PDO continuous process design: calculation of inputs and outputs using the process reaction

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Information for PDO process design

- **PDO process reaction at μ = 0.0245 h^{-1}**

$$-1.295\ C_6H_{12}O_6 - 0.218\ NH_3 - 2.6255\ O_2 + \underbrace{\mathbf{1}\ C_3H_8O_2}_{\text{PDO}} + \underbrace{1.090\ C_1H_{1.80}O_{0.50}N_{0.20}}_{\text{biomass}} + 3.680\ CO_2 + 3.116\ H_2O + 1181\ \text{kJ heat}$$

$$\mathbf{C_s} = 85 \cdot 10^{-6}\ \frac{\text{mol glucose}}{\text{kg broth}},\quad \mathbf{q_p} = 0.02248\ \frac{\text{mol PDO/h}}{\text{mol x}},\quad -\mathbf{q_s} = 0.02911\ \frac{\text{mol glucose/h}}{\text{mol x}}$$

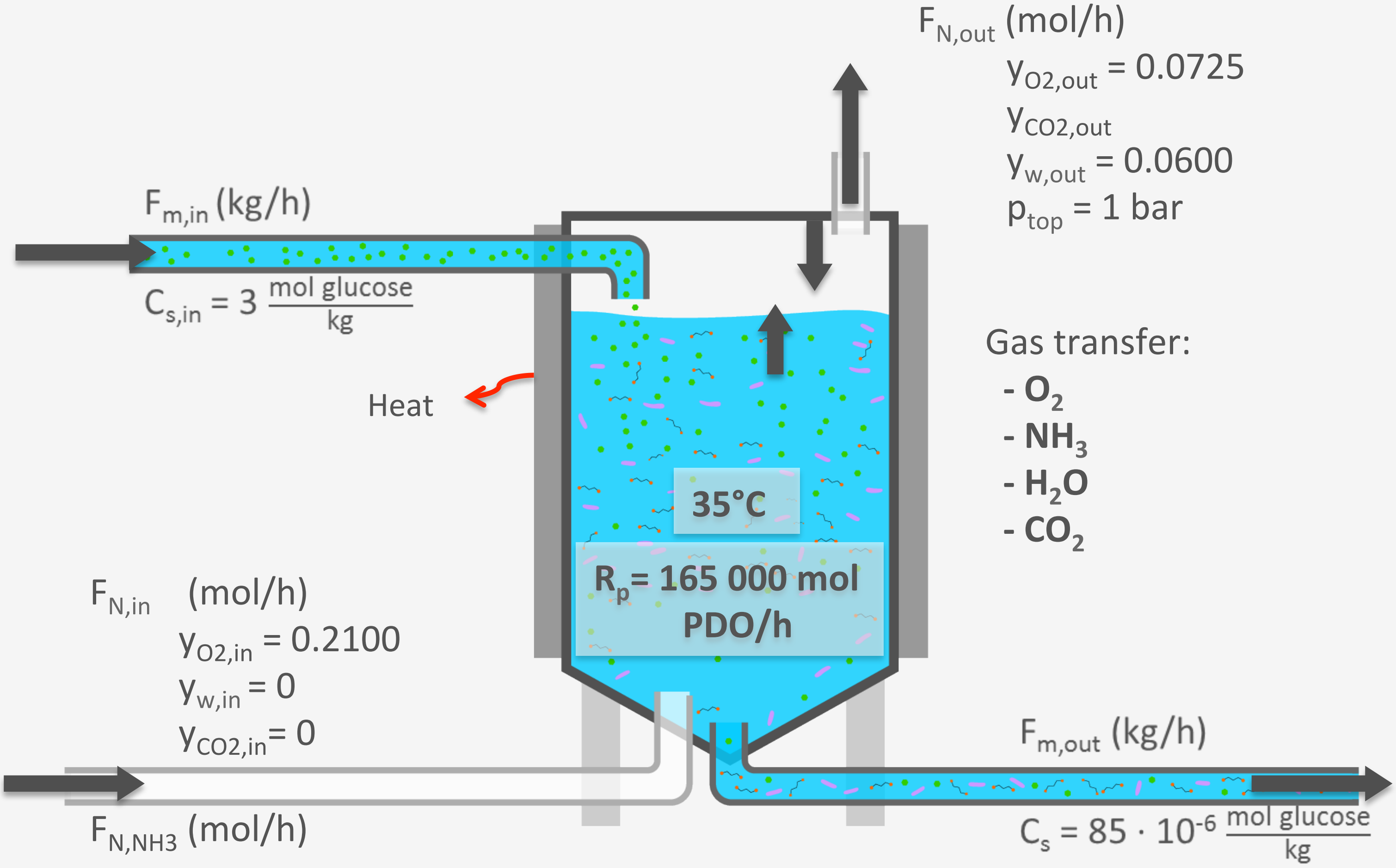
