Gas transport

Technology for biobased products

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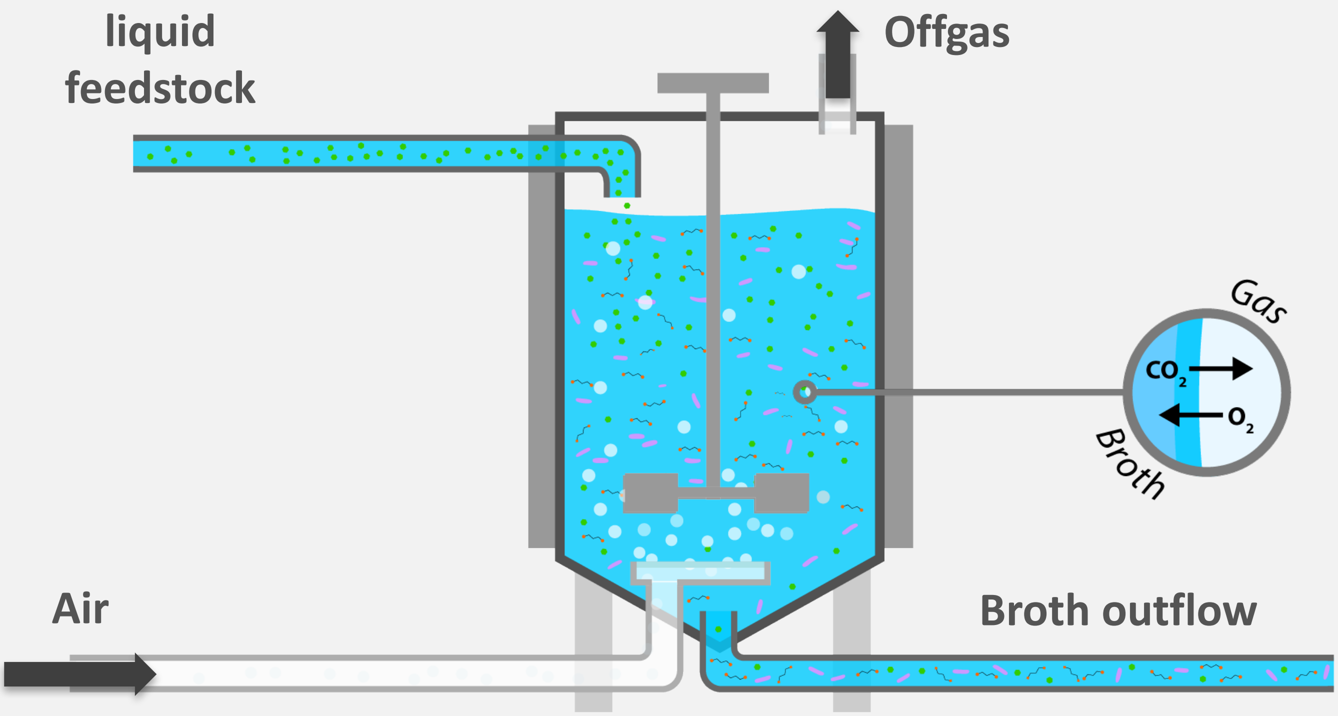
Two of four key transport-limiting steps: O_2 supply and CO_2 removal



O_2 and CO_2 in biological processes

O_2 is an electron acceptor for energy production

1 glucose + 6 O_2 → 6 CO_2 + 6 H_2O

192 g (O_2) / 180 g (glucose) = 1.07 g (O_2) / g (glucose)

