Reactor Engineering Week 6 Problem Set

Question 1a - Parallel Plug Flow
Jeremy has been conducting the following isothermal, liquid-phase reaction

$$\mathrm{A} \xrightarrow{\mathrm{k_2}} \mathrm{B} \tag{1}$$

inside his favourite plug flow reactor, the PFR-3000®. The reaction is second order in A with reaction rate constant k_2, the inlet concentration of A into the plug flow reactor is C_{A0}, the reactor volume is V, and the volumetric flow rate is υ. However, two new miniature PFR's - the all new PFR-1500®! - have just arrived in the post, and as his sister is away on summer camp, her bedroom is free for him to set up a new experiment! He is interested in modifying his reactor as follows. He will replace his single plug flow reactor with two smaller plug flow reactors, each of which is half the size of his original reactor (i.e. each has volume $V/2$), and they will operate in parallel. In particular, the inlet stream will be split into 2 streams of equal flow rate (each will have flow of $\upsilon/2$). One stream will be the inlet stream to one reactor, and the other stream will be the inlet to the other reactor. The two reactor outlet streams will be combined to form an overall outlet stream.

Find an expression for the overall conversion provided by these two reactors-in-parallel. How does it compare with the original, single reactor? Is this an intuitively obvious result?

Question 1b - Fancy Parallel Plug Flow
Jeremy has decided to make the system we described above a little more sophisticated. Rather than splitting the stream evenly between the two reactors (so each has volumetric flow rate of $\upsilon/2$) he is going to split the two streams unevenly, so one has volumetric flow rate of $\xi\upsilon$ and the other $(1-\xi)\upsilon$, where $0 \leq \xi \leq 1$. Nothing else is changed from part (a). Find an expression for the overall conversion of A once the outlet streams of the two reactors are recombined. Is there an optimal splitting ratio ξ that will maximise the conversion?

Question 2a - Parallel Mixed Flow
Jeremy was so interested in his findings above, he wants to repeat them with some mixed flow reactors! Suppose that the reaction, reactor and feed conditions are the same as in question 1(a), except the PFR of volume V is replaced by a CSTR of volume V, and the two small PFR's of volume $V/2$ are replaced by two small CSTR's of volume $V/2$. If the stream is split evenly between the two CSTR's in parallel (so each have inlet volumetric flow rate $\upsilon/2$) how does the overall reaction conversion once the outlet streams are recombined compare with the outlet conversion from the single, larger CSTR reactor? Once again, is this result intuitively obvious?

Question 2b - Fancy Parallel Mixed Flow
What if the stream is split unevenly, and so the volumetric flow rate to one reactor is $\xi\upsilon$, and the flow to the other is $(1-\xi)\upsilon$? Is there an optimal splitting ratio υ that maximises the overall conversion once the two outlet streams are recombined?

Question 2c - Parallel Mixed Flow vs Series Mixed Flow
How do the CSTR's in parallel compare with the same CSTR's placed in series instead (with the overall flow rate υ held constant)? Does the optimal parallel set-up found in part 2(b) achieve better conversion than if the CSTR's were placed in series instead?

Question 2d - Parallel Plug Flow vs Series Plug Flow
Why didn't I bother asking an equivalent of question 2(c) for the plug flow reactor system? :)

Question 3a - Modifying MFR Reactor Flows

A mixed flow reactor of volume V has an inlet stream of volumetric flow rate υ which contains A at initial concentration C_{A0}. The following liquid phase reaction occurs inside the reactor:

$$\mathrm{A} \xrightarrow{\mathrm{k_1}} \mathrm{B} \tag{2}$$

This reaction is first order in A with reaction rate constant k_1. If the outlet conversion of A is currently X_A, and the volumetric flow rate is changed to $\alpha\upsilon$ ($\alpha > 0$) but nothing else is changed, find an expression for the new outlet conversion, $X_{A,\mathrm{new}}$.

Question 3b - Modifying MFR Kinetics

Consider the MFR reactor under the same conditions as described in part (a) (with volumetric flow rate υ). A catalyst is added to the inlet stream which increases the reaction rate to βk_1 ($\beta > 0$). If the conversion before the catalyst was added was X_A, find an expression for the new outlet conversion, $X_{A,\mathrm{catalysed}}$.

Question 3c - Modifying Reaction Mechanisms

Consider the MFR reactor under the same conditions as described in part (a), except consider a general, nth order reaction with nth order reaction rate constant k_n. Find a general expression relating C_{A0}, the outlet conversion X_A, and the space-time τ. If an MFR is conducting a reaction which undergoes only a very, very small degree of conversion X_A (as might happen if the product is only produced in trace amounts) show that

$$X_A = \frac{\tau k_n C_{A0}^{n-1}}{1 + n\tau k_n C_{A0}^{n-1}} \tag{3}$$

Fun-and-Insightful-Fredo-Frog-Challenge-Question

Note: This is a challenging question. Any student who can solve this question within a week will be eligible for a Fredo Frog.

Alice is back on the hunt for a get-rich-quick scheme with yet another creative idea! Her company conducts the following isothermal, liquid phase reaction in an ideal plug-flow reactor:

$$\mathrm{A} + \mathrm{B} \xrightarrow{\mathrm{k_2}} \mathrm{C} \tag{4}$$

The reaction is first order in both A and B, with second-order reaction rate constant k_2. The reactor has two feed streams, one containing A and one containing B, and these are mixed together at the entrance of the reactor. The initial concentration of A and B in their individual feed streams (before the streams are mixed at the inlet of the reactor) are C_{A0} and C_{B0} respectively, and the volumetric flow rates of these individual feed streams (υ_A and υ_B) are chosen so there is an equimolar flow of A and B into the reactor.

