,

$$C_2(0) = 0$$

$$\dot{C}_2(0) = 0$$

$$C_1(0) = 0$$

$$\dot{C}_1(0) = 2\tau$$

$$C_0(t_0) = 2\tau^2$$

Deduct 2 points for missing for missing implicit constraint $(4'')$, which automatically gives wrong equations for the initial conditions.

Deduct at most 4 points for missing the other implicit constraint and other math errors.

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

Solution: As we know from lecture, we want to satisfy the implicit constraints when solving higher index problems. However, the implicit constraints overspecify the problem such that we have more equations than unknowns. For this problem, we have the original equations

(1), (2), and (3) and implicit constraints (3′) and (4″)

$$\dot{C}_1(t) = \frac{C_0(t) - C_1(t)}{\tau} - k_1 C_1(t) \tag{1}$$

$$\dot{C}_2(t) = \frac{C_1(t) - C_2(t)}{\tau} - k_2 C_2(t) \tag{2}$$

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

$$\dot{C}_2(t) = \dot{g}(t) \tag{3$'$}$$

$$\ddot{g}(t) = \frac{1}{\tau}\Big(\dot{C}_1(t) - \dot{C}_2(t)\Big) - k_2 \dot{C}_2(t) \tag{4$''$}$$

One way to get around this is to use the method of auxiliary (dummy) variables. Here, we have two implicit constraints such that we need to replace two derivatives with auxiliary variables. Only two derivatives appear in these equations such that we must replace $\dot{C}_1(t)$ with some new variable $C_1'(t)$ and $\dot{C}_2(t)$ with some new variable $C_2'(t)$.

$$C_1'(t) = \frac{C_0(t) - C_1(t)}{\tau} - k_1 C_1(t)$$

$$C_2'(t) = \frac{C_1(t) - C_2(t)}{\tau} - k_2 C_2(t)$$

$$C_2(t) = g(t)$$

$$C_2'(t) = \dot{g}(t)$$

$$\ddot{g}(t) = \frac{1}{\tau}\Big(C_1'(t) - C_2'(t)\Big) - k_2 C_2'(t)$$

In this case, we are left with only algebraic equations such that we can solve for all of these variables analytically

$$C_0(t) = \tau^2 \ddot{g}(t) + \Big[\tau(1 + k_1\tau) + \tau(1 + k_2\tau)\Big]\dot{g}(t) + (1 + k_1\tau)(1 + k_2\tau)g(t)$$

$$C_1(t) = \tau\dot{g}(t) + (1 + k_2\tau)g(t)$$

$$C_1'(t) = \tau\ddot{g}(t) + (1 + k_2\tau)\dot{g}(t)$$

$$C_2(t) = g(t)$$

$$C_2'(t) = \dot{g}(t)$$

The system of purely algebraic equations (that are uniquely solvable) is an index-1 DAE since a single derivative results in an equivalent ODE set.

Deduct 5 points for missing both implicit constraint (3′) and (4″) if included elsewhere in the problem. Only deduct 3 points if missing (3′) when included elsewhere in the problem. Deduct 1 point for missing implicit constraint (4″) if not included elsewhere in the problem.

Deduct 2 points for not having a well-posed set of equations.

Deduct 1 point for not verifying your derived DAE was index-1.

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:

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

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

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 $\mathbf{u}(x)$.

   Solution: Let $\mathbf{u} = [\frac{dC}{dx},\ C]^T$. Then the first-order ODE system is

   $$\frac{d\mathbf{u}}{dx} = \begin{bmatrix} \frac{v}{D}u_1 - \frac{kC_{A0}}{D}u_2 \\ u_1 \end{bmatrix} = \mathbf{A}\mathbf{u},$$

   where $\mathbf{A} = \begin{bmatrix} \frac{v}{D} & \frac{-kC_{A0}}{D} \\ 1 & 0 \end{bmatrix}$.

   Deduct at most 3 points for incorrect u

   Deduct at most 2 points for math error in deriving A

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 $\mathbf{b}$.

