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Examples and exercise problems – Reactors

The following examples and exercises are grouped by the generally accepted reactor categories. Depending on the mode of operation, a tank reactor (typically stirred, perfect mixing in ideal cases) can be classified as:

- batch (no input or output during the reaction),
- semi-batch (at least one component is added or removed either continuously or after a delay),
- continuous (the ideal version, assuming perfect mixing, is the so-called continuous stirred tank reactor or CSTR).

The other group of reactors comprises (continuous) tubular reactors. Ideal tubular reactors exhibit plug flow.

Based on heat transfer, reactors can be classified as:

- isothermal,
- adiabatic,
- polytropic (a cooled or heated reactor in which temperature varies over time or by location). Strictly speaking, most real reactors belong in this category.

Based on the number of phases, reactors/reactions can be categorized as:

- single phase, i.e. homogeneous (gas, liquid, supercritical fluid),
- two or more phases, i.e. heterogeneous (gas–liquid, gas–solid, liquid–solid, liquid–liquid, gas–liquid–solid etc.)

All examples and exercises are grouped by reactor type and involve only homogeneous reactions.

Example problems: stirred batch reactors

Example 1: Isothermal batch reactor, first-order reaction

An isomerization reaction is carried out in a batch reactor. The reaction is first-order, both isomers are liquids with a density of 900 kg/m^3 at $163 \text{ }^\circ\text{C}$. The reactor is filled in 10 minutes and emptied in 12 minutes. During the 14 minutes required to heat up the reactor, the reaction is negligible, it can be assumed to begin only when $163 \text{ }^\circ\text{C}$ is reached. 900 t of product must be synthesized in 7000 hours of operation per year. Conversion is 97%.

What is the required volume of the stirred batch reactor operated isothermally at $163 \text{ }^\circ\text{C}$? The reaction rate coefficient is $0,8 \text{ 1/h}$.

$$V \approx 0,74 \text{ m}^3$$

Example 2: Isothermal batch reactor, second-order reaction

The reaction $\text{A} + 2\text{B} \rightarrow \text{C} + 2\text{D}$ is carried out in an isothermal, perfectly stirred batch reactor at $80 \text{ }^\circ\text{C}$. The reaction rate can be described as second-order, i.e. $r = k \cdot c_{\text{A}} \cdot c_{\text{B}}$, where $k = 0,058 \text{ m}^3/(\text{kmol} \cdot \text{min})$.

At $80 \text{ }^\circ\text{C}$, 200 kg of material A ($M_{\text{A}}=90 \text{ g/mol}$) and 400 kg of material B ($M_{\text{B}}=90 \text{ g/mol}$) is measured into the reactor. At this point, the (liquid) reaction mixture has a volume of 850 dm^3 . The reaction does not change the volume. What conversion can be achieved in 35 minutes?

$$X = 0,914$$

Example 3: Isothermal, second-order reaction

The reaction $A+B \rightarrow C+D$ is carried out at 80°C in an isothermal, perfectly stirred tank reactor. The reaction rate can be described as second-order, where $k = 0,058 \text{ m}^3/(\text{kmol}\cdot\text{min})$.

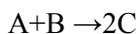
At 80°C , 240 kg of material A ($M_A=60 \text{ g/mol}$) and 400 kg of material B ($M_B=90 \text{ g/mol}$) is measured into the stirred tank. At this point, the volume of the (liquid) reaction mixture is 900 dm^3 . The reaction does not change the volume. How much time is required to reach 95% conversion?

Solution

$$t = 9,96 \text{ min}$$

Example 4: Isothermal, pseudo-first-order reaction

The hydrolysis of acetic anhydride in a dilute aqueous solution appears to be a first-order reaction:



In a dilute solution ($c_A < 0.2 \text{ mol/dm}^3$) the reaction rate coefficient can be calculated with the following equation:

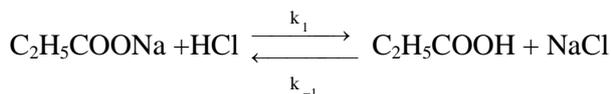
$$k = 9,2335 \cdot 10^6 \cdot e^{\frac{-5335}{T}} \frac{1}{\text{min}}$$

If 200 kg/h acetic acid must be produced at 35°C with an initial anhydride concentration of 0.2 mol/dm^3 , what is the required volume of the reactor? Servicing time is 15 min per batch. The desired conversion is 98%.

$$V = 4,25 \text{ m}^3$$

Example 5: Isothermal, equilibrium reaction

Propanoic acid is synthesized in the following reaction:



In aqueous solution, the reaction is reversible and second-order. A series of isothermal experiments with 2.7 mol/dm^3 initial concentration were performed in a laboratory-scale batch reactor to determine the reaction rate coefficient. A sample was taken from the reactor every 10 minutes, and the conversion of sodium propanoate was determined:

time	(min)	0	10	20	30	50	∞
Conversion	(%)	0	39	55	64	72,5	80

Based on the data in the table, design an isothermal batch reactor to produce 1360 kg/h propanoic acid. Servicing time (loading, heating, cooling and emptying) is 45 minutes per batch. Since the equilibrium conversion of sodium propanoate is 80%, use an operating conversion of 75%. Initial concentrations in the industrial reactor are 323 kg/m^3 sodium propanoate and 123.4 kg/m^3 hydrochloric acid (100% HCl). The density of the reaction mixture is constant, 1200 kg/m^3 .

$$V = 11,8 \text{ m}^3$$

Example 6: Isothermal batch reactor, equilibrium reaction

In an equilibrium reaction, ethyl acetate is synthesized from ethanol and acetic acid in an isothermal batch reactor at 100°C , in the presence of hydrochloric acid as catalyst. An aqueous solution containing 23 m/m% acetic acid, 46 m/m% ethanol and no ethyl acetate is measured into the reactor.

The average density of the solution is 1020 kg/m^3 . When the reaction is stopped, conversion is 35%. The value of the equilibrium constant K_c is 2.39. The reaction rate coefficient k_f is $7.93 \cdot 10^{-6} \text{ m}^3/\text{kmol}\cdot\text{s}$. From the start of the reaction, how much time is required to reach the desired conversion?
2.1 hours.

