UNIVERSITEIT GENT

BIOMATH
Department of Applied Mathematics,
Biometrics and Process Control

Modelling, control and optimization of autotrophic nitrogen removal

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Outline

- Introduction
- Lab scale SHARON reactor
- Modelling autotrophic nitrogen removal
- Control of the SHARON process
- Conclusions and perspectives

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Introduction

- BIOMATH mission statement:

> *"The development and application of <u>mathematical methods</u> for the analysis, understanding and optimization of <u>bioprocess</u>-related systems"*

Introduction

- BIOMATH project workpackages in IcoN:
  - Integrated and validated mathematical model for autotrophic nitrogen removal process in general and Anammox in particular
  - Control strategy development for optimal "exploitation" of Anammox

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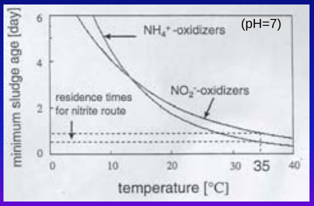
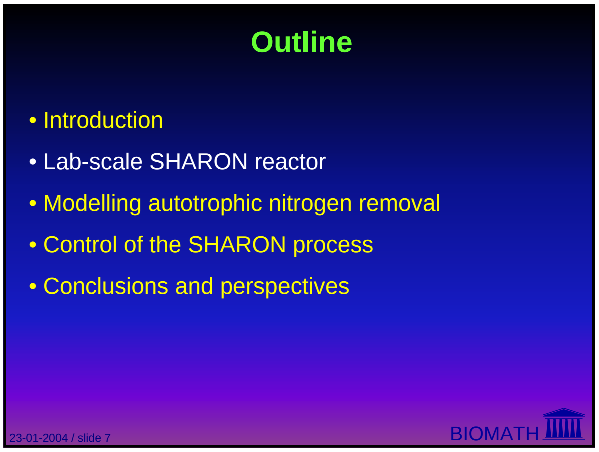
Introduction

- Get an Anammox suited effluent (50/50 NH_4^+/NO_2^-): try to outcompete the nitrite oxidisers
  - High temperature (30-35°C) in <u>chemostat</u> : SHARON



=> Nitrite oxidizers are washed out for suitable dilution rate



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- Lab-scale SHARON reactor
- Modelling autotrophic nitrogen removal
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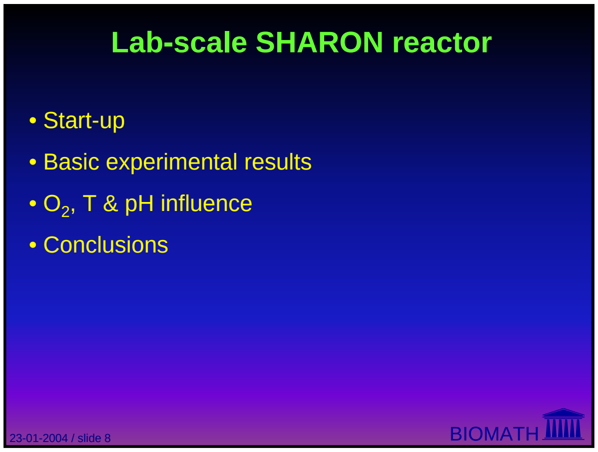
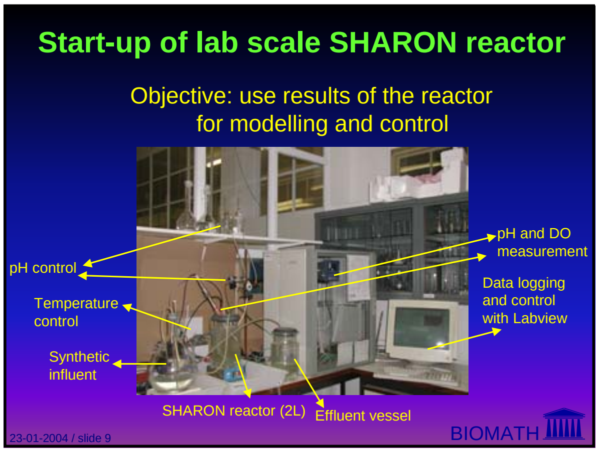
- Conclusions and perspectives



