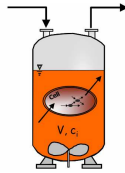


Material und Energiebilanzen



Grundlagen der Bioprozesstechnik

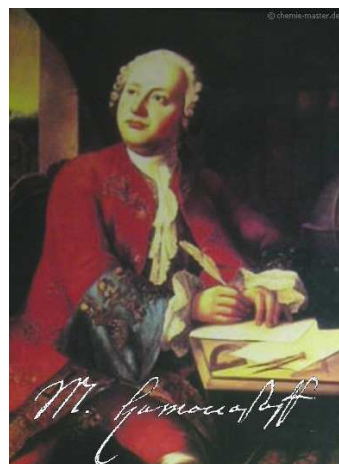
Materialbilanzen

Gesetz von der Erhaltung der Masse
(Lomonossow 1748)

Erstes chemisches Grundgesetz

Bei einer chemischen Reaktion bleibt die Gesamtmasse der beteiligten Stoffe unverändert. Die Summe der Massen der Reaktionsprodukte ist also gleich der Summe der Massen der Ausgangsstoffe.

**Masse der Ausgangsstoffe = Masse
der entstehenden Stoffe**



Grundlagen der Bioprozesstechnik

Materialbilanzen

LAW OF CONSERVATION OF MASS

Mass is conserved in ordinary chemical and physical processes.

Consider the system operating as a continuous process with input and output streams containing glucose.

$$\left(\begin{array}{c} \text{mass} \\ \text{accumulated} \\ \text{within} \\ \text{system} \end{array} \right) = \left(\begin{array}{c} \text{mass in} \\ \text{through system} \\ \text{boundaries} \end{array} \right) - \left(\begin{array}{c} \text{mass out} \\ \text{through system} \\ \text{boundaries} \end{array} \right) + \left(\begin{array}{c} \text{mass} \\ \text{generated} \\ \text{within} \\ \text{system} \end{array} \right) - \left(\begin{array}{c} \text{mass} \\ \text{consumed} \\ \text{within} \\ \text{system} \end{array} \right)$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Terminologie und Prinzipien aus der Thermodynamik

SYSTEM

In thermodynamics, a system consists of any matter identified for investigation. The system is set apart from the surroundings, which are the remainder of the universe, by a system boundary. The system boundary may be real and tangible, such as the walls of a beaker or fermenter, or imaginary. If the boundary does not allow mass to pass from system to surroundings and vice versa, the system is a closed system with constant mass. Conversely, a system able to exchange mass with its surroundings is an open system.

PROCESS

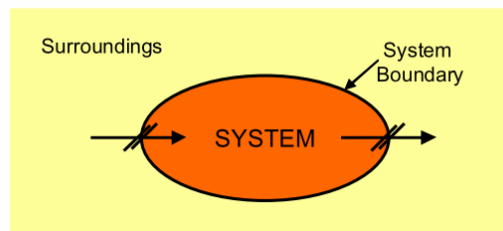
A process causes changes in the system or surroundings. Several terms are commonly used to describe processes.

Grundlagen der Bioprozesstechnik

Materialbilanzen

BATCH PROCESS

All materials are added to the system at the start of the process; the system is then closed and products removed only when the process is complete

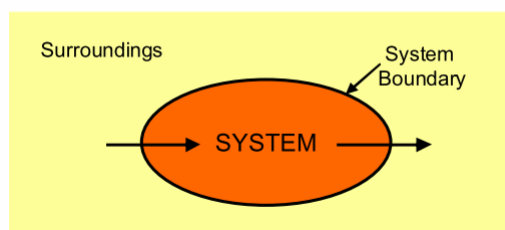


Grundlagen der Bioprozesstechnik

Materialbilanzen

SEMI-BATCH PROCESS

allows either input or output of mass, but not both

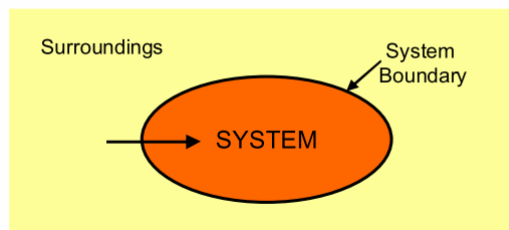


Grundlagen der Bioprozesstechnik

Materialbilanzen

FED-BATCH PROCESS

allows input of material to the system
but not output

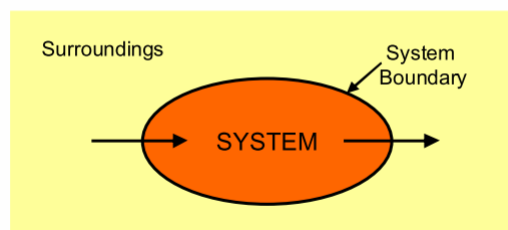


Grundlagen der Bioprozesstechnik

Materialbilanzen

CONTINUOUS PROCESS

allows matter to flow in and out of the system; If
rates of mass input and output are equal,
continuous processes can be operated indefinitely.