Example 7: Isothermal gas phase reaction, changing number of moles

Determine the reaction rate coefficient for the gas phase decomposition of dimethyl ether, based on the pressure change measured in a constant volume reactor! The reaction is first-order and irreversible:



The measurement was carried out by filling the reactor with pure dimethyl ether at time $t = 0$ and measuring the increase in pressure at a constant temperature of $504 \text{ }^\circ\text{C}$.

time	(s)	390	777	1195	3155	∞
pressure change	(mmHg)	96	176	250	476	619

$$k = 0,0005 \text{ 1/s.}$$

Example 8: Adiabatic reaction, batch reactor, first-order reaction

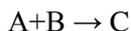
An isomerization reaction is carried out in a batch reactor. The reaction is first-order, both isomers are liquids and have a density of 900 kg/m^3 (density can be considered to be constant). The reaction rate coefficient is 0.8 h^{-1} at $163 \text{ }^\circ\text{C}$. The reaction has an enthalpy of -347.5 J/g and an activation energy of $1.21 \cdot 10^5 \text{ J/mol}$. The molar mass of the material is 250 g/mol . Loading and emptying the reactor takes 10 and 12 minutes, respectively. During the 14 minutes required to heat up the reactor, the reaction is negligible, it can be assumed to begin only when $163 \text{ }^\circ\text{C}$ is reached. 900 t of product must be synthesized in 7000 operating hours per year. Conversion is 97%.

What is the required volume of the stirred tank reactor operated adiabatically?

$$V = 0,11 \text{ m}^3$$

Example 9: Adiabatic, second-order reaction

A Diels–Alder reaction is carried out in an adiabatic batch reactor. Symbolically:



Benzene is used for solvent, the initial concentration of the components is 0.15 kmol/m^3 . The initial temperature of the reaction mixture is $25 \text{ }^\circ\text{C}$. How much time is required to reach 50% conversion?
Data:

$$k = 3,1623 \cdot 10^6 \cdot e^{\frac{-5834}{T}} \frac{\text{m}^3}{\text{kmol}\cdot\text{s}}$$

$$\Delta H_R = -72,8 \frac{\text{kJ}}{\text{mol}}$$

The density and heat capacity of the solution can be considered to be constant. Since the solutions are dilute, the data for benzene can be used for calculations:

$$c_p = 1,75 \text{ kJ}/(\text{kg}\cdot\text{K}), \rho = 880 \text{ kg/m}^3$$

10 min.

Example problems: continuous stirred tank reactors

Example 10: Isothermal continuous stirred tank reactor, irreversible reaction

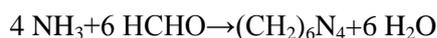
The hydrolysis of acetic anhydride is carried in a continuous stirred tank reactor at 25°C. The reaction is pseudo-first-order. The feed stream (0.6 m³/h) is a 0.9 kmol/m³ solution of acetic anhydride. The reaction rate coefficient is 0.0806 min⁻¹. The desired conversion is 97%. Calculate the required volume of the reactor!

Solution

$$V = 4 \text{ m}^3$$

Example 11: Isothermal continuous tank reactor, irreversible reaction

The laboratory synthesis of hexamethylene tetramine (C) from aqueous solutions of ammonia (A) and formaldehyde (B) proceeds at 36 °C, in a continuous stirred tank reactor (CSTR). The mixing can be considered as ideal. The reactor has a useful volume of 490 cm³. The density of the reaction mixture does not change. The feed streams enter the reactor via two separate pipes at a rate of 1.5 cm³/s each. Stream A contains 4.06 mol/dm³ of ammonia, stream B contains 6.32 mol/dm³ formaldehyde. The consumption rate of A can be calculated with the formula $r_A = k \cdot c_A \cdot c_B^2$. The reaction rate constant is given by $k = 1,42 \cdot 10^3 e^{-\frac{3090}{T}} \frac{\text{dm}^6}{\text{mol}^2 \text{s}}$, where T denotes the absolute temperature. The reaction equation is as follows:



Calculate the outlet concentrations and the conversion at steady state!

Solution

$$X = 0,821, c_B = 0,66 \text{ mol/dm}^3, c_C = 0,417 \text{ mol/dm}^3.$$

Example 12: Isothermal, irreversible first-order reaction

An A→B reaction which is first-order with respect to A is carried out in an isothermal, continuously stirred tank reactor, in dilute solution. The reaction rate constant can be calculated with the Arrhenius equation, and at 150 °C $k = 15.53 \text{ h}^{-1}$. The feed concentration of component A is 0.250 mol/dm³, at a rate of 0.35 dm³/min. $E = 4752.6 \text{ J/mol}$.

Calculate the conversion for the reaction

- carried out at 20 °C,
- carried out at 150 °C.

Solution

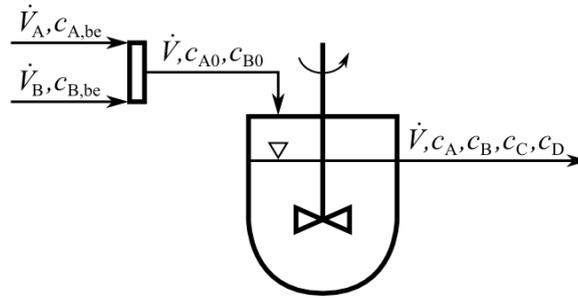
$$X = 0,67$$

$$X = 0,787.$$

Example 13: Isothermal equilibrium reaction

An equilibrium reaction of the type $\text{A} + \text{B} \xrightleftharpoons[k_{-1}]{k_1} \text{C} + \text{D}$ is carried out in a 0.12 m³ continuous stirred tank reactor. The desired conversion is 75 %. Feed streams are equal and contain only one component each. Stream A contains 2.8 mol/dm³ of component A, stream B contains 1.6 mol/dm³ of component B. The value of k_1 is 7 dm³/(mol·min), the value of k_{-1} is 3 dm³/(mol·min). What is the required feed rate?

Solution



$$\dot{V}_A = \dot{V}_B = \frac{\dot{V}}{2} = 4 \frac{\text{dm}^3}{\text{min}}$$

Example 14: Adiabatic reaction, first-order irreversible reaction

An irreversible $A \rightarrow B$ reaction is carried out in a perfectly stirred continuous adiabatic reactor. The reaction enthalpy is -12800 kJ/kmol , the reaction rate constant can be calculated with the formula $8.41 \cdot 10^4 \cdot e^{-49200/RT} \text{ (s}^{-1}\text{)}$. The mixture has an average specific heat capacity of $2440 \text{ J/(kg}\cdot\text{K)}$ and a density of 800 kg/m^3 . The feed concentration of A is 12 kmol/m^3 . The reaction enthalpy and the specific heat capacity of the materials do not depend on the temperature.