O_2 has low solubility in aqueous broth

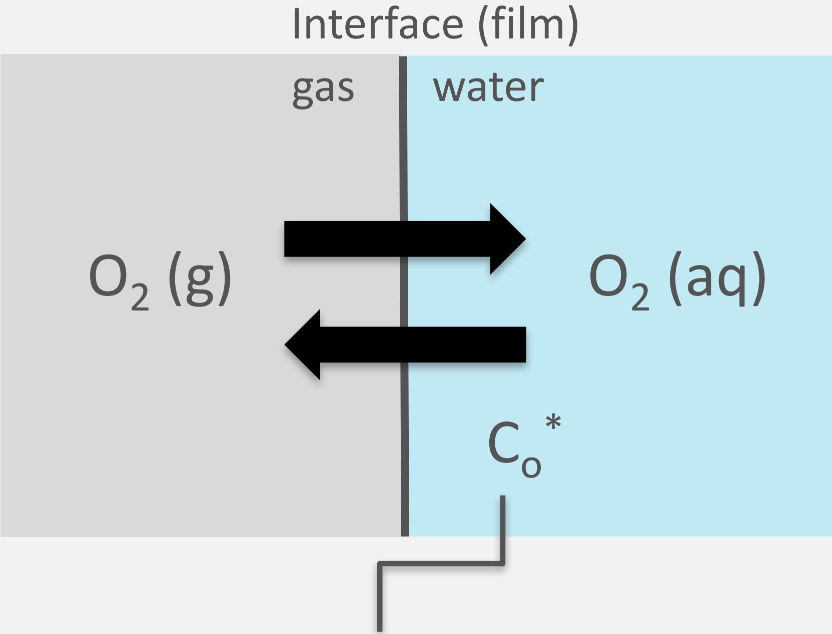
21% O_2 in air at 1 bar, 25 °C

0.24 mol/m^3 ≈ 7 mg (O_2) / L (broth)

