Black box models: The PDO process reaction as function of μ

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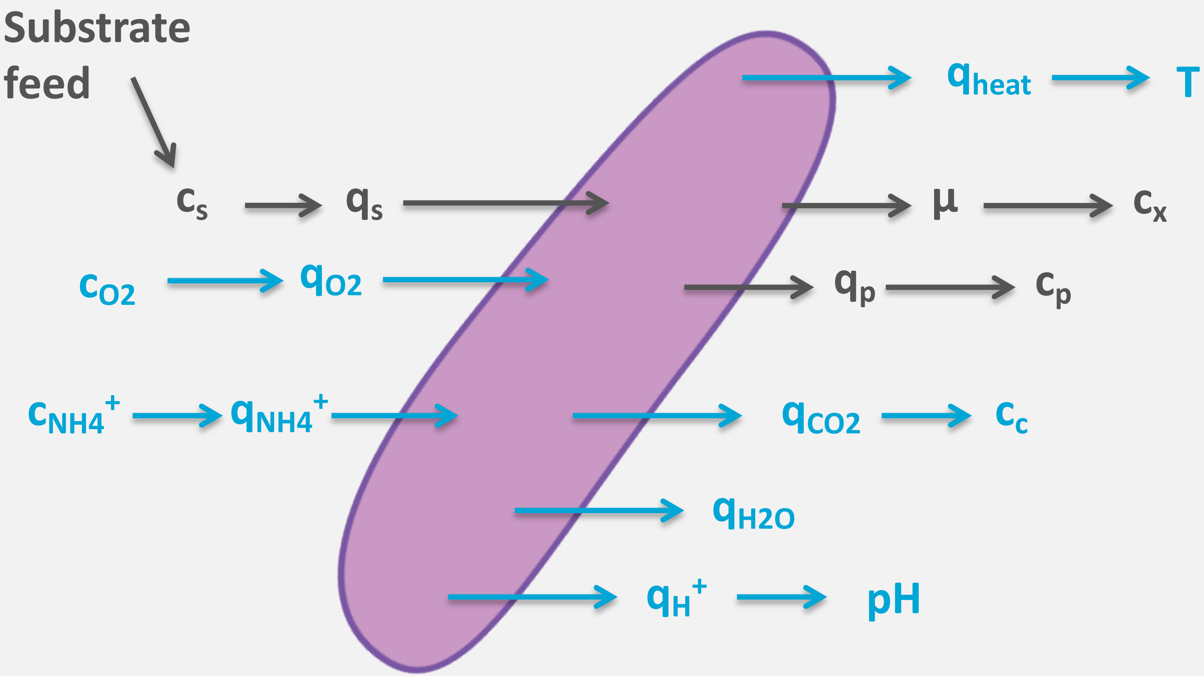
Challenge the future

Expanding the black box model with other q-rates: use conservation principles

There are many more q-rates needed for process design than μ, q_s and q_p

We can calculate them from μ, q_s and q_p using **conservation principles**



Setting up reactions from the Herbert-Pirt relation of the PDO Black Box model

Herbert-Pirt relation:

$$q_s = -0.25\,\mu - 0.80\,q_p - 0.005$$

$\left[\frac{mol_s}{mol_x}\right]$ $\left[\frac{mol_s}{mol_p}\right]$

Biomass reaction (rate: μ)

- 0.25 $C_6H_{12}O_6$ + $\mathbf{a_n}$ NH_4^+ + $\mathbf{a_o}$ O_2 + **1** $C_1H_{1.8}O_{0.5}N_{0.2}$ + $\mathbf{a_c}$ CO_2 + $\mathbf{a_w}$ H_2O + $\mathbf{a_h}$ H^+

Product reaction (rate: q_p)

- 0.80 $C_6H_{12}O_6$ + **1** $C_3H_8O_2$ + $\mathbf{b_o}$ O_2 + $\mathbf{b_c}$ CO_2 + $\mathbf{b_w}$ H_2O+ $\mathbf{b_h}$ H^+

Maintenance (rate: - m_s = 0.005)

- 1 $C_6H_{12}O_6$ – **6** O_2 + **6** CO_2 + **6** H_2O

The unknown stoichiometric coefficient a_i and b_i can be calculated with conservation principles

Using conservation relations to the BB model reactions (I/II): the biomass reaction