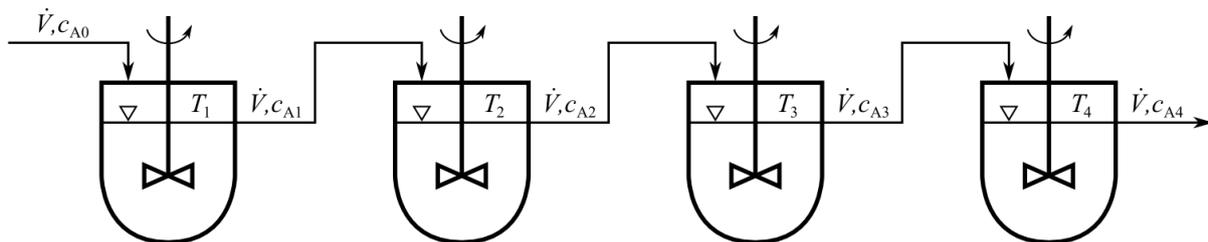
- Calculate the conversion and the reactor temperature, if the initial mixture is fed into a reactor with 3.9 m^3 useful volume at 303 K , at a rate of $0.006 \text{ m}^3/\text{s}$!
- Calculate the conversion and the reactor temperature, if the initial mixture is fed into a reactor with 3.25 m^3 useful volume at 283 K ! The average residence time is kept equal to that in part a).

Solution

Example 15: Tank reactor cascade, pseudo-first-order reaction

The hydrolysis of acetic anhydride (a pseudo-first-order reaction) is carried out in a cascade of four stirred tank reactors of equal volume. The consecutive tanks are operated at progressively higher temperatures ($10 \text{ }^\circ\text{C}$, $15 \text{ }^\circ\text{C}$, $25 \text{ }^\circ\text{C}$, $40 \text{ }^\circ\text{C}$). The reaction rate constant can be determined from the Arrhenius equation. The value of the preexponential factor is $22655200 \text{ min}^{-1}$, the activation energy is 46311.15 J/mol . The desired conversion is 91% . The feed rate is $0.1 \text{ m}^3/\text{min}$. Calculate the volume of the reactors.

Solution



$$V = \dot{V} \cdot \bar{t} = 0,1 \frac{\text{m}^3}{\text{min}} \cdot 5 \text{ min} = 0,5 \text{ m}^3$$

Example 16: Cooled tank reactor

A liquid phase, irreversible, first-order reaction is carried out in a continuous stirred tank reactor. The feed temperature is 293 K , the average residence time is 1200 s , the maximal adiabatic temperature increase is 165.9 K , the value of the preexponential factor is 32500 s^{-1} , the activation energy is 45.66 kJ/mol , the cooling parameter is $1,482$, the feed concentration is 8 kmol/m^3 . determine the stationary operating point of the reactor for average coolant temperatures of 273.45 K and 289.2 K .

Check if the criteria of dynamic stability are satisfied for the given operating parameters.

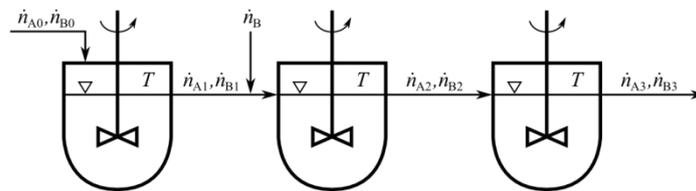
Solution

Example 17: Tank reactor cascade, second-order irreversible reaction

A second-order irreversible reaction of the form $A+B \rightarrow C+D$ is carried out in a cascade of 3 tank reactors with 2 m^3 useful volume in each reactor. 333 kg/h of A and 111 kg/h of B are fed into the first reactor, and an additional 148 kg/h of B is fed into the second reactor along with the stream arriving from the first reactor. The molar masses of the components are: $M_A = 222 \text{ g/mol}$, $M_B = 74 \text{ g/mol}$, $M_C = 278 \text{ g/mol}$, $M_D = 18 \text{ g/mol}$. The feed streams are perfectly mixed as soon as they are fed into the reactors, each reactor can be regarded as a perfectly mixed tank reactor. The density of the reaction mixture is 1058 kg/m^3 and remains constant during the reaction. Each element in the cascade operates under isothermal conditions at $40 \text{ }^\circ\text{C}$. The reaction rate constant is $1.25 \cdot 10^{-3} \text{ m}^3/(\text{kmol} \cdot \text{min})$.

- How many kg of C is produced per hour?
- How many kg of product is obtained every hour if the cascade is replaced by a single 2 m^3 tubular reactor with feed streams of 333 kg/h A and 111 kg/h B?

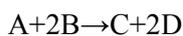
Solution



Example problems: tubular reactors

Example 18: Isothermal tubular reactor, gas phase reaction, no change in the number of moles

Methane and sulphur react in gas phase at $600 \text{ }^\circ\text{C}$ and atmospheric pressure, yielding carbon disulphide and hydrogen sulfide. The reaction is carried out in an isothermal tubular reactor. The reaction rate of sulphur can be described with the equation $k \cdot c_A \cdot c_B$ ($k = 119,8 \text{ m}^3/\text{mol} \cdot \text{h}$), provided that the reaction equation is the following:



The feed is stoichiometric, the feed rate of methane is $23,8 \text{ mol/h}$.

What is the required residence time to achieve an 18% conversion of methane? What is the required size of the reactor?

Example 19: Isothermal, gas phase reaction, no change in the number of moles

The following second-order reaction is carried out in an isothermal, ideal tubular reactor.



The feed contains only reactants. The pressure and temperature in the reactor are 1.3 bar and $500 \text{ }^\circ\text{C}$.

- The feed stream contains the component is stoichiometric ratio. What percent conversion can be achieved with a residence time of 8 s??
- What is the required residence time if twice the required amount of component A is added, and 40% percent conversion is desired? What percent is the flow rate of that in part a)?

