Calibration and validation of model describing complete autotrophic nitrogen removal in granular sludge

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Publication date:
2012

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Vangsgaard, A. K., Mutlu, A. G., Gernaey, K., Smets, B. F., & Sin, G. (2012). Calibration and validation of model describing complete autotrophic nitrogen removal in granular sludge [Sound/Visual production (digital)]. IWA Nutrient Removal and Recovery 2012, Harbin, China, 23/09/2012

Calibration and validation of model describing complete autotrophic nitrogen removal in granular sludge

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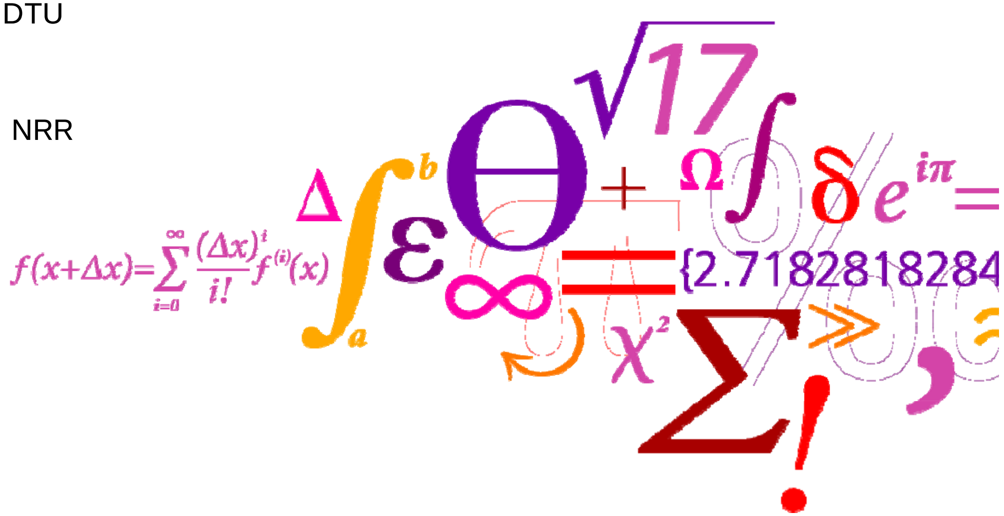
[c]PROCESS - Chemical and Biochemical Engineering - DTU

IWA Nutrient Removal and Recovery 2012: Trends in NRR
September 23-25, 2012. Harbin, China



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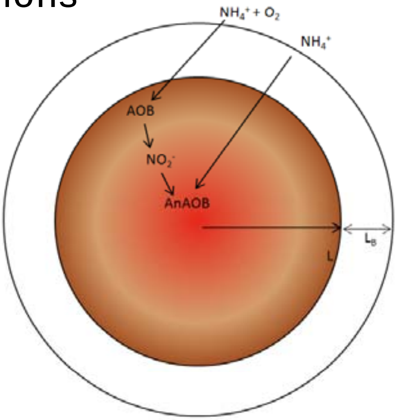
The case

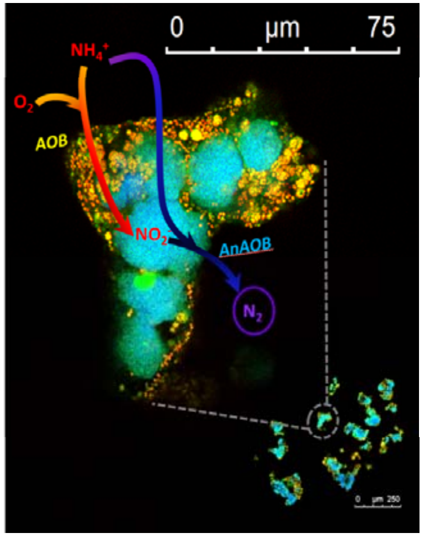
A granular sludge SBR performing N removal through nitritation/anammox

- Calibration methodology developed
- Fast model initialization
- Stoichiometric ratio evaluation

Purpose:

- Experiment planning
- Performance prediction for control applications





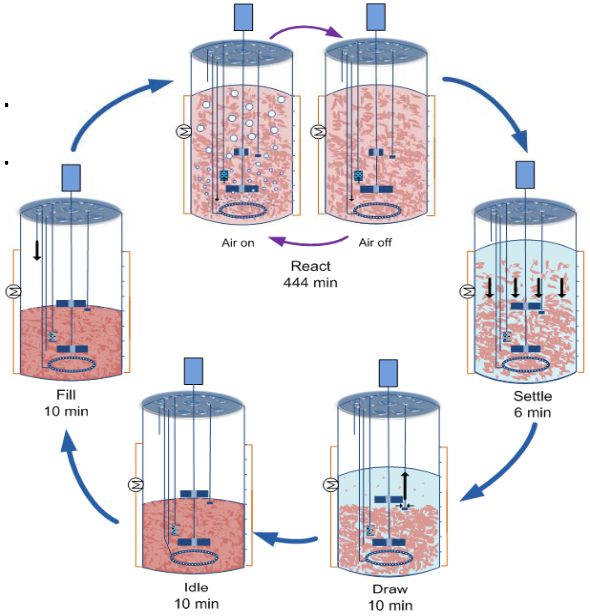
Methods
Physical system

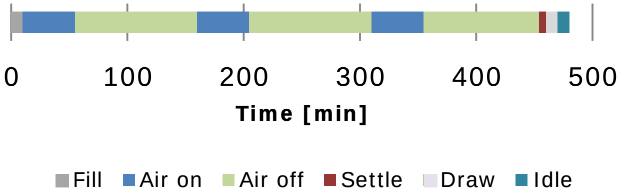
Reactor characteristics:

Volume:	4L
Temperature:	30°C
pH:	7.5±0.3
Mixing:	6-bladed Rushton impeller at 80 rpm + bubble aeration
Solids concentration:	4.2 g VSS/L
Ave. gran. size:	50 µm
Operating time:	11 months

Sequencing batch operation:

Fill:	10 min.
Reaction:	444 min. consisting of three aerated phases and three non-aerated phases
Settling:	6 min.
Draw:	10 min.
Idle:	10 min.