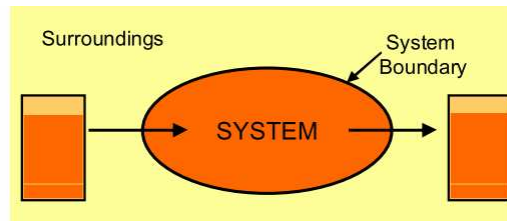


Grundlagen der Bioprozesstechnik

Materialbilanzen

CONTINUOUS PROCESS - STEADY STATE

all system properties (temperature, pressure, concentration, volume, mass etc.) do not vary



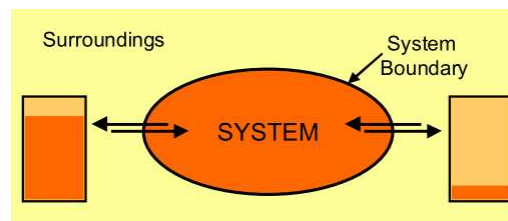
$$\left(\begin{array}{c} \text{Rate of mass flow} \\ \text{into the system} \end{array} \right) = \left(\begin{array}{c} \text{Rate of mass flow} \\ \text{out of the system} \end{array} \right)$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

EQUILIBRIUM

all opposing forces are perfectly counterbalance
no net-change no net-driving force



Grundlagen der Bioprozesstechnik

Materialbilanzen

Types of mass balance equations

Dynamic total mass balances

$$\left(\begin{array}{c} \text{Rate of mass} \\ \text{accumulation} \\ \text{in the} \\ \text{system} \end{array} \right) = \left(\begin{array}{c} \text{Rate of} \\ \text{Mass flow in} \end{array} \right) - \left(\begin{array}{c} \text{Rate of} \\ \text{Mass flow out} \end{array} \right)$$

Steady state balances

$$\left(\begin{array}{c} 0 \end{array} \right) = \left(\begin{array}{c} \text{Rate of} \\ \text{Mass flow in} \end{array} \right) - \left(\begin{array}{c} \text{Rate of} \\ \text{Mass flow out} \end{array} \right)$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Types of mass balance equations

Component Balances

$$\left(\begin{array}{c} \text{Rate of} \\ \text{accumulation of} \\ \text{mass of component} \\ \text{in the system} \end{array} \right) = \left(\begin{array}{c} \text{Mass flow of} \\ \text{the component} \\ \text{in to the system} \end{array} \right) - \left(\begin{array}{c} \text{Mass flow of} \\ \text{the component} \\ \text{out of the system} \end{array} \right)$$

Component balances with reaction

$$\left(\begin{array}{c} \text{Rate of} \\ \text{accumulation of} \\ \text{mass of component} \\ \text{in the system} \end{array} \right) = \left(\begin{array}{c} \text{Mass flow of} \\ \text{the component} \\ \text{in to the system} \end{array} \right) - \left(\begin{array}{c} \text{Mass flow of} \\ \text{the component} \\ \text{out of the system} \end{array} \right) - \left(\begin{array}{c} \text{Rate of} \\ \text{consumption} \\ \text{of the} \\ \text{component} \end{array} \right)$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Types of mass balance equations

Elemental balances

$$\left(\begin{array}{c} \text{Rate of} \\ \text{accumulation of} \\ \text{carbon} \\ \text{in the system} \end{array} \right) = \left(\begin{array}{c} \text{Mass flow of} \\ \text{carbon in to} \\ \text{the system} \end{array} \right) - \left(\begin{array}{c} \text{Mass flow of} \\ \text{carbon out of} \\ \text{the system} \end{array} \right)$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Types of material balances

differential balance

integral balance

Simplification of general mass balance equation

differential balance → mass balance based on rates

integral balance → balance based on mass quantities

Grundlagen der Bioprozesstechnik

Materialbilanzen

Aufstellen von Massenbilanzen

- Definition der Systemgrenzen, Flussdiagramm, Einheiten festlegen
- Festlegung des Systemtyps, Identifikation der Flüsse und Materialströme
- Formulieren der Massebilanz, Annahmen definieren
 - Mathematische Beschreibung Bilanzen
- Implementierung zusätzlicher Zusammenhänge, Identifikation welche Komponenten an Reaktionen beteiligt

