Tut 2

1. For the first order liquid phase reaction A → B occurring in an adiabatic CSTR, the following information is available

Parameter	Value	Units
C_{A_O}	0.1	$mol.L^{-1}$
Q_o	2	$L.s^{-1}$
V	500	L
k_o	20000	s^{-1}
E	55000	$J.mol^{-1}$
$\Delta H_{RX_{298}}$	-30	$kJ.mol^{-1}$
C_{p_A}	157.9	$J.mol^{-1}.K^{-1}$
C_{p_B}	157.9	$J.mol^{-1}.K^{-1}$

a) Given an inlet temperature of 340 K, what is the conversion in the reactor*? (hint: Plot the two equations that you have to solve simultaneously as a function of the two variables, T on x-axis and x on y-axis to "see" the solution. Then fine tune by using fsolve!)*

b) If the inlet flow rate is changed to 0.8 l/s, how will the conversion change? Are there any additional advantages to doing this? *(Now you can use your plots in a) to see the effect of a change in Q on your mole balance – LOVING python).*

c) By how much should the inlet temperature be altered to improve the controllability of the design in (a)? (*I will be OK with an approximate answer here – do not try to "design" a fancy solver. Use the figures you constructed in a))*

d) The student who determined the activation energy of the reaction did not work accurately enough. The real value is closer to $E = 60000\,J.mol^{-1}$. How will this affect the design in (a)? *(Spare a thought for the responsibility you have if you are the one shaping the rate equation of a specific reaction from laboratory data…)*

e) If additional heat was added to the reactor) in (a) by means of a constant temperature utility, what must the utility temperature be to obtain 95% conversion? Are multiple steady states a problem in this case? (Use UA=31.6W/K)

Suggestion: If you have time, use interact from ipywidgets in Python and change Q, $Q, \Delta H. E$ & T_0 in order to see how each of the parameters will affect the plots! Not compulsory, but really cool.

2. The irreversible liquid phase oligomerization reaction where:

$$2A \rightarrow B$$

takes place in two ***adiabatic*** CSTR reactors operated in series (*See Figure*). The volumetric flow rate to the first reactor is $\boldsymbol{Q_o = 5\ \ell.min^{-1}}$. It contains pure A at a concentration of $\boldsymbol{C_{A_o} = 2\ mol.\ell^{-1}}$. The inlet temperature to this first reactor is $\boldsymbol{T_o = 325\ K}$ and its volume is: $\boldsymbol{V_1 = 150\ \ell}$. An elementary rate expression may be assumed for the reaction rate of component A, i.e. $\boldsymbol{r_A = -kC_A^2}$. Additional data on the reaction are given in the table below:

Parameter	Value	Units
k @ 300 K	6.69×10^{-4}	$\ell.mol_A^{-1}.min^{-1}$
E	55000	$J.mol^{-1}$
$\Delta H^*_{RX_{298}}$	-8500	$J.mol_{RX}^{-1}$
C_{p_A}	*55*	$J.mol^{-1}.K^{-1}$
C_{p_B}	*110*	$J.mol^{-1}.K^{-1}$

*Note the units of ΔH_{RX} !

The products from the first reactor are separated by appropriate processing and only the unconverted A is fed to the second reactor. You may assume the separation process to be isothermal (see the illustration given below). Also $\rho_A \approx \rho_B\ kg.m^{-3}$.

a) Can multiple steady states be a problem in RX1? Prove your answer.
b) What must the volume of the second reactor be if the ***overall*** conversion of reactant A (i.e. in the two reactor system) must be 90 %?
c) Compare the conversion of A that can be achieved in an adiabatic PFR with the same volume and inlet conditions as **RX1** (i.e. $\boldsymbol{V = 150\ \ell}$ and with $\boldsymbol{T_o, C_{A_o}, Q_o}$**),** to the conversion that can be achieved in **RX1** (the first adiabatic CSTR). Explain the difference (or similarity) in the calculated conversions (remember a picture paints a thousand words).
d) If you have time: Design an optimal reactor “train” to achieve 90% conversion if you do NOT plan to separate unconverted A from B after the first reactor. (i.e. select reactor types operating in series, size each reactor). Separation is an EXPENSIVE process. Easy to do in a Tut problem, but a few million R in a real-life large-scale plant.