Lab-scale SHARON reactor

- Start-up
- Basic experimental results
- O_2, T & pH influence
- Conclusions



Start-up of lab scale SHARON reactor

Objective: use results of the reactor
for modelling and control

pH control

Temperature control

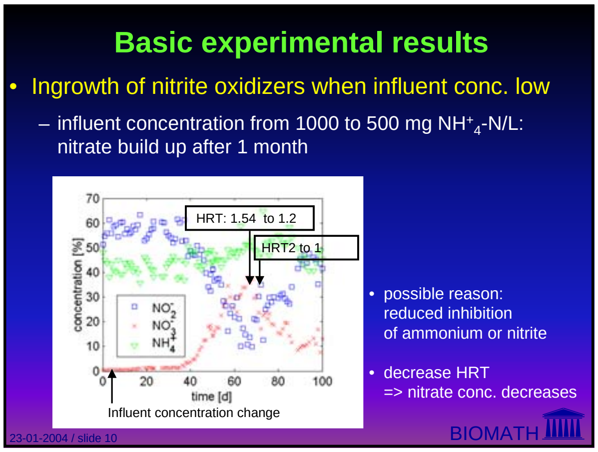
Synthetic influent

pH and DO measurement

Data logging and control with Labview

SHARON reactor (2L)

Effluent vessel



Basic experimental results

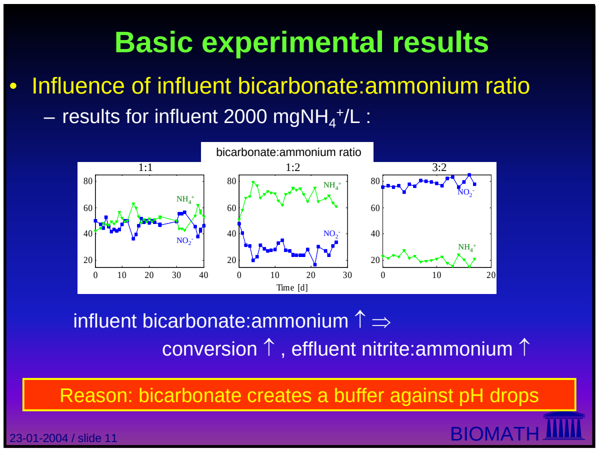
- Ingrowth of nitrite oxidizers when influent conc. low
  - influent concentration from 1000 to 500 mg $NH^+{}_4$-N/L: nitrate build up after 1 month

HRT: 1.54 to 1.2

HRT2 to 1

Influent concentration change

- possible reason: reduced inhibition of ammonium or nitrite
- decrease HRT => nitrate conc. decreases



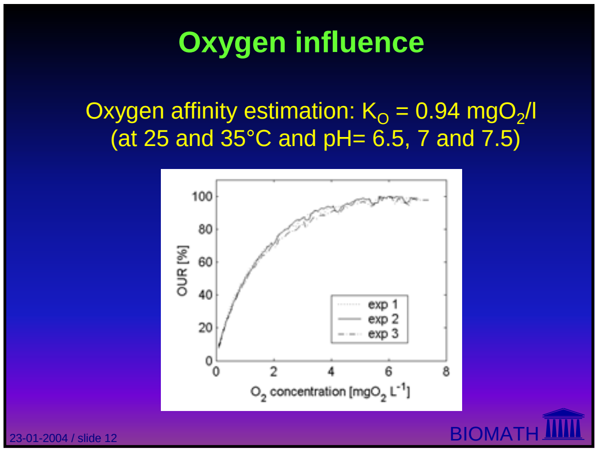
Basic experimental results

- Influence of influent bicarbonate:ammonium ratio
  - results for influent 2000 $mgNH_4^+/L$:

bicarbonate:ammonium ratio

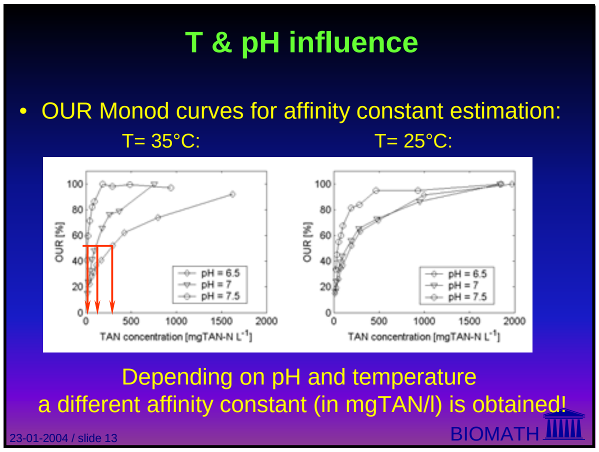
influent bicarbonate:ammonium ↑ ⇒
conversion ↑ , effluent nitrite:ammonium ↑