- **Continuous process**

  R_p = 165000 mol PDO/h (= 10^5 tonnes / year), 8000 hours/year

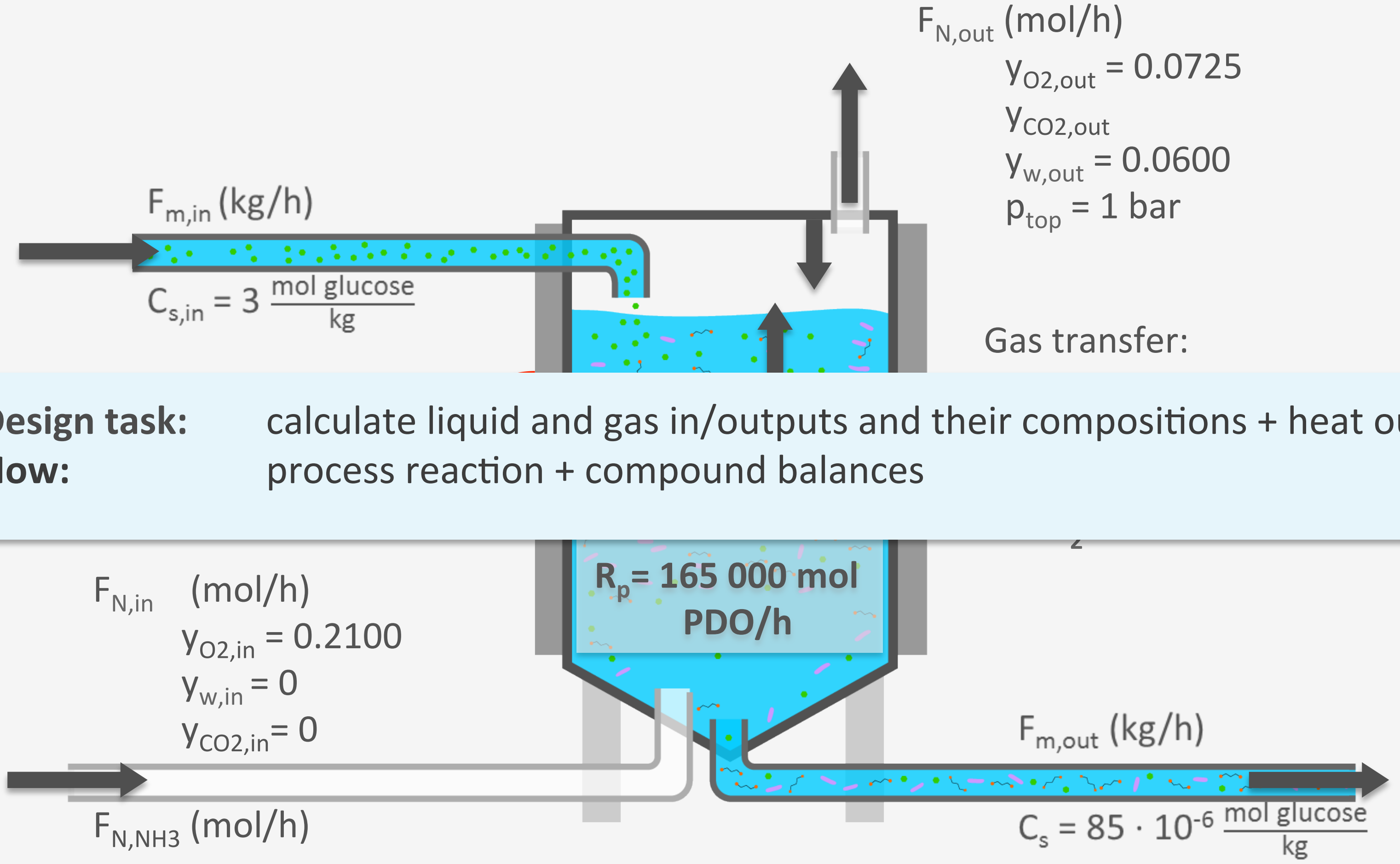
  Fermenter: Bubble column, H = 25m, $y_{O2,out}$ = 0.0725, p_{top} = 1 bar, p_w = 0.06 bar, T = 35 °C

  Feed: C-source, 3.00 mol glucose / kg feed

  N-source, NH_3 gas



$F_{m,in}$ (kg/h)
$C_{s,in} = 3 \frac{\text{mol glucose}}{\text{kg}}$
Heat
$F_{N,in}$ (mol/h)
$y_{O2,in} = 0.2100$
$y_{w,in} = 0$
$y_{CO2,in} = 0$
$F_{N,NH3}$ (mol/h)
35°C
R_p = 165 000 mol PDO/h
$F_{N,out}$ (mol/h)
$y_{O2,out} = 0.0725$
$y_{CO2,out}$
$y_{w,out} = 0.0600$
$p_{top} = 1$ bar
Gas transfer:
- O_2
- NH_3
- H_2O
- CO_2
$F_{m,out}$ (kg/h)
$C_s = 85 \cdot 10^{-6} \frac{\text{mol glucose}}{\text{kg}}$