Grundlagen der Bioprozesstechnik

Materialbilanzen

Definition der Systemgrenzen

Beispiel Rührkessel

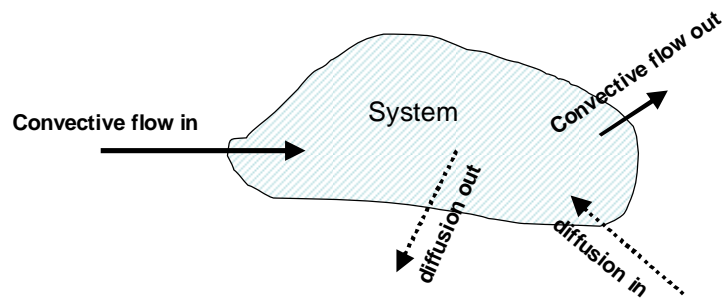
Beispiel Röhrenreaktor

Beispiel Fluss

Grundlagen der Bioprozesstechnik

Materialbilanzen

Identifikation der Flüsse und Materialströme



Grundlagen der Bioprozesstechnik

Materialbilanzen

Formulieren der Massebilanz

$$\left(\begin{array}{c} \text{Rate of} \\ \text{accumulation of} \\ \text{mass of component} \\ \text{in the system} \end{array} \right) = \left(\begin{array}{c} \text{Mass flow of} \\ \text{the component} \\ \text{in to the system} \end{array} \right) - \left(\begin{array}{c} \text{Mass flow of} \\ \text{the component} \\ \text{out of the system} \end{array} \right) - \left(\begin{array}{c} \text{Rate of} \\ \text{consumption} \\ \text{of the} \\ \text{component} \end{array} \right)$$

$$(\text{accumulation}) = (\text{in}) - (\text{out}) - (\text{consumption})$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Mathematische Beschreibung Bilanzen

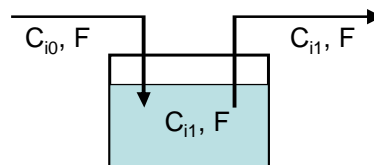
$$\text{Rate of accumulation of mass of component } i \text{ within the system} = \frac{dM_i}{dt}$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Mathematische Beschreibung Bilanzen

$$(\text{Convective mass flow rate}) = (\text{Volumetric flow rate}) \times \left(\frac{\text{Mass}}{\text{Volume}} \right)$$



Grundlagen der Bioprozesstechnik

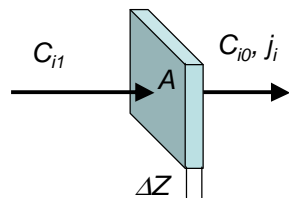
Materialbilanzen

Mathematische Beschreibung Bilanzen

Diffusion of components: Fick's law $j_i = -D_i \frac{dC_i}{dZ_i}$

Total mass flow $= F\rho$

Component mass flow $M_i = FC_i$



Concentration gradient
 $(C_{i0} - C_{i1}) / \Delta Z$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Mathematische Beschreibung Bilanzen

Diffusion of components: Fick's law $j_i = -D_i \frac{dC_i}{dZ_i}$

$$\left(\begin{array}{c} \text{Mass} \\ \text{rate of} \\ \text{component i} \end{array} \right) = \left(\begin{array}{c} \text{Diffusivity of} \\ \text{component i} \end{array} \right) \left(\begin{array}{c} \text{Concentration} \\ \text{gradient of i} \end{array} \right) \left(\begin{array}{c} \text{Area} \\ \text{perpendicular} \\ \text{to transport} \end{array} \right) = -D_i \frac{dC_i}{dZ_i} A$$

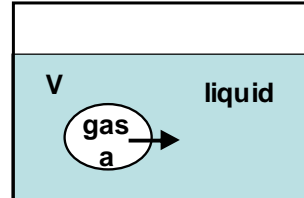
$$j_i = -D_i \frac{\Delta C_i}{\Delta Z} A$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Mathematische Beschreibung Bilanzen

Interphase transport



$$\left(\begin{array}{c} \text{Rate of} \\ \text{accumulation} \\ \text{of the mass of} \\ \text{oxygen in the} \\ \text{gas-phase system} \end{array} \right) = \left(\begin{array}{c} \text{Mass flow} \\ \text{of the oxygen} \\ \text{into the gas} \\ \text{phase} \end{array} \right) - \left(\begin{array}{c} \text{Mass flow} \\ \text{of the oxygen} \\ \text{from the gas} \\ \text{phase} \end{array} \right) - \left(\begin{array}{c} \text{Rate of inter-} \\ \text{facial mass transfer} \\ \text{from the gas phase into} \\ \text{the liquid} \end{array} \right)$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Mathematische Beschreibung Bilanzen