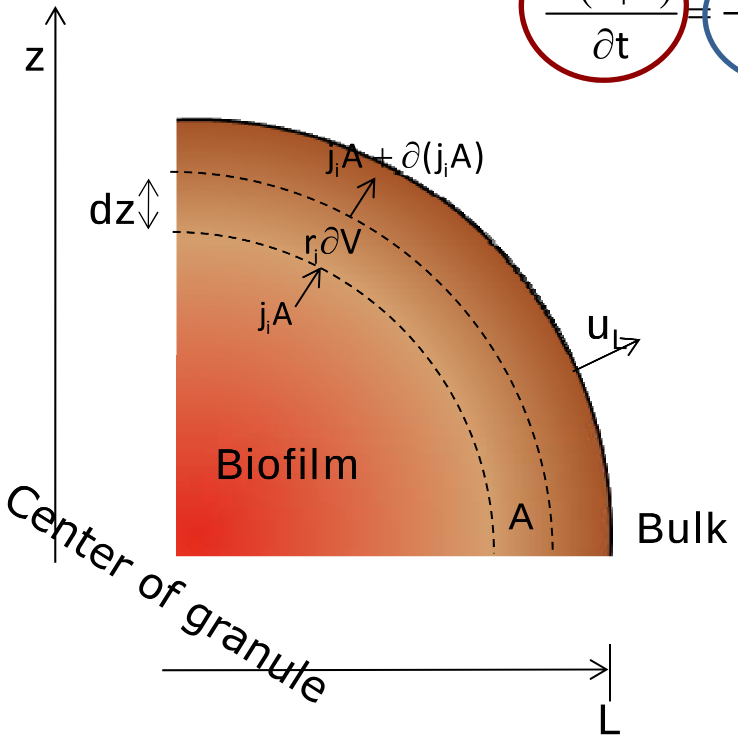


Methods
Model description

Biofilm mass balance equations – Transport and microbial metabolism

Accumulation = Inflow - Outflow + Generation - Consumption

$$\frac{\partial(C_iV)}{\partial t} = -\partial(j_iA) + r_i\partial V \quad < = > \quad \frac{\partial C_i}{\partial t} = \frac{1}{z^2}\frac{\partial}{\partial z}\left(z^2 j_{Ci}\right) + r_i$$



1. Transport of **soluble** compounds is governed by **diffusion** and of **particulate** compounds by **advection**:

$$j_{Si} = D_{bio,i}\frac{\partial S_i}{\partial x} \qquad j_{Xi} = -X_iu_F$$

2. The **granule radius** is a function of the growth and decay of bacteria and a detachment process:

$$\frac{dL}{dt} = u_{F,L} - u_D$$

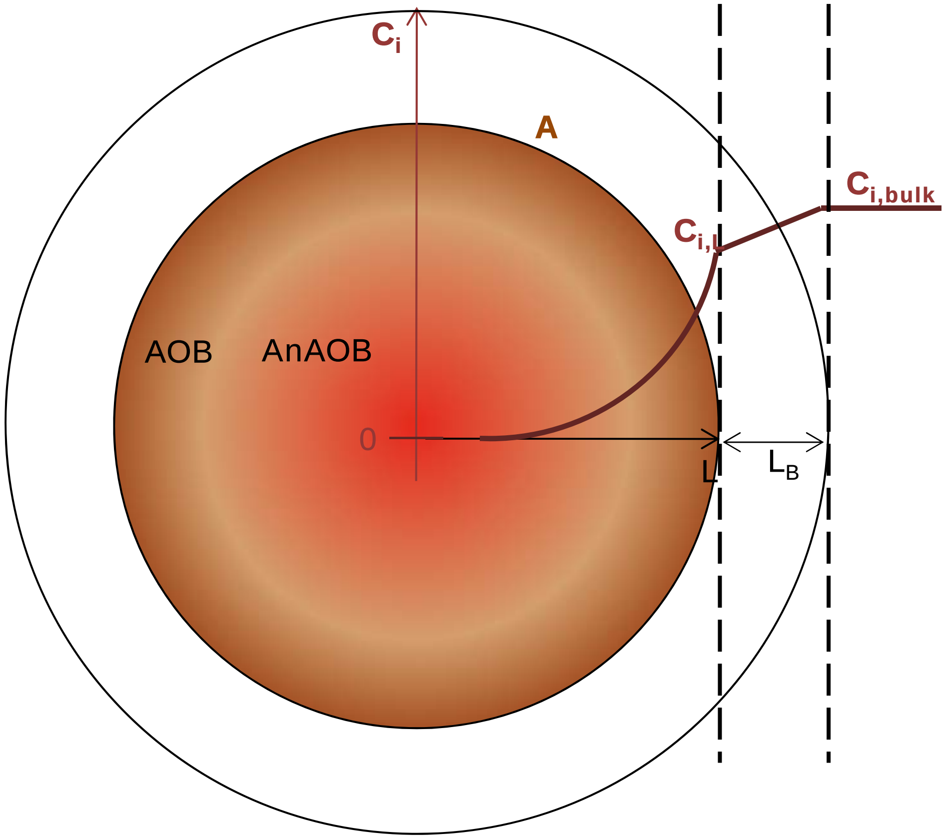
Where the advective velocity is a function of the growth of particulates on the “inside” of a given point k:

$$u_{F,k} = \frac{1}{A_k}\int_0^k A_k\left(\sum_{i=1}^{n_{part}}\frac{r_i}{\rho}\right)_k dz$$

Methods
Model description

Bulk liquid mass balance equations – Transport and microbial metabolism

Accumulation = Inflow - Outflow + Generation - Consumption



$$\frac{dC_i}{dt} = \frac{Q_{in}C_{i,in} - Q_{out}C_{i,bulk} - j_{Ci}A}{V} + r_{Ci}$$

Flux in and out of the biofilm:

