21 SEPTEMBER 2021

10:00 AM CEST

IWA Specialist Group on Modelling and Integrated Assessment Webinar Series

Advancements on N2O Modelling in Water Resource Recovery Facilities

Speakers

Ulf Jeppsson
Lund University

Liu Ye
University of Queensland

Mathieu Sperandio
INSA Toulouse

Eveline Volcke
Ghent University

Saba Daneshgar
Ghent University

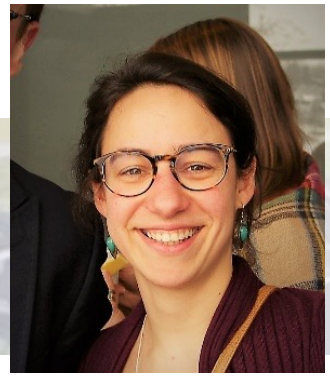
The webinar is going to be recorded and shared on the MIA SG Youtube channel afterward.

MIA Welcome Note

IWA Modelling and Integrated Assessment Specialist Group

Dr. Ulf Jeppsson (Chair of MIA SG)

Dr. Elena Torfs (Vice-chair of MIA SG)



Lund University

Ghent University

inspiring change

MODELLING AND INTEGRATED ASSESSMENT SPECIALIST GROUP (MIA SG)

"This group targets people from research, consulting companies, institutions and operators to think along ***the use of models and computing tools to support the understanding, management and optimization of water systems****."*

PRIORITIES

- Interact with other IWA SGs and other professional organizations
- Organize specialized conferences, sessions and workshops
- Engage and activate YWPs in the domain.

CURRENTLY 1900 MEMBERS

How to find us

Website: http://iwa-mia.org/

https://iwa-connect.org

MIA SG: ACTIVITIES

Task Groups (TGs)

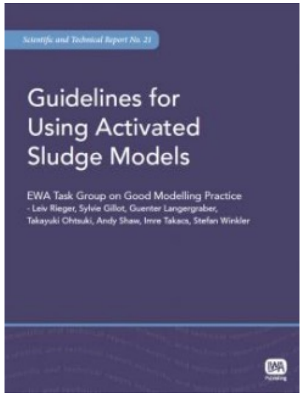
- Benchmarking of Control Strategies for WWTPs (BSM) AND Good Modelling Practice (GMP) (Finished)
- Design and Operations Uncertainty (DOUT)
- Generalised Physicochemical Modelling (PCM)
- Use of Modelling for Minimizing GHG Emissions from Wastewater Systems (GHG)
- Membrane Bioreactor Modelling and Control (MBR)
- Good Modelling Practice in Water Resource Recovery Systems (New)

Working Groups (WGs)

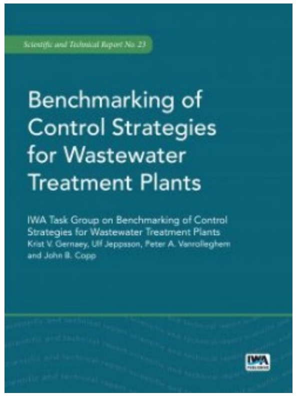
- Integrated Urban Water Systems (IUWS)
- Computational Fluid Dynamics (CFD)
- Good Modelling Practice (GMP)

Conferences / Events

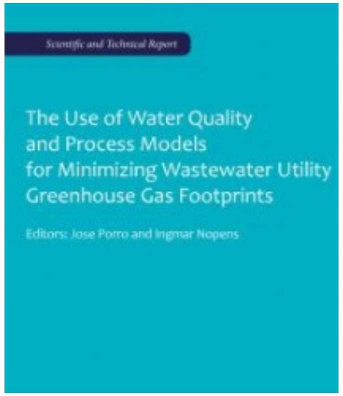
- WRRmod
- Watermatex



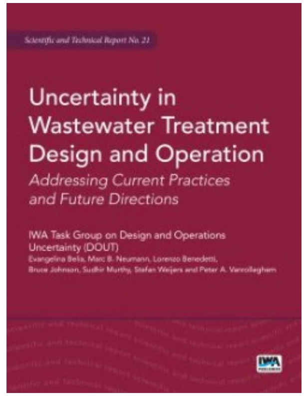
STR
(Sept. 2012)



STR
(Sept. 2014)



STR
(2021)



STR
(2021)

MIA SG: UPCOMING CONFERENCES

8th Water Resource Recovery Modelling seminar (WRRmod2023)

- Location: Stellenbosch, South Africa, January 2023
- Chair: Dr. David Ikumi (Univ. Cape Town)

11th Symposium on Modelling and Integrated Assessment (Watermatex2023)

- Location: Québec City, Canada, summer 2023
- Chair/vice-chair: Prof. Peter Vanrolleghem (Univ. Laval)/Dr. Elena Torfs (Univ. Ghent)

FIND MIA SG ON SOCIAL MEDIA

Follow the Modelling and Integrated Assessment Specialist Group on:

- IWA Connect https://iwa-connect.org/group/modelling-and-integrated-assessment-mia/timeline
- https://www.linkedin.com/company/iwa-mia-specialist-group-on-modelling-and-integrated-assessment
- https://twitter.com/iwa_mia_sg
- **MIA SG open web site** http://iwa-mia.org

to get informed about our latest events, publications and news!

INTRODUCTION TO THE N_2O WEBINAR

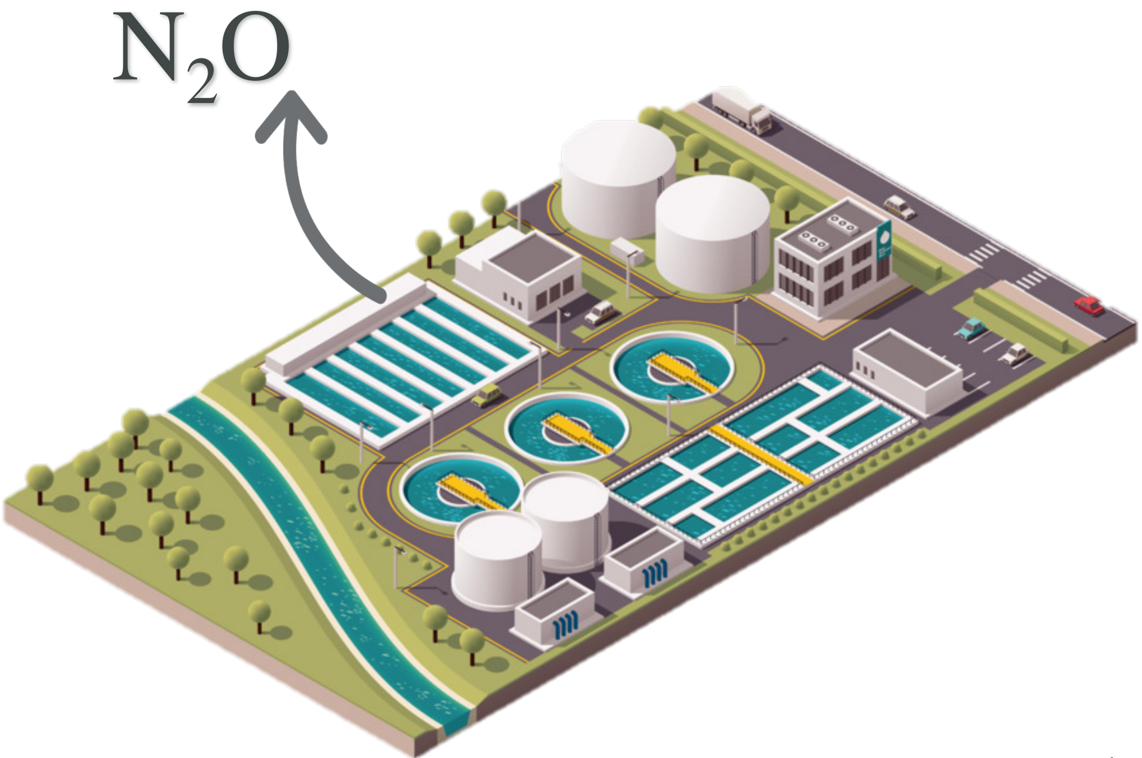
Advancements on N2O Modelling in Water Resource Recovery Facilities

A/Prof Liu Ye (The Univ. of Queensland, Australia)

l.ye@uq.edu.au

IWA GHG TASK GROUP AND N_2O EMISSION

Nitrous Oxide **N_2O**	✓ Impact >**260 times** as strong as CO_2 ✓ Generation during nitrogen conversion



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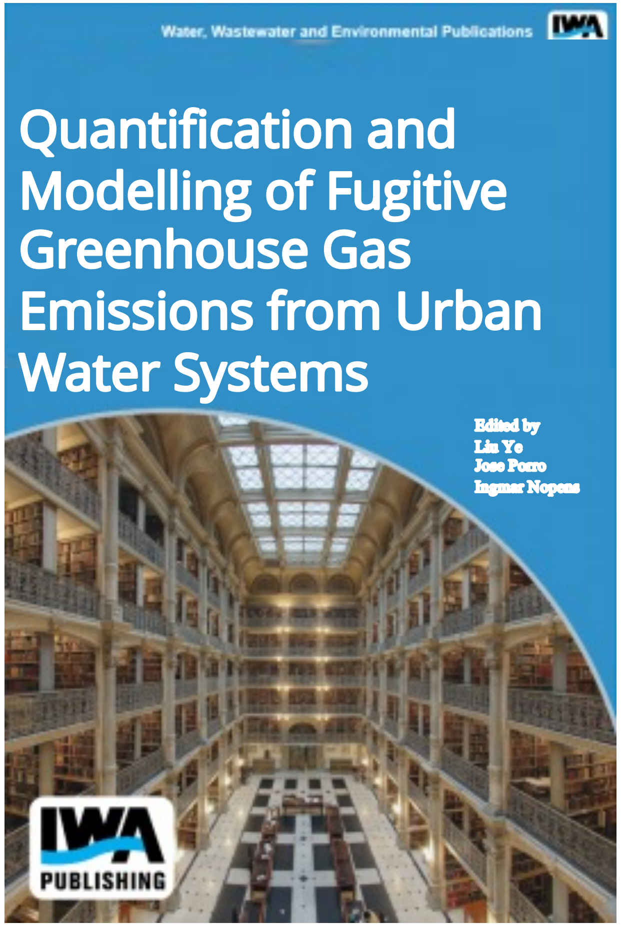

Publication Date:15/11/2021

https://www.iwapublishing.com/books/9781789060454/quantification-and-modelling-fugitive-greenhouse-gas-emissions-urban-water

AGENDA AND HOUSEKEEPING

Speaker 1
Mathieu Sperandio (INSA Toulouse, France)

Speaker 2
Eveline Volcke (Ghent University, Belgium)

Speaker 3
Saba Daneshgar (Ghent University, Belgium)

Q&A Session: *Liu Ye (moderator)*

- This session is being recorded;
- Microphones and cameras have been disabled due to the large number of attendees;
- The normal chat function is disabled;
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History and state of the art of N_2O modelling

Prof. Mathieu Sperandio

DETERMINISTIC N_2O MODELLING
A DECADE HISTORY

- N_2O models related to denitrification
  - **ASMN:** Hiatt and Grady 2008
  - **Other concepts:** Pan et al., 2013 ; Domingo-Félez and Smets 2020

  - **Multistep denitrification (N_2O, NO)**
  - **Electron carriers, other concepts**