O_2 solubility

$$p_o = y_o p$$

- p_o: Partial pressure O_2
- p: Pressure
- y_o: Mol fraction O_2 in gas

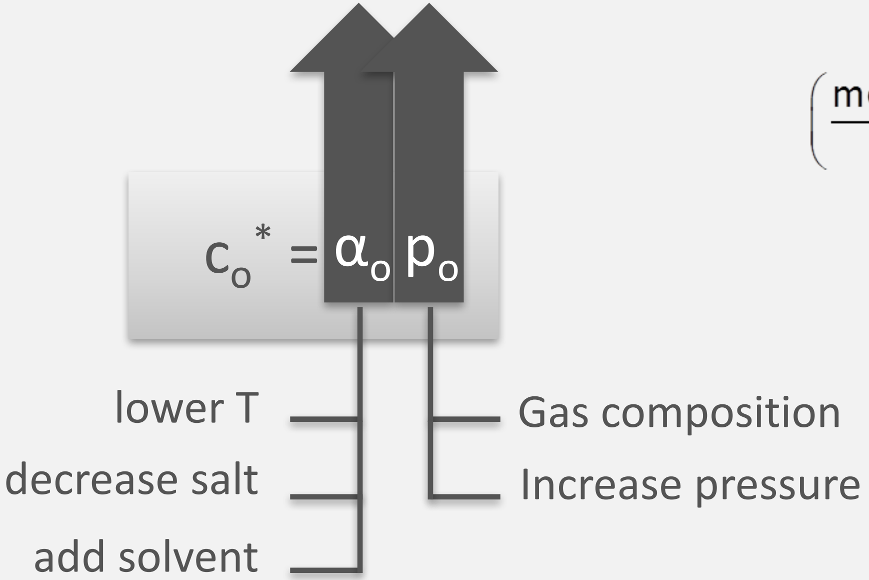


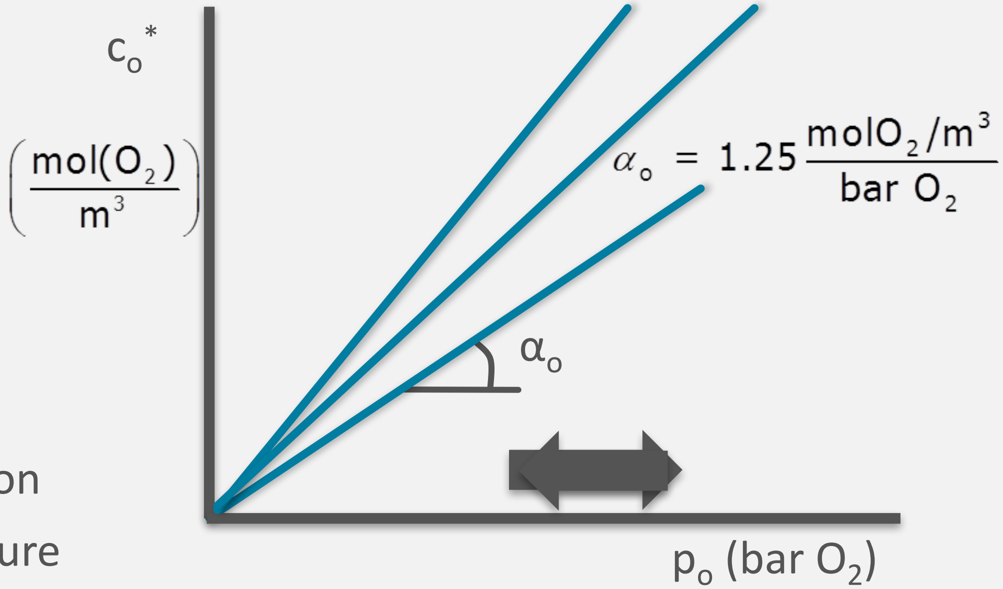
Equilibrium concentration of O_2

O_2-solubility (mol (O_2) / m^3)

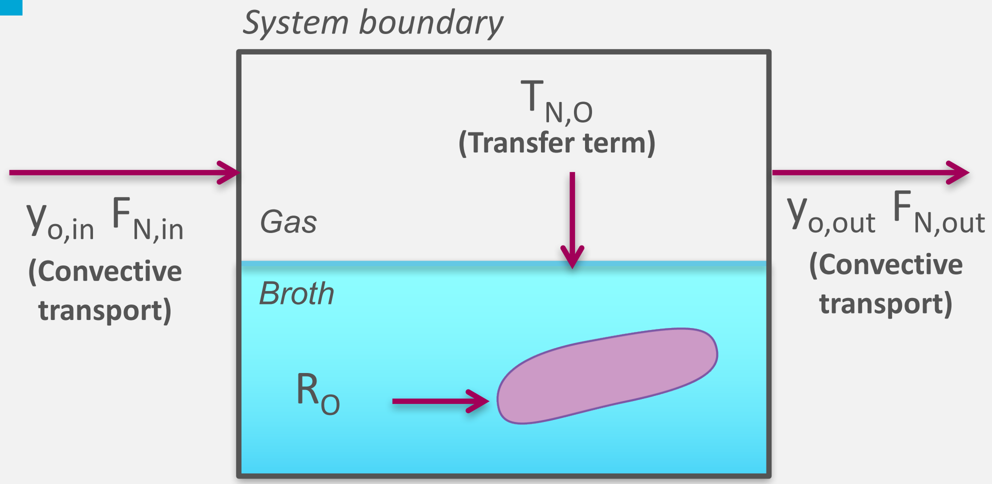
Increasing O_2 solubility

Henry's law





O_2 transfer rate



Transfer rate of O_2 (mol O_2 / h)

Resistance coefficient (m / h)

Total surface area of bubbles (m^2)

$$\frac{T_{N,o}}{V_L} = K_L a (c_o^* - c_o)$$

Concentration in liquid (mol O_2 / m^3)

Solubility (mol O_2 / m^3)

Gas phase $d(N_G y_o)/dt = F_{N,in} y_{o,in} - F_{N,out} y_{o,out} - T_{N,o}$

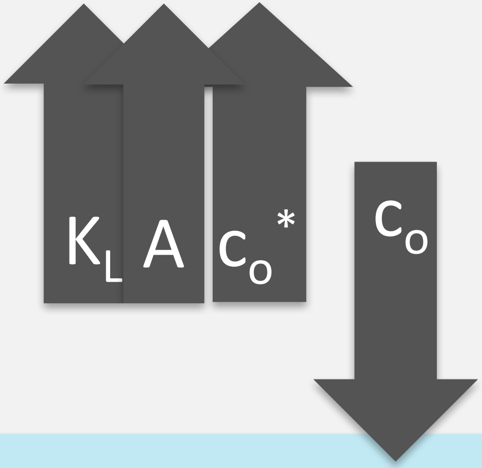
Broth phase $d(V_L c_o)/dt = R_o + T_{N,o}$