   Solution: Boundary conditions in terms of $\mathbf{u}$ are

   $$vu_2(0) - Du_1(0) = 0$$
   $$u_2(L) = c_L$$

   which can be rewritten as

   $$\mathbf{g}(\mathbf{u}(0), \mathbf{u}(L)) = \begin{bmatrix} -D & v \\ 0 & 0 \end{bmatrix}\mathbf{u}(0) + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}\mathbf{u}(L) + \begin{bmatrix} 0 \\ -C_L \end{bmatrix} = \mathbf{0}$$

with $\mathbf{B}_0 = \begin{bmatrix} -D & v \\ 0 & 0 \end{bmatrix}$, $\mathbf{B}_L = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$, and $\mathbf{b} = \begin{bmatrix} 0 \\ -C_L \end{bmatrix}$

Deduct 1 point for incorrect $\mathbf{B}_0$

Deduct 1 point for incorrect $\mathbf{B}_L$

Deduct 1 point for incorrect $\mathbf{b}$

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 $x = L$.

Solution: Let $\mathbf{u}(0) = \mathbf{c}$. Initialize $\mathbf{c}(0) = \mathbf{c}_0$ where $\mathbf{c}_0$ is some constant. During any kth iteration of the shooting method, solve the IVP problem,

$$\frac{d\mathbf{u}}{dx} = \mathbf{A}\mathbf{u}, \quad \mathbf{u}(0) = \mathbf{c}_k.$$

Refer to the IVP solution at $x = L$ as $\mathbf{u}(L; \mathbf{c}_k)$. Then calculate the next boundary condition at $x = 0$ based on both boundary conditions by solving the equation,

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

using Newton's method. The Jacobian required for Newton's method is then

$$\mathbf{J} = \frac{\partial \mathbf{g}}{\partial \mathbf{c}} = \mathbf{B}_0 + \mathbf{B}_L \frac{\partial \mathbf{u}(L; \mathbf{c})}{\partial \mathbf{c}}.$$

We can compute the Newton's step for $\Delta \mathbf{c}_k$ with $\mathbf{J}\Delta c_k = -\mathbf{g}$. Using this, we update the boundary condition at $x = 0$ as $\mathbf{c}_k := \Delta \mathbf{c}_k + \alpha \Delta \mathbf{c}$, where α is the damping factor. This new $\mathbf{c}_k$ is then fed to the IVP problem, and the procedure is repeated at the next iteration until the desired tolerance is met.

Deduct 1 point for not initializing shooting method.

Deduct 1 point for not stating the IVP equation.

Deduct 1 point for not defining input and output to function $\mathbf{g}(\mathbf{c}, \mathbf{u}(L; \mathbf{c}))$.

Deduct 1 point for Jacobian in Newton's method.

Deduct 1 point for step size equation.

Deduct 1 point for the update rule in Newton's method.

Deduct 1 point for termination of algorithm.

(Note: Deducted at most 3 points for not connecting IVP solution to Newton's method)

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.

Solution: Check the stability of the original IVP problem by calculating the eigenvalues, λ_1 and λ_2, of $\mathbf{A}$:

$$\det \begin{bmatrix} \frac{v}{D} - \lambda & \frac{-kC_{A0}}{D} \\ 1 & -\lambda \end{bmatrix} = 0$$

$$\lambda_{1,2} = \frac{v}{2D} \pm \frac{1}{2}\sqrt{\left(\frac{v}{D}\right)^2 - 4\frac{kC_{A0}}{D}}$$

For any parameter values that result in eigenvalue with imaginary part, the real part $v/(2D)$ is positive for all positive parameter values. For all positive parameter values in which the eigenvalues are real, $\max\left|\frac{1}{2}\sqrt{\left(\frac{v}{D}\right)^2 - 4\frac{kC_{A0}}{D}}\right| < \frac{v}{2D}$. Hence the real part of both eigenvalues $\lambda_{1,2}$ is greater than zero for all positive parameter values. Hence the forward Euler method would be unstable for any choice of $\Delta x > 0$.

Deduct at most 3 points for incorrect eigenvalues of A.

Deduct 2 points for not showing forward Euler stability condition $|1 + \Delta x\lambda| \leq 1$.

Deduct 1 point for not showing that both eigenvalues have positive real parts.

Deduct 1 point for not stating positive eigenvalues of A lead to unstable forward Euler for any choice of 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?