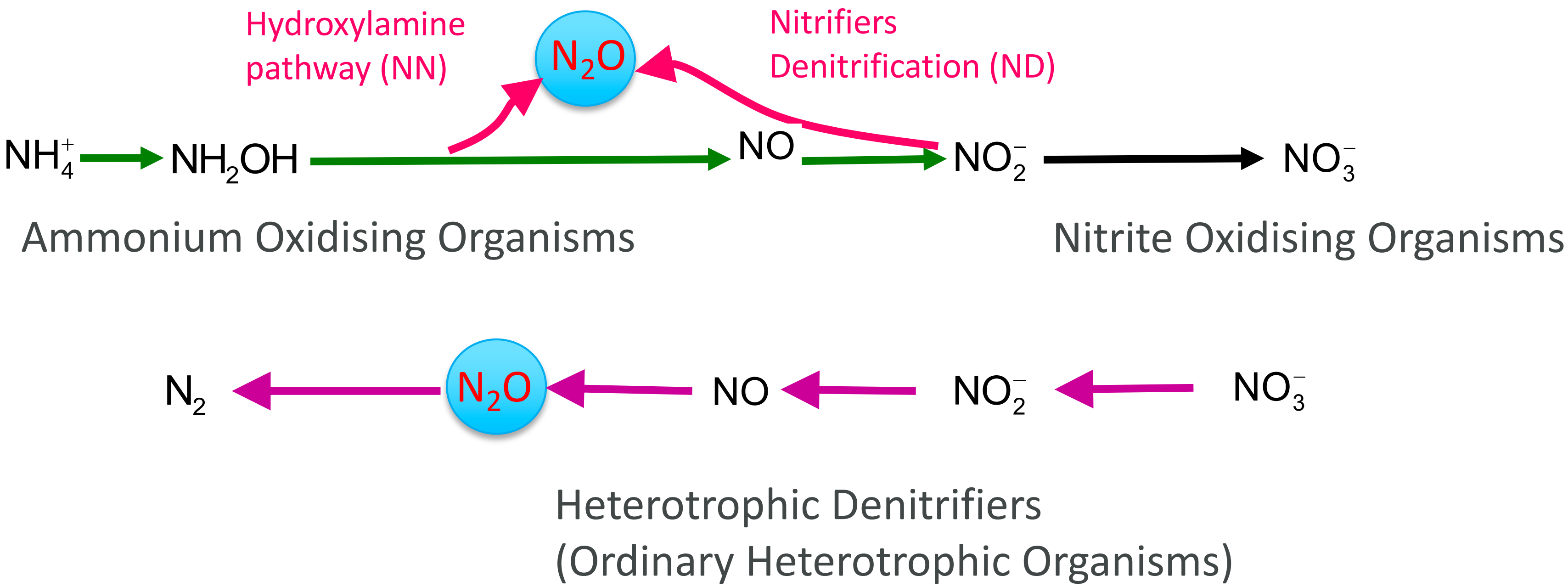
- N_2O models related to nitrification
  - **Single pathway (Nitrifier denitrification – ND):** Ni *et al.*, 2011; Mampaey *et al.*, 2013; Pocquet *et al.*, 2013; Guo and Vanrolleghem, 2014
  - **Single pathway (Hydroxylamine pathway – NN):** Law *et al.*, 2012; Ni *et al.*, 2013
  - **Comparison**: Sperandio *et al.*, 2016
  - **Multiple pathways :** Ni *et al.*, 2014; Peng *et al.*, 2015; Pocquet *et al.*, 2016; Domingo-Félez and Smets, 2016

  - **New intermediates in nitrification (NH_2OH, NO, N_2O)**
  - **Combination with ASM**
  - **Difficulty to represent various situations with single pathway**
  - **Coupling red.ox. pathways**
  - **Electron or energy carriers, other concepts**

- N_2O models related to chemical pathways
  - Harper *et al.*, 2015 ; Su *et al.*, 2019

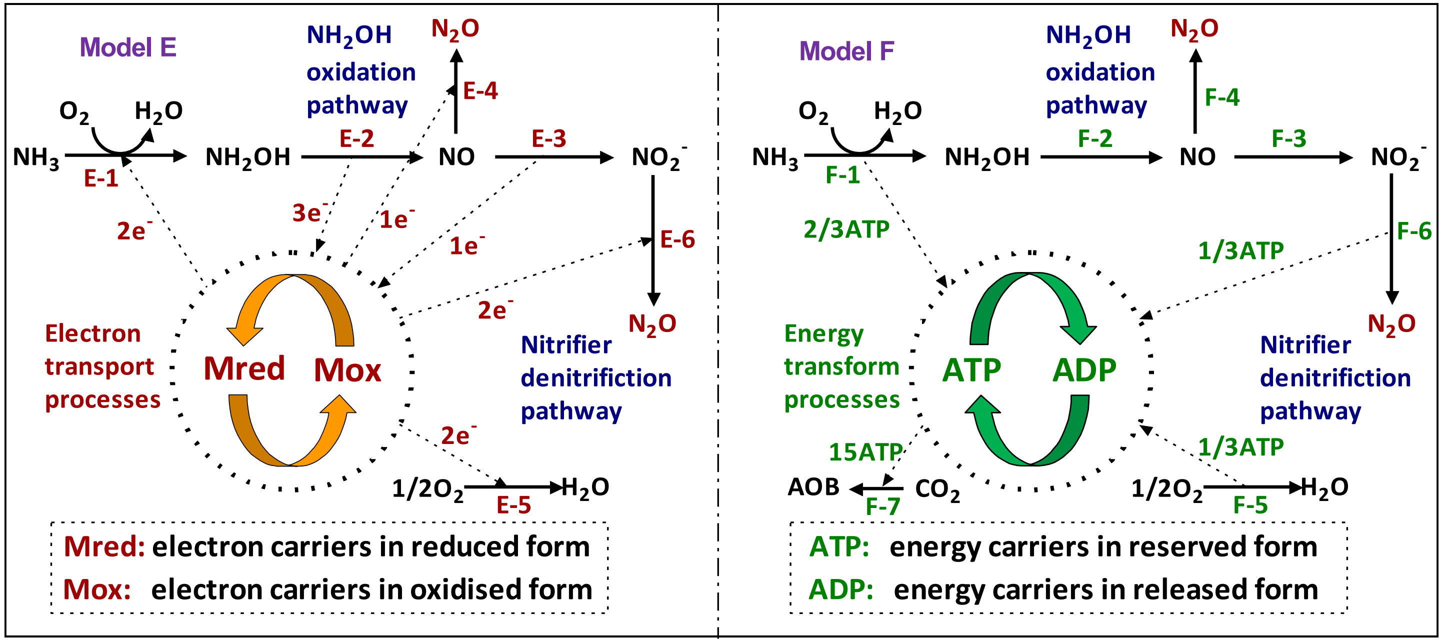
  - **less important than biological**

BIOLOGICAL PATHWAYS



THE ELECTRON PUZZLE AND RED-OX. CONCEPTS (NITRIFICATION)

- Examples: 2-pathway AOB models based on electron carriers or ATP/ADP exchanges

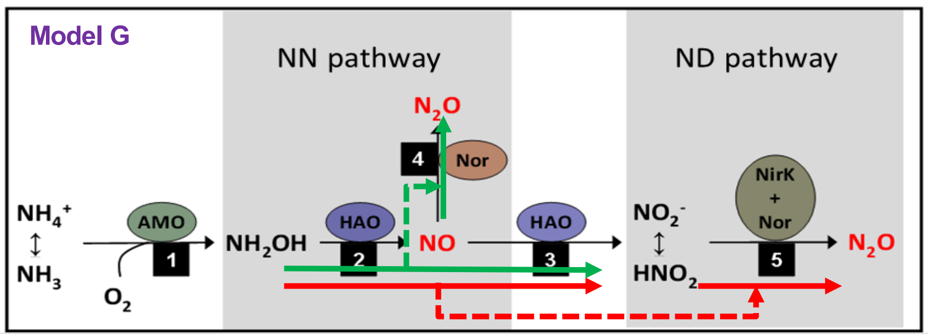


Model E **Ni et al., 2014**	**Using S_{NH4} and S_{NO2};** **With electron carriers.**	**Three-step NH_4^+ oxidation;** **One-step NO_2^- reduction;** **Without cell growth.**	**Applying electron competition concept;** **Without oxygen inhibition;** **Without anoxic reduction factor.**
Model F **Peng et al., 2015**	Mostly same as Model E; With S_{CO2}; With energy carriers.	Mostly same as Model E; With energy carriers involved; With cell growth considered.	Mostly same as Model E; With energy carriers involved; With effect of inorganic carbon considered.

COUPLING REDUCTION AND OXIDATION (NITRIFICATION)

- Similarly to ASM concepts, oxidation and reduction can be pooled in single kinetic rates
- Hydroxylamine is the electron donor

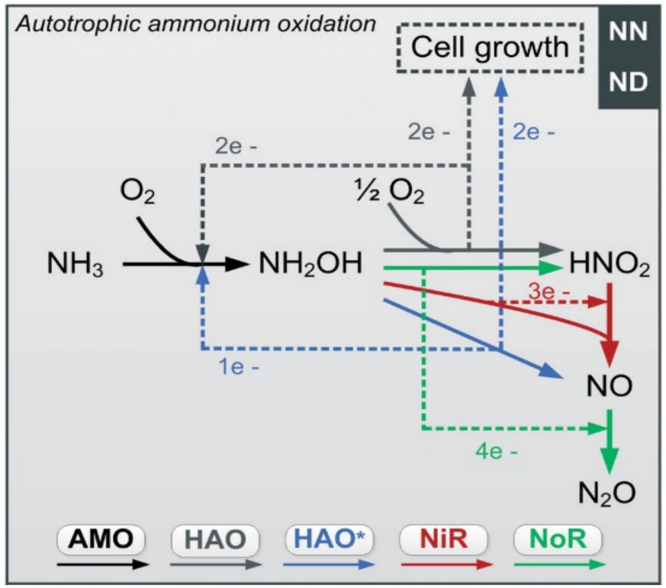
2-pathway model (Pocquet et al., 2016)



Stoichiometry of the 2 pathway model (Gujer matrix).