Alice has noticed that C_{A0} is much greater than C_{B0}, and so (to ensure equimolar flow) υ_B is much greater than υ_A. She believes that the large volume of the stream containing B is diluting the stream containing A, and is slowing down the reaction. She proposes her company exchange their standard plug flow reactor with her new (and outrageously expensive) design, the Alice-the-Great-Injecto-Wizard-4000®.

In Alice's design, the two streams are not completely combined at the entrance of the reactor. Instead, the more dilute stream (in this case, the stream containing B) is injected at various points along the length of the reactor. More precisely: $1/n$th of the stream containing B is combined with the stream containing A at the reactor inlet, while the rest of the stream containing B is injected in equal amounts at $n-1$ injection points evenly spaced along the length of the reactor. The overall molar flow of A and B remain identical, the only difference being that all of A is injected at the reactor entrance, while B is injected at n locations simultaneously. In this way, Alice hopes to increase the average concentration of A, which should speed up the reaction and reduce the overall reactor volume.

If a conversion of A of X_A is required at the reactor outlet, find an expression for the ratio of the volume of Alice's new design, V_{Alice}, to the volume of the original reactor, V_{PFR}. Under what conditions, if any, will Alice's design reduce the reactor volume?

Bonus: *Are evenly-spaced injection points the most efficient placement? If Alice can position her $n-1$ injection points anywhere along the length of her reactor, where should they be placed to minimise reactor volume for a given reaction conversion at the outlet?*

Solutions

Question 1a

The design equation for a single PFR is:

$$V = C_{A0}\upsilon \int_0^{X_A} \frac{dX_A}{-r_A} \tag{5}$$

and for our system $r_A = -k_2 C_{A0}^2 (1 - X_A)^2$, and so

$$V = C_{A0}\upsilon \int_0^{X_A} \frac{dX_A}{k_2 C_{A0}^2 (1 - X_A)^2} \tag{6}$$

and we can actually just solve the question here. Each reactor is half the volume of the original, so the volume of each small reactor $V_{\text{small}} = V/2$. However, the flow rate is also halved, so $\upsilon_{\text{small}} = \upsilon/2$. But these factors of 1/2 just cancel inside (6), and so the conversion coming out of each of the smaller reactos is exactly the same as the conversion coming out of the single, large PFR. Thus, the two small reactors act exactly the same as a single large reactor. This is intuitively obvious, as the two identical PFR's in parallel can just be thought of as one larger PFR with an axial plate cutting it in half down the middle.

Question 1b

We have to be a little more careful here. The conversion X_{A1} out of the reactor with flow rate $\xi\upsilon$ is related to its volume, $V_{\text{small}} = V/2$, by

$$\frac{k_2 C_{A0} V}{2\xi\upsilon} = \int_0^{X_{A1}} \frac{dX_A}{(1 - X_A)^2} = \frac{X_{A1}}{1 - X_{A1}} \tag{7}$$

In a similar way, in the second reactor

$$\frac{k_2 C_{A0} V}{2(1-\xi)\upsilon} = \int_0^{X_{A2}} \frac{dX_A}{(1 - X_A)^2} = \frac{X_{A2}}{1 - X_{A2}} \tag{8}$$

If we define $\alpha \equiv k_2 C_{A0} V/\upsilon$, then we have

$$X_{A1} = \frac{\alpha/2\xi}{1 + \alpha/2\xi} = \frac{\alpha}{2\xi + \alpha} \tag{9}$$

Similarly,

$$X_{A2} = \frac{\alpha}{2(1-\xi) + \alpha} \tag{10}$$

The overall conversion in the combined stream is calculated by adding the total flow of A in each stream, and dividing by the overall volumetric flow rate. We firstly calculate the overall concetration in the combined outlet stream

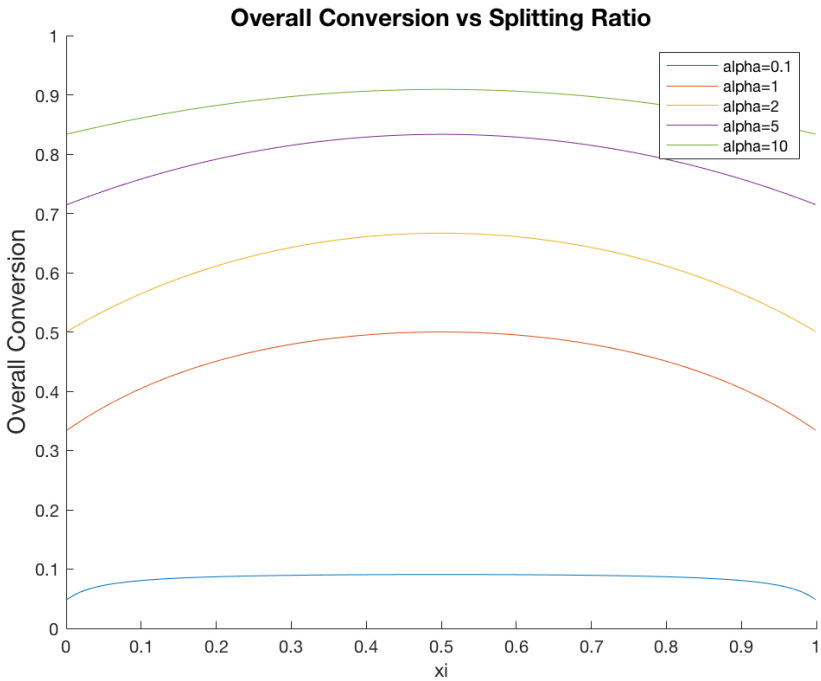
$$C_{A,\text{overall}} = \frac{\xi\upsilon C_{A0}(1 - X_{A1}) + (1-\xi)\upsilon C_{A0}(1 - X_{A2})}{\upsilon} = \xi C_{A0}(1 - X_{A1}) + (1-\xi)C_{A0}(1 - X_{A2}) \tag{11}$$

