Homework 16

Problem 1

Solve the following ODE

$$\frac{dy}{dt} = ye^{-t}$$

to $t = 6$. Plot the resulting function $y(t)$. The initial condition is $y_0 = 1$.

In [ ]:

Problem 2

For the following first order reaction $A \to B$, solve for the concentration of A in time if the initial concentration $A_0 = 1.0$, and the reaction rate is given by

$$\frac{dC_A}{dt} = -kC_A.$$

where k=2.0.

Part a

Make a plot of C_A versus time.

Part b

Calculate the product composition, $C_B(t)$ by solving the additional equation

$$\frac{dC_B}{dt} = kC_A.$$

Include it on the plot of Part a.

In [ ]:

Problem 3

We are performing a chemical reaction as follows.

$$\text{Rxn 1:} \qquad A + B \to C \; \text{Rxn 2:} \qquad B + C \to D$$

Here, symbols A, B, C, D denote species concentrations in mol/L. The initial concentrations are $A_0 = 1$, $B_0 = 1$, $C_0 = 0$, $D_0 = 0$. Also, $k_1 = 1\, L/mol * s$, and $k_2 = 1.5\, L/mol * s$.

Solve for the concentrations of A, B, C, and D as functions of time. Solve at timestep intervals of $dt = 0.2\, s$ and solve to a final time of $t = 3\, s$. Also, solve for the selectivity defined as $S = C/(C + D)$ as a function of time. (S is initially undefined, but you can set it equal to 1 at $t = 0$.) Use ODEINT (not Euler's equation) applied to each d(Species)/dt above.

Plot the concentrations of A, B, C, D, and S as functions of time on the same plot. Label the axes as "time (s)" and “concentration (mol/L)”. You can compare your solution to problem 2 from HW 5 where Euler's method is used to solve the same problem.

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