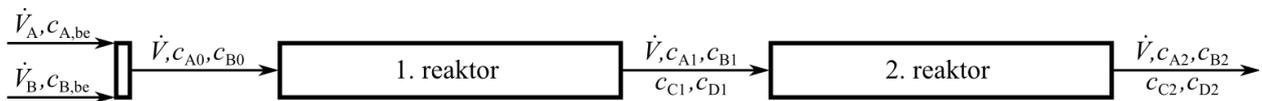
$$\frac{v_2}{v_1} = \frac{L/t_2}{L/t_1} = \frac{t_1}{t_2} = \frac{8 \text{ s}}{5,472 \text{ s}} = 1,46$$

Example 20: Isothermal tubular reactor, homogeneous liquid phase reaction

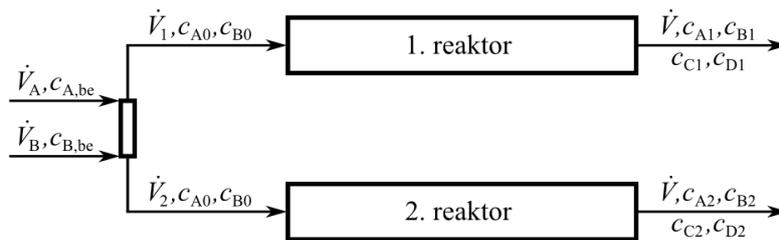
A liquid phase reaction of the type $A+B \rightarrow C$ is to be carried out under isothermal conditions. Two $0,5 \text{ m}^3$ ideal tubular reactors are available. The concentrations of the components in the 25 kmol/h feed stream is $20\text{--}20 \text{ kmol/m}^3$. The reaction is second-order. At the feed temperature of $25 \text{ }^\circ\text{C}$, the reaction rate constant is $0.125 \text{ m}^3/(\text{kmol}\cdot\text{h})$.

- What is the conversion in the reactors separately and in total, if they are in series? What is the amount of C in the outlet stream?
- What is the conversion if the two reactors are parallel and divide the feed streams equally?

Solution



$$\dot{n}_c = 8,33 \frac{\text{kmol}}{\text{h}}$$



$$X = 0,33$$

Example 21: Isothermal first-order irreversible reaction

A reaction of the type $A \rightarrow B$, first-order with respect to A, is carried out in dilute solution in an isothermal tubular reactor. The reaction rate constant can be calculated with the Arrhenius equation and at $20 \text{ }^\circ\text{C}$ its value is $k = 8.53 \text{ h}^{-1}$. The feed concentration of component A is 0.250 mol/dm^3 , the feed rate is $0.35 \text{ dm}^3/\text{min}$. $E = 4752.6 \text{ J/mol}$.

Calculate the conversion if

- the reaction is carried out at $20 \text{ }^\circ\text{C}$,
- the reaction is carried out at $150 \text{ }^\circ\text{C}$.

Example 22: Adiabatic reaction, gas phase reaction, no change in the number of moles

Carbon monoxide and water are converted into carbon dioxide and hydrogen at atmospheric pressure in an adiabatic tubular reactor. The reaction goes to equilibrium. The feed temperature is $380 \text{ }^\circ\text{C}$, the feed rate $2.5 \text{ m}^3/\text{s}$. The ratio of CO and H_2O in the feed is 1:4, the feed contains no inert gas of reaction products. The outlet stream temperature is $500 \text{ }^\circ\text{C}$. The reaction enthalpy is $-39,4 \text{ kJ/mol}$, the molar heat capacity of the gas mixture is $34 \text{ kJ}/(\text{kmol}\cdot\text{K})$. Calculate the conversion and the maximal temperature increase for the reaction!

Example 23: Adiabatic reaction, tube reactor, liquid phase second-order reaction

A second-order $A+B \rightarrow C+D$ reaction is carried out in an ideal adiabatic tube reactor with a volume of 0.12 m^3 . The reaction rate constant can be calculated with the equation $6.52 \cdot 10^5 \cdot e^{-42300/RT} \text{ kmol}/(\text{m}^3 \cdot \text{s})$. The initial concentration of both components is $1,1 \text{ kmol}/\text{m}^3$. The feed contains no product, its temperature is $12 \text{ }^\circ\text{C}$, the feed rate is $4 \cdot 10^{-4} \text{ m}^3/\text{s}$. The reaction enthalpy is $-42600 \text{ kJ}/\text{kmol}$, the specific heat capacity of the mixture is $2800 \text{ J}/(\text{kg} \cdot \text{K})$, its density is $840 \text{ kg}/\text{m}^3$. Calculate the conversion!

Example 24: Cooled tubular reactor

The first-order reaction $A \rightarrow R$ is carried out in a tubular reactor at $50 \text{ }^\circ\text{C}$. The reaction is exothermic, thus a heat exchanger is used as a reactor. The reaction mixture flows in the tubes, the coolant (water) flows in the jacket. The molar heat capacity of the reaction mixture is $33.5 \text{ kJ}/(\text{kmol} \cdot \text{ }^\circ\text{C})$, the specific heat capacity of the cooling water is $4,18 \text{ kJ}/(\text{kg} \cdot \text{ }^\circ\text{C})$, the initial concentration is $0.4 \text{ kmol}/\text{m}^3$, the reaction rate coefficient is 0.128 s^{-1} , the feed rate is $10.2 \text{ m}^3/\text{h}$, the overall heat transfer coefficient is $852 \text{ W}/(\text{m}^2 \cdot \text{K})$, the reaction enthalpy is $-8.32 \cdot 10^4 \text{ kJ}/\text{kmol}$, the reaction mixture has a viscosity of $4,4 \text{ mPas}$ and a density of $900 \text{ kg}/\text{m}^3$.

- Calculate the volume for 90% conversion!
- What is the required number and length of tubes, if the inner diameter of the tubes is 2.54 cm ? (Turbulent flow must be maintained in order for the overall heat transfer coefficient not to degrade.)
- Should the heat exchanger be counterflow or coflow? Reason your answer! Calculate the inlet temperature and flow rate of the cooling water!

A reminder: using computed data, the logarithmic temperature difference and geometric data, the heat flow across the wall can be calculated. The wall thickness is again neglected. Let us compare the results:

$$\Delta T_{\text{atl}} = \frac{(T - T_{\text{h,be}}) - (T - T_{\text{h,ki}})}{\ln \frac{T - T_{\text{h,be}}}{T - T_{\text{h,ki}}}} = \frac{(50^\circ\text{C} - 18,6^\circ\text{C}) - (50^\circ\text{C} - 46,86^\circ\text{C})}{\ln \frac{50^\circ\text{C} - 18,6^\circ\text{C}}{50^\circ\text{C} - 46,86^\circ\text{C}}} = 12,27^\circ\text{C}$$

$$\dot{Q} = h \cdot A \cdot \Delta T_{\text{atl}} = h \cdot n \cdot L \cdot (d + e) \cdot \pi \cdot \Delta T_{\text{atl}} = 852 \frac{\text{W}}{\text{m}^2 \cdot \text{K}} \cdot 29 \cdot 3,47 \text{ m} \cdot (0,0254 + 0) \text{ m} \cdot \pi \cdot 12,27^\circ\text{C} = 84 \text{ kW}$$

Of course when designing, the overall heat transfer coefficient is not known with such precision, neither can the wall thickness be neglected (for calculating the heat transfer surface and the outlet temperature). Observe that the estimated value of the heat transfer coefficient influences the calculated average temperature of the coolant, thus causing uncertainty. Do not forget that the flow characteristics of the materials flowing through and around the pipes determine the value of the overall heat transfer coefficient (as detailed in Chemical Unit Operations I.)