$$\frac{C_{A,\text{overall}}}{C_{A0}} = \frac{2\xi^2}{2\xi + \alpha} + \frac{2(1-\xi)^2}{2(1-\xi) + \alpha} \tag{12}$$

and $X_{A,\text{overall}}$ is given by

$$X_{A,\text{overall}} = 1 - \frac{2\xi^2}{2\xi + \alpha} - \frac{2(1-\xi)^2}{2(1-\xi) + \alpha} \tag{13}$$

Now we must look for the value of ξ that maximises the conversion. We should take the derivative and find the point where $\partial X_{A,\text{overall}}/\partial\xi = 0$, however we can get our answer a little quicker by making a plot of $X_{A,\text{overall}}$ against ξ for various values of α. As a side note, you may notice that I'm much quicker in general to make plots rather than to do all the messy calculus. Messy calculus is good and important, and you should be very good at it. However, it's easy to go wrong with messy calculus. You have all the tools at your disposal to make plots of these kinds of functions (MATLAB, Python, Julia, Octave, Excel (if you *must!*), etc.) and you should get in the habit of making a quick plot when you face these kinds of



questions. The plot, shown below, is quite clear - $\xi = 0.5$ maximises our conversion, and so there is no point attempting some assymetrical split, at least in this case with 2nd order reaction.

Question 2a

This question is very similar to question 1a. The design equation for an MFR with 2nd order chemical reaction is

$$\frac{k_2 C_{A0} V}{v} = \frac{X_A}{(1 - X_A)^2} \tag{14}$$

and we see that halving both the V and the flow rate, v, has no effect on the outlet conversion X_A. Once again, then, splitting the stream into two equal streams flowing through two equally sized reactors with half the volume of the original reactor does not affect the overall conversion in any way.

Question 2b

This also flows in a similar way to Question 1b. We again define $\alpha = k_2 C_{A0} V/v$, so that, through the first MFR with volume $V/2$, flow-rate ξv we have

$$\frac{\alpha}{2\xi} = \frac{X_{A1}}{(1 - X_{A1})^2} \tag{15}$$

and

$$\frac{\alpha}{2(1-\xi)} = \frac{X_{A2}}{(1 - X_{A2})^2}. \tag{16}$$

We will express this in terms of the outlet concentration from each of the smaller CSTR's, as this will be what we will use to calculate the average concentration:

$$\frac{\alpha}{2\xi C_{A0}} = \frac{C_{A0} - C_{A1}}{C_{A1}^2} \tag{17}$$

where $C_{A1} = C_{A0}(1 - X_{A1})$ is the concentration coming out of the first CSTR. We also have

$$\frac{\alpha}{2(1-\xi) C_{A0}} = \frac{C_{A0} - C_{A2}}{C_{A2}^2} \tag{18}$$

Rearranging, we get

$$C_{A1}^2 + \frac{2\xi C_{A0}}{\alpha} C_{A1} - \frac{2\xi C_{A0}^2}{\alpha} = 0 \tag{19}$$

and

$$C_{A1} = \frac{-\frac{2\xi C_{A0}}{\alpha} + \sqrt{\left(\frac{2\xi C_{A0}}{\alpha}\right)^2 - 4\frac{2\xi C_{A0}^2}{\alpha}}}{2} = \frac{\xi C_{A0}}{\alpha}\left(-1 + \sqrt{1 + \frac{2\alpha}{\xi}}\right) \tag{20}$$

Similarly,

$$C_{A2} = \frac{(1-\xi)C_{A0}}{\alpha}\left(-1 + \sqrt{1 + \frac{2\alpha}{(1-\xi)}}\right) \tag{21}$$

And the overall average concentration is given by

$$C_{A,\text{overall}} = \frac{\xi v C_{A1} + (1-\xi) v C_{A1}}{v} = \xi C_{A1} + (1-\xi) C_{A1} \tag{22}$$

$$C_{A,\text{overall}} = \frac{\xi^2 C_{A0}}{\alpha}\left(-1 + \sqrt{1 + \frac{2\alpha}{\xi}}\right) + \frac{(1-\xi)^2 C_{A0}}{\alpha}\left(-1 + \sqrt{1 + \frac{2\alpha}{(1-\xi)}}\right) \tag{23}$$

and $X_{A,\text{overall}} = 1 - C_{A,\text{overall}}/C_{A0}$ is given by

$$X_{A,\text{overall}} = 1 - \frac{\xi^2}{\alpha}\left(-1 + \sqrt{1 + \frac{2\alpha}{\xi}}\right) - \frac{(1-\xi)^2}{\alpha}\left(-1 + \sqrt{1 + \frac{2\alpha}{(1-\xi)}}\right) \tag{24}$$