Soluble species

$$j_{Si} = k_i\left(S_{i,bulk} - S_{i,L}\right)$$

where

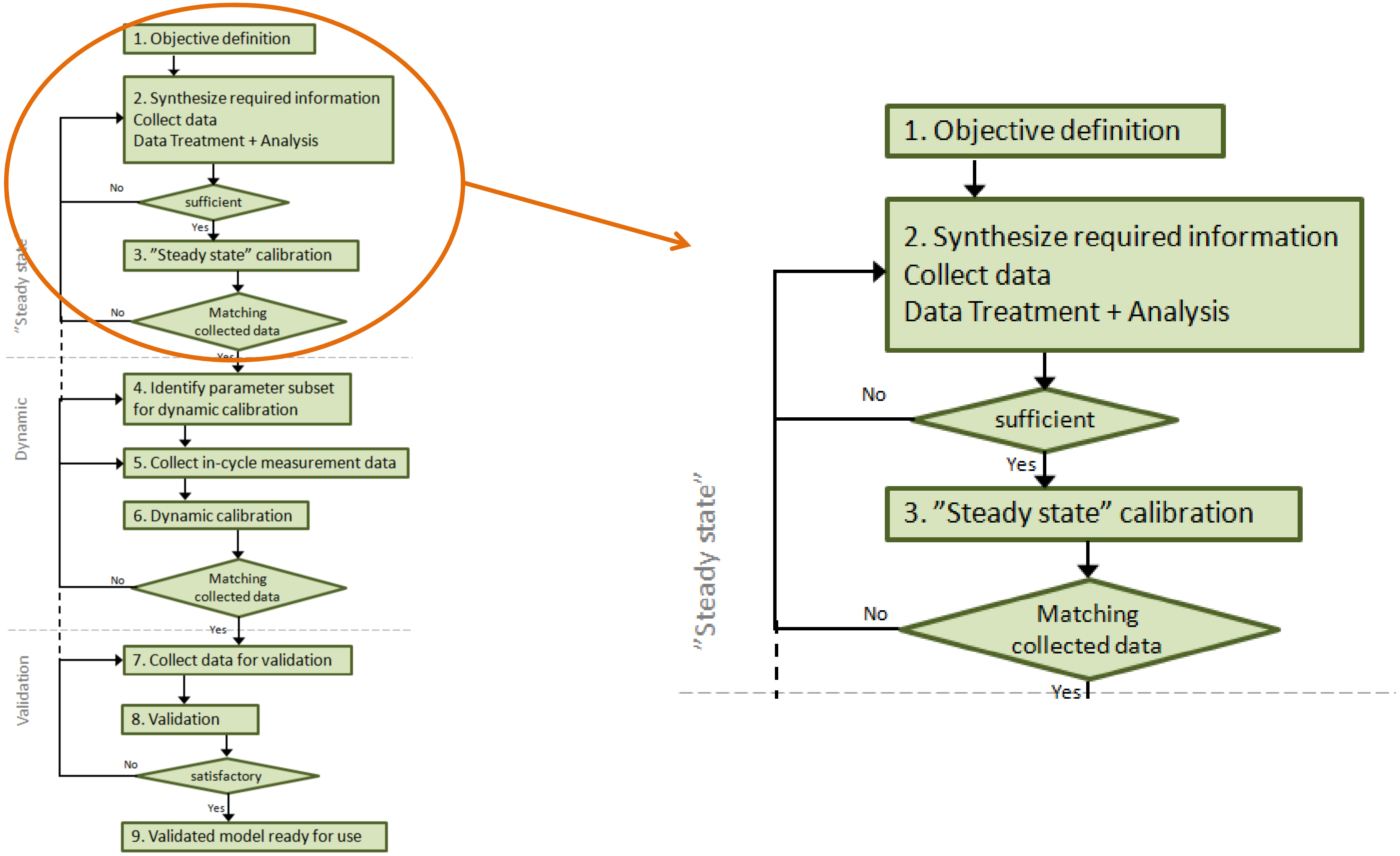
$$k_i = \frac{D_i}{L_B}$$

Particulate species

$$j_{Xi} = -u_D X_{i,L}$$

The mass transfer coefficient is estimated from a semi-empirical correlation considering mixing caused by bubble aeration

Methods
Methodology development



"Steady state"

1. Objective definition

2. Synthesize required information
Collect data
Data Treatment + Analysis

sufficient

No

Yes

3. "Steady state" calibration

Matching collected data

No

Yes

Dynamic

4. Identify parameter subset for dynamic calibration

5. Collect in-cycle measurement data

6. Dynamic calibration

Matching collected data

No

Yes

Validation

7. Collect data for validation

8. Validation

satisfactory

No

Yes

9. Validated model ready for use

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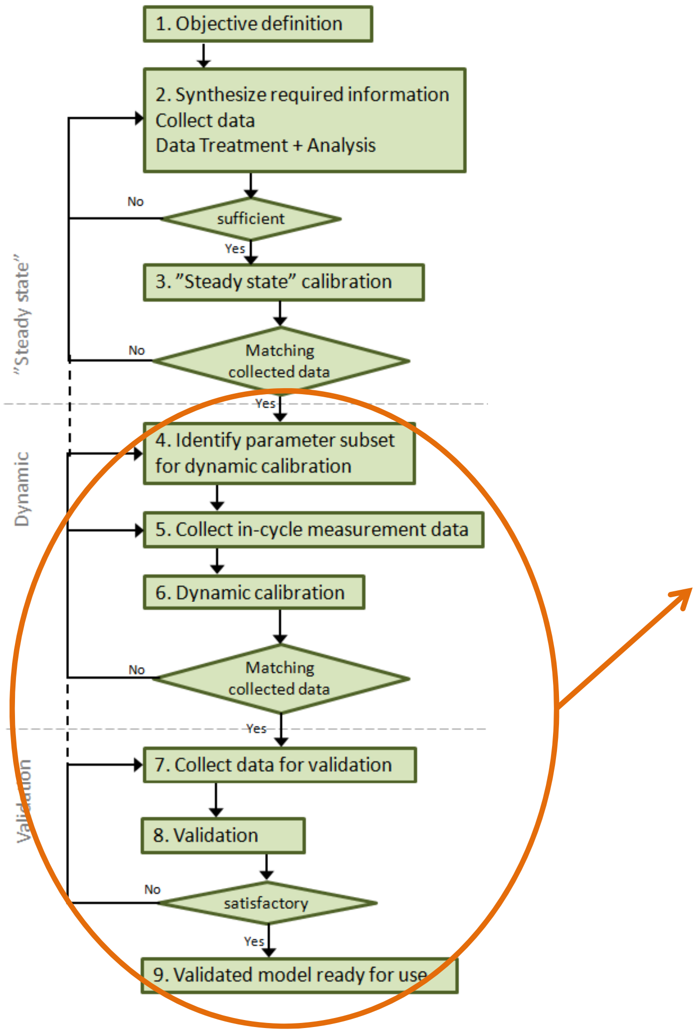

