Kinetics: practical 12 and 13

To answer these kind of questions the first thing we need to do is determining that we have a Batch or PFR Reactor. As stated in the qestion we have an Batch Reactor.We know that batch reactor is a discuntinous reactor that does not have any inlet or outlet stream. To get the rate equations for the Batch rector we could use two different methods which are differential and integral methods. in the differential method we could get the rate equations by differenciating the experimental date, while in the Integral method we can integrate over our material balance(dCA/dt=sum(vi\*ri)) and get kinetic constant and order of the reaction by the best fit of experimental data. For this problem I use the differential method. As the form of the reaction rate did not metion, According to the experimental data, I could assume that we could have three different reactions schemes(A+B>>C, A>B>C,A>B and A>C). According to the experimental data, only the concentration of A is decreasing and the concentration of other species is only increasing, so the only possible reaction scheme is parallel reaction. now, we could implemet data in excel and if r/CA over CA is linear the order of reaction is 1 and k=r/CA. Otherwise, if it was not linear we need to increase the order of the reaction.(dCc/dt = k2 \* CA ; dCB/dt=K1\*CA).

To answer these kind of questions the first thing we need to do is determinng that we have a Batch or PFR Reactor. As stated in the qestion we have an PFR Reactor.this reactor provides the values of concentration over residence time at the outlet of the reactor. To get the rate equations for the PFR rector we could use two different methods which are differential and integral methods. in the differential method we could get the rate euations by differenciating the experimental date, while in the Integral method we can integrate over our material balance(dCA/dt=sum(vi\*ri)) and get kinetic constant and order of the reaction by the best fit of experimental data. One thing that need to be remember is that to use the differental method for PFR reactor the conversion must be less than 5%. in this way the reaction rate is roughly constant inside the reactor volume. The best procedure for the PFR reactor is to determmine the order of the reaction by differential method and get the kinetic constant by integral approach. According to the problem, we have an catalytic reaction. So, the first assuumption is that we are in homogenous and chemical regim. To consider the void fraction our eqation would be(ACC=0> IN-OUT+P=0). dCA/dtau=-kcA^n\*(1-epsi). So in this way we only consider the volume of reactor which the reaction is occring. Then we need to calculate the residence time for every tempearature, because the voumetric flow rate is changing with the temperature. we get the order of the reaction from differential method which is 1 and we know that this is not changing with the temperature. now, we use that to get k from integral method. we know that k=k0\*exp(-E/RT)>> lnK=Ln(K0)-(E/R)\*1/T. so with plotting the ln(k0) over -1/T, we could get our reaction rate.

Gas/Liquid: practical 11

When we are dealing with gas/liquid reactors, we know that the species A is in the gas phase and B is a non-volatile liquid and the reaction is only happening in the liquid phase. The overal rate of the reaction is: rAv= PA/[(1/KG\*a)+(HA/E\*a\*KL)+(HA/Kr\*fL)], PA is partial pressure of A and can be calculated as PA=CA\*HA, KGa\*a and KL\*a are mass transfer coeffiecent, and Kr is the kinetic constant of the reaction. To get the overall rate of the reaction we need to have enhancement factor and Kr. Also, because the reaction rate as stated by the question is in the unit of liquid volume we need to times it with fL to convert it to volume of reactor(r=r\*fL). As in the question the concentration of A is small and the concentraation of B is very big, the CA is our limiting species and the whole reacion rate is depended to only CA. So we need to rewrite the reaction rate: r=Kl\*CA\*CB^2\* >> r=Kr\*CA and Kr=Kl\*CB^2. For the enhancement factor, it varys according to the reaction rate. if we have an slow reaction the E=1, and for intermidiate reactions the E=1+MH^2/3. for Fast reactions the E=1+(va/vb)\*(Db/Da)\*(CB/CA) and CA=PA/HA. So to get the enhancement factor we need to have hatta value which is MH=detaL\*sqrt(Kr/DL)=sqrt(Kr\*DL/KL). now we could impement these date into Matlab and get the overal reaction rate, enhacement factor, and local resistance. If the hatta or E is small it means we have an slow reaction and it better to use tank reactor with significant liquid holdup, because the reaction is occuring in the volume of the liquid. However, if the hatta is large the reaction is occuring in the interface and its better to use the packed or spray column.