- Biomass reaction (rate: μ)

$$-\mathbf{0.25}\ C_6H_{12}O_6 + \mathbf{a_n}\ NH_4^+ + \mathbf{a_o}\ O_2 + \mathbf{1}\ C_1H_{1.80}O_{0.50}N_{0.20} + \mathbf{a_c}\ CO_2 + \mathbf{a_w}\ H_2O + \mathbf{a_h}\ H^+ + \mathbf{b_Q}\ \text{heat}$$

- Conservation relations

C	$-\mathbf{0.25} \cdot 6 + \mathbf{1} \cdot 1 + \mathbf{a_c} \cdot 1 = 0$
H	$-\mathbf{0.25} \cdot 12 + \mathbf{a_n} \cdot 4 + \mathbf{1} \cdot 1.80 + \mathbf{a_w} \cdot 2 + \mathbf{a_h} \cdot 1 = 0$
O	$-\mathbf{0.25} \cdot 6 + \mathbf{a_o} \cdot 2 + \mathbf{1} \cdot 0.50 + \mathbf{a_c} \cdot 2 + \mathbf{a_w} \cdot 1 = 0$
N	$\mathbf{a_n} \cdot 1 + \mathbf{1} \cdot 0.20 = 0$
Charge	$\mathbf{a_n} \cdot \mathbf{(+1)} \cdot \quad + \mathbf{a_h} \cdot \mathbf{(+1)} = 0$

- 5 Linear relations with 5 unknowns can be solved

Using conservation relations to the BB model reactions (II/II): the product reaction

- Product reaction (rate: q_p)

$$-\mathbf{0.80}\ C_6H_{12}O_6 + \mathbf{1}\ C_3H_8O_2 + \mathbf{b_o}\ O_2 + \mathbf{b_c}\ CO_2 + \mathbf{b_w}\ H_2O + \mathbf{b_h}\ H^+$$

- Conservation relations

C	$-\mathbf{0.80} \cdot 6 + \mathbf{1} \cdot 3 + \mathbf{b_c} \cdot 1 = 0$
H	$-\mathbf{0.80} \cdot 12 + \mathbf{1} \cdot 8 + \mathbf{b_w} \cdot 2 + \mathbf{b_h} \cdot 1 = 0$
O	$-\mathbf{0.80} \cdot 6 + 1 \cdot 2 + \mathbf{b_o} \cdot 2 + \mathbf{b_c} \cdot 2 + \mathbf{b_w} \cdot 1 = 0$
Charge	$\mathbf{b_h} \cdot 1 = 0$

- 4 Linear relations with 4 unknowns can be solved

The other Herbert-Pirt relations

- **Biomass reaction (rate μ)**

$$\mathbf{-\,0.25}\ C_6H_{12}O_6\ \mathbf{-\,0.20}\ NH_4^+\ \mathbf{-\,0.45}\ O_2 + \mathbf{1}\ C_1H_{1.8}O_{0.5}N_{0.2} + \mathbf{0.50}\ CO_2 + \mathbf{0.90}\ H_2O + \mathbf{0.20}\ H^+ + 202.5\ \text{kJ heat}$$

- **PDO reaction (rate q_p)**

$$\mathbf{-\,0.80}\ C_6H_{12}O_6 + \mathbf{1}\ C_3H_8O_2\ \mathbf{-\,0.80}\ O_2 + \mathbf{1.80}\ CO_2 + \mathbf{0.80}\ H_2O + \mathbf{0}\ H^+ + 360\ \text{kJ heat}$$

- **Maintenance reaction (rate 0.0050)**

$$\mathbf{-\,1}\ C_6H_{12}O_6 - \mathbf{6}\ O_2 + \mathbf{6}\ CO_2 + \mathbf{6}\ H_2O + 2700\ \text{kJ heat}$$

- **Herbert-Pirt relations**

$$q_s = -0.25\,\mu - 0.80\,q_p - 1 \cdot 0.0050$$
$$q_{O2} = -0.45\,\mu - 0.80\,q_p - 6 \cdot 0.0050$$
$$q_w = ?\ \mu + ?\ q_p + ?$$
$$q_Q = ?\ \mu + ?\ q_p + ?$$

$$q_n = ?\ \mu + ?\ q_p + ?$$
$$q_h = ?\ \mu + ?\ q_p + ?$$
$$q_{CO2} = ?\ \mu + ?\ q_p + ?$$

growth — product — maintenance

growth — product — maintenance

The PDO process reaction depends only on μ (I)

