Aerobic PDO process: improving sustainability

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Challenge the future

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

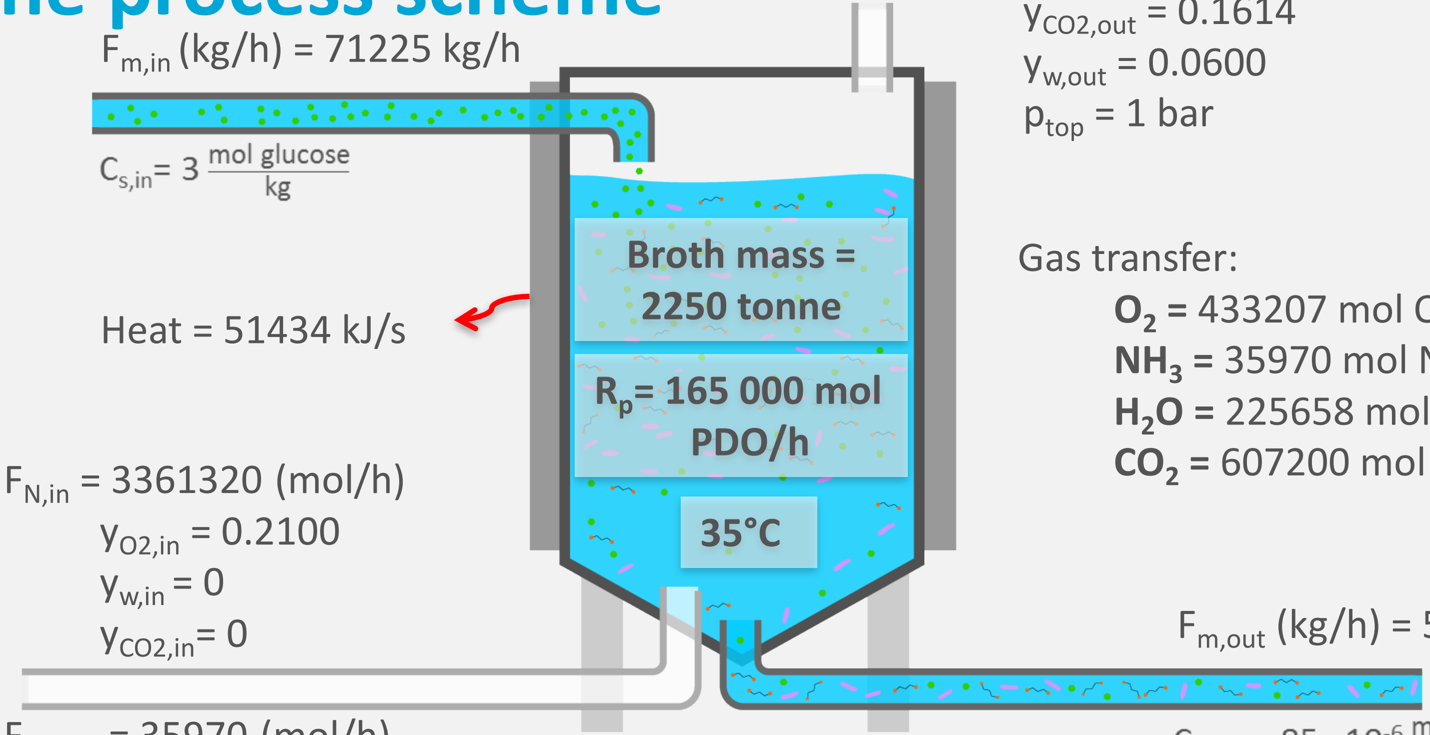
$F_{N,in}$ = 3361320 (mol/h)

$y_{O2,in}$ = 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

More sustainable: “pushing the limits”

Less consumption/production per mol PDO of everything

- Lower coefficients in the process reaction (lower variable cost)

Lower DSP cost: Higher PDO concentration in broth

- Glucose in feed at solubility limit

Lower capital cost: Smaller fermenters

- High O_2 transport rate in the fermenter: week 4
- Low O_2/PDO ratio in process reaction