Fluidizied bed: practical 10

As mentioned in the question we use three phase Kunii-Levenspiel model with Geldart A paticles. Geldart A particles makes a homogeneous fluidization at the vmf and then the bubbles are formed when the bubbling velocity is reached. In this method we assume that the bubble rise velocity is higher with respect to the velocity of the gas percolating through the emulsion at minimum fluidization conditions. Hence, the bubbles are surrounded by thin clouds of recirculating gas. Also, the wakes of the bubbles are considered one region together with cloud. As mentioned in the question we can assume a CSTR like behavior of the emulsion phase. At the end we need to check this hypothesis. To get the fraction of the molar gas and the mass fraction of n-butane in the reactor we need to write mass balance for species i in three phases of bubble, cloud/wake, and emulsion. According to the equation we have here, we need to find Vmf, Vt, Ki,bc, Ki,ce, gamma(b,c, and e), velocity of bubble, density of gas, volume fraction of bubble-could-and emulsion, and height of the bed. We know that Vmf is the superficial gas velocity at which the drag force of the upward moving gas becomes equal to the weight of the particles in the bed. So, to get this one we could say that the pressure drop from Ergun equation is equal to the W/A, and rewrite the equations to get a second order equation for Vmf(A\*Vmf^2+B\*Vmf+C=0). For the density of gas as mentioned in the question we could consider this a mixture of ideal gas and get the density. For the Vt, it is equal to the free fall velocity of the particle and we could get it by the mentioned equation. Cd in this equation is a function of Re of particle and consequently the terminal velocity. We have two relations for Cd and with solving them we could get the Vt. For the velocity of the bubble it is a function of Vmf, Vin, and Vbr. To have the Vbr we need the diameter of bubble, and because we are using Geldart A particles this can be considered constant scaling from pilot to industrial scale reactor. For the reaction rates the first thing that we need to do is to identify the number of the species (in this case 7), and write their stochiometric coefficient. Then we also need to calculate the Mw of mixture, inlet molar and mass fractions. At the end we need to rewrite the reaction rates from partial pressure to total pressure. Now, all the other parameters that we need, according to the equation that have been given to us could be solved. Between these parameters only the mass transfer coefficients need to be solved for each species separately. Now, we have three equation and three unknowns and we could get the mass fraction of any species in the reactor. A slug flow is a condition of a fluidized bed in which large bubbles of gas form, which makes lumps of particles move. To check if slugging mode can occur or not, we need to calculate the maximum diameter of the bubble and compare it with the diameter of the reactor. If this was bigger than the diameter of reactor slugging could happen. Otherwise, no slugging occurring in the reactor. The dbmax=3.07 m and smaller than 5m, so slugging not happening here. As we know the static condition means that we have PFR behavior in the emulsion phase. So in this way because a CSTR behavior is replacing with a PFR, obviously the conversion increase in the reactor.