Production rate

$$\left(\begin{array}{c} \text{Rate of} \\ \text{accumulation of} \\ \text{mass of component} \\ \text{in the system} \end{array} \right) = \left(\begin{array}{c} \text{Mass flow of} \\ \text{the component} \\ \text{in to the system} \end{array} \right) - \left(\begin{array}{c} \text{Mass flow of} \\ \text{the component} \\ \text{out of the system} \end{array} \right) + \left(\begin{array}{c} \text{Rate of} \\ \text{production} \\ \text{of the} \\ \text{component} \end{array} \right)$$

$$\left(\begin{array}{c} \text{Mass rate} \\ \text{production of} \\ \text{component A} \end{array} \right) = r_A V = \left(\begin{array}{c} \text{Reaction rate} \\ \text{per volume} \end{array} \right) \left(\begin{array}{c} \text{Volume of the system} \end{array} \right)$$

$$\frac{kg}{s} = \frac{kg}{sm^3} m^3$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Mathematische Beschreibung Bilanzen

Growth rate

$$\left(\begin{array}{c} \text{Mass rate of} \\ \text{biomass} \\ \text{production} \end{array} \right) = r_x V = \left(\begin{array}{c} \text{Growth rate} \\ \text{per volume} \end{array} \right) \left(\begin{array}{c} \text{Volume of the system} \end{array} \right)$$

Substrate consumption rate, r_s directly correlated to cell growth by glucose yield coefficient $Y_{x/s}$

$$\left(\begin{array}{c} \text{Mass rate of} \\ \text{substrate} \\ \text{consumption} \end{array} \right) = \left(\begin{array}{c} \text{Growth rate} \\ \text{per volume} \end{array} \right) \left(\begin{array}{c} \frac{1}{\text{Biomasse Substrat yield}} \end{array} \right) \left(\begin{array}{c} \text{Volume} \end{array} \right)$$

$$r_s V = - \frac{r_x}{Y_{x/s}} V$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Mathematische Beschreibung zusätzliche Zusammenhänge

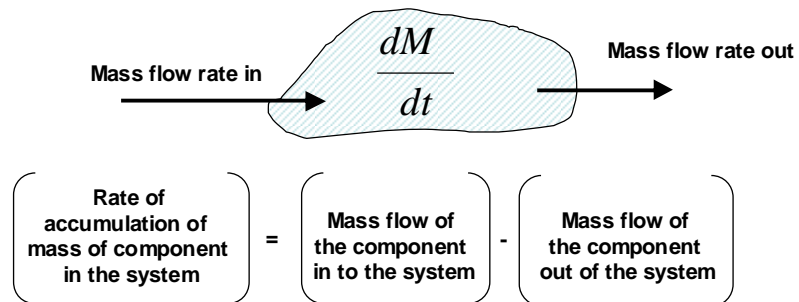
- Reaktionsraten als Funktion der Zeit, Konzentration, Temperatur..
- Stöchiometrische Zusammenhänge
- Ideales Gasverhalten
- Physikalische Eigenschaften in Abhängigkeit von Konzentration
- Druck in Abhängigkeit von Fluss
- Instrument Responszeit
- Gleichgewichtsbedingungen (Henry's Law)
- Regler
-

**JEDE UNBEKANNTE VARIABLE MUSS MIT EINER GLEICHUNG
BESCHRIEBEN WERDEN KÖNNEN**

Grundlagen der Bioprozesstechnik

Materialbilanzen

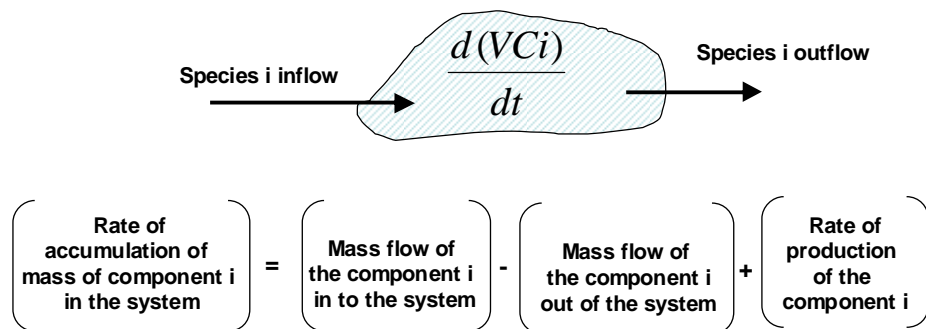
Totale Massenbilanz



Grundlagen der Bioprozesstechnik

Materialbilanzen

Komponentenbilanz für System mit Reaktion



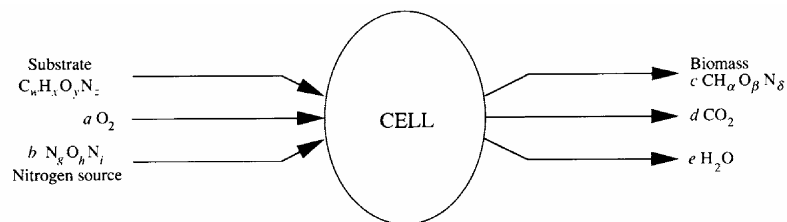
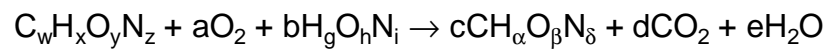
$$\frac{d(VC_i)}{dt} = (F_0 C_{i0}) - (F_1 C_{i1}) + (r_i V)$$

