## 1. seminar: calculation of batch ractors: isotherm and adiabatic cases

## R1. Problem

$\mathrm{An} \mathrm{A}+\mathrm{B} \rightarrow \mathrm{C}+\mathrm{D}$ type reaction is performed in an isotherm, mixed, batch tank reactor at $80^{\circ} \mathrm{C}$. The initial concentrations of both A and $B$ components are $5.2 \mathrm{~mol} / \mathrm{dm}^{3}$. The volume of the reaction mixture is constant during the whole reaction. How long does it take to reach $85 \%$ conversion? The reaction can be described with second order kinetics, thus $r=k \cdot c_{A} \cdot c_{B}$, where $k=0.058 \frac{\mathrm{~m}^{3}}{\mathrm{kmol} \cdot \min }$

| Data given in the example (including reaction order and reversibility) |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



| Mode of operation |  |  |
| :---: | :---: | :---: |
| Isothermal | Adiabatic |  |

## R2. Problem

A perfectly mixed adiabatic bath reactor, with $2.5 \mathrm{~m}^{3}$ inner volume, is installed for an $\mathrm{A} \rightarrow \mathrm{B}$ type irreversible liquid phase reaction. The initial reaction mixture is at $25^{\circ} \mathrm{C}$, it contains 11.25 kmol A component, and no B component. The enthalpy of reaction is $20 \mathrm{MJ} / \mathrm{kmol}$, the specific heat capacity of the mixture is $2200 \mathrm{~J} /(\mathrm{kg} \cdot \mathrm{K})$, density is $850 \mathrm{~kg} / \mathrm{m}^{3}$. The reaction is stopped at $70^{\circ} \mathrm{C}$. The reaction rate coefficient can be calculated by the following equation: $k=10^{13} \cdot e^{-\frac{12000}{T}} S^{-1}$.
Calculate the conversion! Homework: calculate the reaction time!

| Data given in the example (including reaction order and reversibility) |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



|  | Mode of operation |
| :---: | :---: |
| Isothermal | Adiabatic |

## 2. seminar: isothermal and adiabatic plug flow reactors

## R3. problem

A pseudo-first order reaction is performed in an ideal plug flow rector of $3 \mathrm{~m}^{3}$ inner volume. The reaction rate coefficient is $0.0806 \mathrm{~min}^{-1}$. Calculate the conversion if the flow rate of the feed is $0.1 \mathrm{~m}^{3} / \mathrm{min}$ or is it is $0.15 \mathrm{~m}^{3} / \mathrm{min}$ !

| Data given in the example (including reaction order and reversibility) |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



| Mode of operation |  |  |
| :---: | :---: | :---: |
| Isothermal | Adiabatic |  |

## R4. problem

An adiabatic plug flow reactor is used for a second order reaction. The flow rate of the feed A at $20^{\circ} \mathrm{C}$ is $10 \mathrm{dm}^{3} / \mathrm{s}$, containing $7.5 \mathrm{~mol} / \mathrm{dm}^{3} \mathrm{~A}$. The flow rate of the feed B at $20^{\circ} \mathrm{C}$ is $20 \mathrm{dm}^{3} / \mathrm{s}$, containing $3.75 \mathrm{~mol} / \mathrm{dm}^{3} \mathrm{~B}$. The type of reaction is: $\mathrm{A}+\mathrm{B} \rightarrow 2 \mathrm{R}$. Conversion should be $95 \%$. The enthalpy of reaction is $-82 \mathrm{~kJ} / \mathrm{mol}$, density of the mixture is $1050 \mathrm{~kg} / \mathrm{m}^{3}$, specific heat capacity is $3.5 \mathrm{~kJ} /(\mathrm{kg} \cdot \mathrm{K})$. The reaction rate coefficient can be calculated by the following equation: $k=1.63 \cdot 10^{10} \cdot e^{-\frac{8100}{T}} \frac{\mathrm{dm}^{3}}{\mathrm{~mol} \cdot \mathrm{~s}}$ Calculate the necessary reactor volume!

| Data given in the example (including reaction order and reversibility) |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



| Mode of operation |  |
| :---: | :---: |
| Isothermal | Adiabatic |

## 3. seminar: CSTR (isothermal and adiabatic), consultation

## R5. Problem

An $\mathrm{A}+\mathrm{B} \underset{k_{-1}}{\stackrel{k_{1}}{\longrightarrow}} \mathrm{C}+\mathrm{D}$ type equilibrium reaction is performed in a continuously stirred tank reactor of $0.12 \mathrm{~m}^{3}$ inner volume. The conversion should be $75 \%$. The feed flow rates are equal and contain only one of the substrates. The concentration of feed A is $2.8 \mathrm{~mol} / \mathrm{dm}^{3}$, the concentration of feed B is $1.6 \mathrm{~mol} / \mathrm{dm}^{3} \cdot \mathrm{k}_{1}=7 \mathrm{dm}^{3} / \mathrm{mol} \cdot \mathrm{min}, \mathrm{k}_{-1}=3 \mathrm{dm}^{3} / \mathrm{mol} \cdot \mathrm{min}$ at $60^{\circ} \mathrm{C} . \mathrm{k}_{1}=6.3 \mathrm{dm} / \mathrm{mol} \cdot \mathrm{min}$, and $\mathrm{k}_{-1}=2.8 \mathrm{dm}^{3} / \mathrm{mol} \cdot \mathrm{min}$ at $40^{\circ} \mathrm{C}$. Calculate the maximal flow rate in order to achieve the required conversion at $60^{\circ} \mathrm{C}$ and at $80^{\circ} \mathrm{C}$ (homework).