Example problems: semi-batch reactors

Example 25: Semi-batch reactor, pseudo-first-order reaction

An irreversible $A+B \rightarrow 2C$ reaction is carried out in a mixed tank reactor. In a semi-batch operation, 5.5 kmol of pure component B is fed into the reactor and over the course of 2 hours, 5 kmol of pure component A is added at a constant feed rate. Component B is in excess throughout, thus the reaction is pseudo-first-order, the reaction rate coefficient is 7.5 h^{-1} . The molar volumes of all components is $0.06 \text{ m}^3/\text{kmol}$. What is the conversion when all component A has been added?

Solution

$$X = 0.933$$

Example problem: combinations of different reactor types

Example 26: Batch reactor and tubular reactor

The liquid phase reaction $A \rightarrow T$ is irreversible and first-order. The concentration of component A at the time of starting and stopping the reactor, the reaction time and the amount of heat subtracted in order to maintain an isothermal operation were measured in a 2 l isothermal batch reactor.

T (°C)	70	100
c_{A0} (kmol/m ³)	3	3
t (min)	40	34
c_A (kmol/m ³)	2,1	0,9
Q (kJ)	302,4	705,6

What is the required volume of an adiabatic tubular reactor to obtain 17.1 kmol/h of product T, if the reactor is to be operated at 90% conversion? The available concentration of material A is 3 kmol/m³, the inlet temperature of the reactor is 70 °C. The density of the mixture is 1 g/ml, its specific heat capacity is 3.5 kJ/kgK.

Solution

$$\dot{n}_C = 17,1 \frac{\text{kmol}}{\text{h}} = 0,285 \frac{\text{kmol}}{\text{min}}$$
$$\dot{V} = \frac{\dot{n}_{A0}}{c_{A0}} = \frac{\dot{n}_C}{X \cdot c_{A0}} = \frac{0,285 \frac{\text{kmol}}{\text{min}}}{0,95 \cdot 3 \frac{\text{kmol}}{\text{m}^3}} = 0,1 \frac{\text{m}^3}{\text{min}}$$
$$V = \dot{V} \cdot t = 2,38 \text{m}^3$$

Example 27: Comparison of continuous mixed tank reactor and tubular reactor. Isothermal and adiabatic reaction.

10 dm³/s ($c_A = 7,5 \text{ mol/dm}^3$) of material A and 20 dm³/h ($c_B = 3,75 \text{ mol/dm}^3$) of material B is fed into a continuous reactor. The feed temperature is 20 °C and contains no reaction products. The required conversion is 95%. The second-order reaction is of type $A+B \rightarrow 2R$. The reaction rate coefficient can be calculated by the following equation:

$$k = 1,63 \cdot 10^{10} \cdot e^{-\frac{8100}{T}} \frac{\text{dm}^3}{\text{mol} \cdot \text{s}}$$

The reaction enthalpy is -82 kJ/mol, the reaction mixture has a density of 1050 kg/m³ and a specific heat capacity of 3.5 kJ/(kg·K). The density and specific heat capacity can be considered to remain constant during the reaction.

- How much product is obtained in each hour?
- If the reaction is to be carried out in a continuous stirred tank reactor in adiabatic mode, what is the required volume of the reactor?
- What is the required volume of an ideal displacement tubular reactor in adiabatic mode?

Solution

$$\dot{n}_R = 540 \frac{\text{kmol}}{\text{h}}$$

b)

$$\bar{t} = \frac{1}{k \cdot c_{A0}} \cdot \frac{X}{(1-X)^2} = 135,6 \text{ s}$$

$$V = \bar{t} \cdot \dot{V} = 135,6 \text{ s} \cdot 30 \frac{\text{dm}^3}{\text{s}} = 4067,8 \text{ dm}^3 \approx 4,1 \text{ m}^3$$

c)

$$V = \bar{t} \cdot \dot{V} = 17,4 \text{ s} \cdot 30 \frac{\text{dm}^3}{\text{s}} = 522 \text{ dm}^3 \approx 0,522 \text{ m}^3$$

Practice problems

Problem 1

An isomerisation reaction is to be carried out in an perfectly stirred, isothermal batch reactor. The reaction is first-order. The density of the mixture can be approximated as 865 kg/m^3 , independent of temperature. The preexponential factor is 45.46 h^{-1} , the activation energy is 14742.5 J/mol . Filling the reactor requires 20 minutes, emptying requires 10 minutes. The temperature adjustment requires 10 minutes (during which the reaction can be considered to not run). 1500 t of product must be obtained in 6800 operational hours per year. Conversion is 99%.

What is the required volume of the stirred batch reactor for operating temperatures of 80 and 120 °C?
(4 m^3 , 1.43 m^3)

Problem 2

Design a reactor capable of synthesizing three different products. For each product, the required design capacity, reaction type and order and the required temperature are shown in the following table.

Parameter	product	product	product
Reaction type	A+B→T	A→T	2A→T
Yearly hours of operation	2500	1000	3500
Yearly production	50 kmol	200 kmol	80 kmol
Temperature (°C)	110	130	160
Reaction rate coefficient	$0.1 \text{ m}^3/(\text{kmol} \cdot \text{h})$	$0.2 \text{ m}^3/(\text{kmol} \cdot \text{h})$	0.5 1/h
Conversion	92%	99%	95%

Reactants are fed into the reactor at 20 °C. The average rate at which the reactor can be heated is 5 °C/min . Loading takes 10 minutes, emptying and cleaning takes 60 minutes. Assume that the reaction starts only upon reaching the required temperature. Reacting components are available in 1 kmol/m^3 concentration. Reactants are fed into the reactor in stoichiometric ratio.