Process	S_{NH}	S_{NH2OH}	S_{NO}	$S_{NO_2^-}$	S_{N2O}	S_{O2}	X_{AOB}
	Model Components – 2-P model						
1	-1	1				$-8/7$	
2	$-i_{N,BM}$	$-1/Y_{AOB}$	$1/Y_{AOB}$			$-\left({}^{12}/_{7} - Y_{AOB}\right)/Y_{AOB}$	1
3			-1	1		$-4/7$	
NN 4		-1	-4	1	4		
ND 5		-1		-1	2		

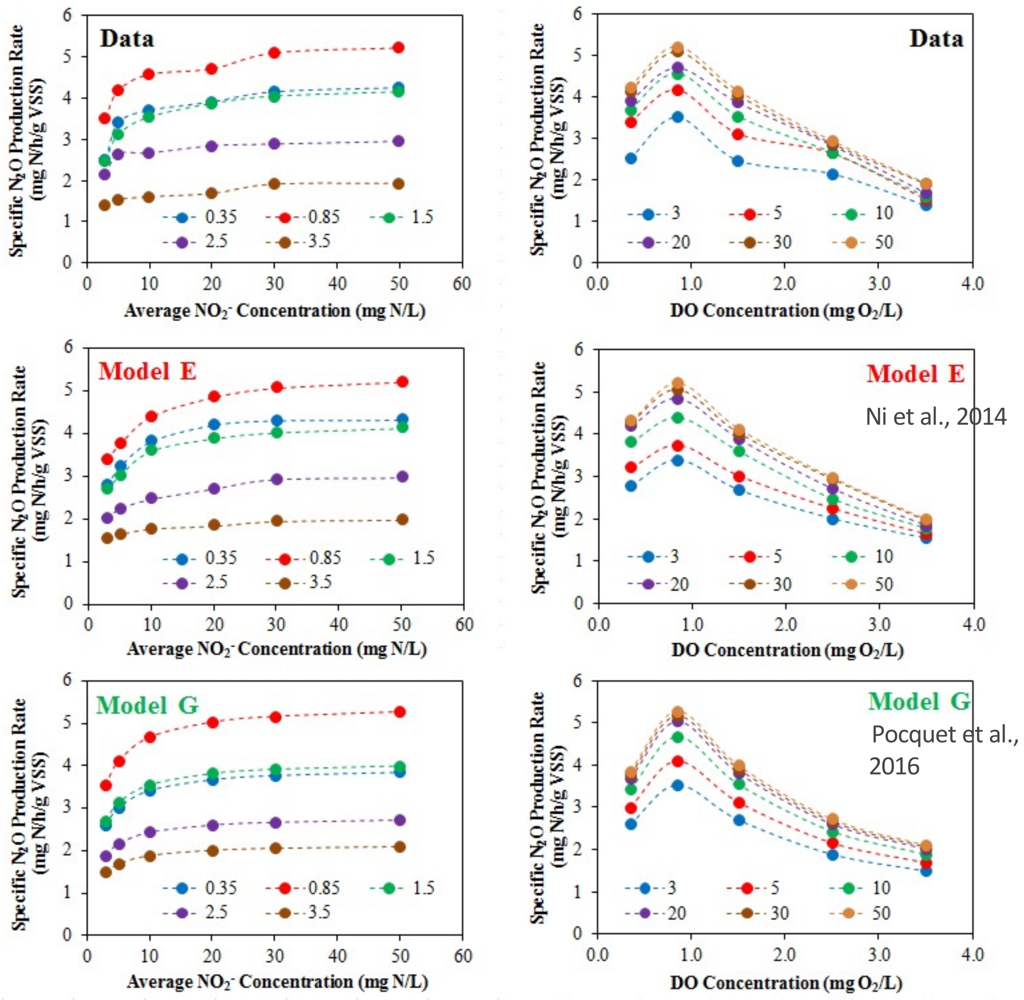
2-Pathway model
Domingo-Félez and Smets, 2016



PREDICTION OF COMBINED EFFECT OF DISSOLVED OXYGEN AND NITRITE (NITRIFICATION)

Effect of NO_2 for different DO

Effect of DO for different NO_2

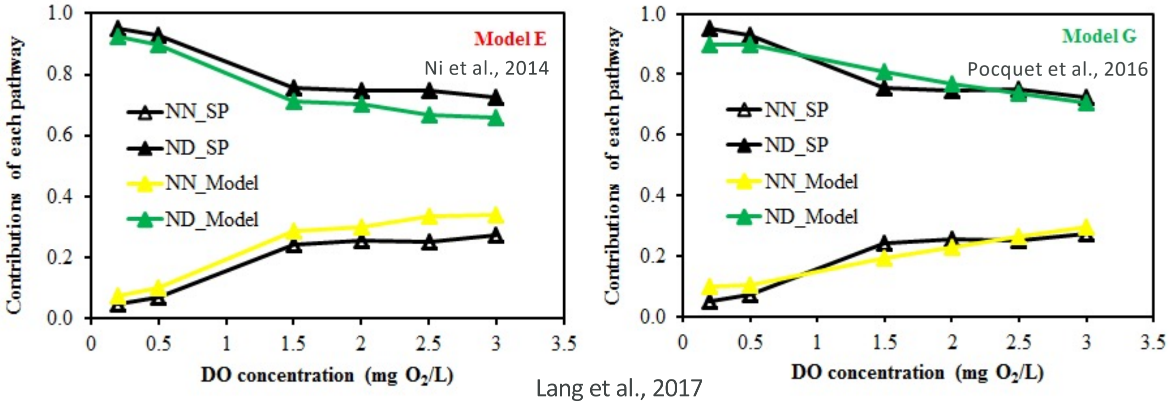


Lang et al., 2017

- Importance of combined effect of DO and Nitrite
- Inhibition terms and kinetic competition
- Electron carriers model (E) and coupled redox model (G) can give similar prediction
- The relative effect of pH can be included by NO_2^- / HNO_2 dissociation

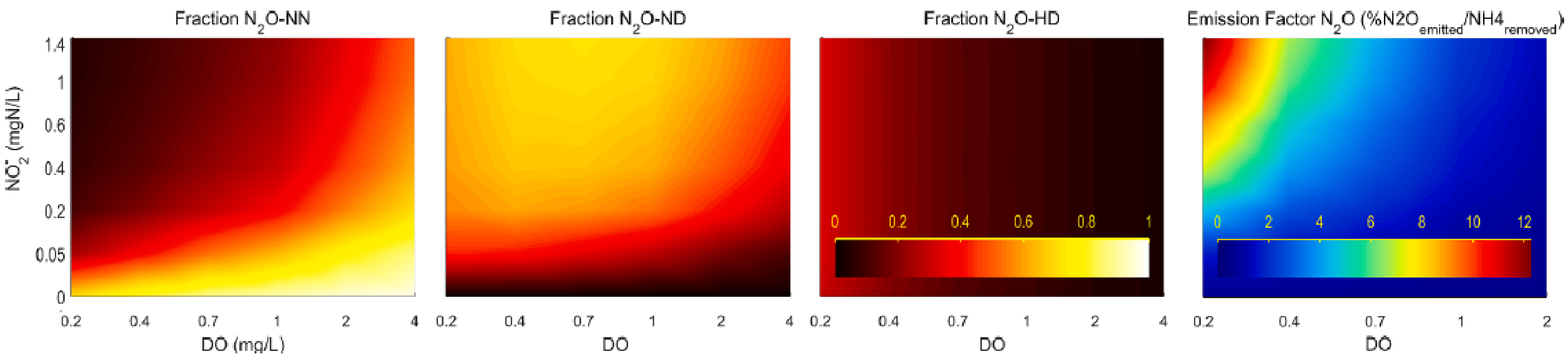
PREDICTION OF PATHWAYS CONTRIBUTION (NITRIFICATION)

Effect of DO on respective contribution of NN and ND



- Pathways measured by isotopomers signature preference (SP)
- Multiple pathways models can predict their contributions
- DO ↑ : less ND and more NN
- NO_2 ↑ : less NN and more ND

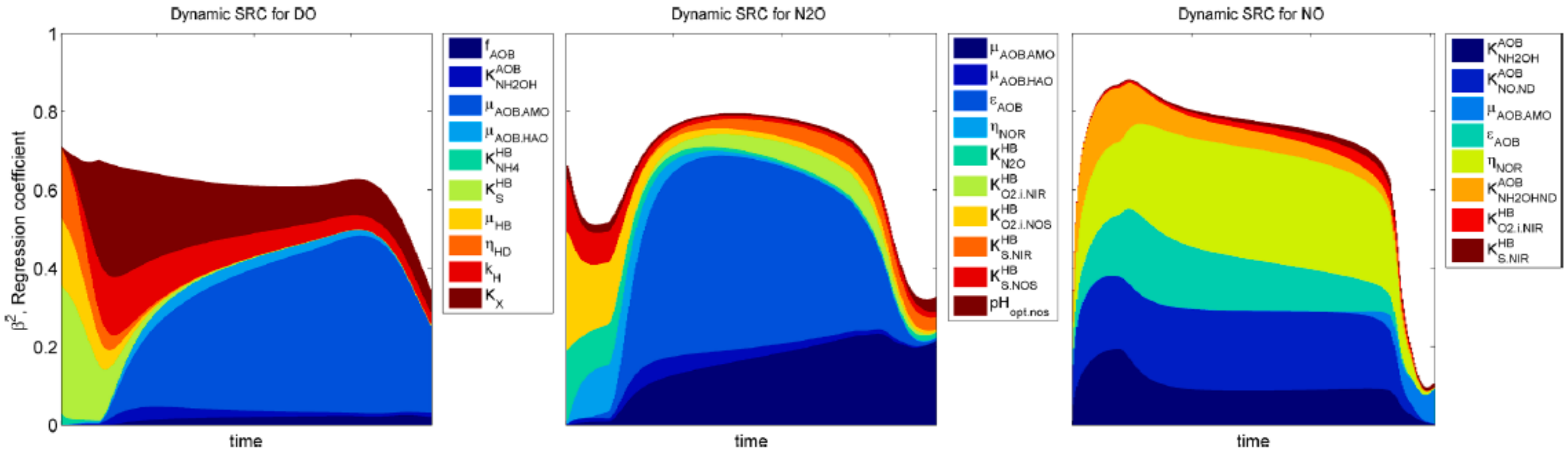
Good for understanding microbial pathways regulation !



Domingo-Felez and Smets, 2020

CALIBRATION CHALLENGES

- Increasing number of intermediates and parameters makes calibration more complex
- Multiple step vs. One step calibration (Fiat et al., 2021; Wan et al., submitted)
- Importance of measuring more intermediates like NO (Pocquet et al., 2016)
- Importance of dynamic sensitivity analysis and uncertainty analysis (Domingo-Félez and Smets, 2020)



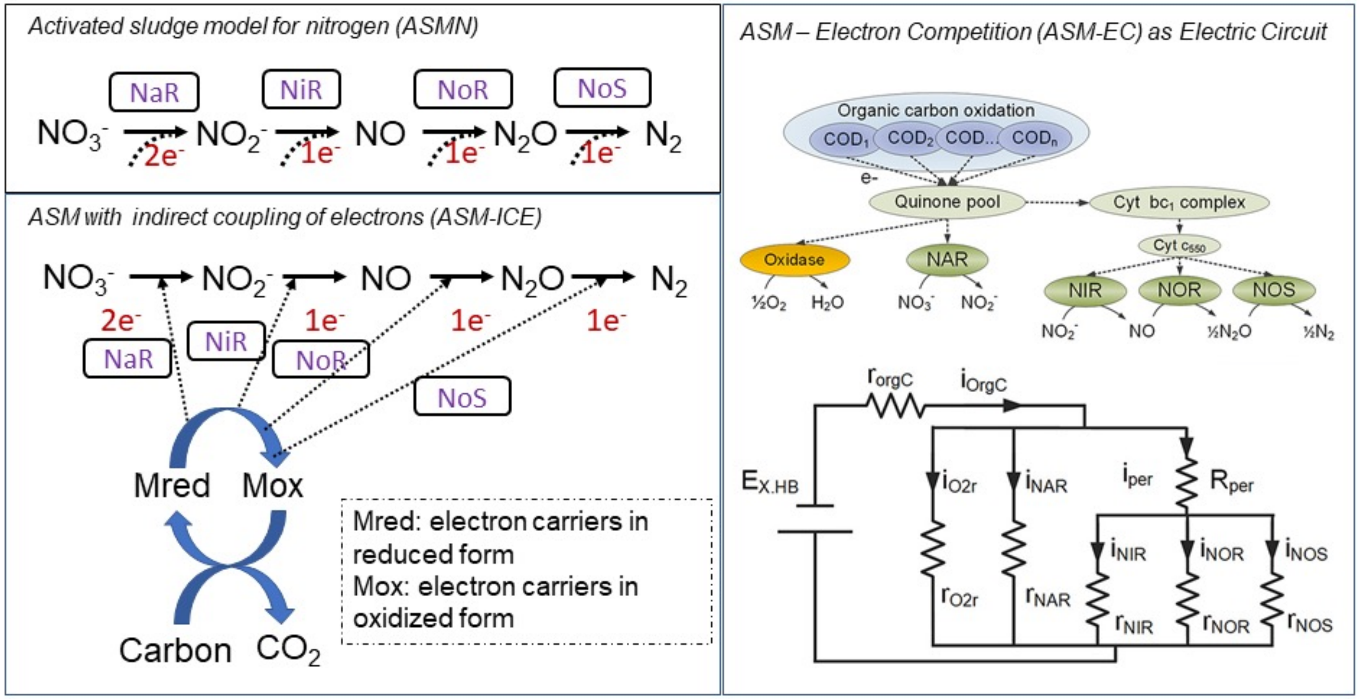
(Domingo-Félez and Smets, 2020)