1D pseudo-homogeneous model: practical 6

As mentioned in the question we want to produce PA from the oxidation of o-xylene in a catalytic bed reactor. As requested by the question I use the 1D pseudo-homogeneous model with the heat transfer computed through the Dixon-Specchia correlation. This model based on the assumption that concentration and temperature gradients only occur in the axial direction and the only transport mechanism in this direction of flow itself. To get the number of tubes needed for this question, we could calculate the productivity for one tube and with the goal that we want from this unit which is 8000 ton/year we could get the total number of tubes needed. To get the productivity of tube we need to know conversion, selectivity and yield in the reactor. Also, there is a limit on the system that the maximum pressure drop per meter is not be more than 0.1 bar/m. So, to get these values we need to have the concentration, Temperature and pressure gradients, and for that we could write a mass, energy, and mechanical energy balance on the system, and get these equations. According to the equations that we have and the data which are given we could modify them and write them based on G=4900 kg/h/m2. We also need to get the values for their boundary condition. We know that at z=0 T=T0=335 C, P=P0=P\_ outlet + delta P=1.3 bar, and for mass fraction in the inlet we need to calculate it. First, we need to identify the species which are 6. Then, according to question we are diluting the o-x with air so the inlet moles are only N2, O-X, and O2 [0.79 0.013 0.21 0 0 0]. With having these moles, we could calculate the molar fraction. Now with multiplying them with their molecular weight we could get the mass of every species and at the end calculate the inlet mass fraction. Now, according to the equation we could calculate void fraction, surface per unit volume, and overall heat transfer coefficients. To get the gas density, because we have an ideal gas mixture we could use ideal gas rule, and get the molar gas density. with multiplying it with 10^-3 and mw, we turn it to mass gas density. To get the superficial velocity, we need to do this: G/mass gas density/3600 and get v with the unit of m/s. Now, we need to find the stochiometric coefficients and modify the reaction rate. Stochiometric coefficients are achievable from the three reaction scheme that we have. The reaction rate should be written in terms of total pressure(bar) and mol fraction of species in the reactor. Now, we only have three equations and three unknowns and could get the change in mass fraction of any species in the reactor, the thermal profile, the conversion, selectivity and yield. The parameters that we could change to reduce the number of tubes are inlet pressure and temperature, flow rate, o-x concentration, and external temperature. With increasing the pressure, the gas density and reaction rate increases. This will enhance the productivity and reduce the number of tubes. But it cannot reduce it under 9000 tubes, because the reaction rate which is exothermic is increasing in the reactor, and as we only have one hot spot, the thermal run away happen and the reactor design collapse. The same thing happens when we increase the other parameters. The best procedure is to dilute the catalytic bed and divide it into two sections according to the first hot spot that we have making two hot spots in the reactor. The first section should be diluted to decrease the reaction happening their and the second one only have the catalyst to make the reaction increase and make the second hot spot. Now we could easily increase the pressure or o-x concentration without reaching thermal runway and exceed the limit of the previous design.

1D heterogeneous model:practica7

As mentioned in the question we want to produce PA from the oxidation of o-xylene in a catalytic bed reactor. As requested by the question I use the 1D heterogeneous model with the heat transfer computed through the Dixon-Specchia correlation. In this model, the presence of reaction and transport in parallel could create the occurrence of gradients between the catalyst and the gas phase. So, due to the difference in the concentration of species and the temperature in the gas phase and on the catalyst surface, we need two equation for concentration gradients and two for the temperature gradients. We only need one equation for pressure. With these 5 equations and their boundary conditions that we wrote, we could determine the axial evolution of temperature and concentration for both the gas and the solid phase. To get the number of tubes needed for this question, we could calculate the productivity for one tube and with the goal that we want from this unit which is 8000 ton/year we could get the total number of tubes needed. To get the productivity of tube we need to know conversion, selectivity and yield in the reactor. Also, there is a limit on the system that the maximum pressure drop per meter is not be more than 0.1 bar/m. According to the equations that we have and the data which are given we could modify them and write them based on G=4900 kg/h/m2. We also need to get the values for their boundary condition. We know that at z=0 T=T0=335 C, P=P0=P\_ outlet + delta P=1.3 bar, and for mass fraction in the inlet we need to calculate it. First, we need to identify the species which are 6. Then, according to question we are diluting the o-x with air so the inlet moles are only N2, O-X, and O2 [0.79 0.013 0.21 0 0 0]. With having these moles, we could calculate the molar fraction. Now with multiplying them with their molecular weight we could get the mass of every species and at the end calculate the inlet mass fraction. Now, according to the equation that we have, we need to identify the av, epsi, ki, h, U, pg, stochiometric coefficients, reaction rates, delta\_ H, and superficial velocity. To identify each of these parameters we have some related equations and data that we could use. We should really be careful for the units when we are converting it. For the mass gas density we could use the assumption according to the question that we have an ideal gas and calculate it (density mass gas=(P/R\*T)\*10^-3\*mw\_ average). The superficial velocity could be calculate it from the inlet flow rate(V=G/density mass gas/3600). Now, we need to find the stochiometric coefficients and modify the reaction rate. Stochiometric coefficients are achievable from the three reaction scheme that we have. The reaction rate should be written in terms of total pressure(bar) and mol fraction of species on the catalyst surface. Now, we only have five equations and five unknowns and could get the change in mass fraction of any species in the reactor, the thermal profile, the conversion, selectivity and yield. The parameters that we could change to reduce the number of tubes are inlet pressure and temperature, flow rate, o-x concentration, and external temperature. With increasing the pressure, the gas density and reaction rate increases. This will enhance the productivity and reduce the number of tubes. But it cannot reduce it under 9000 tubes, because the reaction rate which is exothermic is increasing in the reactor, and as we only have one hot spot, the thermal run away happen and the reactor design collapse. The same thing happens when we increase the other parameters. The best procedure is to dilute the catalytic bed and divide it into two sections according to the first hot spot that we have making two hot spots in the reactor. The first section should be diluted to decrease the reaction happening their and the second one only have the catalyst to make the reaction increase and make the second hot spot. Now we could easily increase the pressure or o-x concentration without reaching thermal runway and exceed the limit of the previous design.