Reason: bicarbonate creates a buffer against pH drops



Oxygen influence

Oxygen affinity estimation: $K_O = 0.94\ mgO_2/l$
(at 25 and 35°C and pH= 6.5, 7 and 7.5)

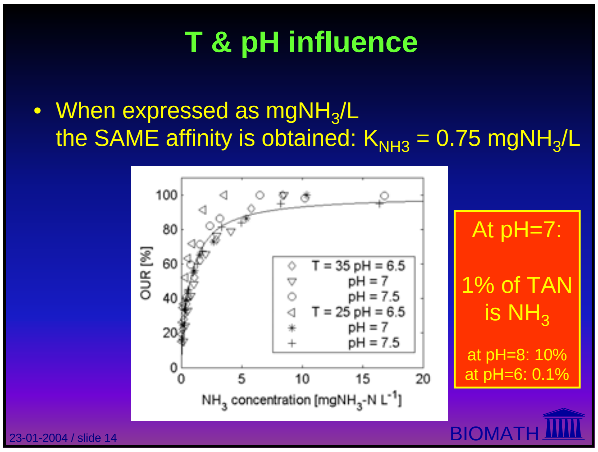


T & pH influence

- OUR Monod curves for affinity constant estimation:

T= 35°C: T= 25°C:

Depending on pH and temperature
a different affinity constant (in mgTAN/l) is obtained!



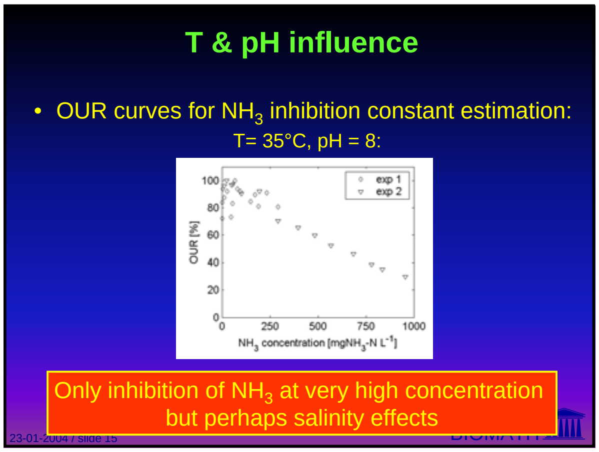
T & pH influence

- When expressed as mgNH$_3$/L
the SAME affinity is obtained: K_{NH3} = 0.75 mgNH$_3$/L

At pH=7:

1% of TAN is NH$_3$

at pH=8: 10%
at pH=6: 0.1%

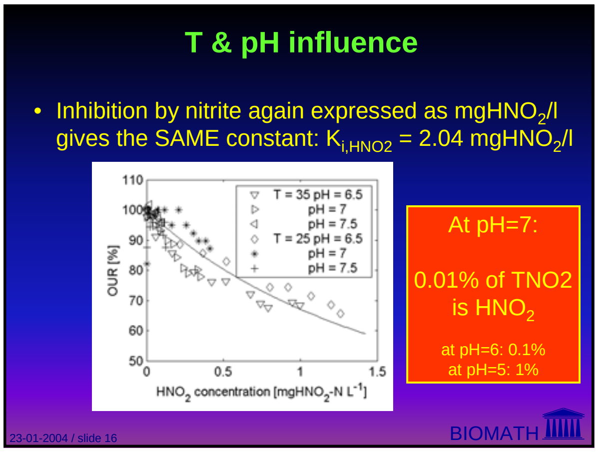


T & pH influence

- OUR curves for NH$_3$ inhibition constant estimation:

T= 35°C, pH = 8:

Only inhibition of NH$_3$ at very high concentration
but perhaps salinity effects



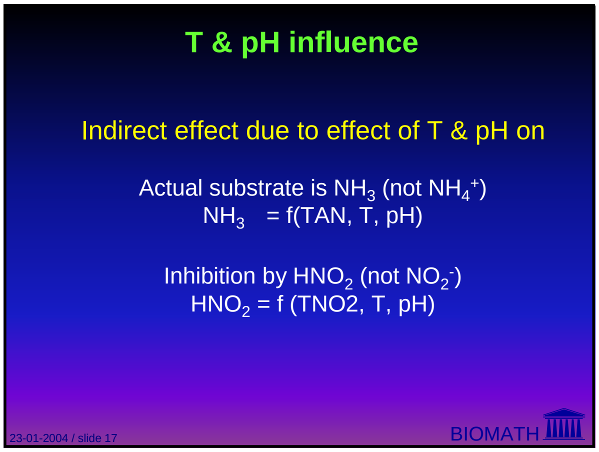
T & pH influence

- Inhibition by nitrite again expressed as mgHNO$_2$/l
gives the SAME constant: $K_{i,HNO2}$ = 2.04 mgHNO$_2$/l

At pH=7:

0.01% of TNO2 is HNO$_2$

at pH=6: 0.1%
at pH=5: 1%

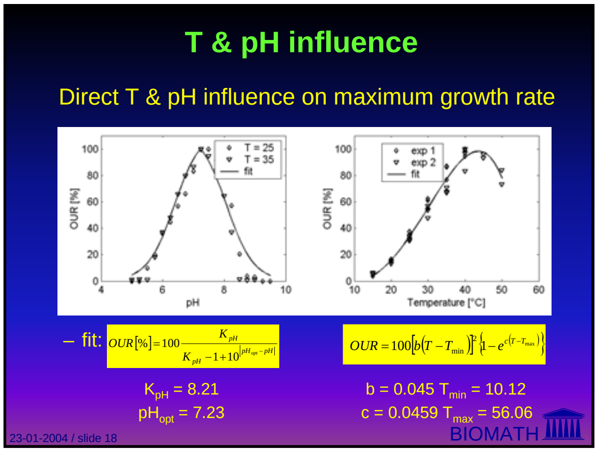


T & pH influence

Indirect effect due to effect of T & pH on

Actual substrate is NH$_3$ (not NH$_4^+$)
NH$_3$ = f(TAN, T, pH)

Inhibition by HNO$_2$ (not NO$_2^-$)
HNO$_2$ = f (TNO2, T, pH)



T & pH influence

Direct T & pH influence on maximum growth rate

– fit: $OUR[\%] = 100 \dfrac{K_{pH}}{K_{pH} - 1 + 10^{|pH_{opt} - pH|}}$ $OUR = 100\left[b\left(T - T_{\min}\right)\right]^2 \left\{1 - e^{c\left(T - T_{\max}\right)}\right\}$

K_{pH} = 8.21
pH_{opt} = 7.23

b = 0.045 T_{min} = 10.12
c = 0.0459 T_{max} = 56.06

Conclusion lab-scale SHARON reactor

- Nitrite:ammonium ratio produced by SHARON
  is influenced by
  - influent bicarbonate:ammonium ratio
  - influent ammonium load
- NH_3 and HNO_2 are the actual substrates/inhibitors
- T & pH have a large influence
  on the SHARON nitritation process

⇒ in practice, it will be necessary to monitor / control the SHARON reactor to <u>always</u> obtain the desired nitrite:ammonium ratio for Anammox

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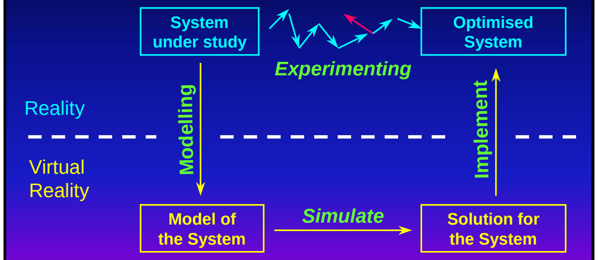
Modelling autotrophic N-removal

- Why modelling?
- Modelling the SHARON process
- Modelling the Anammox process

Why modelling?