Grundlagen der Bioprozesstechnik

Materialbilanzen

Stöchiometrie und Elementarbilanzen

Grundlegende Bilanzgleichung für das Wachstum von Organismen



Grundlagen der Bioprozesstechnik

Materialbilanzen

Elementar - Bilanzen

C-Bilanz	$w = c + d$
H-Bilanz	$x + bg = c \alpha + 2e$
O-Bilanz	$y + 2a + bh = c \beta + 2d + e$
N-Bilanz	$z + bi = c \delta$

4 Gleichungen, aber 5 Koeffizienten a, b, c, d, e sind unbekannt
 → zusätzliche Information Respiratorischer Quotient, RQ

Grundlagen der Bioprozesstechnik

Materialbilanzen

Beispiele für Elementar - Bilanzen

Table 4.3 Elemental composition and degree of reduction for selected organisms

(From J.A. Roels, 1980, *Application of macroscopic principles to microbial metabolism*, Biotechnol. Bioeng. 22, 2457–2514)

Organism	Elemental formula	Degree of reduction γ (relative to NH_3)
<i>Escherichia coli</i>	$\text{CH}_{1.77}\text{O}_{0.49}\text{N}_{0.24}$	4.07
<i>Klebsiella aerogenes</i>	$\text{CH}_{1.75}\text{O}_{0.43}\text{N}_{0.22}$	4.23
<i>Kl. aerogenes</i>	$\text{CH}_{1.73}\text{O}_{0.43}\text{N}_{0.24}$	4.15
<i>Kl. aerogenes</i>	$\text{CH}_{1.75}\text{O}_{0.47}\text{N}_{0.17}$	4.30
<i>Kl. aerogenes</i>	$\text{CH}_{1.73}\text{O}_{0.43}\text{N}_{0.24}$	4.15
<i>Pseudomonas C₁₂B</i>	$\text{CH}_{2.00}\text{O}_{0.52}\text{N}_{0.23}$	4.27
<i>Aerobacter aerogenes</i>	$\text{CH}_{1.83}\text{O}_{0.55}\text{N}_{0.25}$	3.98
<i>Paracoccus denitrificans</i>	$\text{CH}_{1.81}\text{O}_{0.51}\text{N}_{0.20}$	4.19
<i>P. denitrificans</i>	$\text{CH}_{1.51}\text{O}_{0.46}\text{N}_{0.19}$	3.96
<i>Saccharomyces cerevisiae</i>	$\text{CH}_{1.64}\text{O}_{0.52}\text{N}_{0.16}$	4.12
<i>S. cerevisiae</i>	$\text{CH}_{1.83}\text{O}_{0.56}\text{N}_{0.17}$	4.20
<i>S. cerevisiae</i>	$\text{CH}_{1.81}\text{O}_{0.51}\text{N}_{0.17}$	4.28
<i>Candida utilis</i>	$\text{CH}_{1.83}\text{O}_{0.54}\text{N}_{0.10}$	4.45
<i>C. utilis</i>	$\text{CH}_{1.87}\text{O}_{0.56}\text{N}_{0.20}$	4.15
<i>C. utilis</i>	$\text{CH}_{1.83}\text{O}_{0.46}\text{N}_{0.19}$	4.34
<i>C. utilis</i>	$\text{CH}_{1.87}\text{O}_{0.56}\text{N}_{0.20}$	4.15
Average	$\text{CH}_{1.79}\text{O}_{0.50}\text{N}_{0.20}$	4.19

Grundlagen der Bioprozesstechnik

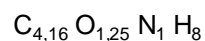
Materialbilanzen

Berechnung der molekularen Zusammensetzung der Biomasse aus der Elementarzusammensetzung

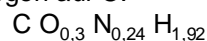
Angabe in % Trockensubstanz			
C	50	K	1
O	20	Na	1
N	14	Ca	0,5
H	8	Mg	0,5
P	3	Cl	0,5
S	1	Fe	0,2

100 g Biomasse enthalten: 50 g C, 20g O, 14 g N, 8 g H

→ molekulare Zusammensetzung



→ bezogen auf C:

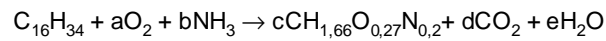


→ Molmasse der Biomasse : 22,06

Grundlagen der Bioprozesstechnik

Materialbilanzen

Beispiel: Wachstum auf Hexadekan $C_{16}H_{34}$



$$\text{C-Bilanz } 16 = c + d$$

$$\text{H-Bilanz } 34 + 3b = 1,66c + 2e$$

$$\text{O-Bilanz } 2a = 0,27c + 2d + e$$

$$\text{N-Bilanz } b = 0,2c$$

$$RQ = 0,43 \quad RQ = d/a$$

$$d = 16 - c \quad a = d/0,43 = 2,326 d$$

$$a = 2,326 (16 - c)$$

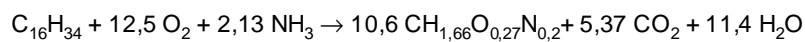
$$a = 37,22 - 2,326 c$$

$$34 + 3(0,2c) = 1,66c + 2e \rightarrow 34 = 1,06c + 2e \rightarrow e = 17 - 0,53c$$

$$2(37,22 - 2,326c) = 0,27c + 2(16 - c) + 17 - 0,53c \rightarrow 25,44 = 2,39c$$

$$c = 10,64$$

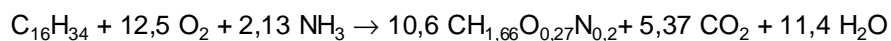
$$a = 12,48; b = 2,13; c = 10,64; e = 11,36$$



Grundlagen der Bioprozesstechnik

Materialbilanzen

Bilanzgleichung für Hexadekan-Verwertung



Ermittlung des Sauerstoffbedarfes :

$$O_2 \text{ Bedarf : } 12,5 O_2 = 12,5 \cdot 32 = 400$$

$$\text{Gebildete Biomasse: } 10,6 \cdot (12 + 1,66 + 16 \cdot 0,27 + 14 \cdot 0,2) = 220,2 \text{ g BTS}$$

→ spezifischer Sauerstoffbedarf 1,8 g O_2 /g BTS

Stöchiometrische Verteilung des verbrauchten Sauerstoffs (12,5 Mol):

Biomasse:	45,8
CO ₂	171,8
H ₂ O	182,4
Summe	400,0

Grundlagen der Bioprozesstechnik

Materialbilanzen

Konzept der verfügbaren Elektronen - Elektronen Bilanz

„Verfügbare Elektronen“ sind jene, die auf Sauerstoff übertragen werden können bei der Verbrennung einer Substanz zu CO_2 , H_2O und N-Verbindungen.

Anzahl verfügbarer Elektronen errechnet sich aus Valenzen der einzelnen Elemente:
4 für C, 1 für H, -2 für O, 5 für P, 6 für S, N hängt von der Verbindung ab, -3 für Ammoniak

Reduktionsgrad γ ist definiert als die Anzahl von Elektronen, die in der 1 g C-Atom äquivalenten Substanzmenge verfügbar sind,

z.B. Substrat $\text{C}_w\text{H}_x\text{O}_y\text{N}_z$ verfügbare Elektronen $(4w+x-2y-3z)/w$

Verfügbare Elektronen für die Übertragung auf Sauerstoff:

Elektronenbilanz: $w\gamma_S - 4a = c\gamma_B$ γ_S und $\gamma_B =$ Reduktionsgrad von
Substrat und Biomasse

Grundlagen der Bioprozesstechnik

Materialbilanzen

Berechnung des Sauerstoffbedarfs aus Reduktionsgrad:

$$w\gamma_S - 4a = c\gamma_B$$

a: Sauerstoffbedarf

$$a = 1/4 (w\gamma_S - c\gamma_B)$$

c: Ausbeute an Biomasse

Beispiel: Hefe *Candida utilis*, C-Quelle Glucose

Zellzusammensetzung $\text{CH}_{1,84}\text{O}_{0,55}\text{N}_{0,2}$ plus 5% Asche, $Y_{x/s} = 0,5$, N-Quelle = NH_3

MW Biomasse = 25,44 + Asche \rightarrow MW = 25,44/0,95 = 26,78

$$\gamma_S = 4 \quad (\text{C}_w\text{H}_x\text{O}_y\text{N}_z \quad (4w+x-2y-3z)/w, \text{ für } \text{C}_6\text{H}_{12}\text{O}_6 \quad (4 \cdot 6 + 12 - 12) = 4)$$

$$\gamma_B = 4,14 \quad (4 \cdot 1 + 1 \cdot 1,84 - 2 \cdot 0,55 - 3 \cdot 0,2) = 4,14$$

$$Y_{x/s} = 0,5 \text{ g/g} \quad \text{Umwandlung Masse in molare Ausbeute } 0,5(180/26,78) = 3,36 = c$$

$$a = 1/4 (w\gamma_S - c\gamma_B) \rightarrow a = 1/4 (6 \cdot 4 - 3,36 \cdot 4,14) = 2,52 \text{ g mol O}_2$$

pro mol Glucose verbraucht

Grundlagen der Bioprozesstechnik

Materialbilanzen

Table 4.4 Thermodynamic maximum biomass yields

(Adapted from L.E. Erickson, I.G. Minkovich and V.K. Eroshin, 1978, Application of mass and energy balance regularities in fermentation, Biotechnol. Bioeng. 20, 1595–1621)