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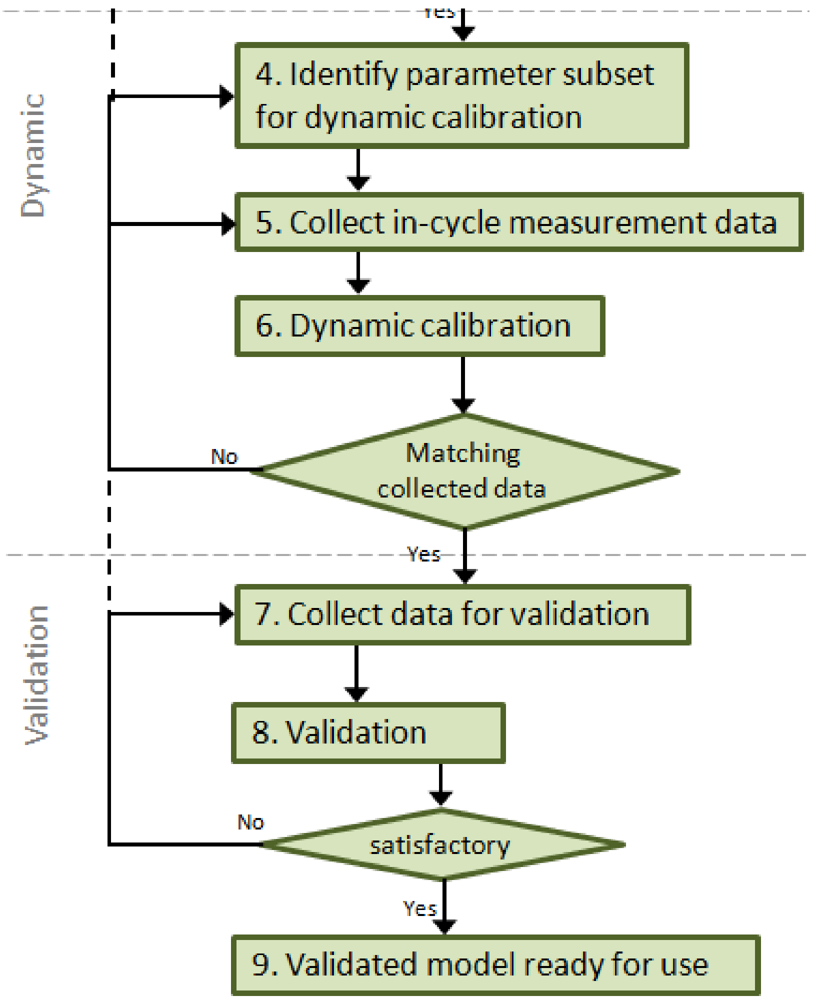

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Results
Steady state calibration

- Step 1:

Determine bulk liquid soluble N species concentrations

- Step 2:

Capturing overall reactor performance through five evaluation criteria:
Three ratios and two efficiencies:

$R1 = \frac{\Delta NO_2^-}{\Delta NH_4^+}$ ⟶ AOB vs. AnAOB + NOB → relative activity

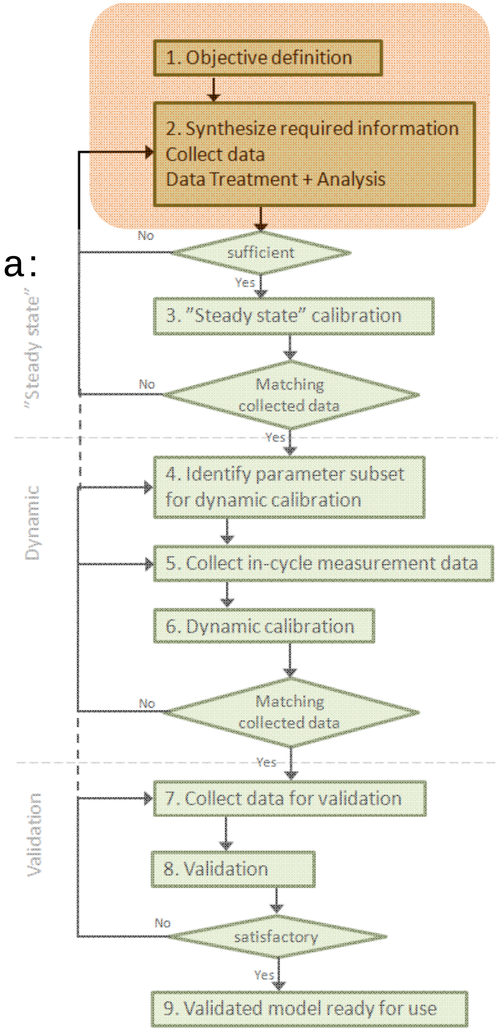
$R2 = \frac{\Delta NH_4^+}{\Delta TN}$ ⟶ AnAOB vs. AOB → relative activity

$R3 = \frac{\Delta NO_3^-}{\Delta NH_4^+}$ ⟶ AnAOB vs. NOB → relative activity

$E1 = \frac{\Delta NH_4^+}{NH_{4,in}^+}$

$E2 = \frac{\Delta TN}{TN_{in}}$

⟶ Absolute microbial activity



Mutlu et al., 2012. WWC Proceedings

Results
Steady state calibration

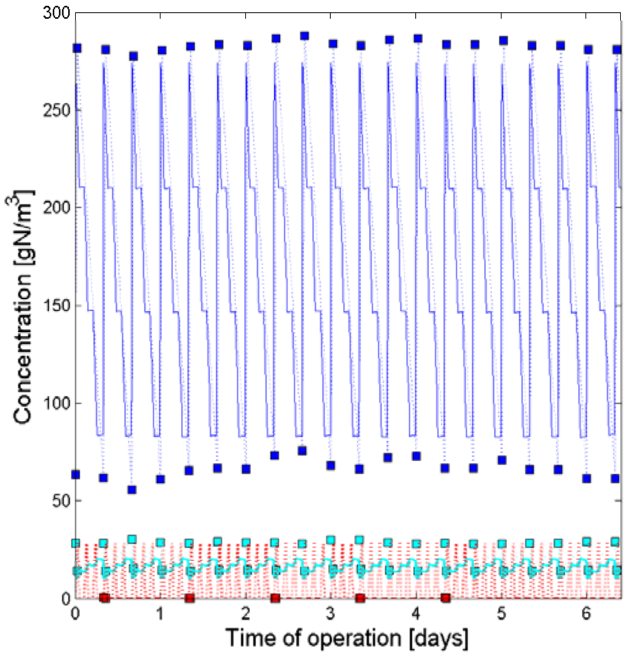
- Step 3:

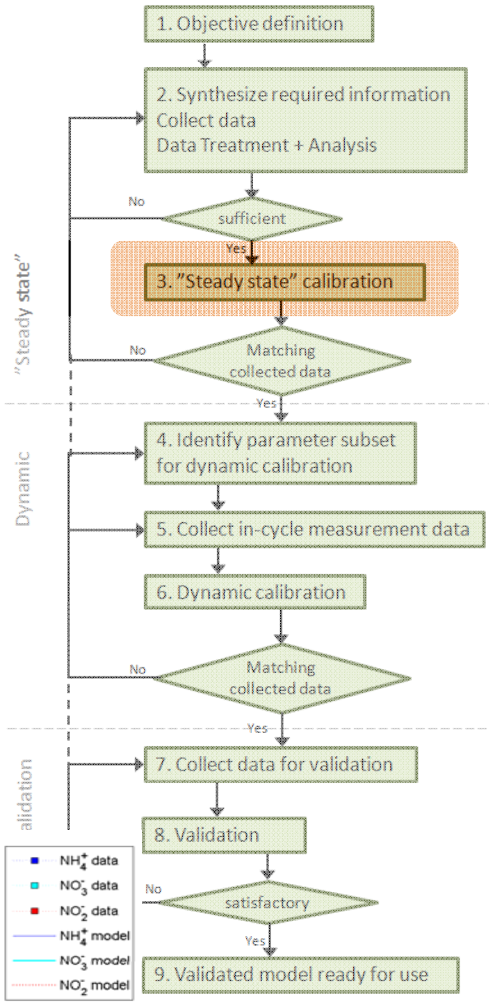
Since oxygen k_La could not be experimentally estimated, this was calibrated based on the five evaluation criteria:

	k_La d^{-1}	R1 $\Delta NO_2^-/\Delta NH_4^+$	R2 $\Delta NH_4^+/\Delta TN$	R3 $\Delta NO_3^-/\Delta TN$	NH_4^+ removal %	TN removal %
Simulation	524.4	0.000	1.052	0.049	79.25	74.32
Experimental	-	0.001	1.072	0.071	80.80	71.52

Experimental values were obtained as an average of one week of ”steady state” operation.

Model was initialized by simulating continuous operation for 1000 days, which was then followed by 10 days of SBR operation of which the results from the last cycle were used for the steady state model evaluation.





1. Objective definition

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Collect data
Data Treatment + Analysis

sufficient

3. ”Steady state” calibration

Matching collected data

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5. Collect in-cycle measurement data

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satisfactory

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Results
Dynamic calibration

- Step 4: Parameter subset identification

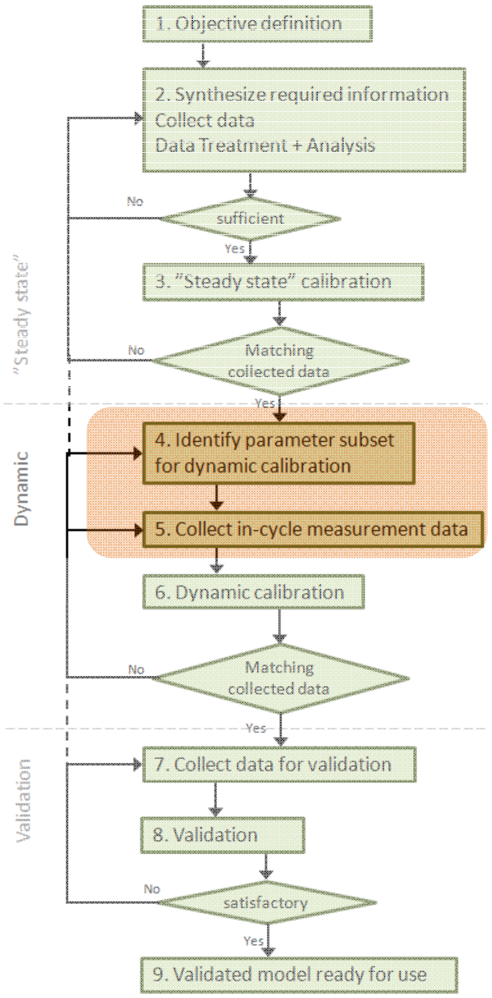
Based on global sensitivity analysis:

	$\mu_{max,AOB}$ d^{-1}	$K_{O2,AOB}$ $gCOD/m^3$	b_{AOB} d^{-1}	$\mu_{max,AnAOB}$ d^{-1}	$K_{O2,AnAOB}$ $gCOD/m^3$	Y_{AnAOB} $gCOD/gN$
Default value	2.050	0.300	0.130	0.073	0.010	0.160
Lower bound	1.538	0.150	0.098	0.055	0.005	0.152
Upper bound	2.563	0.450	0.163	0.091	0.015	0.168

- Step 5: In-cycle data collection

Samples from bulk liquid were manually collected every 15 min. and analyzed for soluble N species.

Analysis results from three cycles were used for calibration.



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Matching collected data

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"Steady state"

Dynamic

Validation

Vangsgaard et al., 2012. Bioresource Technol.

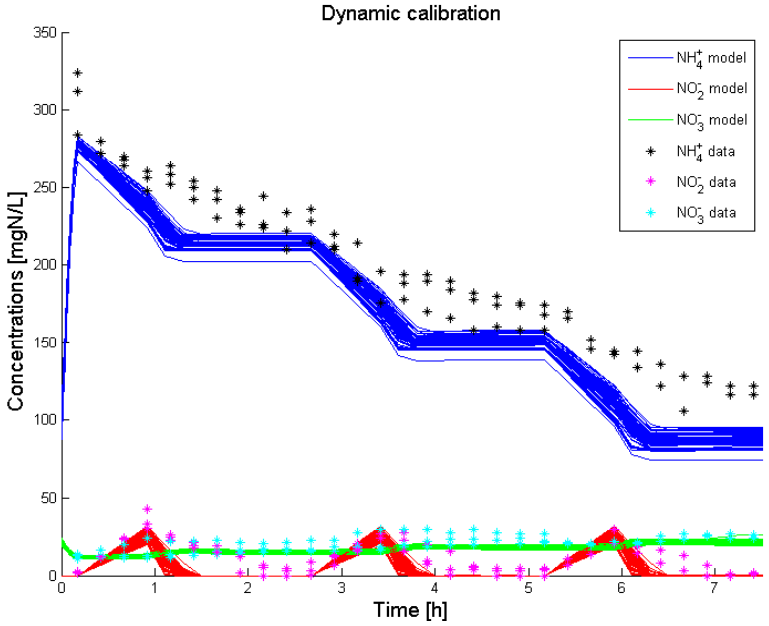
Results
Dynamic calibration

- Step 6: Calibration

Based on pragmatic Monte Carlo method, which was evaluated by WSSE:

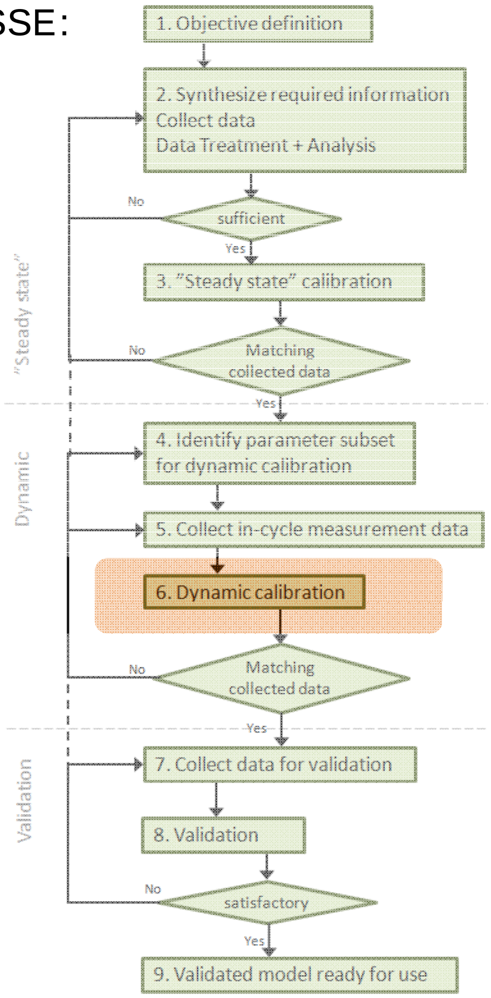
$$\mathrm{WSSE} = \sum_{k=1}^{m}\sum_{i=1}^{n}\left(\frac{y_{\mathrm{meas},k}(t) - y_{\mathrm{model},k}(t,\theta)}{\sigma_k}\right)^2$$

	$\mu_{\mathrm{max,AOB}}$ d^{-1}	$K_{\mathrm{O2,AOB}}$ $\mathrm{gCOD/m^3}$	b_{AOB} d^{-1}	$\mu_{\mathrm{max,AnAOB}}$ d^{-1}	$K_{\mathrm{O2,AnAOB}}$ $\mathrm{gCOD/m^3}$	Y_{AnAOB} gCOD/gN
Default value	2.050	0.300	0.130	0.073	0.010	0.160
Lower bound	1.538	0.150	0.098	0.055	0.005	0.152
Upper bound	2.563	0.450	0.163	0.091	0.015	0.168
Calibrated value	2.450	0.165	0.136	0.068	0.011	0.166



However, all MC sims have an offset compared to the collected data

→ Iteration of step 4-6, in accordance with the methodology



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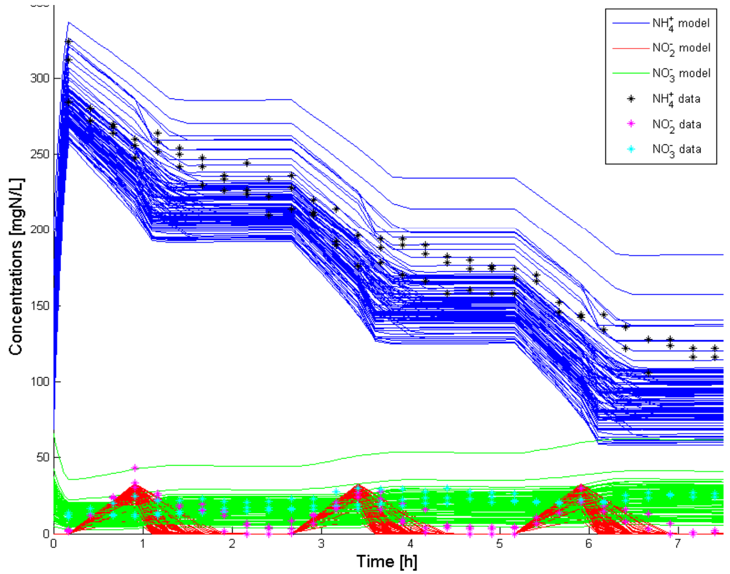
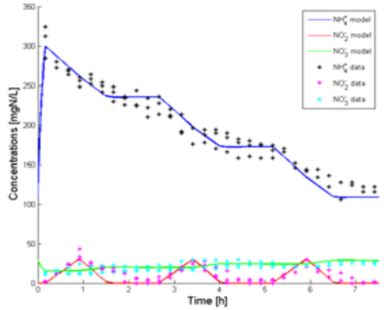
Results
Dynamic calibration

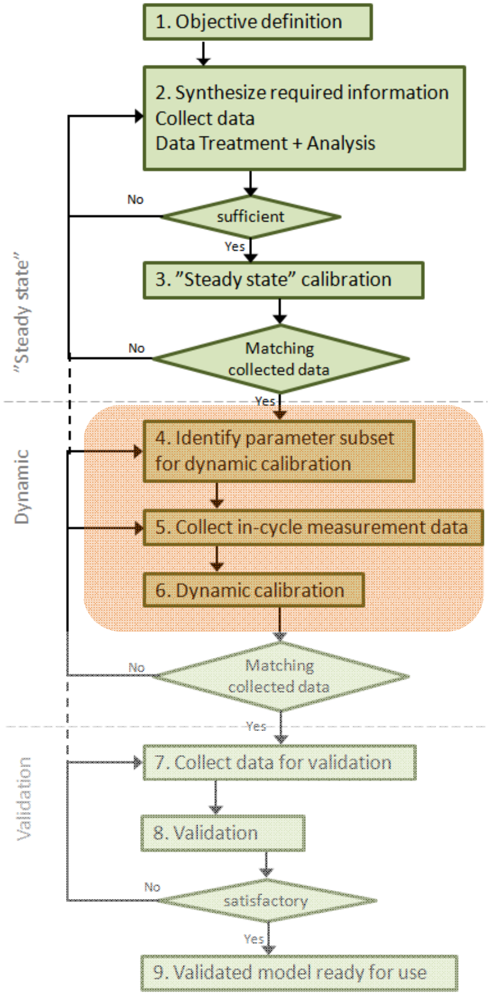
- Step 4-6 - iterated: Parameter subset and sampling space were expanded

	Unit	Default value	Lower bound	Upper bound	Calibrated value
$\mu_{max,AOB}$	d^{-1}	2.050	1.025	3.075	2.064
$K_{O2,AOB}$	$gCOD/m^3$	0.300	0.150	0.450	0.332
b_{AOB}	d^{-1}	0.130	0.065	0.195	0.150
$\mu_{max,NOB}$	d^{-1}	1.454	0.727	2.181	0.974
$K_{O2,NOB}$	$gCOD/m^3$	1.100	0.550	1.650	0.752
b_{NOB}	d^{-1}	0.061	0.030	0.091	0.069
$\mu_{max,AnAOB}$	d^{-1}	0.073	0.037	0.110	0.088
$K_{O2,AnAOB}$	$gCOD/m^3$	0.010	0.005	0.015	0.013
$K_{HNO2,AnAOB}$	gN/m^3	2.81e-6	1.41e-6	4.22e-6	2.92e-6
Y_{AOB}	gCOD/gN	0.210	0.105	0.315	0.292
Y_{AnAOB}	gCOD/gN	0.160	0.080	0.240	0.124
D_{NO2}	m^2/d	2.60e-4	1.30e-4	3.90e-4	1.70e-4
L_B	m	1.76e-5	8.80e-6	2.64e-5	2.26e-5



Among the new MC sims, the subset sample giving the smallest error fitted much better to the data than the previous.