| Data given in the example (including reaction order and reversibility) |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



|  | Mode of operation |
| :---: | :---: | :---: |
| Isothermal | Adiabatic |

## R6. Problem

An adiabatic, continuously stirred tank reactor is used for a second order reaction. The flow rate of the feed A at $20^{\circ} \mathrm{C}$ is $10 \mathrm{dm}^{3} / \mathrm{s}$, containing $7.5 \mathrm{~mol} / \mathrm{dm}^{3} \mathrm{~A}$. The flow rate of the feed B at $20^{\circ} \mathrm{C}$ is $20 \mathrm{dm}^{3} / \mathrm{s}$, containing $3.75 \mathrm{~mol} / \mathrm{dm}^{3} \mathrm{~B}$. The type of reaction is: $\mathrm{A}+\mathrm{B} \rightarrow 2 \mathrm{R}$. Conversion should be $95 \%$. The enthaply of reaction is $-82 \mathrm{~kJ} / \mathrm{mol}$, density of the mixture is $1050 \mathrm{~kg} / \mathrm{m} 3$, specific heat capacity is $3.5 \mathrm{~kJ} /(\mathrm{kg} \cdot \mathrm{K})$. The reaction rate coefficient can be calculated by the following equation: $k=1.63 \cdot 10^{10} \cdot e^{-\frac{8100}{T}} \frac{\mathrm{dm}}{\mathrm{mol} \cdot \mathrm{s}}$ Calculate the necessary reactor volume! Compare your result with the result of the R4 problem. Consulation.

| Data given in the example (including reaction order and reversibility) |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



| Mode of operation |  |
| :---: | :---: |
| Isothermal | Adiabatic |

## R7. Problem

A liquid phase $A+B \rightarrow C+D$ reaction is performed under isotherm conditions. Two ideal tubular reactors are available with a volume of $0.5 \mathrm{~m}^{3}$ each. The flowrate of the feeding streams is $25 \mathrm{kmol} / \mathrm{h}$ each, while the concentration of the reagents is $20 \mathrm{kmol} / \mathrm{m}^{3}$. The reaction can be considered second order. At inlet temperature, $25^{\circ} \mathrm{C}$, the value of the reaction rate coefficient is 0.125 $\mathrm{m}^{3} /(\mathrm{kmol} \cdot \mathrm{h})$.
a) Calculate conversion in the reactors separately and summarized if the reactors are connected consecutively. Calculate the quantity of component C leaving the reactors.
b) What conversion can be reached by connecting the reactors parallelly and dividing the feed streams equally between them?

| c) Data given in the example (including reaction order and reversibility) |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



|  | Mode of operation |
| :---: | :---: | :---: |
| Isothermal | Adiabatic |

## R8 problem

An $A+B \rightarrow C+D$ type, second order, irreversible reaction is conducted in a three element cascade consisting of vessels with a useful volume of $2 \mathrm{~m}^{3}$ each. The first reactor is fed with $333 \mathrm{~kg} / \mathrm{h}$ of A and $111 \mathrm{~kg} / \mathrm{h}$ of B. Besides the stream arriving from the first reactor, $148 \mathrm{~kg} / \mathrm{h} \mathrm{B}$ is also filled into the second vessel. The molar masses of the components: $\mathrm{M}_{\mathrm{A}}=222 \mathrm{~g} / \mathrm{mol}, \mathrm{M}_{\mathrm{B}}=74 \mathrm{~g} / \mathrm{mol}$, $\mathrm{M}_{\mathrm{C}}=278 \mathrm{~g} / \mathrm{mol}, \mathrm{M}_{\mathrm{D}}=18 \mathrm{~g} / \mathrm{mol}$. Upon entering the reactor, the feed streams mix immediately and completely and all of the reactor vessels can be considered perfectly mixed tank reactors. The density of the reaction mixture is $1058 \mathrm{~kg} / \mathrm{m}^{3}$, remaining constant during the reaction. Every element of the cascade is operating under isotherm conditions, at $40^{\circ} \mathrm{C}$. The reaction rate coefficient is $1.25 \cdot 10^{-3} \mathrm{~m}^{3} /(\mathrm{kmol} \cdot \mathrm{min})$.
a) Determine the mass of product C forming in an hour.
b) How many kg of product can be formed if one single $2 \mathrm{~m}^{3}$ reactor is applied instead of the cascade? Feeding streams remain the same: $333 \mathrm{~kg} / \mathrm{h}$ of A and $111 \mathrm{~kg} / \mathrm{h}$ of B.