As in question 1b, we could take a derivative here to work out the maximum, but it's a little simpler just to make a plot. Once again, we see that the optimal splitting ratio is $\xi = 0.5$, where we split the flow 50/50. When this is the case

$$X_{A,\text{overall}} = 1 - \frac{1}{2\alpha}\left(-1 + \sqrt{1 + 4\alpha}\right) \tag{25}$$

On the other hand, for a single CSTR of volume V and flow rate v, we have

$$\alpha = \frac{X_A}{(1 - X_A)^2} \tag{26}$$

and so

$$X_A^2 - 2X_A + 1 - \frac{X_A}{\alpha} = X_A^2 - \frac{2\alpha + 1}{\alpha} X_A + 1 = 0 \tag{27}$$

So

$$X_A = \frac{\frac{2\alpha+1}{\alpha} - \sqrt{\left(\frac{2\alpha+1}{\alpha}\right)^2 - 4}}{2} = \frac{2\alpha+1}{2\alpha} - \sqrt{\left(\frac{2\alpha+1}{2\alpha}\right)^2 - 1} \tag{28}$$

$$X_A = 1 + \frac{1}{2\alpha} - \sqrt{\frac{1}{\alpha} + \frac{1}{4\alpha^2}} = 1 - \frac{1}{2\alpha}(-1 + \sqrt{1 + 4\alpha}) \tag{29}$$

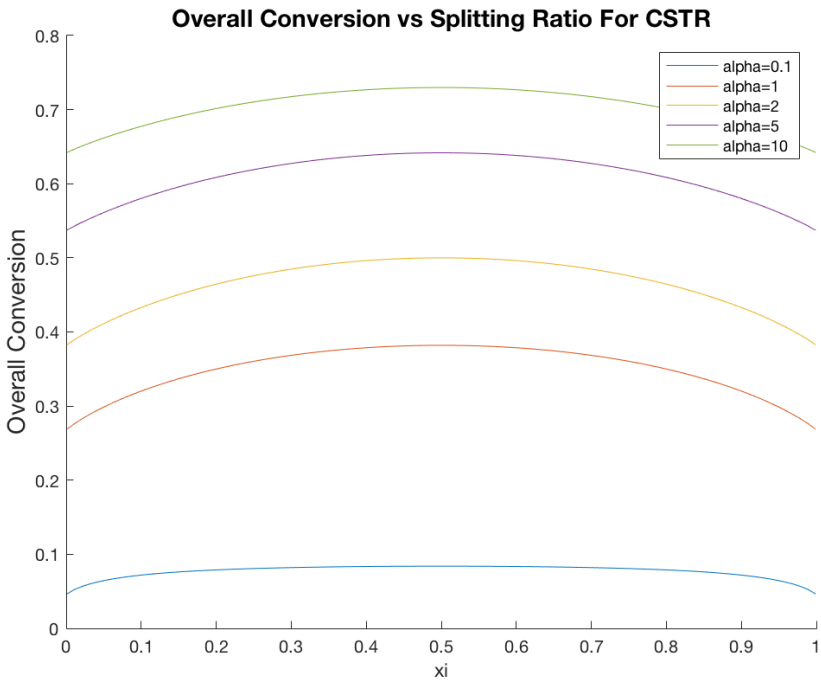
exactly as we found in (25) for $\xi = 0.5$. This confirms Q2a a little more explicitly (though no more rigorously!)

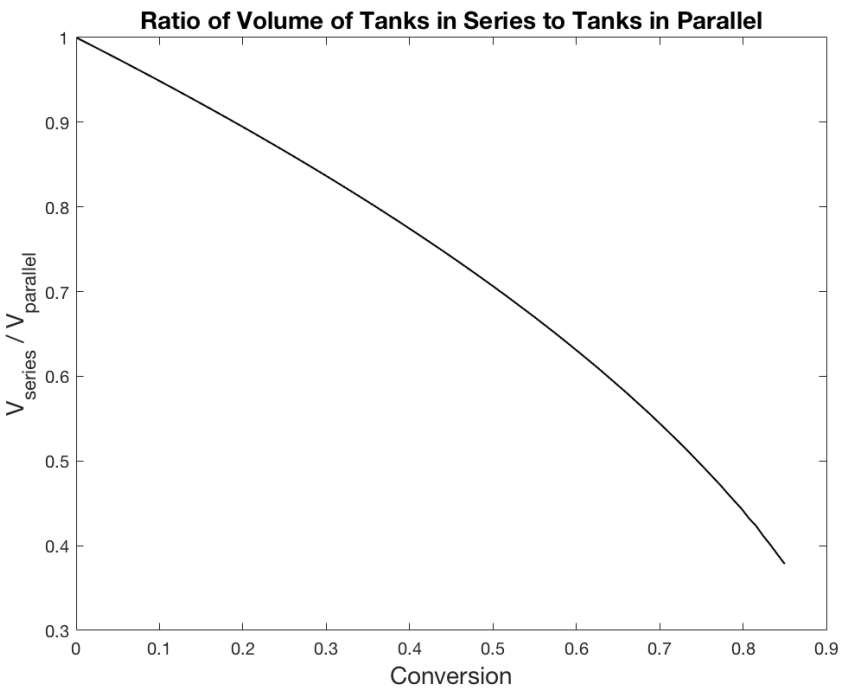
Question 2c

We reference the solution from Week 5, Question 1a. For two equal-volumed CSTR's in series, the conversion, X_A, is related to $\alpha = k_2 C_{A0} V/v$ (where V is the overall volume of both reactors combined) is:

$$\alpha/2 = \frac{\left(X_A - \alpha(1 - X_A)^2/2\right)}{\left(1 - (X_A - \alpha(1 - X_A)^2/2)\right)^2} \tag{30}$$