Note: gas phase $O_2/CO_2/N_2$ balances (see unit "Learning about the process: Gas phase balances" in week 2)

O_2 transfer rate

Increase power input

0.2 – 2 m/h
set by the bubble size



$$T_{N,o} = K_L A \, (c_o^* - c_o)$$

limited by the microorganism

Maximum O_2 transfer rate occurs at $c_o = 0$

$$T_{N,o,max} = K_L A \, c_o^*$$

Transfer of CO_2

$$T_{N,c} = (K_L A)_c (c_c - c_c^*)$$

CO_2 transfer (mol CO_2 / m^3) is opposite to O_2

CO_2 solubility

$$\alpha_C = 38 \frac{mol(CO_2)/m^3(broth)}{bar(CO_2)}$$

30 x larger

CO_2 inhibition

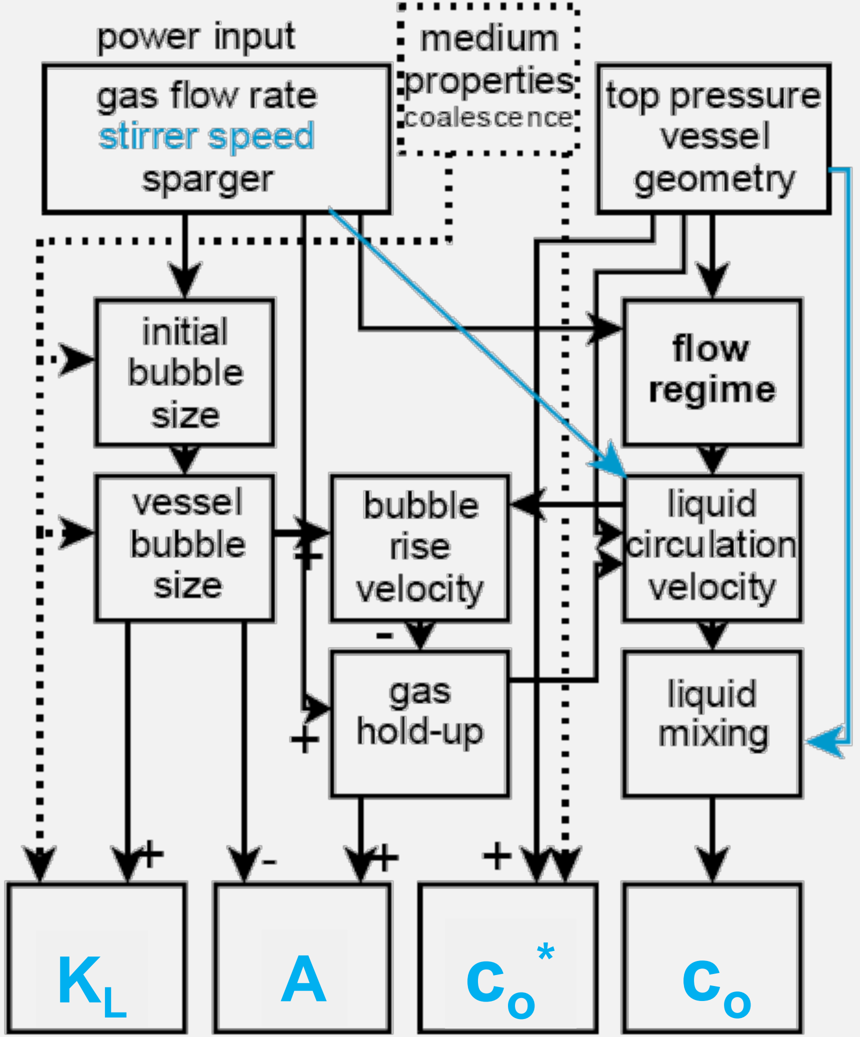
O_2 solubility

$$\alpha_o = 1.25 \frac{mol(O_2)/m^3(broth)}{bar(O_2)}$$

Note: gas phase O_2/CO_2/N_2 balances (see unit "Learning about the process: Gas phase balances" in week 2)