1D+1D pseudo-homogeneous model: practical 8

As mentioned in the question we want to produce PA from the oxidation of o-xylene in a catalytic bed reactor. As requested by the question I use the 1D+1D pseudo-homogeneous model with the heat transfer computed through the Dixon-Specchia correlation. This model based on the combination of a pseudo-homogenous 1D model with considering the internal limitation inside the pellet. So, in this model we assume that there is no transfer of mass and energy between the catalyst and gas phase, and the reactions are occurring in the catalytic particles. To account for the internal gradient of concentration and temperature, we could write a mass and energy balance for the pellet. So, in total we have 5 general equations, in which two of them are for the concentration gradients in the gas phase and inside the pellet, two for the temperature in the gas and pellet and one for pressure. One of the other important parameters in the internal limitation is effectiveness factor. This parameter is the ratio between the rate of the reaction in the pellet with pore resistance and the rate of reaction in the absence of pore resistance and its value is between 0 and 1. With this parameter we could couple the equation from pseudo1D and Htero1D with the equation for internal regime. To get the number of tubes needed for this question, we could calculate the productivity for one tube and with the goal that we want from this unit which is 8000 ton/year we could get the total number of tubes needed. To get the productivity of tube we need to know conversion, selectivity and yield in the reactor. Also, there is a limit on the system that the maximum pressure drop per meter is not be more than 0.1 bar/m. According to the equations that we have and the data which are given we could modify them and write them based on G=4900 kg/h/m2. We also need to get the values for their boundary condition. We know that at z=0 T=T0=335 C, P=P0=P\_ outlet + delta P=1.3 bar, and for mass fraction in the inlet we need to calculate it. First, we need to identify the species which are 6. Then, according to question we are diluting the o-x with air so the inlet moles are only N2, O-X, and O2 [0.79 0.013 0.21 0 0 0]. With having these moles, we could calculate the molar fraction. Now with multiplying them with their molecular weight we could get the mass of every species and at the end calculate the inlet mass fraction. To get the values that we are seeking for, we need to know the epsi, U, delta\_ HR, stochiometric coefficients, mass density of gas, superficial velocity, and the effective diffusion coefficient. To identify each of these parameters we have some related equations and data that we could use. We should really be careful for the units when we are converting it. For the mass gas density, we could use the assumption according to the question that we have an ideal gas and calculate it (density mass gas=(P/R\*T) \*10^-3\*mw\_ average). The superficial velocity could be calculated from the inlet flow rate (V=G/density mass gas/3600). Now, we need to find the stochiometric coefficients and modify the reaction rate. Stochiometric coefficients are achievable from the three reaction scheme that we have. The reaction rate should be written in terms of total pressure(bar) and mol fraction of species in the pellet. To get the Di,eff, we know that it is the function of continuum and Knudsen diffusion. So, we could calculate it easily. Now, we could implement theses data and equation in Matlab to get what we wanted. Due to the complex nature of the equation for the internal regime, we replace derivatives in them with some finite difference approximation. Now, we only have five equations and five unknowns and could get the change in mass fraction of any species in the gas phase and in the pellet, the thermal profile in gas and solid phase, the conversion, selectivity, yield, and catalyst efficiency. The catalyst efficiency increases when we have an eggshell configuration instead of a spherical one. Because in this way we have less active site in the catalyst and sort of diluted the pellet. But, this decrease the productivity and less amount of PA will be produce. To solve this we could increase the o-x ratio.