We can compare this with the expression for the optimal solution for parallel CSTR's when $\xi = 0.5$, given by (25). We then plot the ratio of the α values in parallel and in series (α is proportional the total volumes) for various conversions. Looking at the plot below, we see that two equal-volume reactors in series are always substantially smaller than two equal-volume reactors-in-parallel, especially at high conversions (where one reactor can be used to conduct the fast, low-conversion reaction, and the other to conduct the slow reaction at higher conversion.) Further, we reference Week 5 Question 1 to note that two equal-volume CSTRs in series may not be as efficient as, for example, a 40/60 split of the CSTR


Overall Conversion vs Splitting Ratio For CSTR
alpha=0.1
alpha=1
alpha=2
alpha=5
alpha=10
Overall Conversion
xi
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Ratio of Volume of Tanks in Series to Tanks in Parallel
V_series / V_parallel
Conversion
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9

volumes (so the first tank is smaller than the second.) When this is accounted for, the series reactors perform even better.

Question 2d
I didn't bother asking because we already know that identical PFR's in series are equivalent to a single plug flow reactor. This isn't the case for a CSTR system.

Question 3a
We know that for an MFR with a first-order reaction and flow rate υ

$$\frac{V}{\upsilon} = \frac{C_{A0}X_A}{-r_A} = \frac{X_{A,\upsilon}}{k_1(1-X_{A,\upsilon})} \tag{31}$$

$$\frac{Vk_1}{\upsilon} = \frac{X_{A,\upsilon}}{(1-X_{A,\upsilon})} \tag{32}$$

$$X_{A,\upsilon} = \frac{Vk_1}{\upsilon + Vk_1} \tag{33}$$

The conversion when the flow rate is changed to $\alpha\upsilon$ is given by

$$X_{A,\alpha\upsilon} = \frac{Vk_1}{\alpha\upsilon + Vk_1} = X_{A,\upsilon}\left(\frac{\upsilon + Vk_1}{\alpha\upsilon + Vk_1}\right) = X_{A,\upsilon}\left(\frac{1+\tau}{\alpha+\tau}\right) \tag{34}$$

where $\tau = V/\upsilon$. Thus increasing the volumetric flow rate decreases the conversion, as would be expected.

Question 3b
Once again we have the following conversion when the reaction rate constant is k_1:

$$X_{A,k_1} = \frac{Vk_1}{\upsilon + Vk_1} \tag{35}$$

whereas for reaction rate equal to βk_1,

$$X_{A,\beta k_1} = \frac{V\beta k_1}{\upsilon + V\beta k_1} = \frac{Vk_1}{\upsilon/\beta + Vk_1} = X_{A,k_1}\left(\frac{\upsilon + Vk_1}{\upsilon/\beta + Vk_1}\right) = X_{A,k_1}\left(\frac{1+\tau}{1/\beta+\tau}\right) \tag{36}$$

where $\tau = V/\upsilon$. Thus increasing the reaction rate constant k_1 increases the conversion, as would be expected.

Question 3c
For an MFR with an nth order reaction,

$$\frac{\tau}{C_{A0}} = \frac{X_A}{-r_A} = \frac{X_A}{k_n C_{A0}^n (1-X_A)^n} \tag{37}$$

Or

$$\tau k_n C_{A0}^{n-1} = \frac{X_A}{(1-X_A)^n} \tag{38}$$

This is difficult/impossible to analytically solve for general n, however when $X_A \ll 1$, we have $(1-X_A)^n \approx 1 - nX_A$. Thus

$$\tau k_n C_{A0}^{n-1} = \frac{X_A}{(1-nX_A)} \tag{39}$$

which, when rearranged, gives

$$X_A = \frac{\tau k_n C_{A0}^{n-1}}{1 + n\tau k_n C_{A0}^{n-1}}. \tag{40}$$

Challenge Question

To get us started, lets solve the reference case: a standard plug flow reactor. When the two streams are combined, the inlet concentration of A and B, $C_{A,0}^{\mathrm{PFR}}$ and $C_{B,0}^{\mathrm{PFR}}$, are equal and they are both equal to:

$$C_{A,0}^{\mathrm{PFR}} = C_{B,0}^{\mathrm{PFR}} = \frac{C_{A0}\upsilon_A}{\upsilon_A + \upsilon_B} = \frac{C_{B0}\upsilon_B}{\upsilon_A + \upsilon_B}. \tag{41}$$

The equality is guaranteed by the equimolar flow condition, whch requires $C_{A0}\upsilon_A = C_{B0}\upsilon_B$. Along the length of the reactor we have $C_A = C_B$, and so:

$$\tau = \int_{C_A}^{C_{A,0}^{\mathrm{PFR}}} \frac{dC_A}{-r_A} = \int_{C_A}^{C_{A,0}^{\mathrm{PFR}}} \frac{dC_A}{k_2 C_A^2} \tag{42}$$

where $\tau = V_{\mathrm{PFR}}/(\upsilon_A + \upsilon_B)$. Integrating,

$$k_2\tau = \frac{1}{C_A} - \frac{1}{C_{A,0}^{\mathrm{PFR}}} \tag{43}$$

and so

$$\frac{C_A}{C_{A,0}^{\mathrm{PFR}}} = \frac{1}{\alpha + 1} \tag{44}$$

or

$$X_A = \frac{\alpha}{\alpha + 1} \tag{45}$$

where $\alpha = k_2\tau C_{A,0}^{\mathrm{PFR}} = k_2 V_{\mathrm{PFR}} C_{A,0}^{\mathrm{PFR}}/(\upsilon_A + \upsilon_B)$.