HETEROTROPHIC DENITRIFICATION CHALLENGES

- Heterotrophic denitrification (OHO) is the only process able to either consume or produce N_2O: very important to consider for mitigation strategies!
- New concepts may be necessary for differentiating the effect of C source (COD)

ASMN: Hiatt and Grady (2008)

ASM-ICE: Pan et al. (2013)



ASM-EC; Electric circuit analogy: Domingo-Félez and Smets (2020)

CONCLUSIONS

- N_2O models reach the age of maturity (13-15 years)
- Very useful for identifying influencing factors, understanding pathways and developping control stragegies
- Still questionable about their quantitative prediction ability in full scale

ON GOING AND FUTURE RESEARCH TRENDS

- Microbial

NO and N_2O loops between heterotrophs and autotrophs and anammox, enzymes regulation

- Heterogeneity description

CFD coupled with biokinetics, biofilm 1..-D models

- Non deterministic models

Hybrid models, data driven, fuzzy logic, neuronal

- Calibration and observation methodology

Real time, software sensors

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Mathieu Sperandio

Mathieu Spérandio

TBI-SYMBIOSE RESEARCH GROUP

TOULOUSE

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THANK YOU FOR YOUR ATTENTION !

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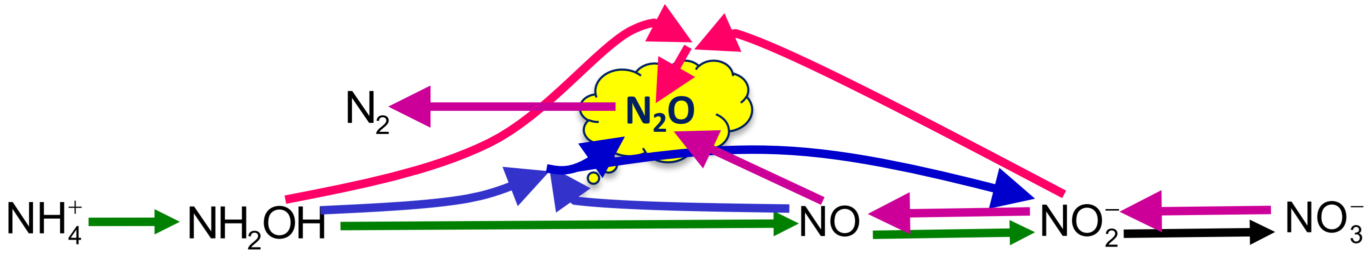
Potential of N_2O emission models for full-scale applications

Eveline Volcke

BIOLOGICAL N_2O CONVERSIONS - MODELS



by AOB: direct N_2O production pathway
= NH_2OH pathway

Pocquet et al., Water Res., 2016

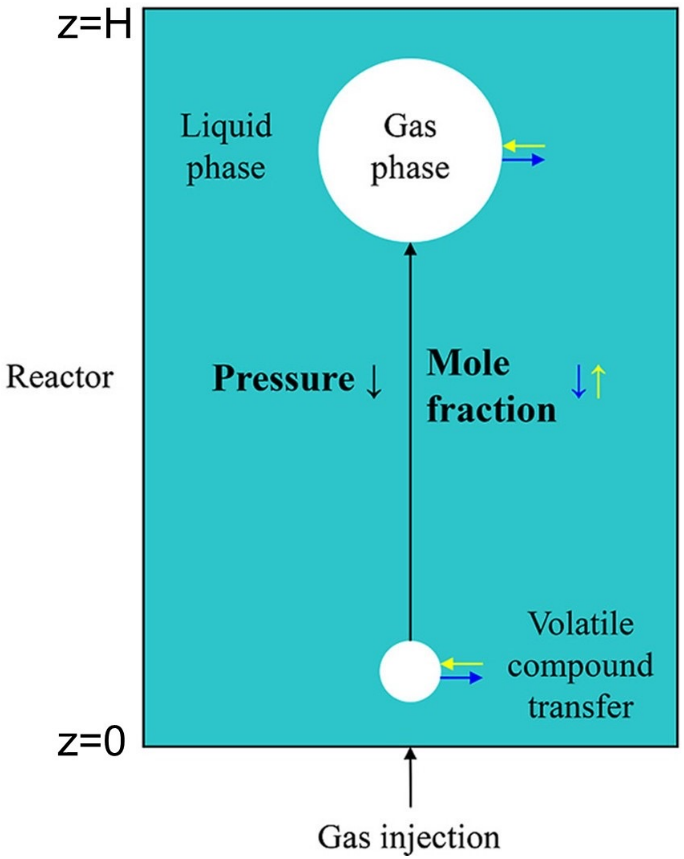
by AOB: autotrophic denitrification
= nitrifier denitrification = indirect pathway
- with O_2 inhibition

Pocquet et al., Water Res., 2016

heterotrophic denitrification

Hiatt & Grady, Water Environ. Res., 2008

LIQUID-GAS TRANSFER MODELLING



Check it yourself with our spreadsheet tool!

Baeten et al., Water Res. 2020

Liquid-gas transfer rate along reactor height influenced by
- pressure
- gas and liquid composition
- kLa

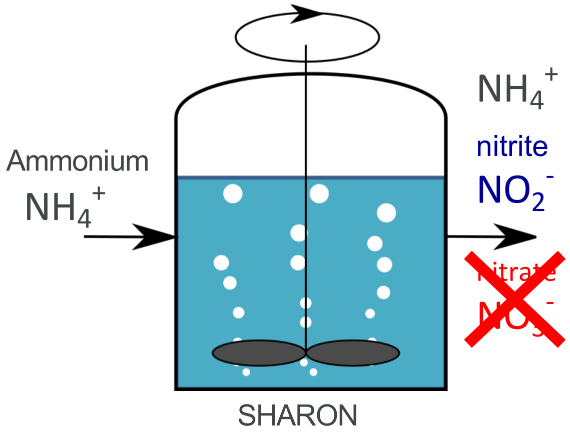
Simplified expressions can be used depending on
- component
- reactor design
- operating conditions

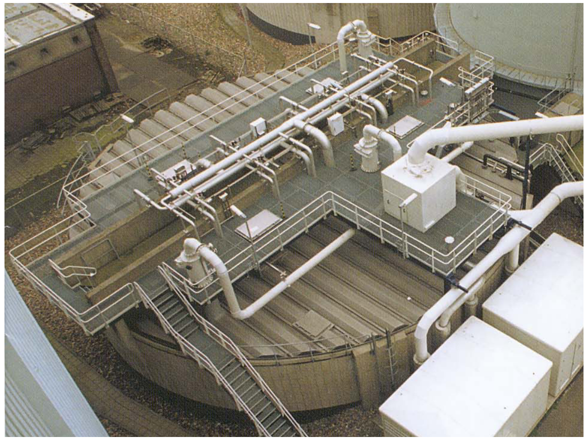
O_2: pressure !

N_2O: mole fraction !

Case study 1:

Modelling N_2O emissions from a full-scale partial nitritation reactor (suspended sludge)





Mampaey et al., 2019. Biochem. Eng. J.

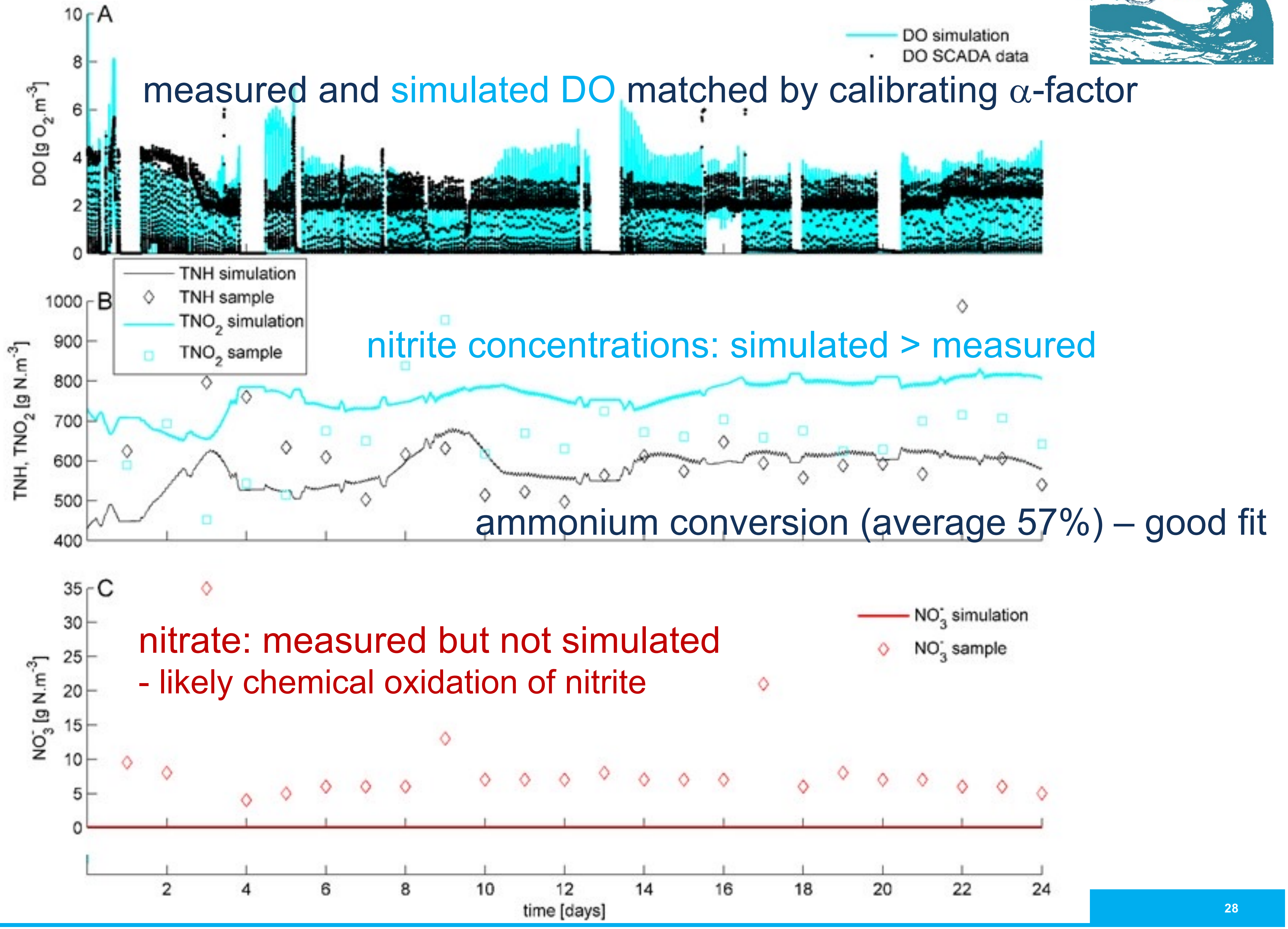
PROCEDURE

Mampaey et al., 2019. Biochem. Eng. J.