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Matching collected data
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Validation

Results
Validation

- Step 7: Data collection for validation

Samples were collected during one cycle under slightly different conditions compared to the calibration cycles. The solids concentration was 4.4 g VSS/L and average granule size was 35 µm.

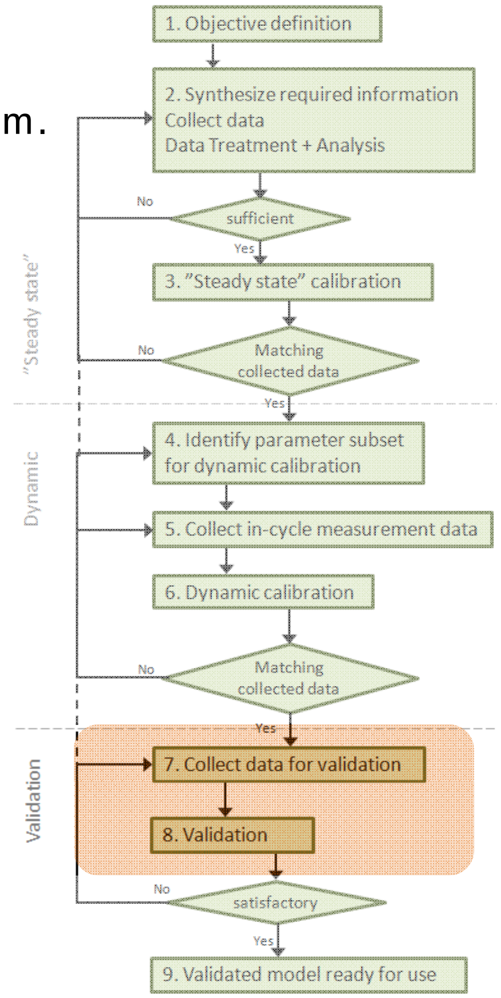
- Step 8: Validation

The validation was evaluated by the Janus coefficient:

$$J^2 = \frac{\frac{1}{n_{val}} \sum_{i=1}^{n_{val}} \left(y_{meas,i} - y_{model}\left(t_i, \theta\right) \right)^2}{\frac{1}{n_{cal}} \sum_{i=1}^{n_{cal}} \left(y_{meas,i} - y_{model}\left(t_i, \theta\right) \right)^2}$$

	MAE		RMSE		Janus coefficient
Model output	**Calibration**	**Validation**	**Calibration**	**Validation**	
NH_4^+	0.030	0.053	0.039	0.057	1.478
NO_2^-	0.265	0.116	0.366	0.173	0.473
NO_3^-	0.131	0.080	0.171	0.093	0.544

J is relatively close to 1 for all model outputs, which implies a good model fit.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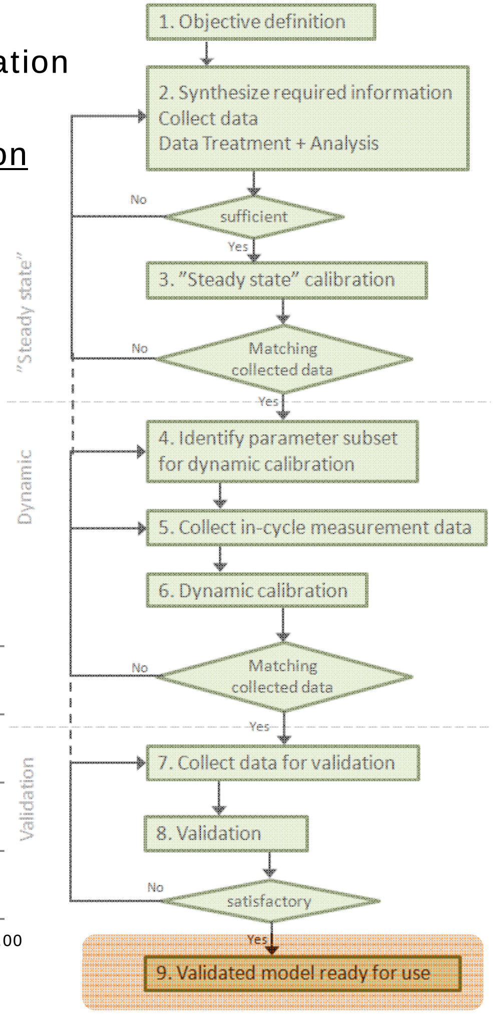
Perspectives

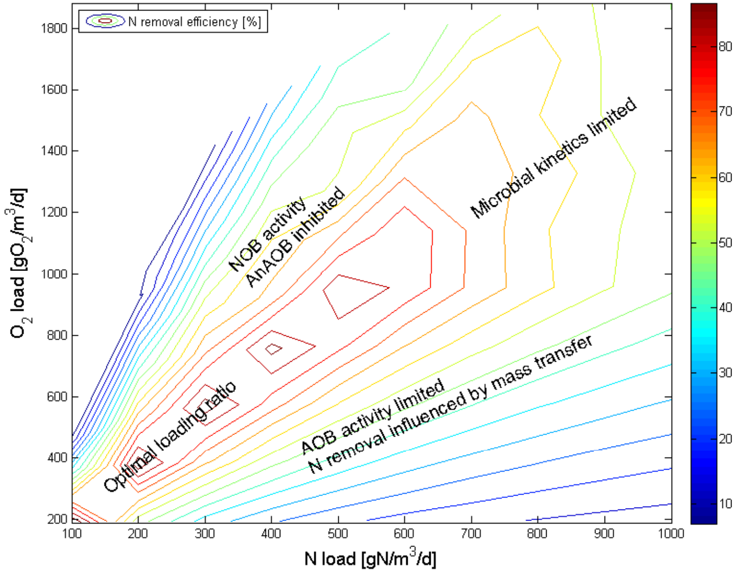
- The validated model will be used for two purposes:

1) design of future lab-scale experiments in the form of perturbations in the operation

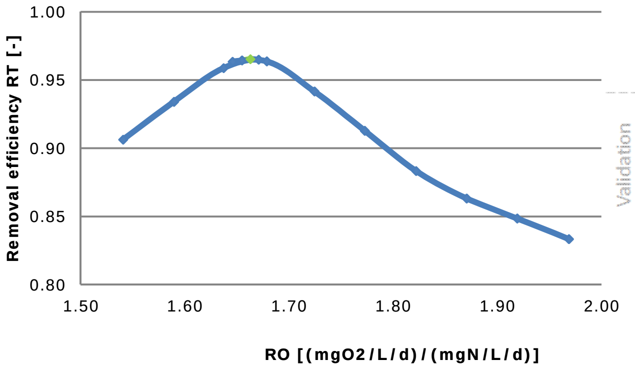
2) for predicting the process performance, which is important in future optimization and process control applications and in up-scaling of the system



Process optimization (based on results from Vangsgaard et al., 2012)



Analysis on calibrated model



Vangsgaard et al., 2012. Bioresource Technol.

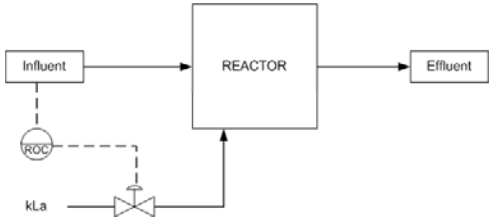
Perspectives

2) for predicting the process performance, which is important in future optimization and process control applications and in up-scaling of the system

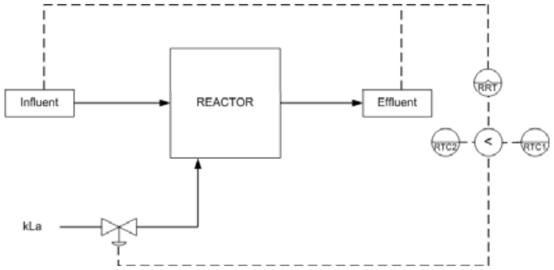
Control implementation:

Three different control strategies have been developed and analyzed on the calibrated model.

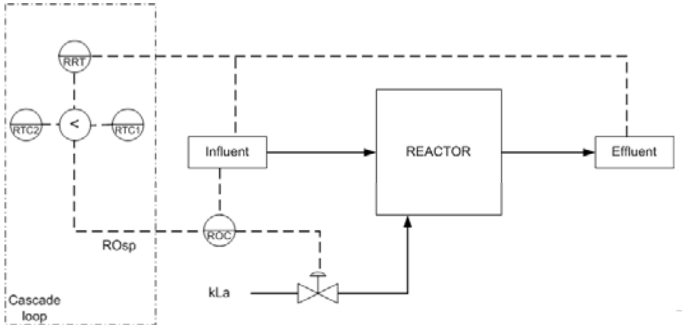
1. Feedforward based on oxygen/nitrogen loading ratio (Vangsgaard et al., 2012)



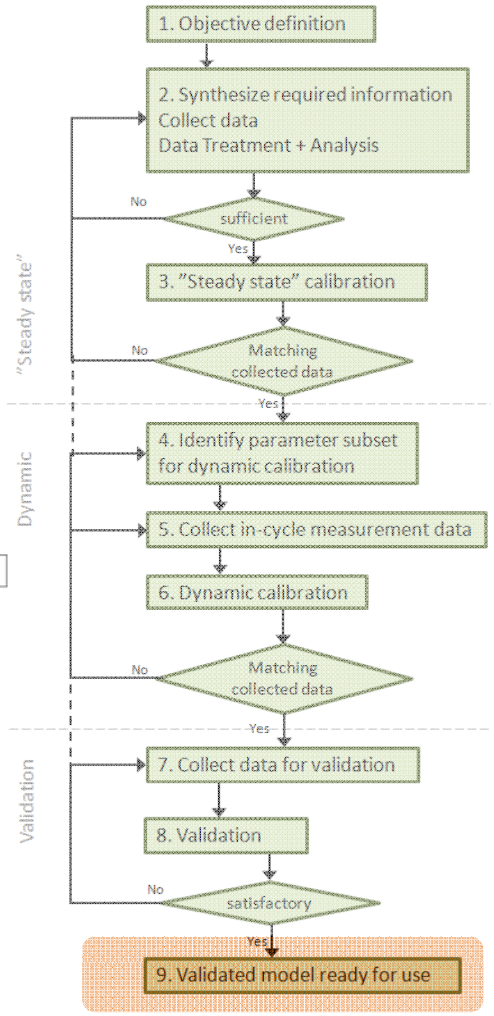
2. Feedforward + feedback based on stoichiometric rules (Mutlu et al., 2012):



3. Cascade control as a combination of 1. and 2.



As future extension of the current work, the developed control strategy will be experimentally tested in the lab-scale reactors.



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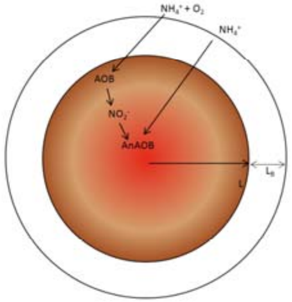
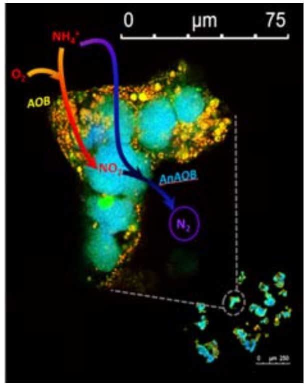
Vangsgaard et al., 2012. Bioresource Technol. *Mutlu et al., 2012. WWC Proceedings*

Conclusions / wrap-up

- The model was successfully calibrated and validated by following a developed methodology:
  - First, k_La was calibrated to long term ”steady state” data by using novel evaluation criteria of **stoichiometric ratios** indicating the relative activity of the microbial groups.
  - Second, a subset of parameters were calibrated through dynamic calibration to in-cycle data.
  - An iteration of the second step was performed before a satisfactory result was obtained.
- A fast and efficient novel **initialization process** was developed
  - Simulating 1000 days of continuous operation before SBR operation.
- The model is now being used for optimization and control structure analyses.





Thanks for your attention!

Acknowledgements to:

All the supervisors and the Danish Agency for Science, Technology and Innovation through the Research Centre for Design of Microbial Communities in Membrane Bioreactors (09-067230) for funding of the project

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