Assignment 3

Fall, 2024 **06-606**

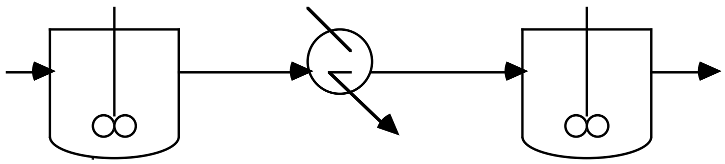
Nonlinear Optimization in Process Systems Engineering

Due: 10/1/24

1. Using Taylor series expansion and the chain rule for partial differentiation for $dy/dx = f(x, y)$, derive the implicit 2nd order Gauss formula

$$y_{n+1} = y_n + k_1$$
$$k_1 = h\, f(x_n+h/2,\ y_n + k_1/2)$$

2. The reaction $A \rightarrow B$ takes place at steady state in two isothermal CSTR reactors in series as shown below in the figure, with a constant flowrate of 100 ft^3/min. Obtain the concentrations C_{A1}, C_{A2} as a function of time given that the inlet concentration C_{A0} is perturbed from 1.5 to 2.0 moles/ft^3. Integrate for the first ten minutes using your favorite method. Plot your results and compare them with the analytical solution.



$V_1 = 500\ ft^3$ $\qquad$ $V_2 = 20\ ft^3$

$k_1 = 0.05\ min^{-1}$ $\qquad$ $k_2 = 38\ min^{-1}$

3. Show that the trapezoidal rule: $y_{n+1} = y_n + h/2\ \{f(x_n,y_n) + f(x_{n+1},y_{n+1})\}$
also corresponds to a 2nd order implicit Runge-Kutta method, and obtain its coefficients in the Butcher block matrix.

4. Show that for any v, the following Runge-Kutta method, is consistent of order 2.

$$y_{n+1} = y_n + 1/2\ (k_2 + k_3),$$
$$k_1 = hf(x_n, y_n)$$
$$k_2 = hf(x_n + vh,\ y_n + v\ k_1)$$
$$k_3 = hf(x_n + (1-v)h,\ y_n + (1-v)\ k_1)$$

5. Investigate the numerical stability of the following methods for $y' = \lambda y$, $\lambda < 0$

i) $y_{n+1} = y_n + h/12[\ 5f_{n+1} + 8f_n - f_{n-1}]$ (3rd Order Adams-Moulton Corrector)
ii) $y_{n+1} = y_{n-1} + h/3[\ f_{n+1} + 4f_n + f_{n-1}]$ (Milne-Simpson Formula)
iii) $y_{n+1} = y_{n-1} + h/2[\ f_n + 3f_{n-1}]$

6. The equation $y' = -Ay + B$ has a general solution $y(x) = c\ e^{-Ax} + B/A$ where c is an arbitrary constant and thus $y(x) \dashrightarrow B/A$ as x goes to infinity. If Euler's method is applied to this equation, show that $y_n \dashrightarrow B/A$ as n goes to infinity only if $h < 2/A$.

7. Consider the system

$y_1' = -0.1\ y_1 - 49.9\ y_2 \qquad y_1(0) = 3$
$y_2' = -50\ y_2 \qquad y_2(0) = 1.5$
$y_3' = 70\ y_2 - 120\ y_3 \quad y_3(0) = 3$

a) Calculate the stiffness ratio and the eigenvalues for this system
b) Find the analytic solution.
c) Find the maximum value for which h is stable for a fourth order explicit Runge-Kutta method (see Carnahan and Wilkes paper on website for the stability plot.)