   Solution: For the backwards shooting method, define $\bar{x} = L - x$, and rewrite the first ODE system for $\bar{\mathbf{u}} = \left[\frac{dC}{d\bar{x}}, C\right]^T$ as

$$\frac{d\bar{\mathbf{u}}}{d\bar{x}} = \bar{\mathbf{A}}\bar{\mathbf{u}},$$

   where $\bar{\mathbf{A}} = \begin{bmatrix} \frac{-v}{D} & \frac{-kC_{A0}}{D} \\ 1 & 0 \end{bmatrix}$. The eigenvalues of $\bar{\mathbf{A}}$ are

$$\lambda_{1,2} = -\frac{v}{2D} \pm \frac{1}{2}\sqrt{\left(\frac{v}{D}\right)^2 - 4\frac{kC_{A0}}{D}}$$

   Now the real part of both eigenvalues $\lambda_{1,2}$ is negative for all positive parameter values, using similar argument as in the previous section. Hence, we can choose some Δx so that the forward Euler integration is stable, making the backward shooting method more numerically advantageous than the forward shooting method for this problem. For the forward Euler integration to be (absolutely) stable requires $|1 + \lambda_{1,2}\Delta x| \leq 1$.

   To derive Δx, we have to consider two cases inside the square root term:

   (a) If $\left(\frac{v}{D}\right)^2 - 4\frac{kC_{A0}}{D} < 0$, then both eigenvalues are complex conjugates. Since $\lambda_{1,2}$ could be complex values in this case, write it as $\lambda_i = a \pm bi$, where $a, b \in \mathbb{R}$ such that $a \equiv \text{Re}(\lambda_i)$ and $b \equiv \text{Im}(\lambda_i)$ Then the stability condition yields,

$$|1 + (a \pm bi)\Delta x| \leq 1$$

   or

$$\sqrt{(1 + a\Delta x)^2 + b^2(\Delta x)^2} \leq 1$$

   We can square both sides and get

$$(1 + a\Delta x)^2 + b^2(\Delta x)^2 \leq 1$$

which gives

$$2a\Delta x + (a^2 + b^2)(\Delta x)^2 \leq 0$$

which since $\Delta x > 0$, simplifies to

$$2a + (a^2 + b^2)\Delta x \leq 0$$

or

$$\Delta x \leq -\frac{2a}{(a^2 + b^2)}.$$

In this case, the real part, $a = -\frac{v}{2D}$, is negative. Let's define $\hat{a} = -a = \frac{v}{2D} > 0$. Then the stability criterion for the step size is

$$\Delta x \leq \frac{2\hat{a}}{(\hat{a}^2 + b^2)}.$$

or

$$\Delta x \leq \frac{2|\text{Re}(\lambda_i)|}{|\lambda_i|^2}$$

since $|\lambda_i|^2 \equiv a^2 + b^2 = \hat{a}^2 + b^2$. We plug in the values for $\hat{a}$ and b to derive the step size in terms of the given parameters.

$$\hat{a} = \frac{v}{2D}$$
$$b = \frac{1}{2}\sqrt{4\frac{kC_{A0}}{D} - \left(\frac{v}{D}\right)^2}$$
$$\Delta x \leq \frac{2\left(\frac{v}{2D}\right)}{\left(\frac{v}{2D}\right)^2 + \frac{1}{4}\left[-\left(\frac{v}{D}\right)^2 + 4\frac{kC_{A0}}{D}\right]}$$

Simplying the above yields,

$$\Delta x \leq \frac{v}{kC_{A0}}.$$

In this case, the step size is bounded only by the ratio of the convection term to the reaction term.

(b) If $\left(\frac{v}{D}\right)^2 - 4\frac{kC_{A0}}{D} \geq 0$, then both eigenvalues are real. For $\lambda_i \in \mathbb{R}$,

$$-1 \leq 1 + \lambda_i \Delta x \leq 1$$

which yields

$$-2 \leq \lambda_i \Delta x \leq 0.$$

Since the real part of the eigenvalue is negative as discussed earlier,

$$\frac{-2}{\lambda_i} \geq \Delta x \geq 0$$

For any $\Delta x > 0$,

$$\Delta x \leq \frac{2}{|\lambda_i|}$$

The two eigenvalues may not be equal in magnitude unless $\left(\frac{v}{D}\right)^2 - 4\frac{kC_{A0}}{D} = 0$. Hence, our step size is then bounded by the eigenvalue with larger magnitude:

$$\Delta x \leq \frac{2}{\max\{|\lambda_1|, |\lambda_2|\}}$$

Since both eigenvalues are negative, the more negative eigenvalue would be the one that is important in determining the stability criterion for the step size:

$$\Delta x \leq \frac{2}{\left| -\frac{v}{2D} - \frac{1}{2}\sqrt{\left(\frac{v}{D}\right)^2 - 4\frac{kC_{A0}}{D}} \right|}$$

$$\therefore \Delta x \leq \frac{2}{\frac{v}{2D} + \frac{1}{2}\sqrt{\left(\frac{v}{D}\right)^2 - 4\frac{kC_{A0}}{D}}}$$

Deduct 3 points for not defining coordinate transformation.

Deduct 2 points for not calculating correct eigenvalues of the new $\bar{\mathbf{A}}$.

Deduct 1 point for not showing the stability criteria $|1 + \lambda\Delta x| \leq 1$. Also, needed to show that λ must be negative for numerical stability $\rightarrow$ backward Euler is numerically advantageous.

Deduct 3 points for not calculating the step size Δx for the real eigenvalue case.

Deduct 3 points for not calculating the step size Δx for the complex eigenvalue case.

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.

   Solution: We grid the spatial domain with nodes positioned at $i = 0, 1, 2, \ldots, N+1$ that correspond to $0,\ \Delta x,\ 2\Delta x, \ldots,\ L$ in the x-direction. There are a total of $N+2$ points and $N+1$ line segments. Therefore, the spacing between nodes is $\Delta x = \frac{L}{N+1}$.

   The method of lines results in a set of ODEs by approximating the spatial derivatives with a finite difference approximation while keeping the time derivatives. Here, we are told to use second-order accurate in space approximations (i.e., central differences)

$$\left.\frac{\partial n}{\partial x}\right|_{(x_i)} \approx \frac{n(x_i + \Delta x, t) - n(x_i - \Delta x, t)}{2\Delta x} = \frac{n_{i+1}(t) - n_{i-1}(t)}{2\Delta x} \tag{5}$$

$$\left.\frac{\partial^2 n}{\partial x^2}\right|_{(x_i)} \approx \frac{n(x_i + \Delta x, t) - 2n(x_i, t) + n(x_i - \Delta x, t)}{(\Delta x)^2} = \frac{n_{i+1}(t) - 2n_i(t) + n_{i-1}(t)}{(\Delta x)^2} \tag{6}$$

   where $n_i(t) = n(i\Delta x, t)$. Substituting these approximations into the PDE (1) evaluated at each node on the interior gives

$$\frac{dn_i}{dt} = D_n \left[\frac{n_{i+1}(t) - 2n_i(t) + n_{i-1}(t)}{(\Delta x)^2}\right] + v_d \left[\frac{n_{i+1}(t) - n_{i-1}(t)}{2\Delta x}\right] - Bn_i(t) - Kn_i(t)^2 \tag{7}$$

$$\forall i = 1, 2, \ldots, N$$

   We must also include the boundary points $n(0,t) = n_0(t) = \phi_0$ and $n(L,t) = n_{N+1}(t) = \phi_L$.

Substituting these into the MOL equations gives

$$\frac{dn_1}{dt} = D_n\left[\frac{n_2(t) - 2n_1(t) + \phi_0}{(\Delta x)^2}\right] + v_d\left[\frac{n_2(t) - \phi_0}{2\Delta x}\right] - Bn_1(t) - Kn_1(t)^2 \tag{8}$$

$$\frac{dn_i}{dt} = D_n\left[\frac{n_{i+1}(t) - 2n_i(t) + n_{i-1}(t)}{(\Delta x)^2}\right] + v_d\left[\frac{n_{i+1}(t) - n_{i-1}(t)}{2\Delta x}\right] - Bn_i(t) - Kn_i(t)^2 \quad \forall i = 2, 3, \ldots, N-1 \tag{9}$$

$$\frac{dn_N}{dt} = D_n\left[\frac{\phi_L - 2n_N(t) + n_{N-1}(t)}{(\Delta x)^2}\right] + v_d\left[\frac{\phi_L - n_{N-1}(t)}{2\Delta x}\right] - Bn_N(t) - Kn_N(t)^2 \tag{10}$$

From the provided initial condition $n(x, 0) = 0$, we know that the electron concentration is zero at all points in space at $t = 0$. This means we initialize the ODEs using $n_1(0) = n_2(0) = n_3(0) = \cdots = n_N(0) = 0$.

Deduct 2 points for incorrect $\Delta x = \frac{L}{N+1}$.

Deduct 1 point for not stating what type of differencing scheme was used for the spatial derivatives and not stating their accuracy.

Deduct at most 5 points for incorrect MOL equations. Only 1 point was deducted for not including the indices for which the equations are valid.

Deduct at most 2 points for incorrect boundary conditions.

Deduct at most 2 points for incorrect initial conditions (including indices).

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?

   Solution: Again, we grid the spatial domain with nodes positioned at $i = 0, 1, 2, \ldots, N+1$ that must correspond to $0, \Delta x, 2\Delta x, \ldots, L$ in the x-direction (the spacing between nodes is $\Delta x = \frac{L}{N+1}$). We also discretize in time with a step size of Δt.

   In the finite difference method, we approximate all derivatives using finite differences. In this case, we are told to use second-order-in-space (central differences) and first-order-in-time (forward or backward) approximations. For simplicity, we will use a forward difference in time approximation (a backward difference could alternatively be chosen). The derivatives in the PDE are then approximated as

$$\left.\frac{\partial n}{\partial t}\right|_{(x_i,t_j)} \approx \frac{n(x_i, t_j + \Delta t) - n(x_i, t_j)}{\Delta t} = \frac{n_i^{j+1} - n_i^j}{\Delta t} \tag{11}$$

$$\left.\frac{\partial n}{\partial x}\right|_{(x_i,t_j)} \approx \frac{n(x_i + \Delta x, t_j) - n(x_i - \Delta x, t_j)}{2\Delta x} = \frac{n_{i+1}^j - n_{i-1}^j}{2\Delta x} \tag{12}$$

$$\left.\frac{\partial^2 n}{\partial x^2}\right|_{(x_i,t_j)} \approx \frac{n(x_i + \Delta x, t_j) - 2n(x_i, t_j) + n(x_i - \Delta x, t_j)}{(\Delta x)^2} = \frac{n_{i+1}^j - 2n_i^j + n_{i-1}^j}{(\Delta x)^2} \tag{13}$$

where $n_i^j = n(i\Delta x, j\Delta t)$. We can substitute these approximations into the original PDE (1), which gives

$$\frac{n_i^{j+1} - n_i^j}{\Delta t} = D_n\left[\frac{n_{i+1}^j - 2n_i^j + n_{i-1}^j}{(\Delta x)^2}\right] + v_d\left[\frac{n_{i+1}^j - n_{i-1}^j}{2\Delta x}\right] - Bn_i^j - K(n_i^j)^2 \quad (14)$$
$$\forall i = 1, 2, \ldots, N, \quad \forall j \geq 0$$

Our boundary conditions must also be included: $n(0,t) = n_0^j = \phi_0$ and $n(L,t) = n_{N+1}^j = \phi_L$ for all $j \geq 0$. Substituting these boundary conditions into the discretized equation gives

$$\frac{n_1^{j+1} - n_1^j}{\Delta t} = D_n\left[\frac{n_2^j - 2n_1^j + \phi_0}{(\Delta x)^2}\right] + v_d\left[\frac{n_2^j - \phi_0}{2\Delta x}\right] - Bn_1^j - K(n_1^j)^2, \quad \forall j \geq 0 \quad (15)$$

$$\frac{n_i^{j+1} - n_i^j}{\Delta t} = D_n\left[\frac{n_{i+1}^j - 2n_i^j + n_{i-1}^j}{(\Delta x)^2}\right] + v_d\left[\frac{n_{i+1}^j - n_{i-1}^j}{2\Delta x}\right] - Bn_i^j - K(n_i^j)^2 \quad (16)$$
$$\forall i = 2, 3, \ldots, N-1, \quad \forall j \geq 0$$

$$\frac{n_N^{j+1} - n_N^j}{\Delta t} = D_n\left[\frac{\phi_L - 2n_N^j + n_{N-1}^j}{(\Delta x)^2}\right] + v_d\left[\frac{\phi_L - n_{N-1}^j}{2\Delta x}\right] - Bn_N^j - K(n_N^j)^2, \quad \forall j \geq 0 \quad (17)$$