- **Process reaction for 1 mol PDO**

$$\frac{q_s}{q_p} C_6H_{12}O_6 + \frac{q_n}{q_p} NH_4^+ + \frac{q_{O2}}{q_p} O_2 + \frac{\mu}{q_p} C_1H_{1.80}O_{0.50}N_{0.20} + \frac{q_c}{q_p} CO_2$$
$$+ \frac{q_w}{q_p} H_2O + \frac{q_h}{q_p} H^+ + \frac{q_Q}{q_p} \text{kJ heat} + \mathbf{1}\ C_3H_8O_2$$

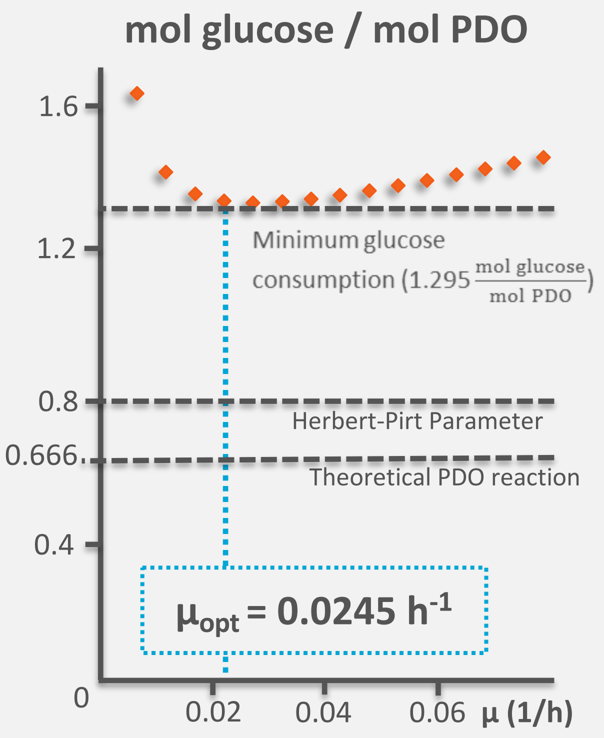
- **$q_p(\mu)$ function**

$$q_p = 0.05 \frac{\mu}{0.03+\mu}$$

- **Substrate Herbert Pirt relation**

$$|q_s| = 0.25\,\mu + 0.80\,q_p + 0.005$$

$$\frac{\text{mol glucose}}{\text{mol PDO}} : \left|\frac{q_s}{q_p}\right| = 1.05 + 5\,\mu + \frac{0.0030}{\mu}$$



The PDO process reaction depends also on μ (II)

Previously: $\frac{\text{mol glucose}}{\text{mol PDO}}: \left|\frac{q_s}{q_p}\right| = 1.05 + 5\,\mu + \frac{0.0030}{\mu}$

Other stoichiometric ratios:

$\left|\frac{q_n}{q_p}\right| = ?$ $\left|\frac{q_{O2}}{q_p}\right| = ?$ $\left|\frac{\mu}{q_p}\right| = ?$ $\left|\frac{q_c}{q_p}\right| = ?$

$\left|\frac{q_w}{q_p}\right| = ?$ $\left|\frac{q_h}{q_p}\right| = ?$ $\left|\frac{q_Q}{q_p}\right| = ?$

Yourself:

- Calculate each stoichiometric ratio as function of μ
- Show them graphically
- For sustainability we want to minimize ratios: calculate μ for each minimum
- Calculate the process reaction stoichiometry at $\mu = 0.0245\ h^{-11}$

The complete PDO black box model

Hyperbolic substrate uptake

$$q_s = -0.20 \frac{c_S}{0.50 + c_S}$$

$q_p(\mu)$ function

$$q_p = 0.05 \frac{\mu}{0.03 + \mu}$$

7 Herbert-Pirt relations

q_s = **- 0.25** μ **- 0.80** q_p **– 1** · 0.0050

q_{O2} = **- 0.45** μ **- 0.80** q_p – **6** · 0.0050

q_{CO2} = ? μ + **?** q_p + ?

q_w = ? μ + **?** q_p + ?

q_n = **?** μ + ? q_p + ?

q_h = ? μ + ? q_p + ?

q_Q = ? μ + ? q_p + ?

1 Free variable, e.g. μ

$\frac{\text{mol glucose}}{\text{mol PDO}}$ is minimal at $\mu_{opt} = 0.0245\ h^{-1}$

→

Process design at $\mu_{opt} = 0.0245\ h^{-1}$

See you in the next unit!