- **Design task:** calculate liquid and gas in/outputs and their compositions + heat output
- **How:** process reaction + compound balances

Calculation of the gas flows $F_{N,in}$, $F_{N,out}$ and their compositions

- **Total gas balance (mol gas / h)**

$$\underbrace{F_{N,in}}_{\text{mol air/h}} + \underbrace{165000 \cdot 3.680}_{\text{mol } CO_2\text{/h}} + \underbrace{0.06\,F_{N,out}}_{\text{mol } H_2O \text{ vapour/h}} = \underbrace{F_{N,out}}_{\text{mol gas/h}} + \underbrace{165000 \cdot 2.6255}_{\text{mol } O_2\text{/h}}$$

- **Gas phase O_2 balance (mol O_2 / h)**

$$\underbrace{0.21\,F_{N,in}}_{\text{mol } O_2\text{/h}} = \underbrace{0.0725\,F_{N,out}}_{\text{mol } O_2\text{/h in off gas}} + \underbrace{165000 \cdot 2.6255}_{\text{mol } O_2\text{/h transferred and consumed by the organism}}$$

- **2 equations, 2 unknowns, which can be solved**

  $F_{N,out}$ = 3760969 mol gas / h

  $F_{N,in}$ = 3361320 mol air / h

- **Question: why is $F_{N,out} > F_{N,in}$?**
- **Calculate y_C in off gas using gas phase CO_2 balance**

Calculation of the liquid flows

Broth glucose balance (mol glucose/h)

$$0 = \underbrace{-165000 \cdot 1.295}_{\text{mol glucose / h consumed}} + \underbrace{F_{m,in} \cdot 3}_{\text{mol glucose / h in feed}} - \underbrace{F_{m,out} \cdot 85 \cdot 10^{-6}}_{\text{mol glucose / h in broth outflow (neglected!)}}$$

$F_{m,in}$ = 71225 kg/h

Total broth mass balance (kg/h)

Feed	+ 71225 kg/h
O_2 input	+ 165000 · 2.6255 · 0.032 = 13863 kg/h
NH_3 input	+ 165000 · 0.218 · 0.017 = 611.5 kg/h
CO_2 loss	- 165000 · 3.68 · 0.044 = 26717 kg/h
Water loss	- 3760969 · 0.060· 0.018 = 4062 kg/h
$F_{m,out}$	**54920 kg/h**

- Note: neglecting glucose in broth outflow, $F_{m,out}C_s$ = 54920 · 85·10^{-6} = 4.7 mol glucose / h, which is indeed negligible compared to a feed of 213675 mol glucose/h

Calculation of the broth outflow biomass and PDO concentration and the fermenter broth mass

- **c_x: use broth biomass balance (mol x / h)**

Accumulation = inflow – outflow + production → $0 = 0 - c_x \cdot F_{m,out} + R_x$

→ Calculate c_x (c_x = 3.275 mol x / kg broth)

- **c_p: use broth PDO balance (mol PDO / h)**

Accumulaton = inflow – outflow + production → $0 = 0 - c_p \cdot F_{m,out} + R_p$

→ Calculate c_p (c_p = 3.00 mol PDO / kg broth)

- **Amount of broth mass M in the fermentor**

$$N_x \text{ (mol x)} = \frac{R_p}{q_p}$$

$$M \text{ (kg broth)} = \frac{N_x}{c_x}$$

R_p → known

q_p → known

c_x → known

→

$$N_x \text{ (mol x)} = 7.34 \cdot 10^6 \text{ mol}$$

$$M \text{ (kg broth)} = 2250 \text{ tonnes}$$

Heat removal

Knowledge needed: from thermodynamic tables heat of water evaporation equals $\Delta H_{vap,w}$ = 43 kJ/mol water

- **Heat balance (in kJ/h):**

Accumulation = Heat of reaction - enthalpy of evaporation + heat from sparged air
- heat removal (cooling) = 0

- **Temperature should be constant so accumulation = 0**

- **Heat from sparged air is neglected**

known known

Heat to be removed = $-(\Delta H_r) \cdot R_p - \Delta H_{vap,w} \cdot y_{w,out} \cdot F_{N,out}$ kJ/h

