RUHR-UNIVERSITÄT BOCHUM

Fakultät Maschinenbau

fortschritt studieren

RUB

Computer-aided Process Design

Handout : Core Metrics of Reactions

Lecture for Master Students

Stochiometric coefficient ν

The stochiometric coefficient ν represents the relative number of moles of a substance involved in a chemical reaction.

- **Positive for products**
- **Negative for reactants**

$$2\ H_2 + (1)\ O_2 \rightarrow 2\ H_2O$$

$$\nu_{H_2} = -2 \qquad \nu_{O_2} = -1 \qquad \nu_{H_2O} = 2$$

Conversion

Conversion = Metric for the Consumption of the (limiting) educt A

$$X_A = \frac{n_{A,0} - n_A}{n_{A,0}}$$

$n_{A,0}$ = **Amount of educt A before the reaction**

n_A = **Amount of educt A after the reaction**

e.g 10 H_2 and 4 O_2 react to form 6 H_2O, 4 H_2 and 1 O_2

$$2\,H_2 + O_2 \rightarrow 2\,H_2O$$

$10\,H_2$, $4\,O_2$ → $4\,H_2$, $1\,O_2$, $6\,H_2O$

$$X_{H_2} = \frac{10 - 4}{10} = 0{,}6 = 60\%$$

$$X_{O_2} = \frac{4 - 1}{4} = 75 = 75\%$$

Yield

Yield = Metric for the product P formed relative to the (limiting) educt A used

$$Y_P = \frac{n_p - n_{p,0}}{n_{A,0}} \cdot \frac{|\nu_A|}{|\nu_P|}$$

$n_{p,0}$ = **Amount of product P before the reaction**

n_p = **Amount of product P after the reaction**

e.g 10 H_2 and 4 O_2 react to form 6 H_2O, 4 H_2 and 1 O_2

$$2\ H_2 + O_2 \rightarrow 2\ H_2O$$

$10\ H_2$, $4\ O_2$ → $4\ H_2$, $1\ O_2$, $6\ H_2O$

$$Y_{H_2O} = \frac{6-0}{4} \cdot \frac{|-1|}{|2|} = 0{,}75 = 75\%$$

$\boldsymbol{n_{A,0} = n_{O_2,0}}$

$\nu_A = \nu_{O_2}$

→ **O_2 is the limiting educt**

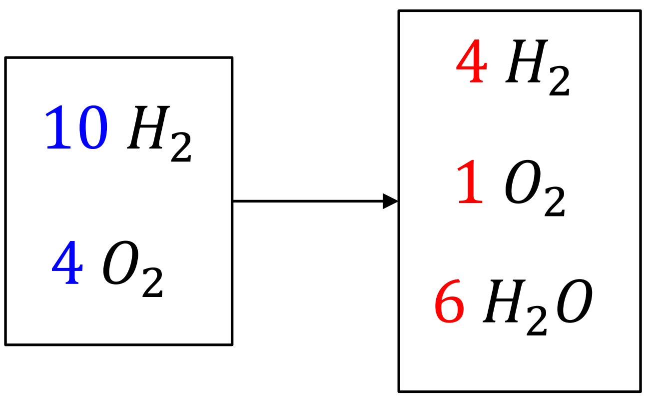
Selectivity

Selectivity = Metric for the <u>product</u> P formed relative to the (limiting) educt A consumed

$$S_P = \frac{n_p - n_{p,0}}{n_{A,0} - n_A} \cdot \frac{|\nu_A|}{|\nu_P|} = \frac{Y_P}{X_A}$$

e.g 10 H_2 and 4 O_2 react to form 6 H_2O, 4 H_2 and 1 O_2

$$2\,H_2 + O_2 \rightarrow 2\,H_2O$$



$$S_{H_2O} = \frac{6-0}{4-1} \cdot \frac{|-1|}{|2|} = 1 = 100\%$$

If there is only 1 reaction, the selectivity is always 1

Kinetic (Reaction rate)

The kinetic of a reaction describes the probability of encounter between reactants