Step 1. Calibration of overall reactor performance

- Model without N_2O formation

OVERALL REACTOR BEHAVIOUR



PROCEDURE

Mampaey et al., 2019. Biochem. Eng. J.

Step 1. Calibration of overall reactor performance

- Model without N_2O formation

Step 2. Qualitative assessment of N_2O formation pathways

- Separate models for individual N_2O formation pathways

Step 3. Model calibration

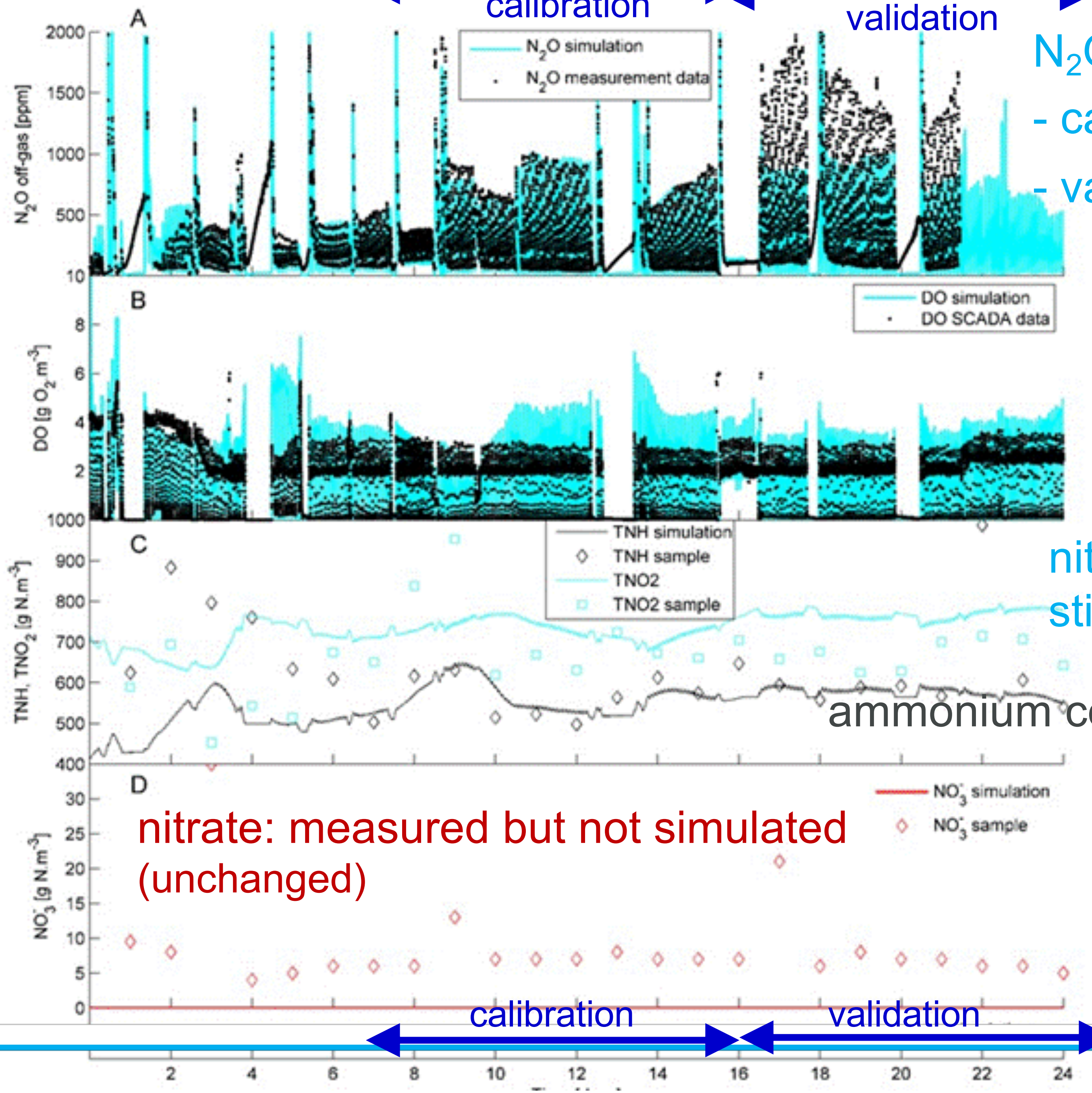
- A single model to which individual N_2O formation pathways are added sequentially

Step 4. Model validation

- A single model with all relevant N_2O formation pathways

OVERALL REACTOR BEHAVIOR INCLUDING N_2O

calibration — validation



N_2O emission
- calibration: good fit
- validation: underprediction

nitrite concentrations:
still overpredicted, but less

ammonium conversion: still good fit

nitrate: measured but not simulated
(unchanged)

calibration — validation

WHAT DID WE LEARN?

Mampaey et al., 2019. Biochem. Eng. J.

- Dynamic reactor behaviour including off-gas N_2O and NO was well-described *qualitatively* – not influenced by N_2O formation

- Identification of N_2O formation pathways

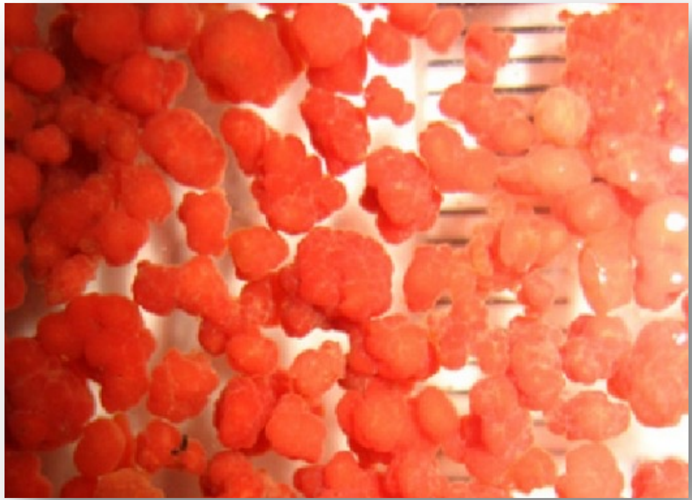
- anoxic: heterotrophic denitrification and AOB indirect pathway
- aerobic: AOB direct pathway (+ AOB indirect pathway)

- Comparison with experimental data allowed model structure identification

- *Quantitative* prediction of N_2O emissions with models remains difficult

Case study 2:

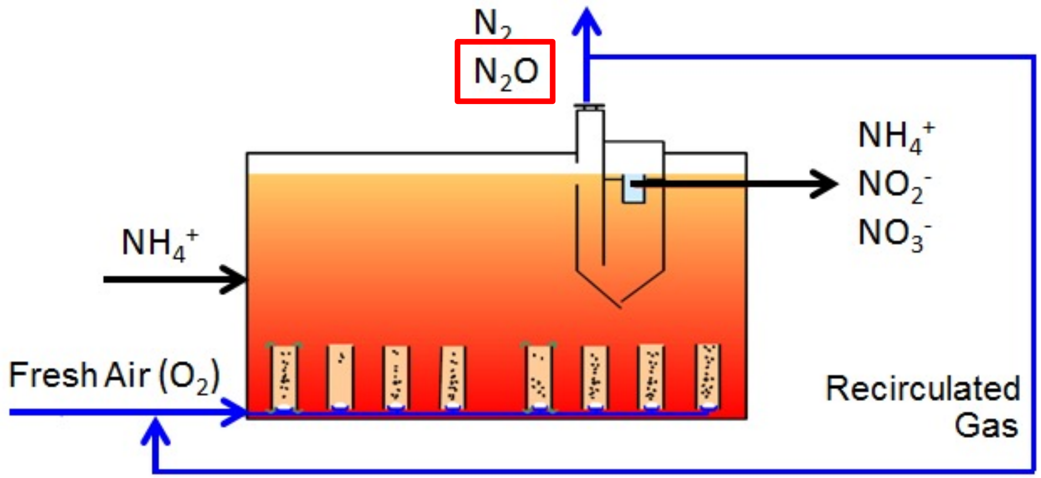
Modelling N_2O emissions from a full-scale partial nitritation – anammox reactor (granular sludge)

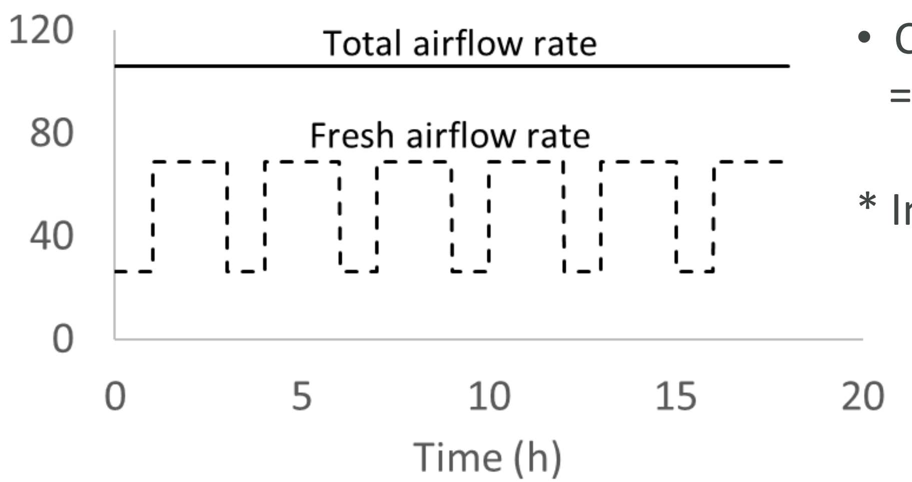


Wan et al., submitted

SYSTEM UNDER STUDY: FULL-SCALE PNA

Air flow rate





- Constant total gas flow in reactor
  = fresh air + recirculated air

* Intermittent high/low amounts of fresh air

Castro-Barros et al., 2015, Water Res.