<u>Solving Problems for complex systems</u>



System under study

Optimised System

Experimenting

Reality

Modelling

Implement

Virtual Reality

Model of the System

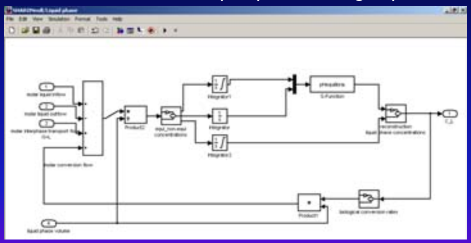
Simulate

Solution for the System

Modelling the SHARON process

Process model in Matlab-Simulink includes:

Mass balances for liquid phase and gas phase



- biological conversion only in liquid phase
- interphase transport of O_2, CO_2 and N_2

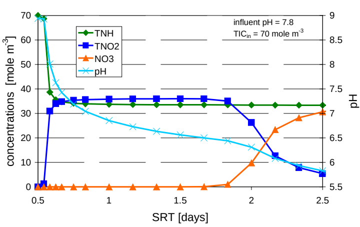
Modelling the SHARON process

Process model in Matlab-Simulink includes:

- Inhibition effects
  - inhibition of ammonia oxidizers by HNO_2
  - inhibition of nitrite oxidizers by NH_3 and HNO_2
- pH effects during nitrification of high loaded N-streams
  - different equilibrium forms are considered (e.g. NH_3 - NH_4^+)
  - every time step pH is calculated (Newton-Raphson algorithm)
- pH dependency of the biomass growth rate
  - explicitly by pH dependency of max. specific growth rate
  - implicitly through concentrations of NH_3 and HNO_2 = f(pH, T)
- no grazing of protozoa
- no decay

Modelling the SHARON process

Influence of SRT (=HRT)



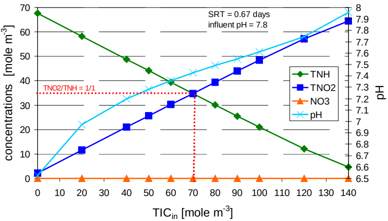
TAN $_{in}$ = 70 mole m^{-3}
TIC$_{in}$ = 70 mole m^{-3}

pH$_{in}$ =7.8

0.65<SRT<1.6 for stable partial nitrification
i.e. influent flow variations hardly effect TNO2/TAN ratio

Modelling the SHARON process

Influence of influent bicarbonate concentration



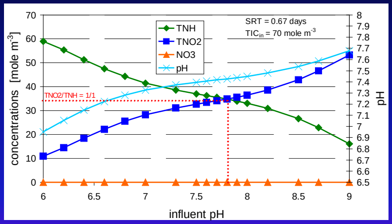
TNH $_{in}$ = 70 mole m^{-3}
TIC$_{in}$ = 0-140 mole m^{-3}

pH$_{in}$ =7.8
SRT=0.67 d

TIC$_{in}$ ↑ ⇒ HCO$_3^-$$_{in}$ ↑
⇒ more protons can be neutralized ⇒ TNO2/TNH ↑

Modelling the SHARON process

Influence of influent pH

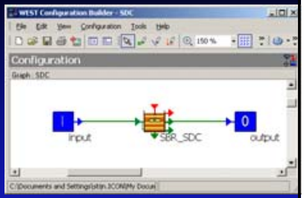


TNH $_{in}$ = 70 mole m^{-3}
TIC$_{in}$ = 70 mole m^{-3}

pH$_{in}$ = 7 - 8.5
SRT= 0.67d

Influent pH ↑ ⇒ HCO$_3^-$$_{in}$/TIC$_{in}$ ↑
⇒ more protons can be neutralized ⇒ TNO2/TNH ↑