| d) Data given in the example (including reaction order and reversibility) |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



|  | Mode of operation |
| :---: | :---: | :---: |
| Isothermal | Adiabatic |

## D1. Problem

10 kmol ethanol - water mixture, with $20 \mathrm{~mol} \%$ ethanol content, is purified until $2 \mathrm{~mol} \%$ ethanol content in the residue by batch distillation. Calculate the molar amount and mass of the distillate and of the residue. Calculate the composition of the distillate.

| Data given in the example |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



## D2. Problem

An ethanol - water mixture ( $100 \mathrm{kmol} / \mathrm{h}$ flow rate, 0.3 molar fraction) is distilled by flash distillation at $86^{\circ} \mathrm{C}$. Calculate the molar flowrate and the composition of the distillate and of the residue. Determine the operational limits of the separation.

| Data given in the example |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |  |
|  |  |  |  |  |
|  |  |  |  |  |
|  |  |  |  |  |
|  |  |  |  |  |
|  |  |  |  |  |



## D3. Problem

A propanol-isopropanol mixture having an isopropanol content of 45 mass percent with a mass flowrate of $2104 \mathrm{~kg} / \mathrm{h}$ is separated on a continuously operating distillation column at ambient pressure. The products contain 90 mass percent of isopropanol and 95 mass percent of propanol respectively. The feed is a boiling liquid and its position is optimal. The mixture of propanol and isopropanol can be considered ideal.
a) How much is molar flowrate of the distillate and the residue?
b) Determine the minimal number of plates.
c) Determine the minimal reflux ratio.

| d) Data given in the example |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



## D4. Problem

At atmospheric pressure $1.2 \mathrm{kmol} / \mathrm{h}$ phenol and metacresol mixture ( $55 \mathrm{~mol} \%$ phenol content) is distilled in a packed distillation column. According to the measurements if the reflux ratio is 6 , the metacresol contamination int he phenol stream is $10 \mathrm{~mol} \%$, while the phenol content of the metacresol stream is $6 \mathrm{~mol} \%$. The column is installed with a partial reboiler. The feed is $20 \%$ vapour, $80 \%$ liquid, its position is optimal.
a) Determine the HETP value if the height of the packing is 3.2 m !
b) Diameter of the column is 25 cm . Calculate the load factor at the bottom of the column! Pressure drop of the column is negligible.

| c) Data given in the example |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |

(

## D5. Problem

$8500 \mathrm{~kg} / \mathrm{h} 50 \mathrm{~mol} \%$ benzene-toluene mixture is separated in a continuous distillation column. Molar fraction of benzene in the distillate is 0.95 while that in the residue is 0.05 .Reflux ratio is $\mathrm{R}=3$. Enthalpy of evaporation: $30336 \mathrm{~kJ} / \mathrm{kmol}$, specific heat capacity: $1,844 \mathrm{~kJ} / \mathrm{kgK}$.
a) Give the mass flow rates of the distillate and of the residue.
b) Give the minimal number of theoretical plates to achieve the certain separation if the feed is liquid, $20^{\circ} \mathrm{C}$.
c) Calculate the number of real plates if the average plate efficiency is $75 \%$. d) Give the diameter of the column, if the average efficiency of plates is $75 \%$, pressure drop is 4 torr/plate and F -factor is $1.4 \mathrm{~Pa}^{1 / 2}$ ?
d) Give the amount of heating water vapour ( 3 bar ) and cooling water consumption, if the inlet temperature of water is $20^{\circ} \mathrm{C}$ and temperature increase have to be below $20^{\circ} \mathrm{C}$.

| Data given in the example |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



## D6. Problem

In a packed column a phenol-metacresol mixture is separated to a phenol stream of $90 \mathrm{~mol} \%$ phenol and to a metacresol stream of $92 \mathrm{~mol} \%$ metacresol content. The molar flow rate of the feed is $1 \mathrm{kmol} / \mathrm{h}$, its phenol content is $40 \mathrm{~mol} \%$. The reflux ratio is 7 . The feed is a mixture of vapour and liquid with $80 \%$ liquid. Position of inlet is optimal. Based on experimental results, the mass transfer coefficient is $0.59 \mathrm{~mol} / \mathrm{m}^{2} \mathrm{~s}$. The diameter of the column is 23.4 cm .
a) Calculate the number of transfer units and the height of the transfer units both in the upper and lower sections of the column! Calculate the height of the column!
b) Calculate the value of the F factor in the bottom and in the top of the column! (homework)

| Data given in the example |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |


| Data to be calculated |  |  |  |
| :---: | :---: | :---: | :---: |
| Name | Notation | Numerical quantity | Unit |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |



