A PDO black box model: experiments for parameter identification

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Summary Black Box Model

Energy consuming product

Aerobic

$$q_s = q_{s,max} \frac{c_S}{K_s + c_s}$$

$$q_s = a\,\mu + b\,q_p + m_S$$

$$q_p = \frac{\alpha\,\mu}{\beta + \mu}$$

1 free variable: μ

Energy producing product

Anaerobic

$$q_s = q_{s,max} \frac{c_S}{K_s + c_s}$$

$$q_s = a\,\mu + m_S$$

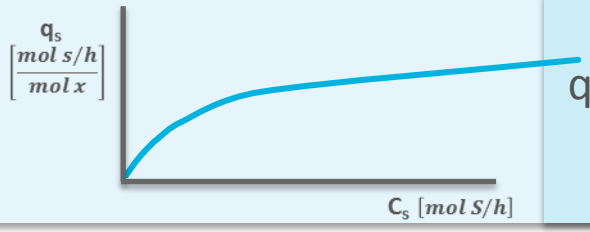
$$q_p = \alpha \cdot \mu + \beta$$

1 free variable: μ

Data needed to determine the parameters for the aerobic BB model

Hyperbolic substrate uptake

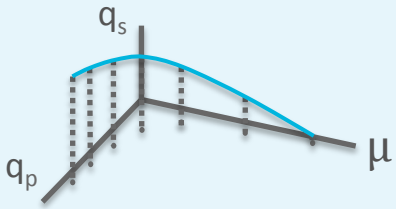
$$q_s = q_{s,max} \frac{c_S}{K_s + c_s}$$



q_s and c_s data needed

Herbert-Pirt

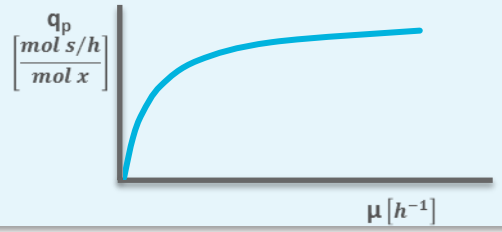
$$q_s = a\,\mu + b\,q_p + m_S$$



q_s, μ and q_p data needed

$q_p(\mu)$ relation

$$q_p = \frac{\alpha\ \mu}{\beta\ +\ \mu}$$



μ and q_p data needed

Parameters are obtained from experiments (example for aerobic model)

Aerobic Black Box Model

Hyperbolic substrate uptake relation:

$$q_s = q_{s,max} \frac{c_s}{c_s + K_s}$$

Herbert-Pirt relation:

$$q_s = a\,\mu + b\,q_p + m_S$$

$q_p(\mu)$ – relation:

$$q_p = \frac{\alpha\ \mu}{\beta + \mu}$$

7 parameters have to be determined experimentally

Experiments should yield sets of c_s, μ, q_p and q_s

Question:
How many experiments do we minimally need to do to obtain the parameters?

Chemostat exp. 1: one set of c_s, μ, q_p and q_s

Exp 1:

Hyperbolic substrate uptake relation:

$$q_s = q_{s,max} \frac{c_s}{c_s + K_s}$$

→ **1** equation, **2** unknowns

Herbert-Pirt relation:

$$q_s = a\,\mu + b\,q_p + m_s$$

→ **1** equation, **3** unknowns

$q_p(\mu)$ – relation:

$$q_p = \frac{\alpha\ \mu}{\beta\ +\ \mu}$$

→ **1** equation, **2** unknowns

Not enough information to find any of the 7 parameters

Chemostat Exp. 2: a new set of c_s, μ, q_p and q_s

Exp 1 + 2:

Hyperbolic substrate uptake relation:

$$q_s = q_{s,max} \frac{c_s}{c_s + K_s}$$

→ **2** equations, **2** unknowns

Herbert-Pirt relation:

$$q_s = a\,\mu + b\,q_p + m_s$$

→ **2** equations, **3** unknowns

$q_p(\mu)$ – relation:

$$q_p = \frac{\alpha\ \mu}{\beta\ +\ \mu}$$

→ **2** equations, **2** unknowns

$q_{s,max}$, K_s and α, β can be found.
Not enough information to find a, b and m_s