Substrate	Formula	γ_s	Thermodynamic maximum yield corresponding to $\zeta_B = 1$	
			Carbon yield ($^{max}f_w$)	Mass yield $Y_{XS,max}$
Alkanes				
Methane	CH_4	8.0	1.9	2.9
Hexane (n)	C_6H_{14}	6.3	1.5	2.6
Hexadecane (n)	$C_{16}H_{34}$	6.1	1.5	2.5
Alcohols				
Methanol	CH_3O	6.0	1.4	1.1
Ethanol	C_2H_5O	6.0	1.4	1.5
Ethylene glycol	$C_2H_4O_2$	5.0	1.2	0.9
Glycerol	$C_3H_8O_3$	4.7	1.1	0.9
Carbohydrates				
Formaldehyde	CH_2O	4.0	0.95	0.8
Glucose	$C_6H_{12}O_6$	4.0	0.95	0.8
Sucrose	$C_{12}H_{22}O_{11}$	4.0	0.95	0.8
Starch	$(C_6H_{10}O_5)_x$	4.0	0.95	0.9
Organic acids				
Formic acid	CH_2O_2	2.0	0.5	0.3
Acetic acid	$C_2H_4O_2$	4.0	0.95	0.8
Propionic acid	$C_3H_6O_2$	4.7	1.1	1.1
Lactic acid	$C_3H_6O_3$	4.0	0.95	0.8
Fumaric acid	$C_4H_4O_4$	3.0	0.7	0.6
Oxalic acid	$C_2H_2O_4$	1.0	0.24	0.1

Grundlagen der Bioprozesstechnik

Energiebilanzen

Bioprozesse sind "nicht" energie-intensiv
 Kultivierung nahe Standardbedingungen
 Energieeintrag im Downstream minimiert um Produkt zu
 schonen
 Jedoch große Bedeutung im Bereich
 Up-scale, Energieeintrag durch Rühren, Kühlung,
 Sterilisation

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Energiebilanzen

Energy takes three forms:

- (i) kinetic energy, E_k ;
- (ii) potential energy, E_p ;
- (iii) internal energy, U .

Kinetic energy is the energy possessed by a moving system because of its velocity.

Potential energy is due to the position of the system in a gravitational or electromagnetic field, or due to the conformation of the system relative to an equilibrium position (e.g. compression of a spring).

Internal energy is the sum of all molecular, atomic and sub-atomic energies of matter. Internal energy cannot be measured directly or known in absolute terms; we can only quantify change in internal energy.

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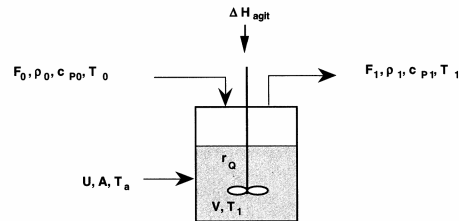
Energiebilanzen

General energy balance equation

$$\left(\begin{array}{c} \text{Accumu-} \\ \text{lation} \\ \text{rate of} \\ \text{Energy} \end{array} \right) = \left(\begin{array}{c} \text{Rate of} \\ \text{energy} \\ \text{in by} \\ \text{flow} \end{array} \right) - \left(\begin{array}{c} \text{Rate of} \\ \text{energy} \\ \text{out by} \\ \text{flow} \end{array} \right) - \left(\begin{array}{c} \text{Rate of} \\ \text{energy} \\ \text{out by} \\ \text{transfer} \end{array} \right) + \left(\begin{array}{c} \text{Rate of} \\ \text{energy} \\ \text{generated} \\ \text{by reaction} \end{array} \right) + \left(\begin{array}{c} \text{Rate of} \\ \text{energy} \\ \text{added by} \\ \text{agitation} \end{array} \right)$$

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$$\sum_{i=1}^S (n_{i1} c_{pi1}) \frac{dT_1}{dt} = F_0 \sum_{i=1}^S (c_{i0} (h_{i0} - h_{i1})) + U A (T_a - T_1) + r_Q V + \Delta H_{agit}$$

n_i is the number of moles of component i ,
 c_{pi} partial molar heat capacities
 h_i partial molar enthalpies
 r_Q the rate of heat production at temperature T_1

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Simplifications:

If the heat capacities, c_{pi} , independent of temperature, the enthalpies at T_1 can be expressed in terms of heat capacities as

$$h_{i1} = h_{i0} + c_{pi} (T_1 - T_0)$$

and with

$$\sum_{i=1}^S n_{i0} c_{pi0} \approx \sum_{i=1}^S n_i c_{pi} = V \rho c_p$$

$$V \rho c_p \frac{dT_1}{dt} = F_0 \rho c_p (T_0 - T_1) + U A (T_a - T_1) + r_Q V + \Delta H_{agit}$$