Lower q_i/q_p ratios: Dissect the process reaction

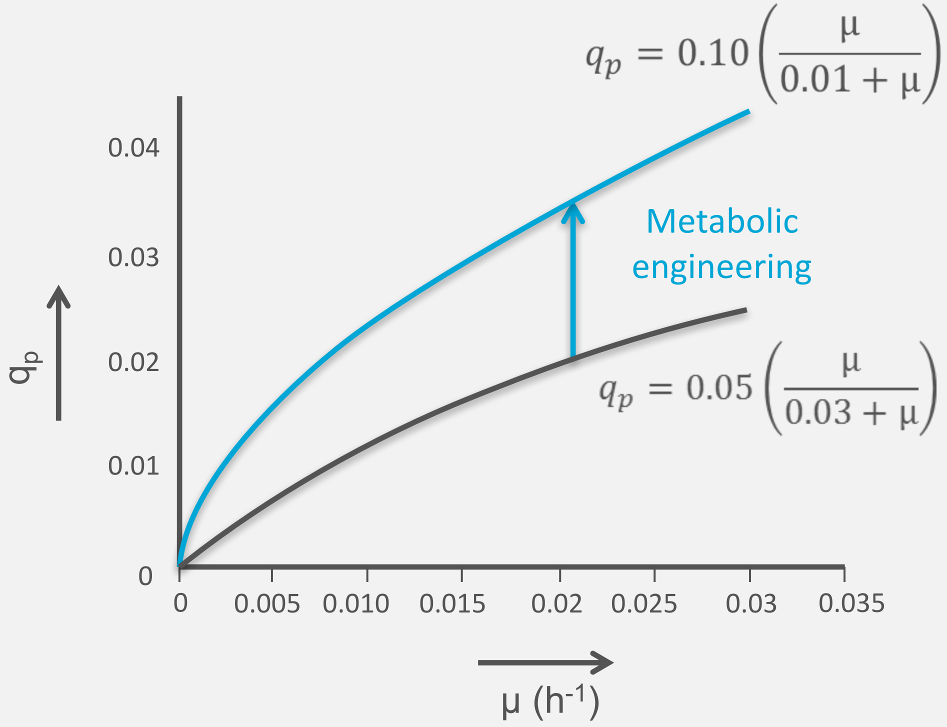
$$\frac{q_s}{q_p} * C_6H_{12}O_6 + \frac{q_{NH_4^+}}{q_p} * NH_4^+ + \frac{q_{O_2}}{q_p} * O_2 + \frac{\mu}{q_p} * C_1H_{1.8}O_{0.5}N_{0.2} + 1 * C_3H_8O_2 + \frac{q_{CO_2}}{q_p} * CO_2 + \frac{q_{H_2O}}{q_p} * H_2O + \frac{q_{H^+}}{q_p} * H^+ + \frac{q_Q}{q_p}(heat)$$

μ/q_p · Biomass reaction
+
(+1) · PDO reaction
+
$(-m_s/q_p)$ · Glucose catabolism

Minimize coefficients by increasing q_p

Lowering q_i/q_p ratios: the kinetic approach by increasing q_p by metabolic engineering

	Wild type	Mutant
$q_{p,max}$ (=α)	**0.05**	**0.10**
μ_{opt}	0.025	0.014
$q_{p,opt}$	0.023	0.059
q_s / q_p	1.295	0.95
μ / q_p	1.09	0.24
q_{O2} / q_p	2.63	1.42
$c_{s,opt}$	$85 \cdot 10^{-6}$	$192 \cdot 10^{-6}$