Transfer in bioreactors

Complex interactions



Bubble types in a fermenter

smaller bubbles (<2 mm) rigid surface

Surface area

9× bubbles of 2 mm =
1× bubble of 6 mm

Volume

27× bubbles of 2 mm =
1× bubble of 6 mm

Non-coalescing

larger bubbles (>6 mm) mobile surface

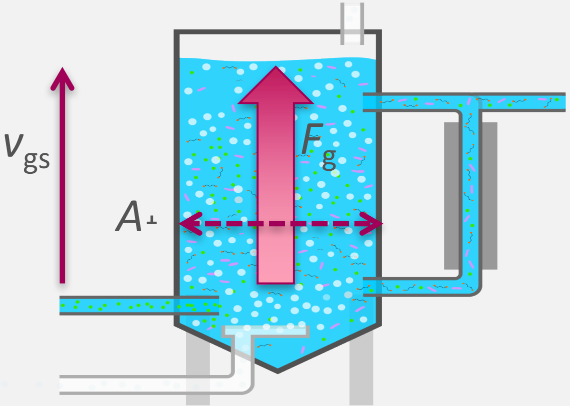
Coalescence reduces A/V 79%

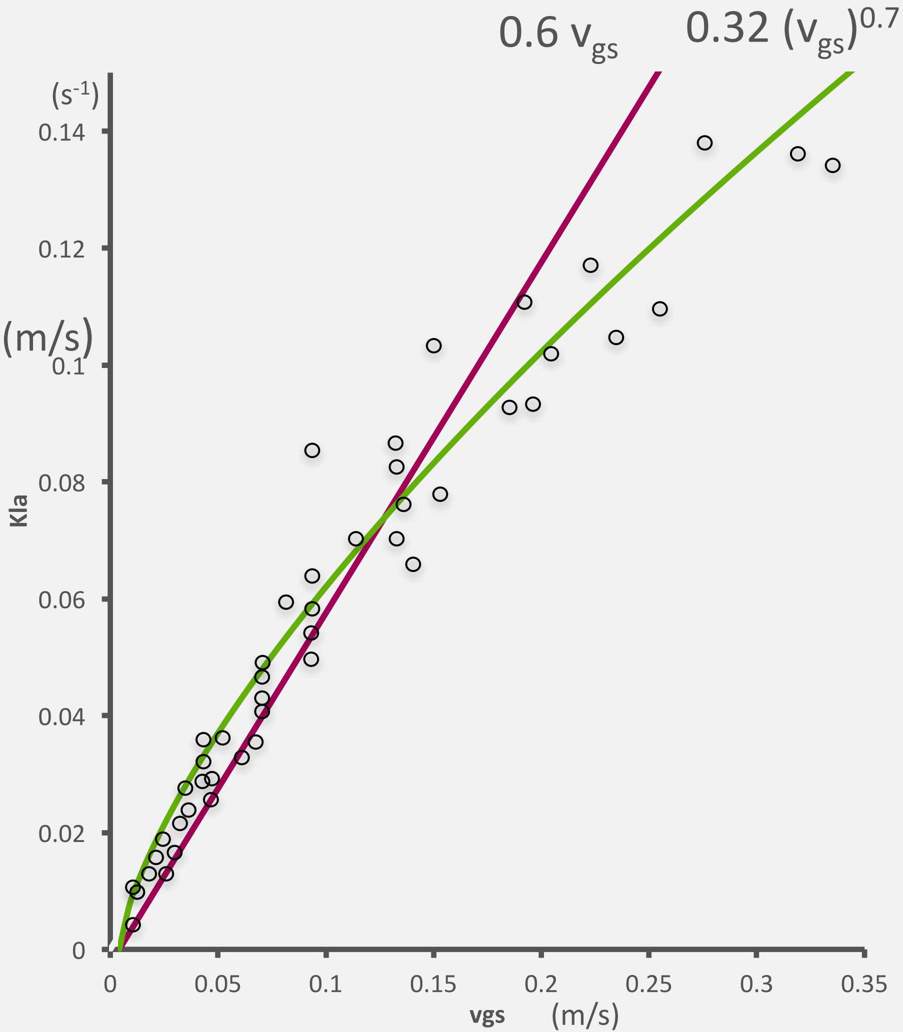
Coalescing

Aeration constant: Bubble column

$$v_{gs} = \frac{F_g}{A_\perp}$$

- v_{gs}: Superficial gas velocity (m/s)
- F_g: Gas flow rate (m^3/s)
- $A_\perp$: Cross-sectional reactor area (m^2)





Aeration constant: Stirred vessel

- single stirrer, standard geometry, coalescing

$$K_L a = 0.026 \left(\frac{P_s}{V_L}\right)^{0.4} v_{gs}^{0.5}$$

K_La (s^{-1})

Power input impeller per volume (W/m^3)

- single stirrer, standard geometry, non-coalescing

~2× better gas transfer than coalescing

$$K_L a = 0.002 \left(\frac{P_s}{V_L}\right)^{0.7} v_{gs}^{0.2}$$

Scale-up: vertical gradient in C_o^*

$c_o^* = \alpha_o\, y_o\, p$

- p: there is a hydrostatic pressure gradient of **0.1 bar** per meter height