SYSTEM UNDER STUDY

I. Calibration of overall reactor performance

Model without N_2O formation

I.1 Parameter selection through sensitivity analysis : steady state + dynamic

I.2 Parameter estimation of most sensitive parameters

- Multiple simulations with increasing number of parameters

II. Calibration of N_2O emissions

Model with N_2O formation

Keep parameters from I. fixed

II.1 Dynamic sensitivity analysis regarding N_2O related parameters

II.2 Model calibration: first separate, then combined pathways

I.+ II. = two-step calibration
bulk liquid - N_2O

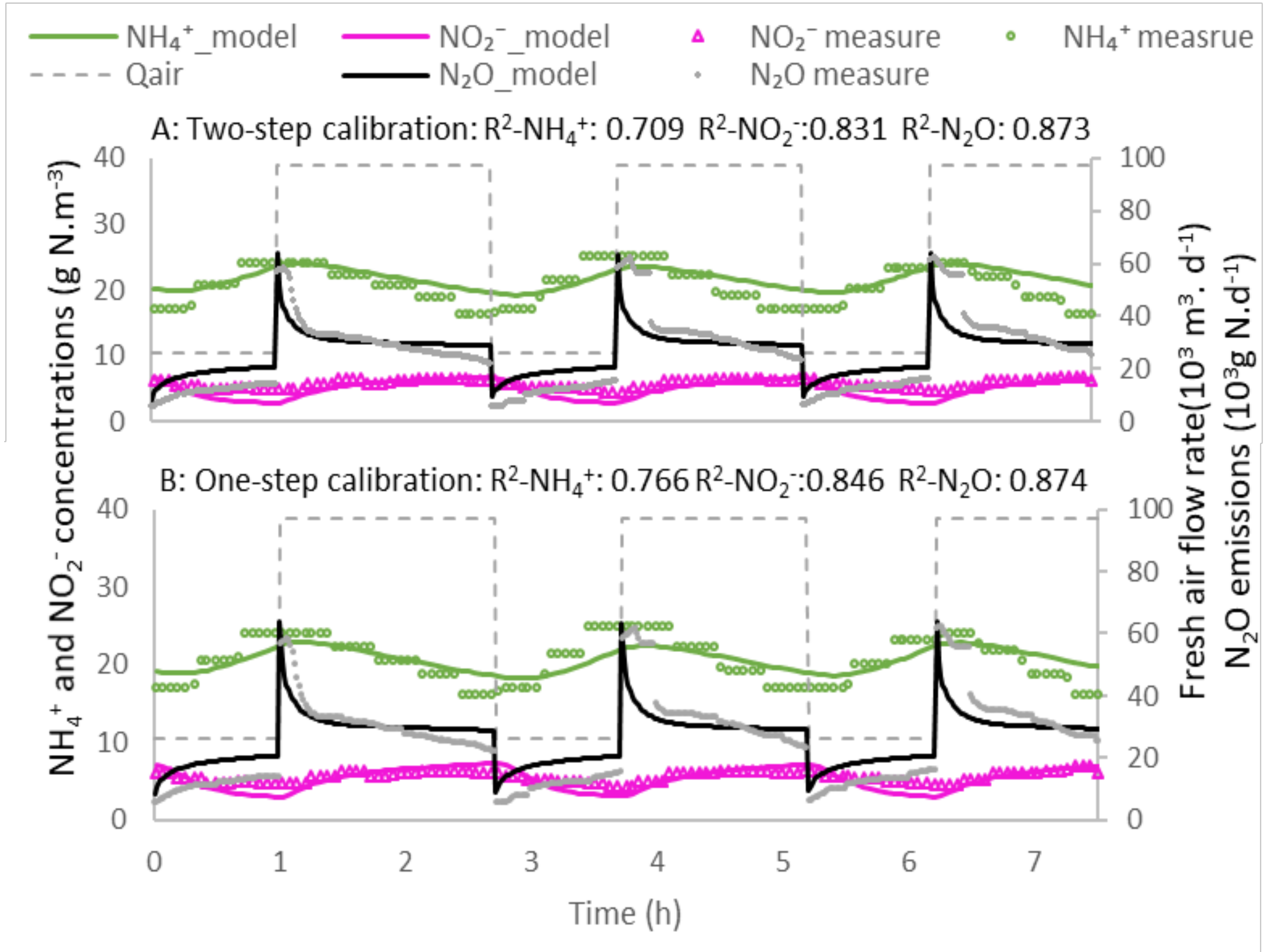
III. One-step calibration

Recalibration of parameters selected in previous steps

Wan et al., submitted

MODEL CALIBRATION RESULTS

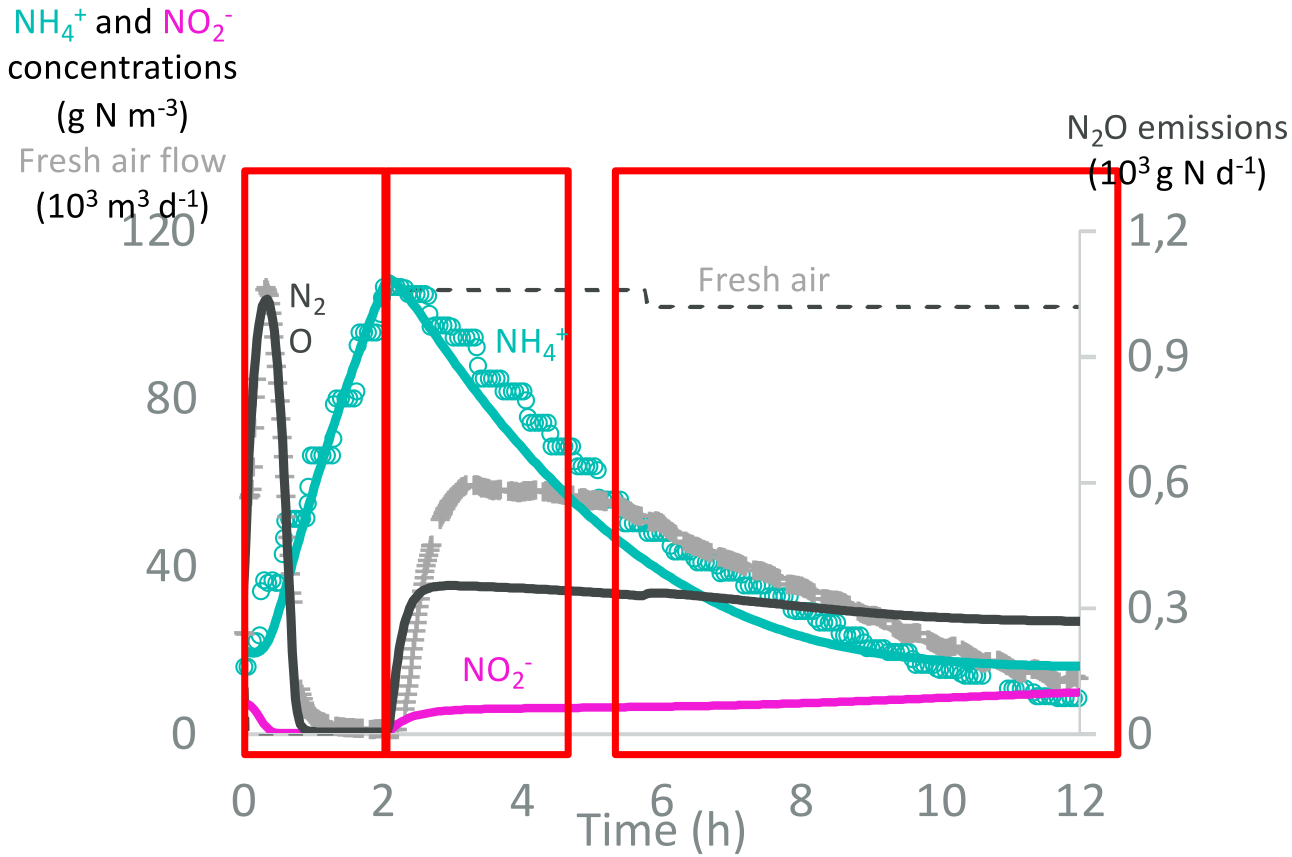
Wan et al., submitted



One-step calibration leads to improved fit !

Wan et al., submitted

MODEL VALIDATION WITH DATA FROM PROLONGED AERATION



- The model can well describe the N_2O at the low aeration phase
- The model predicted lower N_2O at the beginning of high aeration
- The predicted N_2O emissions decreased slower than measurements

Wan et al., submitted

WHAT DID WE LEARN?

Wan et al., submitted

- Calibrated model performance
  - 7 parameters estimated
  - *quantitative* description of average N_2O emissions
  - *qualitative* characterization of the N_2O emission dynamics

- Validation
  - independent data set at different aeration conditions
  - only *qualitatively* prediction of N_2O dynamics

- Identification of N_2O formation pathways
  - nitrifier nitrification pathway was identified as the dominating N_2O production pathway
  - heterotrophic denitrification was a net sink of N_2O.

CONCLUDING STATEMENT

N_2O production models are not suitable for quantitative prediction

⇐ Calibration is not unambiguous

- several parameters sets lead to the same result
- optimal calibration procedure?

⇐ Microbial adaptation is not included in models

still they are useful
for the identification of pathways and influencing factors

leading directly to control strategies for N_2O emission reduction

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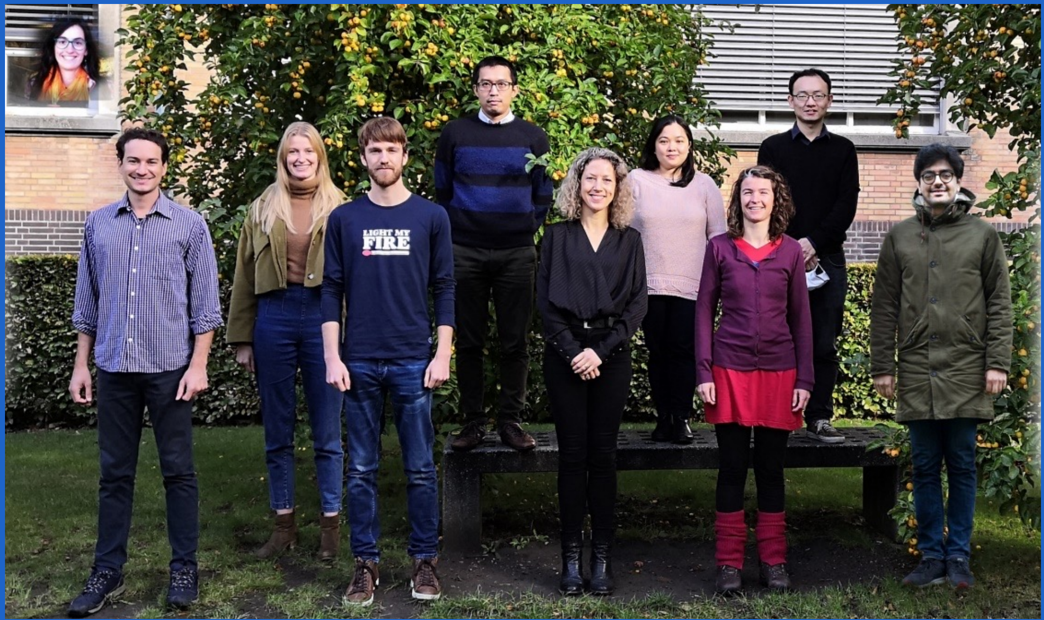


BIOCO RESEARCH GROUP

THANK YOU FOR YOUR ATTENTION !