Now for the more difficult part. Alice's new reactor is divided into n sections, each of which we assume acts as an ideal plug flow reactor with volume V_{Alice}/n and volumetric flow rate υ_n. Just after the beginning of the ith section of the reactor (i.e. just after B has been introduced and has all mixed in) we will say the the concentration of A and B are $C_{A,i}$ and $C_{B,i}$ respectively. The first section is considered the 0th (with $i = 0$), so that at the inlet of the whole reactor we have $C_{A,0}$ and $C_{B,0}$ (not to be confused with C_{A0} and C_{B0}, which are the concentrations before the two inlet streams are mixed). The final section has $i = n - 1$.

It will be helpful to find a general solution to a plug flow reactor undergoing a second order reaction

$$\mathrm{A} + \mathrm{B} \xrightarrow{\mathrm{k_2}} \mathrm{R} \tag{46}$$

for which $mC_{A0} = C_{B0}$ where $m \neq 1$. Then in general throughout the volume of the plug flow reactor $C_B = C_{B0} - (C_{A0} - C_A) = C_A + C_{B0} - C_{A0} = C_A + (m-1)C_{A0}$, and we will have

$$\tau = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A} \tag{47}$$

and so

$$\tau k_2 = \int_{C_A}^{C_{A0}} \frac{dC_A}{C_A(C_A + (m-1)C_{A0})} \tag{48}$$

We need to do some partial fractions here:

$$\frac{1}{C_A(C_A + (m-1)C_{A0})} = \frac{A}{C_A} + \frac{B}{(C_A + (m-1)C_{A0})} = \frac{A(C_A + (m-1)C_{A0}) + BC_A}{C_A(C_A + (m-1)C_{A0})} \tag{49}$$

and so

$$A + B = 0; \quad AC_{A0}(m-1) = 1 \tag{50}$$

and so

$$A = \frac{1}{(m-1)C_{A0}}; \quad B = -\frac{1}{(m-1)C_{A0}}; \tag{51}$$

and

$$\tau k_2 = \int_{C_A}^{C_{A0}} \left(\frac{1}{(m-1)C_{A0}}\right) \frac{dC_A}{C_A} - \int_{C_A}^{C_{A0}} \left(\frac{1}{(m-1)C_{A0}}\right) \frac{dC_A}{(C_A + (m-1)C_{A0})} \tag{52}$$

$$\tau k_2 (m-1)C_{A0} = \int_{C_A}^{C_{A0}} \frac{dC_A}{C_A} - \int_{C_A}^{C_{A0}} \frac{dC_A}{(C_A + (m-1)C_{A0})} \tag{53}$$

$$\tau k_2(m-1)C_{A0} = \ln\frac{C_{A0}}{C_A} + \ln\frac{C_A+(m-1)C_{A0}}{mC_{A0}} = \ln\frac{C_A+(m-1)C_{A0}}{mC_A} \tag{54}$$

The concentration at the outlet, C_A, is then given by

$$C_A = \frac{(1-m)C_{A0}}{1-me^{-\beta}} \tag{55}$$

and

$$C_B = C_A + C_{B0} - C_{A0} = \frac{(1-m)C_{A0}}{1-me^{-\beta}} + C_{B0} - C_{A0} \tag{56}$$

where $\beta \equiv \tau k_2(1-m)C_{A0}$.

Now we're in a position to set up our problem and solve it. Suppose the inlet concentrations to the ith section of Alice's reactor, just after the fresh stream of B has been injected, are $C_{A,i}$ and $C_{B,i}$. Then, according to the solution above, at the very end of the ith section, just before the new B is introduced, the concentrations of A and B are

$$C_{A,i,end} = \frac{(1-m)C_{A,i}}{1-me^{-\beta}} \tag{57}$$

$$C_{B,i,end} = \frac{(1-m)C_{A,i}}{1-me^{-\beta}} + C_{B,i} - C_{A,i} \tag{58}$$

where

$$m = C_{B,i}/C_{A,i} \tag{59}$$

$$\beta = \tau k_2(1-m)C_{A,i} \tag{60}$$

$$\tau = V_{\text{Alice}}/n\upsilon_i. \tag{61}$$

We can then relate these concentrations to the values of $C_{A,i+1}$ and $C_{B,i+1}$, the concentrations just after the new B has been injected. The A simply gets diluted a little, while the B concentration will increase as it gets an extra dose

$$C_{A,i+1} = \frac{C_{A,i,end}\upsilon_i}{\upsilon_{i+1}} \tag{62}$$

$$C_{B,i+1} = \frac{C_{B,i,end}\upsilon_i + \upsilon_B C_{B0}/n}{\upsilon_{i+1}} \tag{63}$$