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Accumulation Term

Densities and heat capacities of liquids can be taken as essentially constant

$$V \rho c_p \frac{dT}{dt}$$

has units:

$$\frac{\text{m}^3 (\text{kg/m}^3) (\text{J/kg K}) \text{K}}{\text{s}} = \frac{\text{kJ}}{\text{s}}$$

Here ($\rho c_p T$) is an energy "concentration" term and has the units

$$\left(\frac{\text{mass}}{\text{volume}} \right) \left(\frac{\text{energy}}{\text{mass degree}} \right) (\text{degree}) = \left(\frac{\text{energy}}{\text{volume}} \right)$$

Thus the accumulation term has the units of energy/time (e.g. J/s)

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Flow Terms

The flow term is $F \rho c_p (T_0 - T_1)$

with the units,
$$\left(\frac{\text{energy}}{\text{volume}} \right) \left(\frac{\text{volume}}{\text{time}} \right) = \left(\frac{\text{energy}}{\text{time}} \right)$$

This term actually describes heating of the stream entering the system with T_0 to the reaction temperature T_1 . It is important to note here that this term is exactly the same for a continuous reactor as for a fed-batch system.

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Heat Transfer Term

The important quantities in this term are the heat transfer area A , the temperature driving force or difference $(T_a - T_1)$, where T_a is the temperature of the heating or cooling source, and the overall heat transfer coefficient, U . The heat transfer coefficient, U , has units of energy/time area degree, e.g. J/s m² °C.

The units for $U A \Delta T$ are thus,

$$(\text{heat transfer rate}) = U A (T_a - T_1)$$

$$\frac{\text{energy}}{\text{time}} = \frac{\text{energy}}{\text{area time degree}} (\text{area}) (\text{degree})$$

The sign of the temperature difference determines the direction of heat flow. Here if $T_a > T_1$ heat flows into the reactor.

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Reaction Heat Term

The term $r_Q V$ gives the rate of heat released by the bioreaction and has the units of

$$\frac{\text{energy}}{\text{volume time}} (\text{volume}) = \frac{\text{energy}}{\text{time}}$$

The rate term r_Q can alternatively be written in various ways as follows: In terms of substrate uptake and a substrate-related heat yield,

$$r_Q = r_S Y_{Q/S}$$

In terms of oxygen uptake and an oxygen-related heat yield, $r_Q = r_{O_2} Y_{Q/O_2}$

In terms of a heat of reaction per mol of substrate and a substrate uptake rate

$$r_Q = \Delta H_{r,S} r_S$$

Here r_S is the substrate uptake rate and $\Delta H_{r,S}$ is the heat of reaction for the Substrate, for example J/mol or kcal/kg. The $r_S \Delta H_{r,S}$ term therefore has dimensions of (energy/time volume) and is equal to r_Q .

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Other Heat Terms

The heat of agitation may be the most important heat effect for slow growing cultures, particularly with viscous cultures. Other terms, such as heat losses from the reactor due to evaporation, can also be important.

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Example

For aerobic fermentation, the heats of reaction per unit volume of reactor are usually directly related to the oxygen uptake rate, r_{O_2} .

Thus for a constant-volume batch reaction with no agitation heat effects, the general energy balance is

$$\left(\begin{array}{c} \text{Accumulation rate} \\ \text{of energy} \end{array} \right) = - \left(\begin{array}{c} \text{Energy out} \\ \text{by transfer} \end{array} \right) + \left(\begin{array}{c} \text{Energy generated} \\ \text{by reaction} \end{array} \right)$$

$$\frac{dT_1}{dt} = \left(\frac{UA}{\rho c_p V} \right) (T_1 - T_a) + r_{O_2} Y_{Q/O_2} \left(\frac{1}{\rho c_p} \right)$$

where Y_{Q/O_2} often has a value near 460 kJ/mol O_2

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If T is constant ($dT/dt = 0$):

$$U A(T_1 - T_a) = r_{O_2} Y_{Q/O_2} V$$

(heat transfer rate) = (rate of heat release)

Using this steady-state energy balance, it is possible to calculate the cooling water temperature (T_a) for a given oxygen uptake rate and cooling device.

Thus,

$$T_a = \frac{-r_{O_2} Y_{Q/O_2} V + U A T_1}{U A}$$

Alternatively this same relation can be used in other ways:

- 1) To calculate the additional heat transfer area required for a known increase in cooling water temperature.
- 2) To calculate the biomass concentration allowable for a given cooling system, knowing the specific oxygen uptake rate ($\text{kg O}_2 / \text{kg biomass h}$).
- 3) To calculate the cooling area required for a continuous fermenter with known volume inlet, temperature, flow rate and biomass production rate.