- y_o: the gas phase is depleted with **0.55%** per meter height
  (J.J.Heijnen, K. van 't Riet (1984), The Chemical Engineering Journal. 28 B21 – B42)

$y_{O_2,in}$	–	$y_{O_2,out}$	=	0.0055 H	
mole fraction O_2 in inlet gas		mole fraction O_2 in outlet gas			unaerated broth height in meters

Example H = 25 m

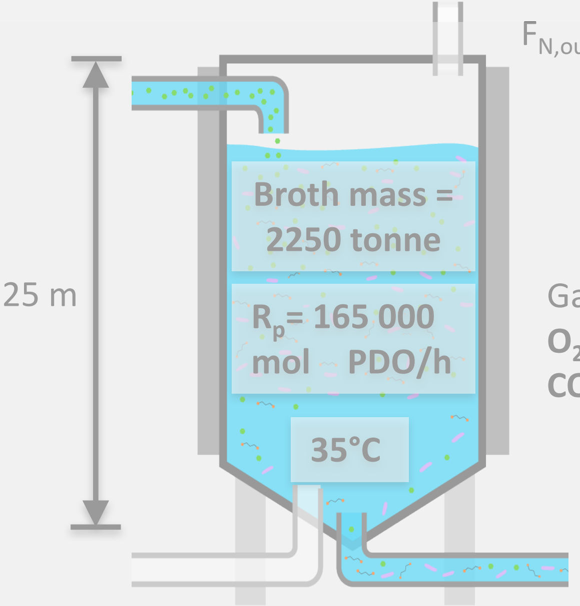
$y_{O_2,out}$ = 0.21 – 0.0055 × 25 = 0.21 – 0.1375 = 0.0725

C_o^* out = 1.25 × 0.0725 × 1 = 0.091 mol/m³

C_o^* in = 1.25 × 0.21 × (1+2.5) = 0.919 mol/m³

Also, there is an opposite gradient in v_{gs} and, hence, K_La (increasing upward)

Average bioreactor geometry, gas transport and mass transfer for the PDO process



$F_{N,out}$ = 3760969 (mol/h)
$y_{O2,out}$ = 0.0725
$y_{CO2,out}$ = 0.1614
p_{top} = 1 bar

Gas transfer:
O_2 = 433207 mol O_2/h
CO_2 = 607200 mol CO_2/h

$F_{N,in}$ = 3361320 (mol/h)
$y_{O2,in}$ = 0.21
$y_{CO2,in}$= 0
P_{bottom} = 1 + 0.1 bar/m·25m = 3.5 bar

Note: required $T_{N,o} > T_{N,o,max}$ so this bioreactor is under-designed → how to improve?