1D+1D heterogenous model: practical 9

As mentioned in the question we want to produce PA from the oxidation of o-xylene in a catalytic bed reactor. As requested by the question I use the 1D+1D heterogenous model with the heat transfer computed through the Dixon-Specchia correlation. This model based on the combination of a heterogenous 1D model with considering the internal limitation inside the pellet. So, in this model, due to the difference in the concentration of species and the temperature in the gas phase and on the catalyst surface we assume that there is a transfer of mass and energy between the catalyst and gas phase, and the reactions are occurring in the catalytic particles. To account for the internal gradient of concentration and temperature, we could write a mass and energy balance for the pellet. So, in total we have 7 general equations, in which three of them are for the concentration gradients in the gas phase, in the interface between gas and solid, and inside the pellet, three for the temperature in the gas phase, on the surface of catalyst, and in the pellet and one for pressure. One of the other important parameters in the internal limitation is effectiveness factor. This parameter is the ratio between the rate of the reaction in the pellet with pore resistance and the rate of reaction in the absence of pore resistance and its value is between 0 and 1. With this parameter we could couple the equation from Htero1D with the equation for internal regime. To calculate the effectiveness factor by using Thiele modulus we assume an isothermal, first-order reaction. The Thiele modulus is a non-dimensional number representing the relationship between the diffusion rate and the reaction rate in a porous catalyst pellet. Another way to estimate the effectiveness factor is by considering the temperature and concentration distributions inside the catalyst particle, known as intraparticle distribution method. In this method, the equations of reaction rates and mass and energy balances are numerically solved to obtain the temperature and concentration distributions and the local reaction rates within the catalyst particle. To get the number of tubes needed for this question, we could calculate the productivity for one tube and with the goal that we want from this unit which is 8000 ton/year we could get the total number of tubes needed. To get the productivity of tube we need to know conversion, selectivity and yield in the reactor. Also, there is a limit on the system that the maximum pressure drop per meter is not be more than 0.1 bar/m. According to the equations that we have and the data which are given we could modify them and write them based on G=4900 kg/h/m2. We also need to get the values for their boundary condition. We know that at z=0 T=T0=335 C, P=P0=P\_ outlet + delta P=1.3 bar, and for mass fraction in the inlet we need to calculate it. First, we need to identify the species which are 6. Then, according to question we are diluting the o-x with air so the inlet moles are only N2, O-X, and O2 [0.79 0.013 0.21 0 0 0]. With having these moles, we could calculate the molar fraction. Now with multiplying them with their molecular weight we could get the mass of every species and at the end calculate the inlet mass fraction. To solve these equations, we need to know av, Ki, molar and mass density of gas, void fraction, h, U, stochiometric coefficients, effective diffusion coefficient, reaction rates, and superficial velocity. To identify each of these parameters we have some related equations and data that we could use. We should really be careful for the units when we are converting it. For the mass gas density we could use the assumption according to the question that we have an ideal gas and calculate it (density mass gas=(P/R\*T) \*10^-3\*mw\_ average). The superficial velocity could be calculated from the inlet flow rate (V=G/density mass gas/3600). Now, we need to find the stochiometric coefficients and modify the reaction rate. Stochiometric coefficients are achievable from the 3 reactions scheme that we have. The reaction rate should be written in terms of total pressure(bar) and mol fraction of species in the pellet. To get the Di,eff, we know that it is the function of continuum and Knudsen diffusion. So, we could calculate it easily. Due to the complex nature of the equation for the internal regime, we replace derivatives in them with some finite difference approximation. Now, we only have 7 equations and 7 unknowns and could get the change in mass fraction of any species in the gas phase, on the catalyst surface, and in the pellet, the thermal profile in gas, surface and solid phase, the conversion, selectivity, yield and catalyst efficiency. The catalyst efficiency increases when we have an eggshell configuration instead of a spherical one. Because in this way we have less active site in the catalyst and sort of diluted the pellet. But, this decrease the productivity and less amount of PA will be produce. To solve this we could increase the o-x ratio.