What is the required volume of the stirred batch tank reactor? ($V_1=2.47 \text{ m}^3$; $V_2=2.27 \text{ m}^3$, $V_3=2.15 \text{ m}^3$, hence 2.5 m^3).

Problem 3

An $A + 2B \rightarrow C + 2D$ reaction is carried out in solution at 90 °C in an isothermal, perfectly stirred batch reactor. The reaction rate can be described as second-order, i.e. $r = kc_Ac_B$, where $k = 0.1 \text{ m}^3/(\text{kmol} \cdot \text{min})$. The solvent is fed into the tank reactor first, then 20 kg of material A ($M_A = 90 \text{ g/mol}$) and 40 kg of material B ($M_B = 90 \text{ g/mol}$) are added. The (liquid) reaction mixture has a volume of 900 dm^3 at this point. The reaction causes no volume change. What is the attainable conversion after 90 minutes? ($X = 81.6\%$)

Problem 4

An $A + 2B \rightarrow C + 2D$ reaction is carried out in solution at $90\text{ }^\circ\text{C}$ in an isothermal, perfectly stirred batch reactor. The reaction rate can be described as second-order, i.e. $r = kc_Ac_B$, where $k = 0.1\text{ m}^3/(\text{kmol}\cdot\text{min})$. The solvent is fed into the tank reactor first, then 20 kg of material A ($M_A = 90\text{ g/mol}$) and 50 kg of material B ($M_B = 90\text{ g/mol}$) are added. The (liquid) reaction mixture has a volume of 900 dm^3 at this point. The reaction causes no volume change. How much time is required to reach 90% conversion? ($t = 166.8\text{ min}$)

Problem 5

An $A + 2B \rightarrow C + 2D$ reaction is carried out in solution at $80\text{ }^\circ\text{C}$ in an isothermal, perfectly stirred batch reactor. The reaction rate can be described as second-order, i.e. $r = kc_Ac_B$, where $k = 0.058\text{ m}^3/(\text{kmol}\cdot\text{min})$. The solvent is fed into the tank reactor first, then 30 kg of material A ($M_A = 90\text{ g/mol}$) and 50 kg of material B ($M_B = 90\text{ g/mol}$) are added. The (liquid) reaction mixture has a volume of 1050 dm^3 at this point. The reaction causes no volume change. How much time is required to reach 90% conversion? ($t = 298.6\text{ min}$)

Problem 6

An $A + B \rightarrow C + D$ reaction is carried out in solution at $80\text{ }^\circ\text{C}$ in an isothermal, perfectly stirred batch reactor. The reaction rate coefficient is $k = 0.058\text{ m}^3/(\text{kmol}\cdot\text{min})$. The solvent is fed into the tank reactor first, then 30.5 kg of material A ($M_A = 90\text{ g/mol}$) and 29.5 kg of material B ($M_B = 90\text{ g/mol}$) are added. The (liquid) reaction mixture has a volume of 890 dm^3 at this point. The reaction causes no volume change. How much time is required to reach 90% conversion? ($t = 337.4\text{ min}$)

Problem 7

Acetic anhydride is hydrolyzed in a continuous stirred tank reactor at $25\text{ }^\circ\text{C}$. The reaction is pseudo-first-order. In the feed stream ($0.4\text{ m}^3/\text{h}$) the concentration of acetic anhydride is 1 kmol/m^3 . The reaction rate coefficient is 0.0806 min^{-1} . The required conversion is 98%. Calculate the required reactor volume! Calculate the daily consumption of acetic anhydride! ($V = 4.05\text{ m}^3, 9.6\text{ kmol/day}$)

How will the conversion change if the feed is increased by 20%? ($X = 0.976$)

Problem 8

A second-order, irreversible reaction ($2A \rightarrow T$) is carried out in a continuous stirred tank reactor. In the feed stream ($0.4\text{ m}^3/\text{h}$) component A is present in a concentration of 1 kmol/m^3 . The reaction rate coefficient is $7.8\text{ m}^3/(\text{kmol}\cdot\text{min})^{-1}$. The required conversion is 98%. Calculate the necessary reactor volume! Calculate the daily feed reactant consumption! ($V = 2.1\text{ m}^3, 9.6\text{ kmol/day}$)

Problem 9

An equilibrium reaction of the type $A+B \xrightleftharpoons[k_{-1}]{k_1} C+D$ is carried out in a 0.2 m^3 continuous stirred tank reactor. The feed streams have equal volumetric flow rates and contain only one component each. Stream A contains 2.8 mol/dm^3 of component A, stream B contains 1.6 mol/dm^3 of component B. The value of k_1 is $7\text{ dm}^3/(\text{mol}\cdot\text{min})$, the value of k_{-1} is $3\text{ dm}^3/(\text{mol}\cdot\text{min})$. What is the equilibrium conversion? ($X = 75.47\%$)

Problem 10

An equilibrium reaction of the type $A+B \xrightleftharpoons[k_{-1}]{k_1} C+D$ is carried out in a 0.2 m^3 continuous stirred tank reactor. The feed streams have equal volumetric flow rates and contain only one component each.

Stream A contains 3.2 mol/dm^3 of component A, stream B contains 2.1 mol/dm^3 of component B. The value of k_1 is $7 \text{ dm}^3/(\text{mol}\cdot\text{min})$, the value of k_{-1} is $3 \text{ dm}^3/(\text{mol}\cdot\text{min})$.

What is the equilibrium conversion? ($X = 72.14\%$)

At what feed rate will the conversion be 70%? ($64.5 \text{ dm}^3/\text{min}$)

Problem 11

An $A + B \rightarrow C + D$ second-order reaction is carried out in a 0.12 m^3 ideal adiabatic tubular reactor. The reaction rate coefficient can be calculated by the formula $6.52 \cdot 10^5 \cdot e^{-42300/RT} \text{ m}^3/(\text{kmol}\cdot\text{s})$. The initial concentration of both A and B is 1.1 kmol/m^3 . The feed contains no product, has a temperature of $12 \text{ }^\circ\text{C}$ and a volumetric flow rate of $4 \cdot 10^{-4} \text{ m}^3/\text{s}$. The reaction enthalpy is -42600 kJ/kmol , the mixture has a specific heat capacity of $2800 \text{ J}/(\text{kg}\cdot\text{K})$ and a density of 840 kg/m^3 . Calculate the conversion! ($X = 88.9\%$)

