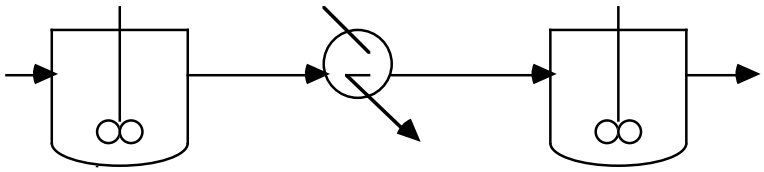
Fall, 2024 **06-606**

Nonlinear Optimization in Process Systems Engineering

Due: 10/24/24

1. The reaction A → B takes place at steady state in two CSTR reactors in series as shown below in the figure. Obtain the concentrations C_{A0} and C_{A1} as a function of time given that the outlet concentration C_{A2} is given as a function of time: $C_{A2} = 0.1 - 0.005t$. Plot your results for the first 10 minutes by solving the problem analytically.

Feed = 100 ft^3/min



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

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

(Isothermal) (Isothermal)

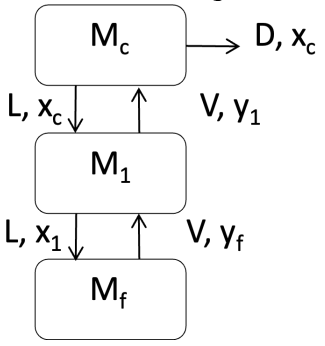
2. Find a consistent initial condition for this system and solve this problem (as stated) using some DAE solver. Which one would you choose?

3. What is the index of the above problem? Using the structure of these equations, reformulate the system to index 1 and solve for the first 10 minutes with your favorite DAE solver.

4. Formulate this problem using an index two (intermediate form) from problem 3. Choose initial conditions that are not consistent and solve the system using your favorite DAE solver.

5. For problems 2. to 4., comment on the performance of your solver for each solution. Compare your results to the analytic solution in problem 1.

6. Consider the model for the binary 2-stage distillation system given below, where α is the relative volatility. The mass balance equations can be written as:



$M_f' = L - V$

$(M_f x_f)' = L x_1 - V y_f$

$(M_1 x_1)' = L (x_c - x_1) + V (y_f - y_1)$

$(M_c)' = V - (L + D)$

$(M_c x_c)' = V y_1 - (L+D) x_c$

$y_1 - \alpha x_1 / [1+ (\alpha - 1) x_1] = 0$

$y_f - \alpha x_f / [1+ (\alpha - 1) x_f] = 0$

$M_f = f_0(t)$, $M_1 = f_1(t)$

$L - 1.5 D = 0$

$V = g(t)$

a) Formulate this problem as a semi-explicit DAE system. What is its index?
b) Reformulate this problem to an index 1 system.