We have one more difference equation for υ_i

$$\upsilon_{i+1} = \upsilon_i + \upsilon_B/n \tag{64}$$

Our initial conditions are:

$$\upsilon_0 = \upsilon_A + \upsilon_B/n \tag{65}$$

$$C_{A,0} = C_{A0}\frac{\upsilon_A}{\upsilon_A+\upsilon_B/n} \tag{66}$$

$$C_{B,0} = C_{B0}\frac{\upsilon_B/n}{\upsilon_A+\upsilon_B/n} \tag{67}$$

We can solve these difference equations (57) to (67) iteratively, from $i = 0, 1, 2, \ldots$ up to $i = n-1$ to calculate $C_{A,n-1,end}$ and $C_{B,n-1,end}$ - the concentrations at the outet of the reactor. Before we do this, we will rearrange the equations so we are dealing with some slightly more insightful dimensionless variables. One dimensionless variables will be n. Another will be the relative flow rate $\xi = \upsilon_A/(\upsilon_A+\upsilon_B)$ In order to conveniently compare our system with a standard PFR, as given by (45), we will also use $\alpha = k_2 V_{\text{Alice}} C_{A,0}^{\text{PFR}}/(\upsilon_A+\upsilon_B)$, where $C_{A,0}^{\text{PFR}}$ is defined in (41). If we then use the following dimensionless variables

$$\bar{C}_{A,i} \equiv \frac{C_{A,i}}{C_{A,0}^{\text{PFR}}} \tag{68}$$

$$\bar{C}_{B,i} \equiv \frac{C_{B,i}}{C_{B,0}^{\text{PFR}}} \tag{69}$$

$$\bar{\upsilon}_i \equiv \frac{\upsilon_i}{\upsilon_A + \upsilon_B} \tag{70}$$

the difference equations (57) to (67) become: for the initial conditions

$$\bar{\upsilon}_0 = \xi + (1-\xi)/n \tag{71}$$

$$\bar{C}_{A,0} = \frac{\upsilon_A + \upsilon_B}{\upsilon_A + \upsilon_B/n} = \frac{1}{\xi + (1-\xi)/n} \tag{72}$$

$$\bar{C}_{B,0} = \frac{(\upsilon_A + \upsilon_B)/n}{\upsilon_A + \upsilon_B/n} = \frac{1/n}{\xi + (1-\xi)/n} \tag{73}$$

and then to calculate the $i+1$th section from the ith section

$$m = \bar{C}_{B,i}/\bar{C}_{A,i} \tag{74}$$

$$\bar{\upsilon}_{i+1} = \bar{\upsilon}_i + (1-\xi)/n \tag{75}$$

$$\beta = \frac{k_2 V_{\text{Alice}}(1-m)C_{A,i}}{n\upsilon_i} = \frac{k_2 V_{\text{Alice}} C_{A,0}^{\text{PFR}}}{\upsilon_A + \upsilon_B} \times \frac{\bar{C}_{A,i}(1-m)}{n\bar{\upsilon}_i} = \frac{\alpha(1-m)\bar{C}_{A,i}}{n\bar{\upsilon}_i} \tag{76}$$

$$\bar{C}_{A,i+1} = \frac{(1-m)\bar{C}_{A,i}}{1-me^{-\beta}}\left(\frac{\bar{\upsilon}_i}{\bar{\upsilon}_{i+1}}\right) \tag{77}$$

$$\bar{C}_{B,i+1} = \left(\frac{(1-m)\bar{C}_{A,i}}{1-me^{-\beta}} + \bar{C}_{B,i} - \bar{C}_{A,i}\right)\left(\frac{\bar{\upsilon}_i}{\bar{\upsilon}_{i+1}}\right) + \frac{1}{n\bar{\upsilon}_{i+1}} \tag{78}$$

The final concentration of A is at the end of the $n-1$th stage. No extra liquid is added at this point, so we can get the answer by calculating $\bar{C}_{A,n}$ and then rescaling:

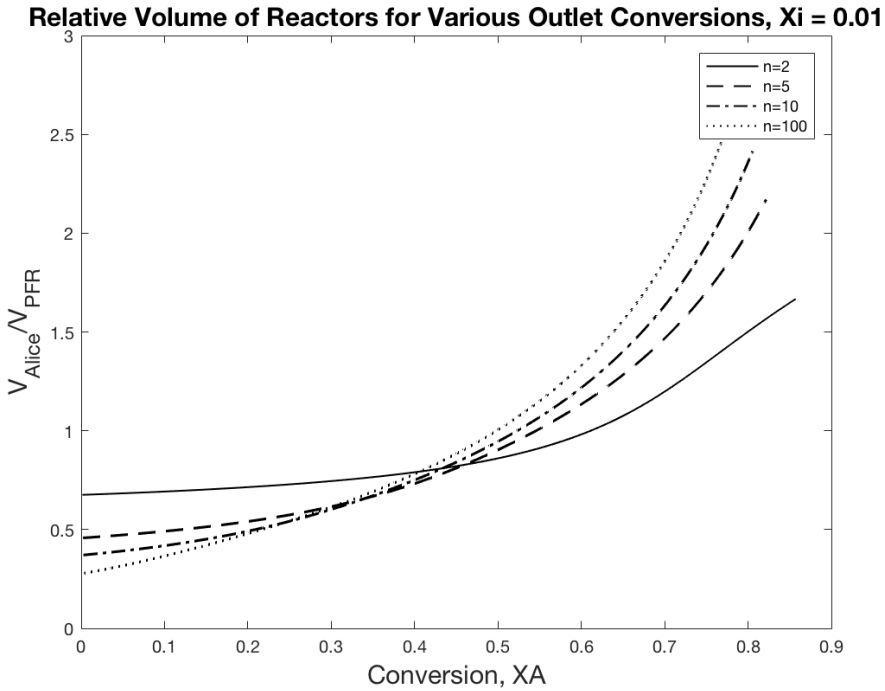
$$\bar{C}_{A,n}\left(\frac{\upsilon_n}{\upsilon_{n-1}}\right) = \bar{C}_{A,n}\left(\frac{1+(1-\xi)/n}{1}\right) \tag{79}$$