Modelling the Anammox process



USC

SBR
system

BIOMATH

WEST
model

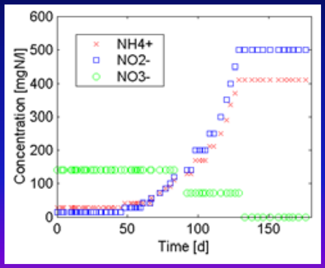
Modelling the Anammox process

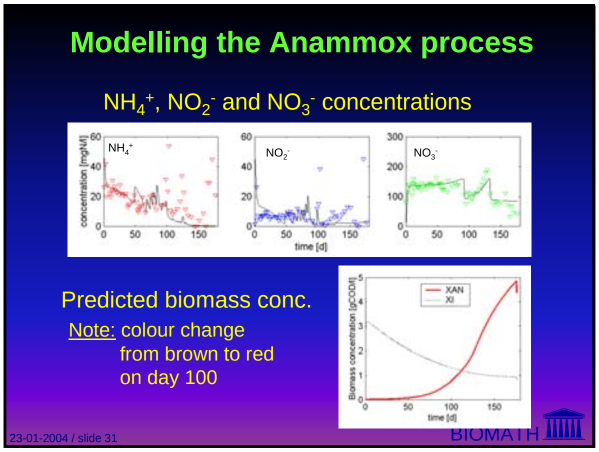
- Inoculated with sludge
  from 3 municipal WWTP in A Coruña (Spain)
- T = 35°C
- pH = 7.8 - 8
- Different phases in the Sequencing Batch Reactor:

Phase	Duration [h]	Flow rate [ml/h]
Fill	5.5	72.8
Reaction	0	0
Settle	0.33	0
Draw	0.17	2400
Idle	0	0

Modelling the Anammox process

Fed with synthetic wastewater (NH$_4^+$, NO$_2^-$, NO$_3^-$):





Modelling the Anammox process

NH_4^+, NO_2^- and NO_3^- concentrations

Predicted biomass conc.

Note: colour change from brown to red on day 100

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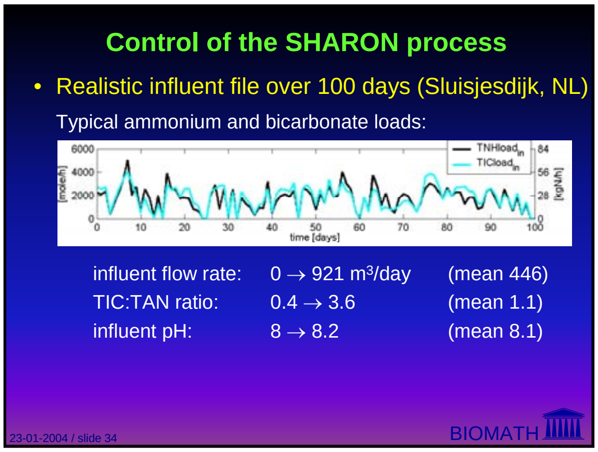
Control of the SHARON process

- Objective: Make sure Anammox works optimally
  i.e. provide it with the optimal NH_4:NO_2 ratio
- Too high => NH_4 is not removed (too little NO_2)
  => discharge of nitrogen
- Too low => NO_2 is not removed (too little NH_4)
  => discharge of nitrogen
  => Anammox inhibition (> 20 mg NO_2-N/L)
  => even slower removal
  => accumulation of NO_2
  => complete inhibition

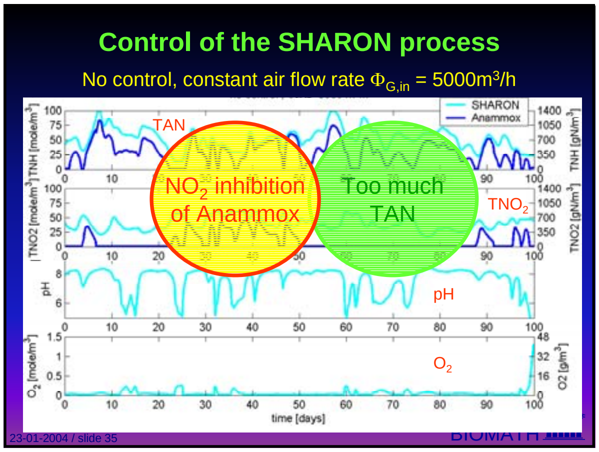


Control of the SHARON process

- Realistic influent file over 100 days (Sluisjesdijk, NL)