AGENDA AND HOUSEKEEPING

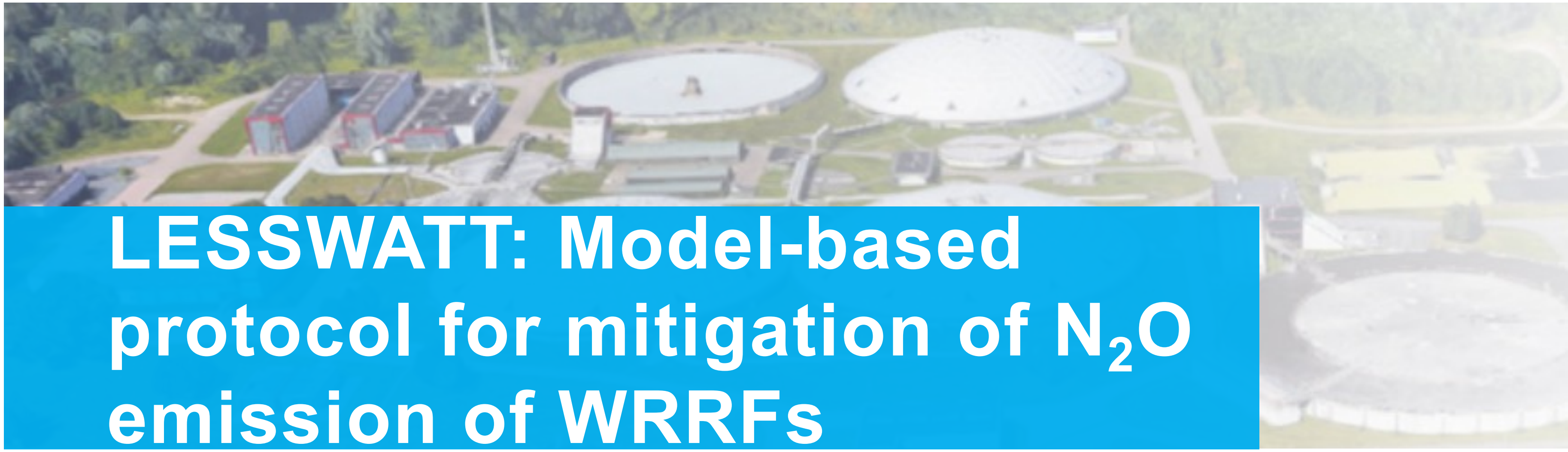
Speaker 1
Mathieu Sperandio (INSA Toulouse, France)

Speaker 2
Eveline Volcke (Ghent University, Belgium)

Speaker 3
Saba Daneshgar (Ghent University, Belgium)

Q&A Session: *Liu Ye (moderator)*

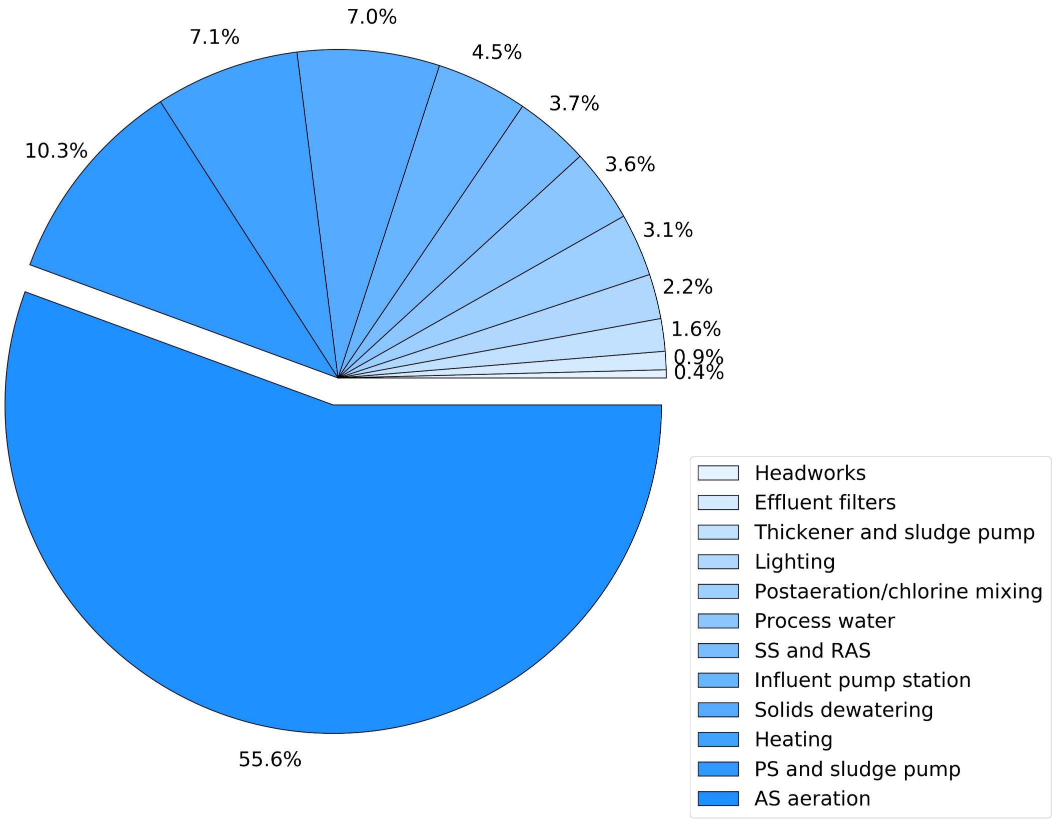
- This session is being recorded;
- Microphones and cameras have been disabled due to the large number of attendees;
- The normal chat function is disabled;
- Please put any questions and comments you may have in the Q&A and we will do our best to answer them during the session (in writing or orally).

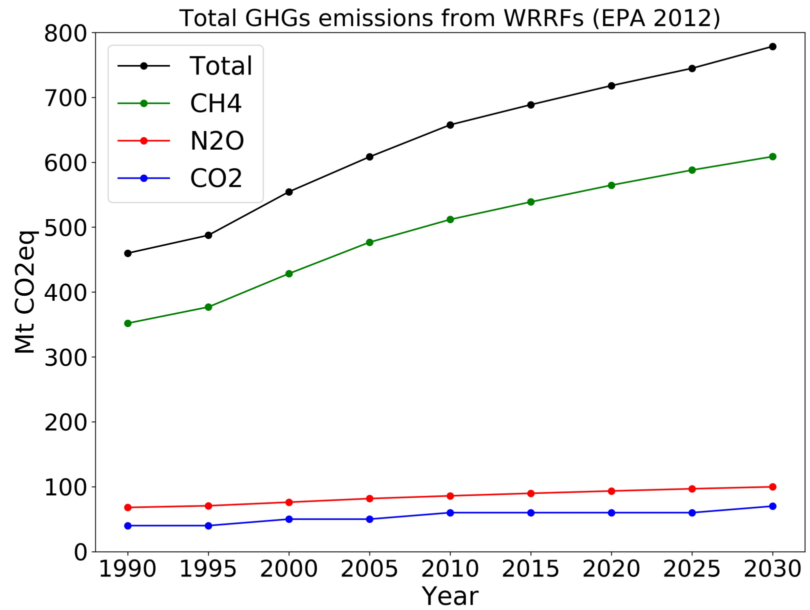


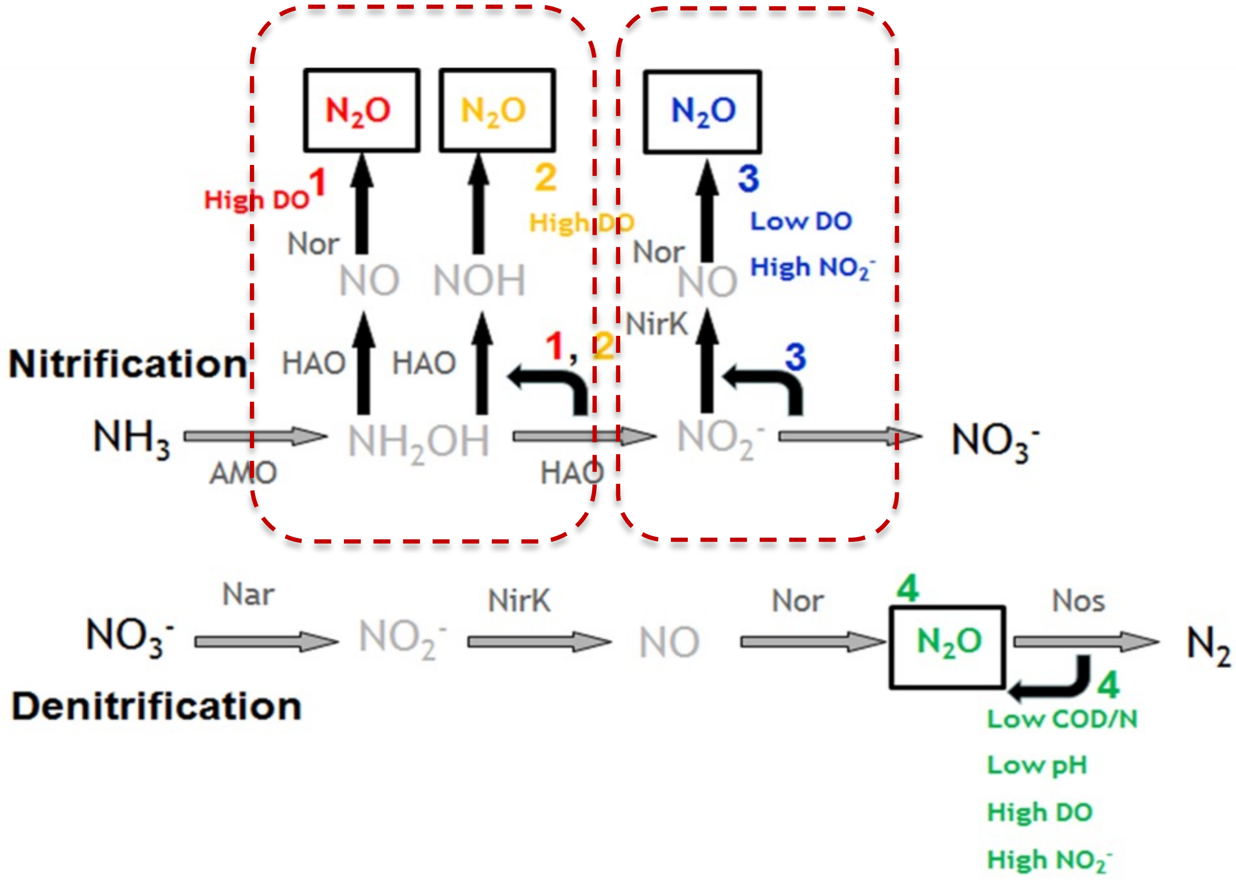
LESSWATT: Model-based protocol for mitigation of N_2O emission of WRRFs

Dr. Saba Daneshgar

INTRODUCTION





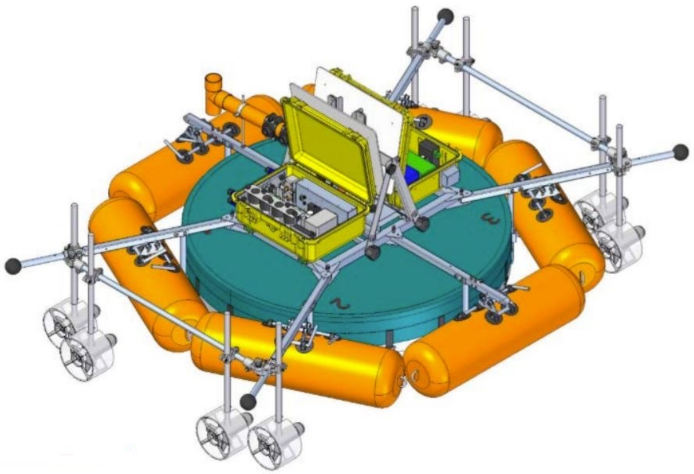


High DO risk: risk of N_2O emission due to high DO concentrations
Low DO risk: risk of N_2O emission due to low DO concentrations

LESSWATT OBJECTIVES

Innovative technologies (LESSDRONE, protocol)	Energy and GHGs reduction	Transferability To other WRRFs

