1) You were lucky enough to be selected for a Summer REU position at Hogwarts School of Witchcraft and Wizardry in the Potion Engineering Department. Upon arrival, you immediately are pulled aside by one of the Cauldron Design TAs, Ron Weasley. He is freaking out because he has no idea what he's doing. He begs for your help in sizing non-isothermal, adiabatic cauldrons (similar to the reactors that muggles use). He says that the liquid-phase, reversible reaction has the chemical equation

$$A + B \leftrightarrow 2C$$

and follows an elementary rate law. The class instructor, Prof. Snape, said the reactor should have an inlet flow rate of 1000 m<sub>3</sub>/hr and equimolar concentrations of A and B equal to 10 mol/L, or else there will be "consequences," whatever that means.

You also know the following information:

 $\begin{array}{lll} C_{P,A} = 140 \ cal/(mol \ K) & kf (30 \ ^{\circ}C) = 1.8 \ L/(mol \ hr) \\ C_{P,B} = 100 \ cal/(mol \ K) & Kc (30 \ ^{\circ}C) = 25.0 \\ C_{P,C} = 120 \ cal/(mol \ K) & H_{rxn}^{\circ}(30 \ ^{\circ}C) = -7.6 \ kcal/mol \\ \end{array}$ 

X	0.1	0.2	0.3	0.4	0.5	0.6
Fao/-ra [m3]						

- **a.** Calculate and tabulate FA0/-rA values for the conversions in the table above and generate a Levenspiel plot. Be sure to label axes appropriately. (Note: deriving each relationship and then using Python to calculate all values at once probably makes life easier)
  - **b.** Assuming the data generated in part (a) sufficiently approximates the Levenspiel plot and that a continuously stirred tank cauldron will be used first, followed by a plug-flow cauldron, what are the volumes of each cauldron such that the total volume is minimized?
  - **c.** Ron was originally going to assume a single plug-flow cauldron would give the smallest volume. How much bigger would a single plug-flow cauldron be compared to the volume of cauldrons in series from your answer in part (b)?

## **4)** The elementary liquid-phase reactions

## A B C

take place in a non-isothermal 100-L CSTR with heat effects. The volumetric feed rate is 1000 L/min at a concentration of A of 0.3 mol/L with an inlet temperature of 20  $^{\circ}$ C.

Additional Information

 $C_{P,A} = C_{P,B} = C_{P,C} = 200 \text{ J/mol} \cdot \text{K}$ 

 $k_1 = 1.3 \text{ min-1}$  at 300 K, with  $E_1 = 11.9 \text{ kcal/mol}$ 

 $k_2 = 3.5 \text{ min-1}$  at 500 K, with  $E_2 = 23.0 \text{ kcal/mol}$ 

 $\Delta H_{Rx1A} = -38.0 \text{ kJ/mol A}$ 

 $\Delta H_{Rx1B} = -65.0 \text{ kJ/mol B}$ 

 $UA = 30.0 \text{ kJ/mol} \cdot \text{K} \text{ with } T_a = 57 \text{ }^{\circ}\text{C}$ 

**a.** At what temperatures are the different steady states and what are the effluent concentrations for each species at each steady state? Be sure to include your plot of G(T), R(T) vs T with properly labeled axes and a legend. (Note: you do not need

polymath to plot G(T) and R(T) vs T, Python can be used to plot them) **b.** By comparing the selectivities of B/C, which steady state would you choose if you wanted to maximize formation of B?