Chemostat Exp. 3: a third set of c_s, μ, q_p and q_s

Exp 1, 2 and 3 :

Hyperbolic substrate uptake relation:

$$q_s = q_{s,max} \frac{c_s}{c_s + K_s}$$

→ **3** equations, **2** unknowns

Herbert-Pirt relation:

$$q_s = a\,\mu + b\,q_p + m_s$$

→ **3** equations, **3** unknowns

$q_p(\mu)$ – relation:

$$q_p = \frac{\alpha\ \mu}{\beta\ +\ \mu}$$

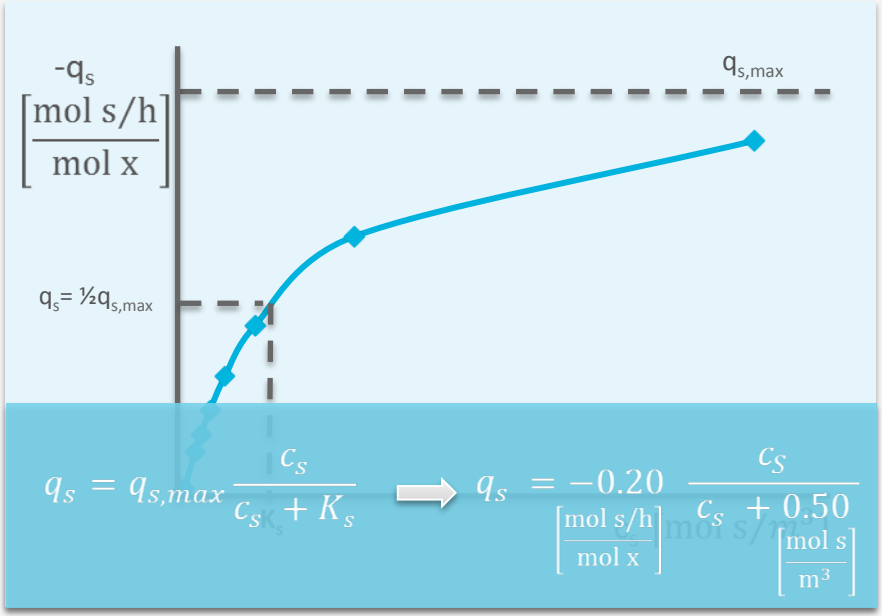
→ **3** equations, **2** unknowns

Enough information to find all 7 parameter values

So **in theory** we need at least **3 experiments** performed at 3 different μ values

Calculating the hyperbolic substrate uptake relation parameters from experimental data

	c_s $\left[\frac{\text{mol s}}{\text{m}^3}\right]$	q_s $\left[\frac{\text{mol s/h}}{\text{mol x}}\right]$	μ $\left[\frac{\text{mol x/h}}{\text{mol x}}\right]$	q_p $\left[\frac{\text{mol p/h}}{\text{mol x}}\right]$
1	0.048	-0.0175	0.0100	0.0125
2	0.075	-0.0260	0.0200	0.0200
3	0.117	-0.0379	0.0400	0.0286
4	0.185	-0.0541	0.0800	0.0364
5	0.324	-0.0787	0.16	0.0421
6	0.7755	-0.1216	0.32	0.0457
7	2.606	-0.1678	0.50	0.0472



With the experimental data we can calculate the parameters α and β of the $q_p(\mu)$ relation