BATCH AND SEMI BATCH REACTOR

To compare the conversion, selectivity, and yield of a Batch reactor and a Semi-Batch reactor in two different cases of lab and industrial scale, we need to write a mass balance and an energy balance for both reactors and get the gradient of temperature and concentration of species. According to the reaction that we have (A🡪P🡪S), the P is the wanted product and S is the unwanted product. According to the text, the kinetic constant and activation energy of the second reaction is much higher than the first reaction, meaning that after that concentration of P reaches to an acceptable amount, in a high temperature it totally converts to the unwanted product of S. To control the temperature of the system, we are using a coolant jacket around the reactor. To solve the equations that we have, we need to know stochiometric coefficients, reaction rates, U, av, delta\_ HR, and the volumetric inlet flow rate. All of these data are given, and it said that our reaction rates are first order. Now, with solving these equations, we could get the concentration gradient of A, P, and S in the reactor, alongside of the temperature in the reactor. As we are changing from lab scale to industrial one in both of the reactors, we could see that the same selectivity and yield decrease a lot. This is due to the fact that the volume of reactor increased, more reaction is happening in the reactor and consequently the temperature is higher. As mentioned before, this would convert the P to S. to solve this problem, the best procedure is that we change the reactor from a batch to a semi-batch reactor. In this way we introducing the A to the system gradually, so the reaction rates are under control and the temperature do not increase a lot to make it possible for the second reaction to take the overall process rate. So, in the end the semi-batch reactor is the better choice when we have series reactions. The other option to increase the selectivity and yield is through changing the time that the coolant goes to the jacket. First we run the experiment to see where we have the maximum amount of P, then we adjust the cooling time around that point to reduce the temperature and do not let the P convert to S.

STR REACTOR

To get the temperature, concentration, and conversion in a CSTR reactor, we need to write a mass and energy balance on the system. We know that a CSTR has continues input and output of material, and it is fully homogenous. So, in this case the control volume is the whole volume of the reactor. According to the equation that we wrote, we need volumetric flow rate, initial concentration of species, delta\_ HR, reaction rate, UA, and the coolant temperature. All of these data are given to us by the problem. So, now we could implement them in Matlab and get the conversion and temperature of the reactor. In this reactor, when we increase the feed temperature, this will result in the increase of reactor temperature and consequently increase the conversion. In this case, the 300k temperature, is an unstable point, because a small increase in this temperature will enhance the conversion a lot, and wise versa. This is due to the fact that this point is in the middle of the intersection of Q\_ gen with Q\_ ext (stability criteria: Q\_ gen< Q\_ ext). Now, if we want to keep the reactor temperature under 340k and have a conversion higher than 80%, we need to control the temperature of the reactor with a cooling jacket which has the temperature of 310k and UA of 9000 w/k. in this way we could work in higher feed temperature, without reaching to temperature higher than 340k in the reactor. In this case, if we reduce the feed temperature, it is obvious that the conversion will drop. To make up for this decrease in feed temperature, we could increase the coolant temperature to 331k resulting in increase of conversion. This is due to the fact that, this increases the Q\_ external and consequently the reactor temperature increase. Changing the inlet flow rate, could have an effect on the conversion and reactor temperature. If we increase the flow rate, more reactant will go to the system, and if the feed temperature would be enough high to initiate the reaction, the temperature increase and result in an increase of conversion. But, if the temperature is not high enough this increase in flow rate transports more heat with itself from the reactor to the outlet, and result in the failure of reactor.