Typical ammonium and bicarbonate loads:

influent flow rate:	0 → 921 m^3/day	(mean 446)
TIC:TAN ratio:	0.4 → 3.6	(mean 1.1)
influent pH:	8 → 8.2	(mean 8.1)



Control of the SHARON process

No control, constant air flow rate $\Phi_{G,in}$ = 5000m^3/h

NO_2 inhibition of Anammox

Too much TAN

Control of the SHARON process

- No control, constant air flow rate $\Phi_{G,in}$ = 5000m^3/h

- Low air flow rate => low O_2 => limit NO_2 production
  => avoid nitrite inhibition in Anammox reactor

- During periods with low influent ammonium loads (e.g. day 25)
  => oxygen supply is no longer limiting
  => too much nitrite is produced and
  => Anammox reaction is strongly inhibited

⇒ highly recommended to strictly control NO_2:NH_4 ratio produced by the SHARON reactor to avoid inhibitory nitrite concentrations

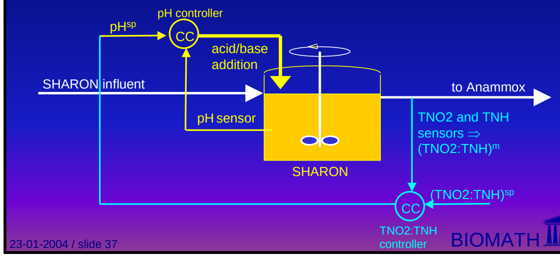
Control of the SHARON process

- Cascade pH control

NO_2:NH_4 ratio produced in SHARON is measured and compared to desired NO_2:NH_4 ratio

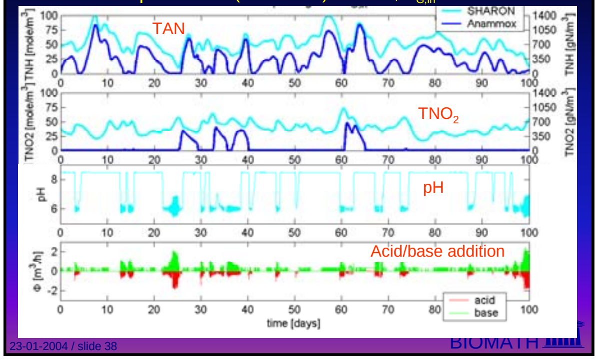
⇒ change in pH required (desired value: $6 < pH^{sp} < 8.5$)

⇒ pH controlled to pH^{sp} by pH controller through acid/base addition


pH controller
pH^{sp}
CC
acid/base addition
SHARON influent
pH sensor
SHARON
to Anammox
TNO2 and TNH sensors ⇒ $(TNO2:TNH)^m$
$(TNO2:TNH)^{sp}$
CC
TNO2:TNH controller

Control of the SHARON process

- Cascade pH control $(TNO2:TNH)^{sp} = 1.2:1$, $\Phi_{G,in} = 5000 m^3/h$



Control of the SHARON process

- Cascade pH control $(TNO2:TNH)^{sp} = 1.2:1$, $\Phi_{G,in} = 5000 m^3/h$

- Better effluent quality than scenario without control but with same constant air flow rate

- However: adding large amounts of acid/base

- Too expensive solution
- Only feasible when permit depends on it !

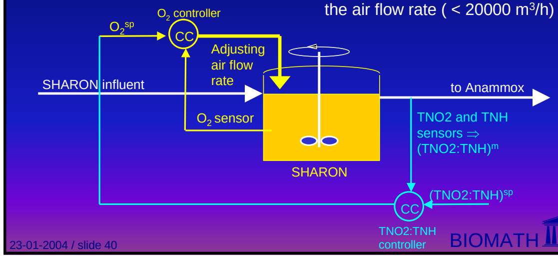
Control of the SHARON process

- Cascade O_2 control

NO_2:NH_4 ratio produced in SHARON process is measured and compared to desired NO_2:NH_4 ratio