(Volumetric) reaction rate of component i :

$$r_i = \frac{1}{V} \cdot \frac{\Delta n_i}{\Delta t}$$

V = **Reaction volume**

Δn_i = **Amount of substance consumed or formed**

Δt = **Time period**

General reaction rate :

$$r = \frac{r_i}{\nu_i}$$

The reaction rate is a function of temperature and concentration

Arrhenius equation

The Arrhenius equation describes the temperature dependence of reaction rates

$$f(t) = k = k_0 \cdot e^{-\frac{E_a}{R \cdot T}}$$

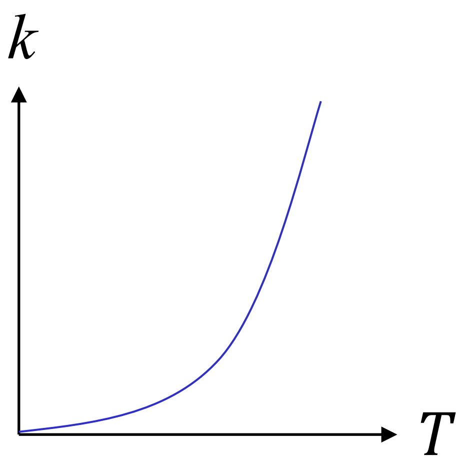
k = **Rate constant**

k_0 = **Pre-exponential factor**

T = **Absolute temperature in K**

R = **Universal gas constant**

E_a = **Activation energy**



⇨ **An increase in temperature leads to an exponential increase in reaction rate**

Rate law

The rate law defines the relationship between the reaction rate and the molar concentrations of reactants

$$\boxed{\nu_1 A + \nu_2 B \rightarrow \nu_3 C + \nu_4 D}$$

$$r = k \cdot c_A^{m_1} \cdot c_B^{m_2}$$

$$m = m_1 + m_2$$

m_1 = **Reaction order in A**

m_2 = **Reaction order in B**

m = **Total reaction order**

c_A = **Concentration of A**

c_A = **Concentration of B**

The reaction order represents the exponential dependence of the reaction rate on the concentration of each reactant

- **A higher reaction order means a decrease in concentration will lead to a higher reduction in reaction rate**

Mass balance

Convection >> Diffusion

$$\frac{dn}{dt} = \dot{N}_{i,conv,in} - \dot{N}_{i,conv,out} + \dot{N}_{i,diff,in} - \dot{N}_{i,diff,out} + \dot{N}_{reaction}$$

Molar flow rate entering / leaving the control volume by convection / diffusion :

$$\dot{N}_{i,conv,in}, \dot{N}_{i,conv,out}, \dot{N}_{i,diff,in}, \dot{N}_{i,diff,out}$$

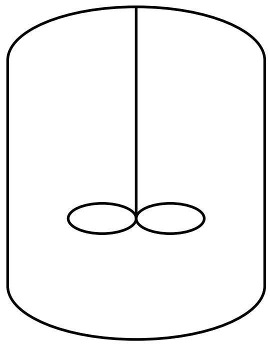
Rate of change of amount of substance due to reaction within the control volume:

$$\dot{N}_{reaction}$$

Rate of change of amount of substance in the control volume:

$$\frac{dn}{dt}$$

Batch Reactor



Properties:

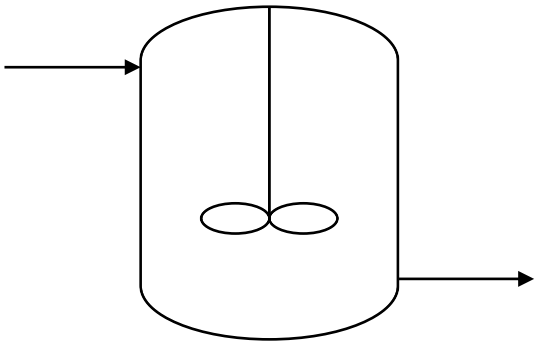
- **Ideally mixed**
- **Transient concentration change**
- **No inlet or outlet stream**