PFR REACTOR

As stated in the question we want to oxidize the inlet gas before entering an absorption tower for the production of nitric acid by a PFR reactor. We need to design the volume of this reactor in a way that the ratio of NO2/NO >= 5. This volume should be calculated in two different cases. The first case is that the temperature and pressure is constant in the reactor. So, for solving the volume of reactor we only need the mass balance on the system. According to the equation that we wrote, we need to know stochiometric coefficients, reaction rate, and the boundary condition. As how we write the equation, the BC is the inlet molar flow rate (kmol/s). we have volumetric flow rate 10^4 (m^3/hr), and if we could calculate the total inlet concentration, we could have the inlet molar flow rate. We could get the total concentration like this (C\_ tot = P/R\*T), and the molar flow rate will be achieved (molar inlet flow rate= Q/3600 \*C\_ tot\*x\_ in). the inlet moles has been given to us, and from that we could get the mol fraction. With looking at the reaction scheme, we could get the stochiometric coefficients for the four species that we have, along side of the reaction rate. So, now we could solve the problem and get the volume of the reactor (V=107.79 m^3). In the second case the temperature is changing inside the reactor, and kr is changing with temperature. So, we need an energy balance on system to find the reactor temperature. According to the energy balance, we need to have delta\_ HR and Cp\_ mix. The question only gave us the Cp of each species and the reference enthalpy. (CP\_ mix =xi \* Cpi and delta\_ HR= delta\_ reference + Cp\_ mix \* (T- T\_ ref)). Now we could put both of the equation in matlab and find the volume of the reactor (V= 51 6.95 m^3). The volume of the reactor when the condition is not isotherm and the temperature is decreasing in the reactor is almost 5 times bigger that an isothermal condition. It is due to the fact that, decrease in the temperature in the second case will result in the decrease in reaction rate and to have the same amount of productivity we need a bigger volume. For the second question, from the ratio between the reaction rates, we could understand that if we want to maximize the yield of the B (A🡪B and A🡪C ; Rb= k\*CA^2, Rc= K\*CA), we should keep the concentration of CA high during the reaction. The best reactor to do this is the ideal PFR, because no dispersion happening in this case and the concentration of A remains high. The other option is the series of CSTR with their volume increasing. Because at the end of reactor the concentration would be low, so it is important to keep the concentration high at the beginning of reaction. The one that would make the yield of B minimize is the CSTR reactor. For the third question, according to the reaction that is happening ( A🡪B , and A🡪C , and A🡪 D; Rb= k\*CA^2, Rc= K\*CA, and Rd=K\*CD^0.5), if we want to maximize the yield of C, the ration between the rc and rb tells us to keep the concentration of A low, while the ratio between rc and rd tells us the opposite. In this case we need to couple a CSTR with a PFR to get the optimal yield of C. first should be the CSTR reactor, because the other unwanted reaction rate is in higher orders of wanted reaction rate and if the concentration of A would be high in beginning, all of them turns to B. also, at the end the concentration would be low so a PFR reactor would be good.

RTD

To get the dispersion coefficient, we need to use the residence time distribution function. This function tells us the fraction of molecules of tracer that has been in the system for the time t and t+ dt. With having the E, we could calculate the mean time and variance (sigma\_ square). The variance tells us how far we are from the Ideal PFR. With having both of them we could calculate the sigma\_ theta \_ square and from that we could get the Pe number. With having the Pe number, velocity and length of the tube the dispersion coefficient will be achieved. We know that the Pe number has an inverse relationship with dispersion coefficient. if the D is high it means a lot of mixing happening in the reactor, and we have diffusion flux in the system.