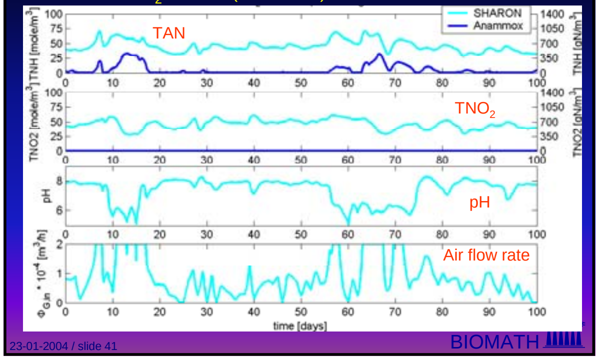
⇒ change in O_2 required (desired value: $0 < O_2^{sp} < 8$ g/m³)

⇒ O_2 controlled to value O_2^{sp} by O_2 controller through adjusting the air flow rate (< 20000 m³/h)


O_2 controller
O_2^{sp}
CC
Adjusting air flow rate
SHARON influent
O_2 sensor
SHARON
to Anammox
TNO2 and TNH sensors ⇒ $(TNO2:TNH)^m$
$(TNO2:TNH)^{sp}$
CC
TNO2:TNH controller

Control of the SHARON process

- Cascade O_2 control $(TNO2:TNH)^{sp} = 1.2:1$



Control of the SHARON process

- Cascade O_2 control $(TNO2:TNH)^{sp} = 1.2:1$

- NO_2:NH_4 ratio produced in SHARON reactor
  remains quite constant
  EVEN IF individual NO_2 and NH_4 concentrations still vary

⇒ Anammox reactor performs very well:
  nitrite concentration stays very low
  NO nitrite inhibition occurs

Control of the SHARON process

- Performance evaluation through operating cost index (OCI)
  includes most important operating cost factors [€/year]

$$OCI = \gamma_1 \cdot EQ + \gamma_2 \cdot AE + \alpha_{acid} \cdot \Phi_{acid} + \alpha_{base} \cdot \Phi_{base}$$

Cost factor (€/year)	economic weight	value	unit
Effluent fines (kg PU/d)	γ_1	50	€/EQ/year
Aeration energy (kWh/d)	γ_2	25	€/AE/year
Acid addition (96% H_2SO_4)	α_{acid}	62.3	€/m^3
Base addition (50% NaOH)	α_{base}	93.4	€/m^3

Control of the SHARON process

- Performance evaluation through operating cost index (OCI)

cost factor (€/year)	no control $\Phi_{G,in} = 5000\ m^3/h.$	cascade pH control	cascade O_2 control
effluent fines	207000	179000	30160
aeration costs	25520	25530	65090
chemical addition	0	117100	0
OCI [€/year]	232480	321600	95250
savings [€/year]	0	-89120	137200

- cascade pH control is not worth implementing
- cascade O2 control warrants investment costs for
  - ammonium and nitrite sensors and
  - equipment for adjusting air flow rate

Control of the SHARON process

- Conclusions
  - Control of NO_2:NH_4 ratio is crucial to avoid Anammox nitrite toxicity and increase overall conversion efficiency
  - Control of NO_2:NH_4 via pH control via acid/base addition only slightly improves SHARON-Anammox performance but is not economically feasible
  - Control of NO_2:NH_4 via O_2 control through air flow rate adjustment provides excellent overall performance and good return on investment
  - Results are sensitive to nitrite inhibition coefficient $K_{i,HNO2}$

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Conclusions

- Successful start-up/operation of the SHARON reactor
  - NH_3 is actual substrate and HNO_2 is actual inhibitor
  - Influent TIC:TAN, SRT, Temperature, oxygen & pH effects
- Validated integrated model of autotrophic N-removal
  - SHARON model in Matlab-Simulink (O_2, T & pH)
  - Anammox model in WEST (Matlab-Simulink ongoing)
- Control of the SHARON reactor is necessary
  - to avoid nitrite inhibition of Anammox and
  - to improve overall conversion efficiency
- Cascade O_2 control provides excellent conversion efficiency and good return on investment

Perspectives

- Scenario-analysis with an Anammox biofilm model
- Further validation of the SHARON Matlab model
  - Steady state sensitivity analysis for model parameters
  - Validation with lab-scale / full-scale SHARON data
- Evaluation of control strategies
  on the integrated SHARON-Anammox process
  - in one simulation environment (Matlab-Simulink)
  - in lab Sharon/Anammox system at BIOMATH
  - in Sluisjesdijk ?
- Further testing of the nitrate biosensor