Problem 12

The liquid-phase first-order irreversible reaction $A \rightarrow T$ is carried out in an isothermal batch reactor having with volume $V = 2 \text{ dm}^3$. The concentration of component A at the start and end of the reaction, the reaction time and the heat removed in order to ensure isothermal conditions were measured at $70 \text{ }^\circ\text{C}$ and at $100 \text{ }^\circ\text{C}$. The results are shown in the following table:

$T \text{ (}^\circ\text{C)}$	70	100
$c_{A0} \text{ (kmol/m}^3)$	3	3
$t \text{ (min)}$	40	34
$c_A \text{ (kmol/m}^3)$	2.1	0.9
$Q \text{ (kJ)}$	302.4	705.6

What volume should an adiabatic tubular reactor have, if 17.1 kmol/h of product T must be synthesized operating at 90% conversion? The available concentration of material A is 3 kmol/m^3 , fed into the reactor at $70 \text{ }^\circ\text{C}$. The density can be approximated as 1000 kg/m^3 , the specific heat capacity is $3500 \text{ J}/(\text{kg}\cdot\text{K})$. ($V = 2.44 \text{ m}^3$)

Problem 13

The reaction $A + B \rightarrow C + D$ is second-order. The initial mixture contains component A 2.5 kmol/m^3 , component B is added in 20% excess. The feed mixture has a flow rate of $4 \text{ m}^3/\text{h}$ and enters the reactor at $20 \text{ }^\circ\text{C}$. The reaction enthalpy is -42 kJ/mol , the density is 900 kg/m^3 , the specific heat capacity is 2.8 kJ/kgK . These parameters do not depend on the temperature.

The reaction rate coefficient can be calculated with the formula $k = 6.5 \cdot 10^6 \cdot e^{\frac{-5000}{T}} \frac{\text{m}^3}{\text{kmol}\cdot\text{min}}$.

What conversion can be achieved in a 2.5 m^3 continuous reactor operating at $65 \text{ }^\circ\text{C}$? The reactor can be charged at most to 80%. ($X = 0,8614$)

In order to maintain $65 \text{ }^\circ\text{C}$, should the reactor be heated or cooled? What is the required heat duty? (requires heating, 91.8 MJ/h)

What conversion can be achieved in a 0.8 m^3 adiabatic tubular reactor? ($X = 0,775$)

Problem 14

The liquid-phase second-order irreversible reaction $A + B \rightarrow C$ is carried out in an adiabatic tubular reactor. The reaction occurs in solution, the concentration of the components in the storage tanks are: solution A 0.2 kg/dm^3 ($M_A = 100 \text{ g/mol}$); solution B 0.112 g/dm^3 ($M_B = 80 \text{ g/mol}$). The solutions are fed into the reactor from the storage tanks at the following rates: solution A at $2 \text{ dm}^3/\text{min}$, solution B at $3 \text{ dm}^3/\text{min}$. The value of the reaction rate coefficient is known at two temperatures: $1.7 \text{ dm}^3/(\text{mol}\cdot\text{h})$ at

20 °C, 10 dm³/(mol·h) at 50 °C. What is the necessary volume of the adiabatic tubular reactor, if the feed temperature is 20 °C and the desired conversion is 90%? What is the hourly production of C? The enthalpy of the reaction is -242 kJ/mol, density is 850 kg/m³, specific heat capacity is 3 kJ/(kg·K). ($V = 120 \text{ dm}^3$, 216 mol C produced every hour).

Problem 15

Materials A and B react in the irreversible second-order reaction $A + B \rightarrow C + D$. Solutions of A and B are fed separately at 30 °C into the continuous stirred tank reactor with a useful volume of 2 dm³. Solution A is fed at a rate of 2 dm³/h and has a concentration of 2 mol/dm³, Solution B is fed at a rate of 3 dm³/h and has a concentration of 2 mol/dm³. Operating the reactor at 30 °C, the outlet concentration of A is 0.06 mol/dm³. The volume of the reaction mixture does not change during the reaction. If the reaction is carried out in an isothermal tubular reactor operating at the same parameters (feed and outlet rates, concentrations, temperatures) as the tank reactor, what should be the volume of that tubular reactor? ($V = 0.3 \text{ dm}^3$)

Problem 16

The following irreversible liquid-phase reaction is second-order: $A + B \rightarrow C + D$; $M_A = 50 \text{ g/mol}$, $M_B = 120 \text{ g/mol}$, $M_C = 100 \text{ g/mol}$, $M_D = 70 \text{ g/mol}$. The following data are available from laboratory experiments:

800 g of 30% pure A and 1200 g of 40% pure B are loaded into a batch reactor. Initially, products C and D are not present in the reaction mixture. The density of the reaction mixture is 1000 kg/m³ and does not change during the operation. Operating the reactor at 20 °C, 11 minutes after the start material C has a concentration of 180 g/dm³.

50 cm³/min of a 5 mol/dm³ solution of A at 20 °C and a solution of B with the same flow rate, concentration and temperature is fed into a continuous tank reactor having a useful volume of 2 dm³. The outlet stream is at 60 °C and contains 0.125 mol/dm³ of A. The reactor can be considered to be perfectly isolated. The reaction mixture has a specific heat capacity of 4.18 kJ/(kg·K).

What is the required volume of an adiabatic, ideal tubular reactor if the required yearly production is 1500 t at 95% conversion? Calculate with 7000 hours of operation per year. The adiabatic tubular reactor is operated with equimolar feed at 20 °C containing 3 mol/dm³ A. ($V = 14.1 \text{ dm}^3$)

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Appendix – Tables

Calculations for isothermal batch reactors and isothermal tubular reactors ($V = \text{constant}$)

$$t = c_{j0} \int_0^X \frac{dX}{-v_j r}$$

The j^{th} component is always the limiting component. In the table, this is always component A. For batch reactors t denotes the reaction time, for tubular reactors t denotes the average residence time.

Table 1. Calculations for isothermal batch tank reactors and isothermal tubular reactors. Integration aid.

