

Tut 2

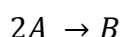
1. For the first order liquid phase reaction $A \rightarrow B$ occurring in an adiabatic CSTR, the following information is available

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	$\text{J. mol}^{-1}. \text{K}^{-1}$
C_{p_B}	157.9	$\text{J. mol}^{-1}. \text{K}^{-1}$

- 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 $E = 60000 \text{ J. mol}^{-1}$. 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 $UA=31.6\text{W/K}$)

Suggestion: If you have time, use interact from ipywidgets in Python and change Q , ΔH , E & T_o 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:



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

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

*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 $\rho_A \approx \rho_B \text{ kg} \cdot \text{m}^{-3}$.

- Can multiple steady states be a problem in RX1? Prove your answer.
- 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 %?
- Compare the conversion of A that can be achieved in an adiabatic PFR with the same volume and inlet conditions as **RX1** (i.e. $V = 150 \ell$ and with 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).
- 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.