	c_s $\left[\frac{\text{mol s}}{\text{m}^3}\right]$	q_s $\left[\frac{\text{mol s/h}}{\text{mol x}}\right]$	μ $\left[\frac{\text{mol x/h}}{\text{mol x}}\right]$	q_p $\left[\frac{\text{mol p/h}}{\text{mol x}}\right]$
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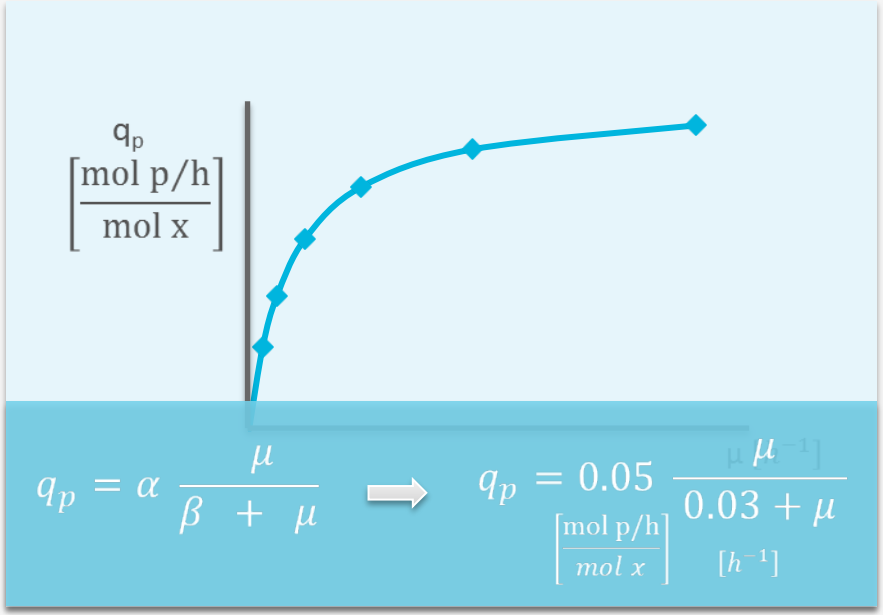

With the experimental data we can calculate the Herbert-Pirt parameters

	c_s $\left[\frac{\text{mol s}}{\text{m}^3}\right]$	q_s $\left[\frac{\text{mol s/h}}{\text{mol x}}\right]$	μ $\left[\frac{\text{mol x/h}}{\text{mol x}}\right]$	q_p $\left[\frac{\text{mol p/h}}{\text{mol x}}\right]$
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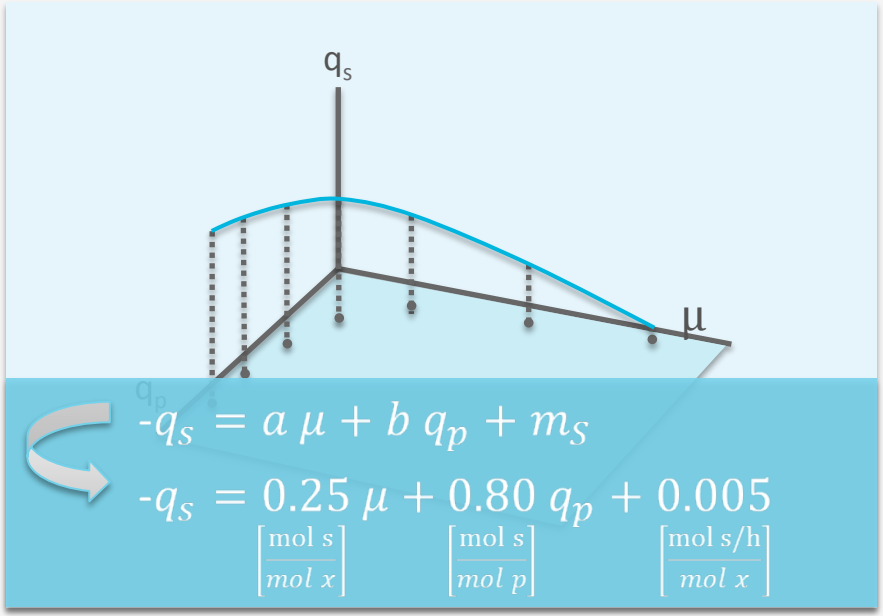

Summarizing parameter estimation in aerobic Black Box models

- **Perform at least 3 chemostat experiments with different μ values**

- **With the resulting datasets of c_s, μ, q_s and q_p:**
  1. Do a graphical evaluation of the parameter values
  2. Use standard (non-)linear parameter fitting programmes to find the relevant parameter values and their errors

- **It is also possible to obtain datasets of c_s, μ, q_s and q_p from fed-batch experiments**

See you in the next unit!