Reaction type and order	Reaction rate equation	$t = c_{A0} \int_0^X \frac{dX}{-v_A r}$ substituted	Value of t after integration	X (by rearranging the previous column)
A → B zero-order	$r = k$	$t = \frac{c_{A0}}{k} \int_0^X dX$	$\frac{c_{A0} \cdot X}{k}$	$\frac{k \cdot t}{c_{A0}}$
A → B first-order	$r = k \cdot c_A = k \cdot c_{A0} \cdot (1 - X)$	$t = \frac{1}{k} \int_0^X \frac{dX}{(1 - X)}$	$-\frac{1}{k} \ln(1 - X)$	$1 - e^{-k \cdot t}$
A → B m-order ($m \neq 1$)	$r = k \cdot c_A^m = k \cdot c_{A0}^m \cdot (1 - X)^m$	$t = \frac{c_{A0}^{1-m}}{k} \int_0^X \frac{dX}{(1 - X)^m}$	$\frac{(1 - X)^{1-m} - 1}{k \cdot c_{A0}^{m-1} \cdot (m - 1)}$	$1 - \left(1 + (m - 1) \cdot k \cdot t \cdot c_{A0}^{m-1}\right)^{\frac{1}{1-m}}$
2A → P v. A + B → P second-order ($c_{A0} = c_{B0}$)	$r = k \cdot c_A^2 = k \cdot c_{A0}^2 \cdot (1 - X)^2$	$t = \frac{1}{k \cdot c_{A0}} \int_0^X \frac{dX}{(1 - X)^2}$	$\frac{(1 - X)^{-1} - 1}{k \cdot c_{A0}} = \frac{1}{k \cdot c_{A0}} \cdot \frac{X}{1 - X}$	$\frac{k \cdot t \cdot c_{A0}}{1 + k \cdot t \cdot c_{A0}}$

$A+B \rightarrow P$ second-order ($c_{A0} < c_{B0}$)	$r = k \cdot c_A \cdot c_B =$ $= k \cdot c_{A0} \cdot (1-X) \cdot (c_{B0} - c_{A0} \cdot X)$	$t = \frac{1}{k} \int_0^X \frac{dX}{(1-X) \cdot (c_{B0} - c_{A0} \cdot X)}$	$= \frac{1}{k \cdot (c_{B0} - c_{A0})} \cdot \ln \frac{c_{B0} - c_{A0} X}{c_{B0} (1-X)}$	$\frac{c_{B0} \cdot (e^{k \cdot (c_{B0} - c_{A0}) t} - 1)}{c_{B0} \cdot e^{k \cdot (c_{B0} - c_{A0}) t} - c_{A0}}$
$A \xrightleftharpoons[k_{-1}]{k_1} B$ $c_{B0} = 0$	$r = k_1 c_A - k_{-1} c_B =$ $= k_1 c_{A0} (1-X) - k_{-1} c_{A0} \cdot X =$ $= c_{A0} \cdot k_1 \left(1 - \frac{k_1 + k_{-1}}{k_1} X\right)$	$t = \frac{1}{k_1} \int_0^X \frac{dX}{\left(1 - \frac{k_1 + k_{-1}}{k_1} X\right)}$	$= \frac{1}{k_1 + k_{-1}} \ln \left(1 - \frac{k_1 + k_{-1}}{k_1} X\right)$	$\frac{k_1}{k_1 + k_{-1}} (1 - e^{-(k_1 + k_{-1}) t})$

Calculations for isothermal, ideally stirred tank reactors

$$V = \dot{V} \cdot \bar{t}$$

$\frac{1}{\bar{t}} \cdot (c_{j0} - c_j) + v_j \cdot r = 0$ in steady state, for reactions without volume change. Substituting the conversion:

$$\frac{1}{\bar{t}} \cdot \frac{(c_{j0} - c_j)}{c_{j0}} + \frac{v_j \cdot r}{c_{j0}} = 0 \Rightarrow \frac{1}{\bar{t}} \cdot X = -\frac{v_j \cdot r}{c_{j0}}$$

The j^{th} component is always the limiting component. In the table, this is always component A.

Table 2. Calculations for an ideally stirred batch reactor

Reaction type and order	Reaction rate equation and substitution	\bar{t} (after substituting the reaction rate and rearranging)	X (by rearranging the previous column)
A → B zero-order	$r = k$ $\frac{1}{\bar{t}} \cdot X = -\frac{-1 \cdot k}{c_{A0}}$	$\frac{c_{A0} \cdot X}{k}$	$\frac{k \cdot \bar{t}}{c_{A0}}$
A → B first-order	$r = k \cdot c_A = k \cdot c_{A0} \cdot (1 - X)$ $\frac{1}{\bar{t}} \cdot X = k \cdot (1 - X)$	$\frac{1}{k} \cdot \frac{X}{1 - X}$	$\frac{k \cdot \bar{t}}{1 + k \cdot \bar{t}}$
A → B m-order (m ≠ 1)	$r = k \cdot c_A^m = k \cdot c_{A0}^m \cdot (1 - X)^m$ $\frac{1}{\bar{t}} \cdot X = \frac{k \cdot c_{A0}^m \cdot (1 - X)^m}{c_{A0}}$	$\frac{1}{k \cdot c_{A0}^{m-1}} \cdot \frac{X}{(1 - X)^m}$	$\frac{k \cdot \bar{t} \cdot c_{A0}^{m-1}}{1 + k \cdot \bar{t} \cdot c_{A0}^{m-1}}$
2A → P v. A+B → P second-order ($c_{A0} = c_{B0}$)	$r = k \cdot c_A^2 = k \cdot c_{A0}^2 \cdot (1 - X)^2$	$\frac{1}{k \cdot c_{A0}} \cdot \frac{X}{(1 - X)^2}$	$\frac{2k \cdot \bar{t} \cdot c_{A0} + 1 - \sqrt{1 + 4k \cdot \bar{t} \cdot c_{A0}}}{2k \cdot \bar{t} \cdot c_{A0}}$

	$\frac{1}{\bar{t}} \cdot X = \frac{k \cdot c_{A0}^2 \cdot (1-X)^2}{c_{A0}}$		
A+B→P second-order ($c_{A0} < c_{B0}$)	$r = k \cdot c_A \cdot c_B =$ $= k \cdot c_{A0} \cdot (1-X) \cdot (c_{B0} - c_{A0} \cdot X)$ <hr/> $\frac{1}{\bar{t}} \cdot X = \frac{k \cdot c_{A0} \cdot (1-X) \cdot (c_{B0} - c_{A0} \cdot X)}{c_{A0}}$	$\frac{1}{k} \cdot \frac{X}{(1-X) \cdot (c_{B0} - c_{A0} \cdot X)}$	$\frac{1 + (c_{B0} + c_{A0}) \cdot k \cdot \bar{t} - \sqrt{(1 + (c_{B0} - c_{A0}) \cdot k \cdot \bar{t})^2 + 4k \cdot \bar{t} \cdot c_{A0}}}{2k \cdot \bar{t} \cdot c_{A0}}$