NH_3 sparging

- **Use NH_3 balance (mol NH_3 / h)**

Accumulation	= inflow – outflow – consumption
0	$= F_{N,NH3} - 0 - 165000 \cdot 0.218$

$$F_{N,NH3} = 35970 \text{ mol } NH_3 / h$$

The process scheme

$F_{m,in}$ (kg/h) = 71225 kg/h

$C_{s,in} = 3 \frac{\text{mol glucose}}{\text{kg}}$

Heat = 51434 kJ/s

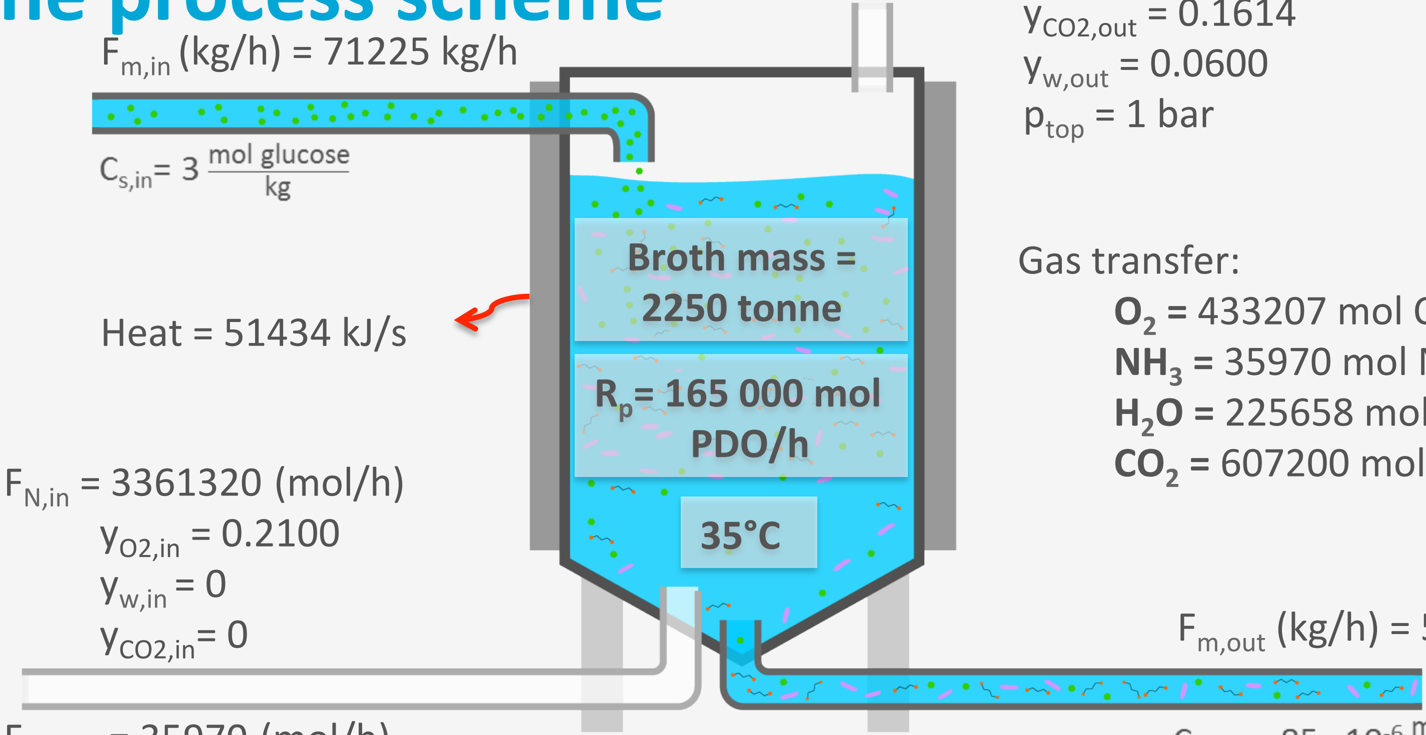
$F_{N,in}$ = 3361320 (mol/h)

$y_{O2,in}$ = 0.2100

$y_{w,in}$ = 0

$y_{CO2,in}$ = 0

$F_{N,NH3}$ = 35970 (mol/h)



$F_{N,out}$ = 3760969 (mol/h)

$y_{O2,out}$ = 0.0725

$y_{CO2,out}$ = 0.1614

$y_{w,out}$ = 0.0600

p_{top} = 1 bar

Gas transfer:

O_2 = 433207 mol O_2/h

NH_3 = 35970 mol NH_3/h

H_2O = 225658 mol H_2O/h

CO_2 = 607200 mol CO_2/h

$F_{m,out}$ (kg/h) = 54920 kg/h

$C_{S,out} = 85 \cdot 10^{-6} \frac{\text{mol glucose}}{\text{kg}}$

$C_{p,out}$ = 3.00 mol PDO/kg

$C_{x,out}$ = 3.275 mol x/kg

See you in the next unit!