Mass balance:

$$\frac{dn}{dt} = \dot{N}_{reaction}$$

$$\Rightarrow \quad \frac{\partial c_i}{\partial t} = V_R \cdot \sum \nu_{i,j} \cdot r_j$$

Continuous stirred tank reactor (CSTR)



Properties:

- **Ideally mixed**
- **Steady-State**
- **Continuous inlet and outlet stream**

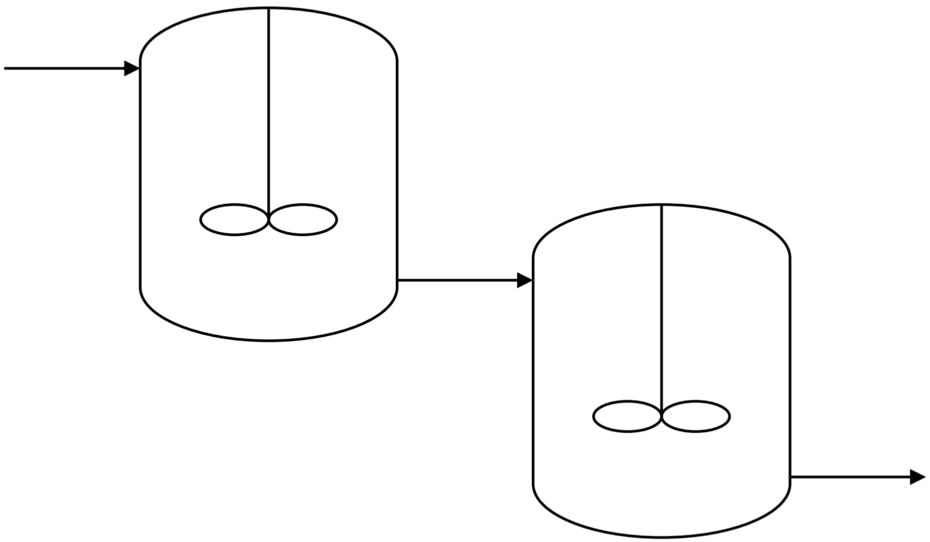
Mass balance:

$$0 = \dot{N}_{i,conv,in} - \dot{N}_{i,conv,out} + \dot{N}_{reaction}$$

$$\Rightarrow \quad 0 = \dot{V} \cdot c_{i,in} - \dot{V} \cdot c_{i,out} + V_R \sum \nu_{i,j} \cdot r_j$$

CSTR cascade

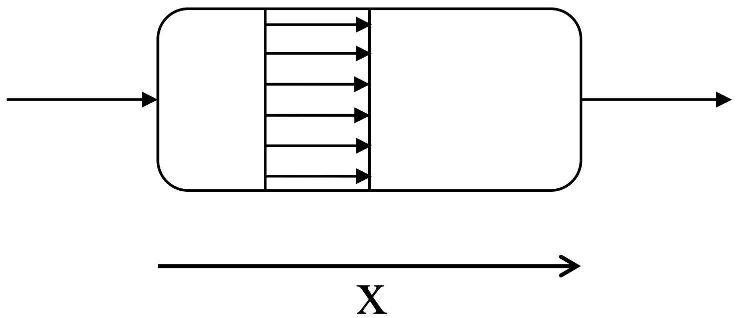
A CSTR cascade (CSTRs) consists of multiple CSTR of equal volume connected in series



A single CSTR operates at exit concentration, resulting in a minimal reaction rate

- **A CSTR cascade achieves a higher conversion while maintaining a smaller total reactor volume**

Plug flow reactor (PFR)



Properties:

- **No backmixing**
- **Steady state with spatial gradients**
- **Continuous inlet and outlet stream**

Mass balance:

$$0 = \dot{N}_{i,conv,in} - \dot{N}_{i,conv,out} + \dot{N}_{reaction}$$

$$\Rightarrow \quad 0 = -u \cdot \frac{\partial c_i}{\partial x} + \sum \nu_{i,j} \cdot r_j$$