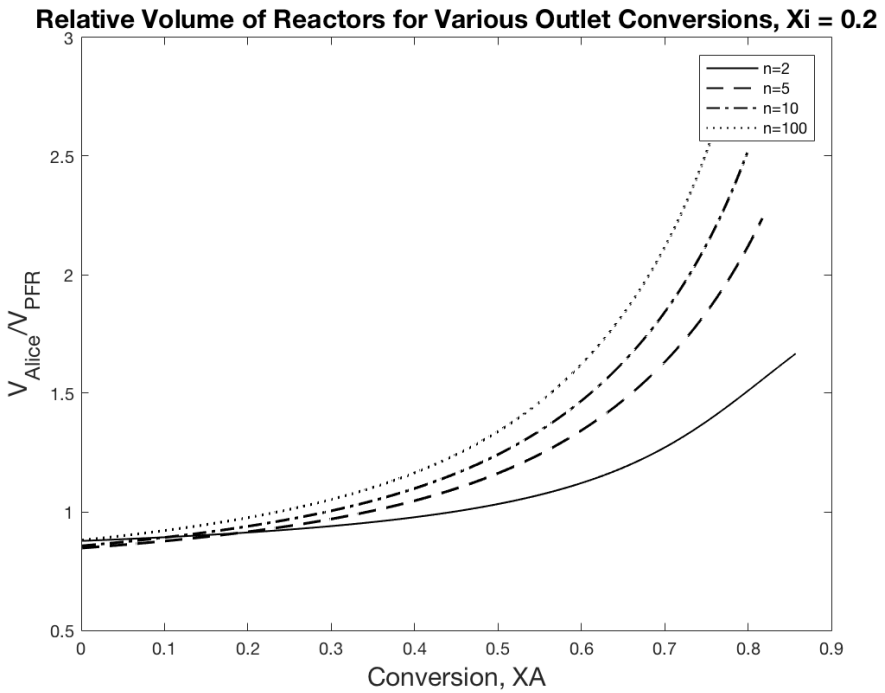
Furthermore, because at the outlet of the reactor the flow rate is $\upsilon_A + \upsilon_B$, the outlet conversion is simply given by

$$X_A^{\text{Alice}} = 1 - \bar{C}_{A,n}. \tag{80}$$

Solving these steps in a for loop in MATLAB, we can calculate X_A^{Alice} and X_A^{PFR} for various values of the relevant dimensionless variables: the number of inlet points n, the relative flow rates of A, ξ, and α, which represents the volume of our reactor relative to the inlet flow rate, concentration and intrinsic reaction rate. When trying to solve these equations, you'll find you get NaN answers for the final stage. That's because, in this final stage, the initial number of moles of A and B will be the same, and so $m = 1$, and the equations above break down. The quick-and-dirty method for getting around this is to add a tiny bit of random error to the m term (and so $m = \bar{C}_{B,i}/\bar{C}_{A,i} +$ `rand()*1e-7`) which will ensure our formulas don't return NaN answers in the final section of the reactor. Alternatively (and more sensibly) you could handle the `m=1` case separately with its own analytical formula (45).

The results for $\xi = 0.01$ and $\xi = 0.2$ and various values of α and n are shown in the figure below. Unsurprisingly, Alice's reactor performs better when ξ is smaller - that is, when stream B is much more dilute than stream A. When only a moderate reaction conversion is desired, Alice's reactor can reduce the overall reactor volume by more than half - especially for large n. On the other hand, Alice's design is not very good when large reaction conversions are required; even for $\xi = 0.01$ (where B is 100 times more concentrated than A) when $X_A > 0.6$ or so, a plain PFR reactor will have smaller volume. This is not too surprising: in Alice's design, we are adding reactants near the very end of the reactor, and it will be difficult to achieve very large conversions when we are doing this. A hybrid design, with unevenly spaced injection points or injection points with varying flow rates (as per the *bonus* question) will likely be able to overcome these deficiencies and increase the overall performance relative to a PFR for any target output conversion. Such an optimisation problem is not particularly difficult: indeed, it would make a good assignment for a reactor engineering or optimisation course.


Relative Volume of Reactors for Various Outlet Conversions, Xi = 0.01
n=2
n=5
n=10
n=100
V_Alice/V_PFR
Conversion, XA
0
0.5
1
1.5
2
2.5
3
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9


Relative Volume of Reactors for Various Outlet Conversions, Xi = 0.2
n=2
n=5
n=10
n=100
V_Alice/V_PFR
Conversion, XA
0.5
1
1.5
2
2.5
3
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9