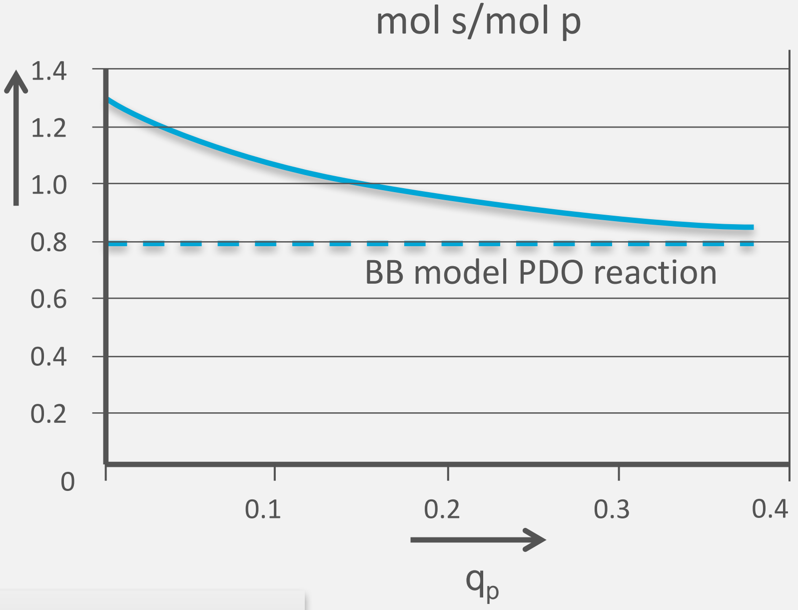


Limit of increasing q_p

Process reaction

strong increasing q_p

BB model PDO reaction is the lower limit



<u>BB model PDO reaction</u>

$$-0.80\ C_6H_{12}O_6 - 0.80\ O_2 + \underbrace{1.00\ C_3H_8O_2}_{\text{PDO}} + 1.80\ CO_2 + H_2O$$

Lowering q_i/q_p ratios: the stoichiometric approach of metabolic engineering

PDO reaction of the Black Box model:

$-0.80\ C_6H_{12}O_6 - 0.80\ O_2 + 1.00\ C_3H_8O_2 + 1.80\ CO_2 + 0.80\ H_2O$

Catabolic part:

$-0.80/6\ C_6H_{12}O_6 \quad -0.80\ O_2 \quad + 0.80/6\ CO_2 \quad + 0.80/6\ H_2O$

Anabolic part, "substract catabolic part from PDO reaction":

$-0.666\ C_6H_{12}O_6 \quad -0\ O_2 \quad + 1.00\ C_3H_8O_2 \quad + 1\ CO_2 \quad + 0\ H_2O$

Limit of stoichiometric approach of metabolic engineering: Anaerobic holy grail

Stoichiometric approach: decrease O_2 stoichiometry

0.80 mol O_2 /mol PDO → 0?

- Improved ATP production / O_2
- Less ATP consumption / mol PDO
- …?

Theoretical PDO reaction

$-0.6666\ C_6H_{12}O_6 - 0\ O_2 + 1\ C_3H_8O_2 + 1CO_2 + 110$ kJ Gibbs energy

Limit of stoichiometric approach of metabolic engineering: Anaerobic holy grail

Theoretical PDO reaction

$-0.6666\ C_6H_{12}O_6 - 0\ O_2 + 1\ C_3H_8O_2 + 1CO_2 + 110$ kJ Gibbs energy

Compare: Theoretical Ethanol reaction

$-0.50\ C_6H_{12}O_6 + 1\ C_2H_6O + 1CO_2 + 112$ kJ Gibbs energy

Anaerobic PDO process in principle possible

- More sustainable!!

Lower DSP cost: focus on less water

High PDO concentration

→ More concentrated glucose solution: operate at glucose solubility limit

→ **water free feedstock**

- Ethanol
- Methanol
- H_2/CO syngas

From sustainable feedstocks

→ High fermentation temperature to increase water evaporation

Big Banana: use mass not volume

For previous calculations we used the volume approach:

- Concentrations in mol/l
- Broth volume V_L (m^3)
- Volume balance

Which is incorrect, minor error in **dilute** systems

However:

- Volume conservation does not exist: *1 l water + 1 l ethanol ≠ 2 l mixture*
- Mass conservation holds: *1 kg water + 1 kg ethanol = 2 kg mixture*

Recommended approach:

- Define concentration in mol/kg liquid
- Use the total broth mass M in the fermenter
- Use the total mass balance to calculate $F_{m,out}$ (kg/h, see PDO case)
- From mass composition and thermodynamic density correlation you can calculate density, volume outflow and broth volume V_L

See you in the next unit!