We can initialize these algebraic equations using the provided initial condition $n(x,0) = 0$. The discretized form is $n(x,0) = n_i^0 = 0, \ \forall i = 1, \ldots, N$ (i.e., $n_1^0 = n_2^0 = n_3^0 = \cdots = n_N^0 = 0$).

Since we used the forward difference for the time derivative, our method is explicit, which is easily verified by looking at the derived algebraic equations where the unknowns n_i^{j+1} for all $i = 1, \ldots, N$ (all spatial points at the next time instant) appear only once on the left-hand side of the equations. If a backward difference approximation was used for the time derivative, we would get an implicit method as the unknowns would appear on both sides of the equations and would need to be computed by solving nonlinear equations.

Deduct 1 point for not stating what type of differencing scheme was used for the temporal derivative and not stating its accuracy.

Deduct 1 point for not stating what type of differencing scheme was used for the spatial derivatives and not stating their accuracy.

Deduct at most 5 points for incorrect finite difference equations. At most 1 point was deducted for not including the indices for which the equations are valid.

Deduct at most 1 point for incorrect boundary conditions.

Deduct at most 2 points for incorrect initial conditions (including indices).

Deduct 2 points for incorrectly identifying your scheme as 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).

Solution: Here, we can use the derived equations from part 2 of the problem. We only have three total points: $i = 0$ corresponds to $x = 0$, $i = 1$ corresponds to $x = L/2$, and $i = 2$ corresponds to $x = L$. Let us evaluate (14) at our midpoint node $i = 1$ i.e.,

$$\frac{n_1^{j+1} - n_1^j}{\Delta t} = D_n\left[\frac{n_2^j - 2n_1^j + n_0^j}{(\Delta x)^2}\right] + v_d\left[\frac{n_2^j - n_0^j}{2\Delta x}\right] - Bn_1^j - K(n_1^j)^2, \quad j \geq 0 \quad (18)$$

We again know from our boundary conditions that $n(0,t) = n_0^j = \phi_0, \; j \geq 0$ and $n(L,t) = n_2^j = \phi_L, \; j \geq 0$. We also know that $\Delta x = L/2$ and $\Delta t = 1$. Substituting these gives us a reduced expression in terms of our known boundary conditions and parameters

$$n_1^{j+1} - n_1^j = \frac{4D_n}{L^2}\Big(\phi_L - 2n_1^j + \phi_0\Big) + \frac{v_d}{L}\Big(\phi_L - \phi_0\Big) - Bn_1^j - K(n_1^j)^2, \quad j \geq 0 \tag{19}$$

As seen in part 2, the initial condition gives us that our middle node has a value of zero initially. As $j = 0$ corresponds to $t = 0$, we know that $n_1^0 = 0$. The midpoint at $t = 1$ is approximately $n(L/2, 1) = n(\Delta x, \Delta t) \approx n_1^1$. Evaluating (19) at $j = 0$, we can get an explicit approximation for n_1^1 i.e.,

$$n_1^1 - \cancelto{0}{n_1^0} = \frac{4D_n}{L^2}\Big(\phi_L - 2\cancelto{0}{n_1^0} + \phi_0\Big) + \frac{v_d}{L}\Big(\phi_L - \phi_0\Big) - B\cancelto{0}{n_1^0} - K(\cancelto{0}{n_1^0})^2 \tag{20}$$

$$n(L/2, 1) \approx n_1^1 = \frac{4D_n}{L^2}\Big(\phi_L + \phi_0\Big) + \frac{v_d}{L}\Big(\phi_L - \phi_0\Big) \tag{21}$$

Deduct 1 point for incorrect substitution of $\Delta x = L/2$.

Deduct 1 point for incorrect substitution of $\Delta t = 1$.

Deduct at most 4 points for incorrect equations and other math errors.