

# Osnovni pojmi

- Konverzija:

$$X_S = \frac{n_{S0} - n_S}{n_{S0}}$$

- Izkoristek

$$\eta_P = \frac{n_P - n_{P0}}{n_{S0}} \left| \frac{\nu_S}{\nu_P} \right|$$

- Selektivnost

$$\sigma_P = \frac{n_P - n_{P0}}{n_{S0} - n_S} \left| \frac{\nu_S}{\nu_P} \right|$$

$$\eta = \sigma \cdot X$$

# Osnovni pojmi

- Enantiomerni presežek (ee):

$$ee_R = \frac{n_R - n_S}{n_R + n_S}$$

- Pretvorbena število

$$tn = \frac{n_P}{n_{cat}} \left| \frac{1}{\nu_P} \right|$$

- Aktivnost encima

$$V = \frac{\partial n_S}{\partial t \cdot m_{cat}} \quad (\text{U/mg, mol/smg})$$

kinetic, thermodynamic and reaction engineering parameters. These together then determine the type of reactor to be chosen and how the down stream processing looks like, thereby forming the total process.

In this chapter some fundamental aspects of reaction engineering, kinetics and enzymatic synthesis are described that are needed for the understanding of the data given in chapter 5.

We will start with definitions of key reaction engineering terms that are used throughout the book. These are followed by an introduction to enzyme biosynthesis and a brief overview of general characteristics of the different enzyme classes. Further topics discussed are the fundamental types of reactors and their mode of operation.

## 4.1 Definitions

### 4.1.1 Conversion

The conversion is the number of converted molecules per number of starting molecules:

$$X_s = \frac{n_{s0} - n_s}{n_{s0}} \quad (1)$$

$X_s$  conversion of substrate  $s$

$n_{s0}$  amount of substrate  $s$  at the start of the reaction (mol)

$n_s$  amount of substrate  $s$  at the end of the reaction (mol)

The conversion has to be maximized firstly to avoid recycling of unconverted reaction solution and secondly to minimize reactor volumes. On the other hand, high conversions can result in long reaction times or high amounts of catalyst being employed. Unwanted subsequent reactions of the product will then result in the formation of by-products.

### 4.1.2 Yield

The yield is the number of synthesized molecules per number of starting molecules:

$$\eta_p = \frac{n_p - n_{p0}}{n_{s0}} \cdot \left| \frac{\nu_s}{\nu_p} \right| \quad (2)$$

In combination with the conversion or the selectivity product molecules are synthesized in relation to the starting molecules. The described yield is the analytical one. The selectivity is given instead, which describes the synthesized amount of product per stream processing. The latter does not help in understanding and developing correct kinetic models. If an entire process is considered, the overall yield can be calculated by multiplication of all selectivities.

### 4.1.3 Selectivity

The selectivity is the number of synthesized product molecules per converted substrate molecules:

$$\sigma_p = \frac{n_p - n_{p0}}{n_{s0} - n_s} \cdot \left| \frac{\nu_s}{\nu_p} \right|$$

$\sigma_p$  selectivity to component  $p$

$n_{s0}$  amount of substrate  $s$  at the start of the reaction (mol)

$n_s$  amount of substrate  $s$  at the end of the reaction (mol)

$n_{p0}$  amount of product  $p$  at the start of the reaction (mol)

$n_p$  amount of product  $p$  at the end of the reaction (mol)

$\nu_s$  stoichiometric factor for substrate  $s$

$\nu_p$  stoichiometric factor for product  $p$

The selectivity describes the synthesized product molecules per converted substrate molecules. Selectivity has to be maximized to avoid waste of educt. It belongs to the most important engineering parameters.

If only a very short reaction course is looked at, the selectivity can be expressed in differential form. This is interesting for gaining information about by-products at every step of conversion. It is decisive for the premature stop of the reaction is efficient with regard to the yield.

The combination of conversion, yield and selectivity is:

$$\eta = \sigma \cdot X$$

### 4.1.8 Deactivation rate

The deactivation rate is defined as the loss of catalyst activity per unit of time:

$$V_1 = V_0 \cdot e^{-k_{deact} \cdot (t_1 - t_0)} \quad (9)$$

$k_{deact}$  deactivation rate ( $\text{min}^{-1}$ ,  $\text{h}^{-1}$ ,  $\text{d}^{-1}$ )

$V_0$  enzyme activity at the start of the measurement ( $\text{U} \cdot \text{mg}^{-1}$ )

$V_1$  enzyme activity at the end of the measurement ( $\text{U} \cdot \text{mg}^{-1}$ )

$t_0$  start time of the measurement (min, h, d)

$t_1$  end time of the measurement (min, h, d)

The deactivation rate expresses the stability of a catalyst.

### 4.1.9 Half life

The half life is defined as the time in which the activity is halved:

$$V_1 = V_0 \cdot e^{-k_{deact} \cdot (t_1 - t_0)} \quad (10)$$

$$V_2 = V_0 \cdot e^{-k_{deact} \cdot (t_2 - t_0)} \quad (11)$$

$$V_1 = \frac{1}{2} \cdot V_2 \quad (12)$$

$$\Rightarrow t_{1/2} = \frac{\ln(2)}{k_{deact}} \quad (13)$$

$t_{1/2}$  half life of catalyst (min, h, d)

$V_1$  enzyme activity at time  $t_1$  ( $\text{U} \cdot \text{mg}^{-1}$ )

$t_1$  time of measurement (min, h, d)

$k_{deact}$  deactivation rate ( $\text{min}^{-1}$ ,  $\text{h}^{-1}$ ,  $\text{d}^{-1}$ )

The half life expresses the stability of a catalyst. The activity usually shows a typical exponential decay. Therefore the half life can be calculated and it gives an extent of the catalyst deactivation independent of considered time differences.

### 4.1.10 Catalyst consumption

$$bc = \frac{m_{catalyst}}{m_{product}}$$

$bc$  biocatalyst consumption ( $\text{g} \cdot \text{kg}^{-1}$  or  $\text{U} \cdot \text{kg}^{-1}$ )

$m_{catalyst}$  mass or activity of catalyst used for synthesized

$m_{product}$  mass of synthesized product (g)

If an expensive catalyst is used, the biocatalyst consumption is as possible to decrease the biocatalyst consumption of pharmaceutical products are valued so high that in direct catalyst can be discarded without recycling. Since the catalyst with conversion due to deactivating by-products, it is necessary to find differential catalyst consumption to find the optimal conditions for the reaction and separating the reaction solution from the

### 4.1.11 Residence time

The residence time ( $\tau$ ) is defined as the quotient of reactor volume and feed rate:

$$\tau = \frac{V_R}{F}$$

$\tau$  residence time or reaction time (h)

$V_R$  reactor volume (L)

$F$  feed rate ( $\text{L} \cdot \text{h}^{-1}$ )

The residence time describes the average time of a molecule in the reactor. Since the residence times of different molecules are not the same, an average residence time is used. Diffusion effects and non-ideal flow in a continuously operated stirred tank reactor (CSTR) or backmixing reactor results in a broad distribution of single residence times. In the case of a batch reactor this distribution has to be taken into account. For one educt molecule could leave the reactor directly after the reaction or it could stay in the reaction system forever. The residence time can be strongly influenced by a broad distribution.

### 4.1.12 Space-time yield

The space-time yield (STY) is the mass of product synthesized per reactor volume and time. It is also named as the **volumetric product**