$$p = \frac{p_{top}+p_{bottom}}{2} = \frac{1+3.5}{2} = 2.25\ bar$$

$$D = \sqrt{\frac{2250\ m^3}{\frac{1}{4}\pi * 25\ m}} = 10.7\ m \rightarrow \quad \frac{H}{D} = \frac{25\ m}{10.7\ m} = 2.34$$

$$\frac{T_{N,o}}{M} = \frac{433207\ mol\ O_2/h}{2250\ tonne} = \mathbf{193}\ \frac{mol\ O_2/h}{tonne} \quad (\rho_{broth} = 1\ tonne/m^3)$$

$$F_N = \frac{3760969+3361320}{2} = 3561145\ \frac{mol}{h} \left(= 11.1\ \frac{m^3}{s}\right)$$

$$v_{gs} = \frac{11.1}{\frac{1}{4}\cdot\pi\cdot 10.7^2} = 0.124\ m/s$$

$$C_o^* = 1.25\ \frac{3.5\cdot 0.21+1\cdot 0.0725}{2} = 0.505\ mol/m^3$$

$$K_L a = 0.32 \cdot 0.124^{\ 0.7} = 0.074\ s^{-1}$$

$$T_{N,o,max} = K_L a \cdot C_o^* = 0.037\ \frac{mol\ O_2/s}{tonne} = \mathbf{135}\ \frac{mol\ O_2/h}{tonne}$$

Conclusions

Design choices and interacting mechanisms

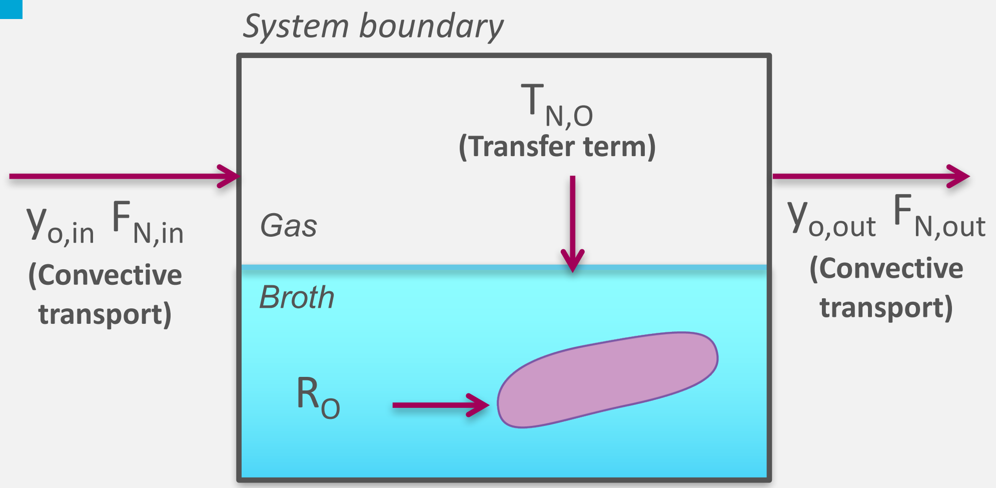
- Gas phase composition and pressure
- Power input
- Interface mobility
- Reactor type
- Reactor geometry and scale
- Gas-liquid flow, gas-liquid mixing and gas hold-up

Mass transfer rate of component ***z***

$$T_{N,z} = (K_L A)_z \, (c_z^* - c_z)$$

See you in the next unit!

O_2 transfer rate



Transfer rate of O_2 (mol O_2 / h)

Resistance coefficient (m / h)

Total surface area of bubbles (m^2)

$$\frac{T_{N,o}}{V_L} = K_L a (c_o^* - c_o)$$

Solubility (mol O_2 / m^3)

Actual conc. in liquid (mol O_2 / m^3)

Gas phase $d(N_G y_o)/dt = F_{N,in} y_{o,in} - F_{N,out} y_{o,out} - T_{N,o}$

Broth phase $d(V_L c_o)/dt = R_o - T_{N,o}$