LESSDRONE

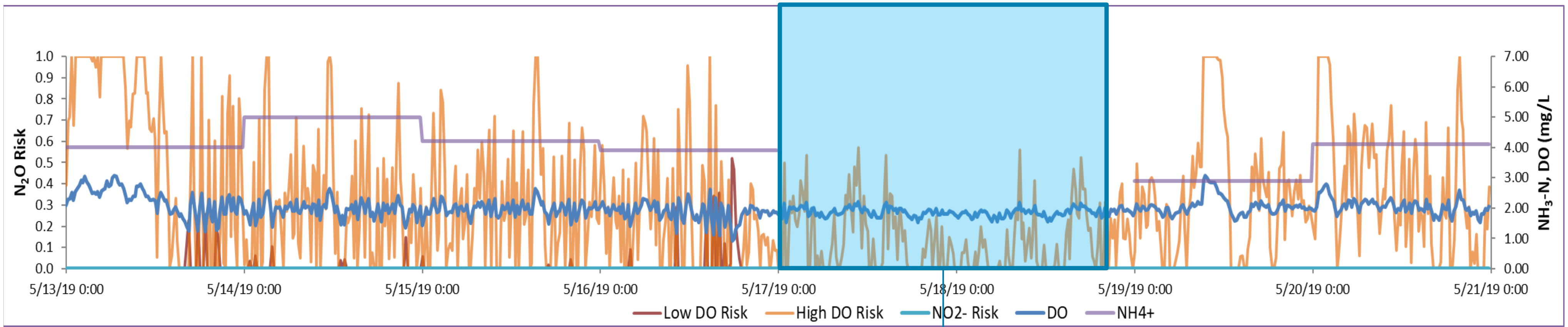


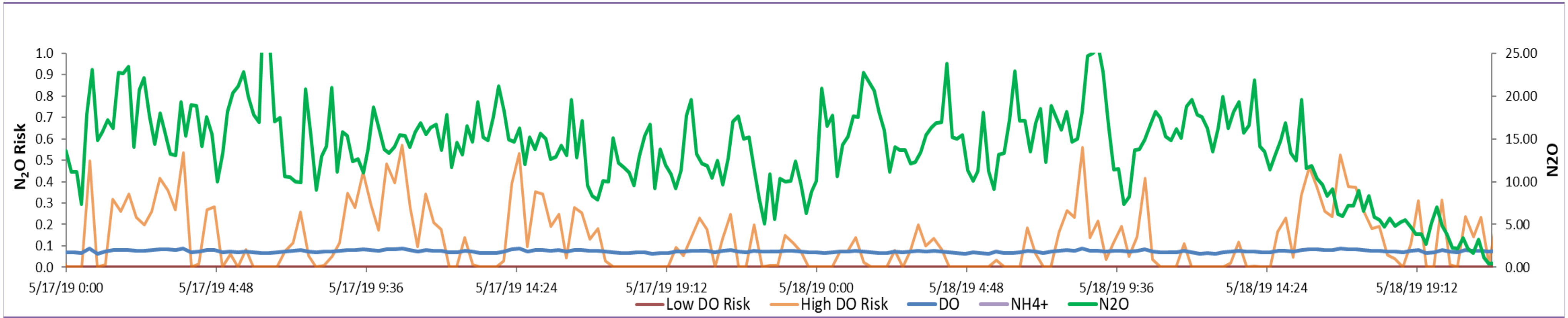
<u>Online Measurements:</u>

- Oxygen transfer rate (OTR)
- Dissolved oxygen
- N_2O emission in off-gas

Cuoiodepur WRRF San Miniato, Italy

N_2O risk assessment model





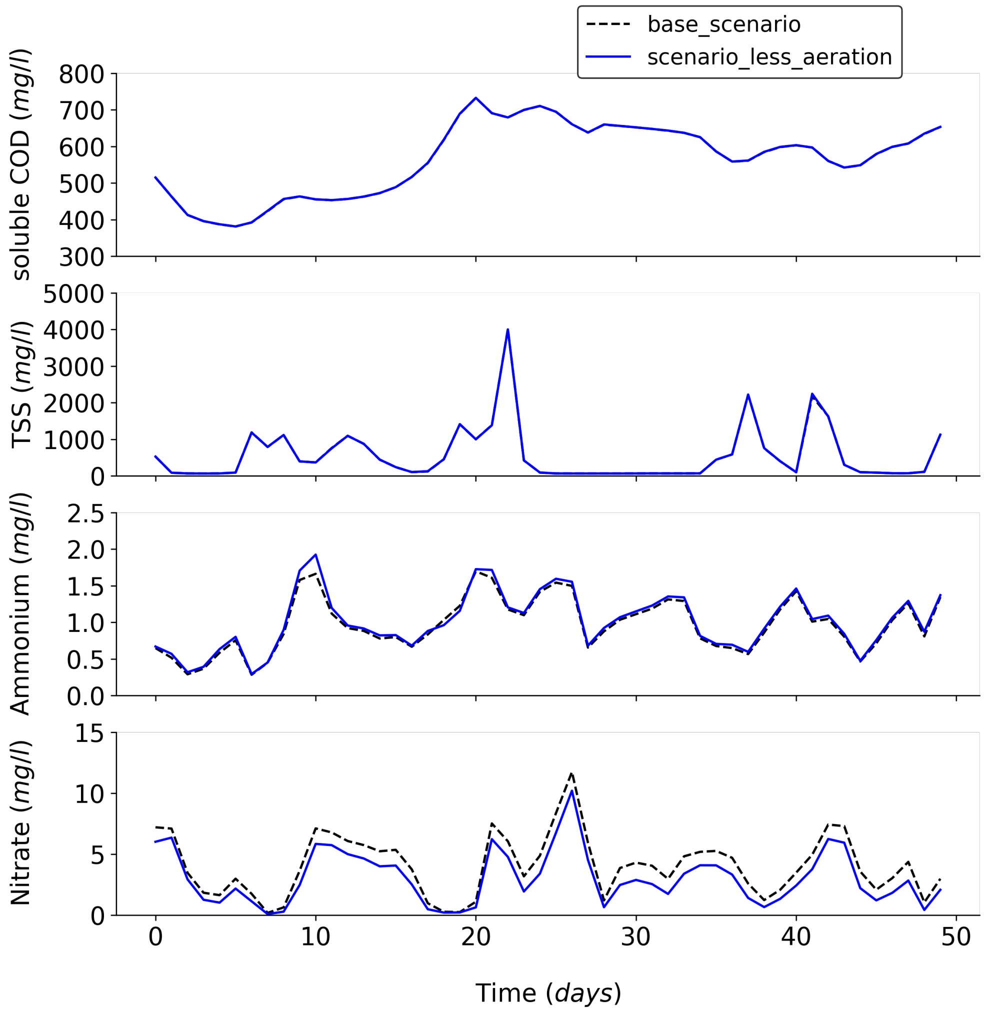
DO is consistently high

High N_2O emission risk caused by high DO

Potential mitigation strategy:
Reducing aeration

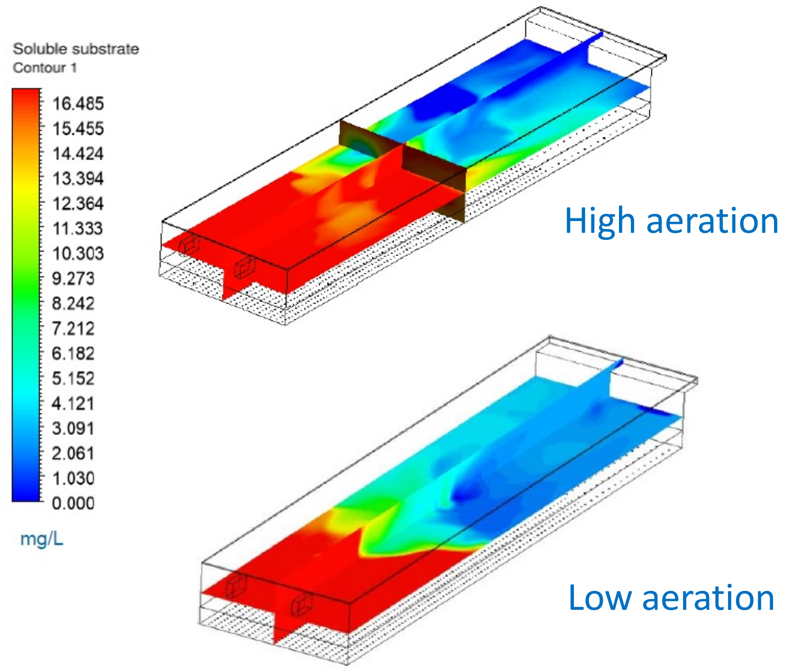
Simulating mitigation strategy

Flow sheet model

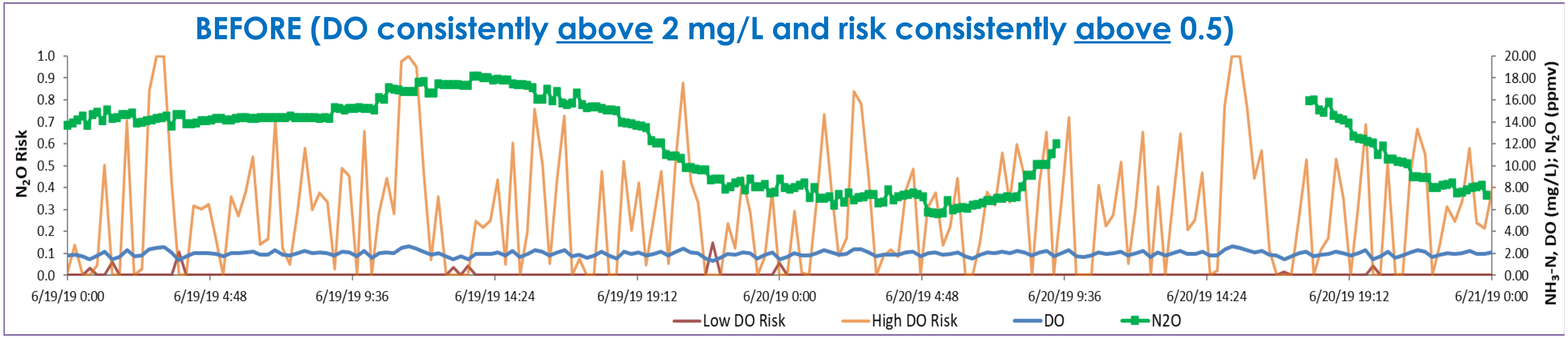


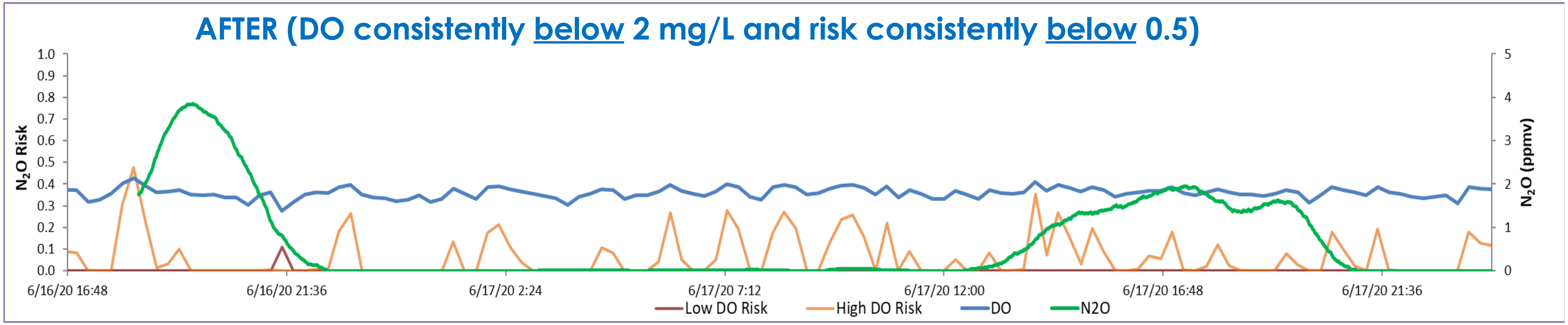
CFD-biokinetic model

Soluble substrate



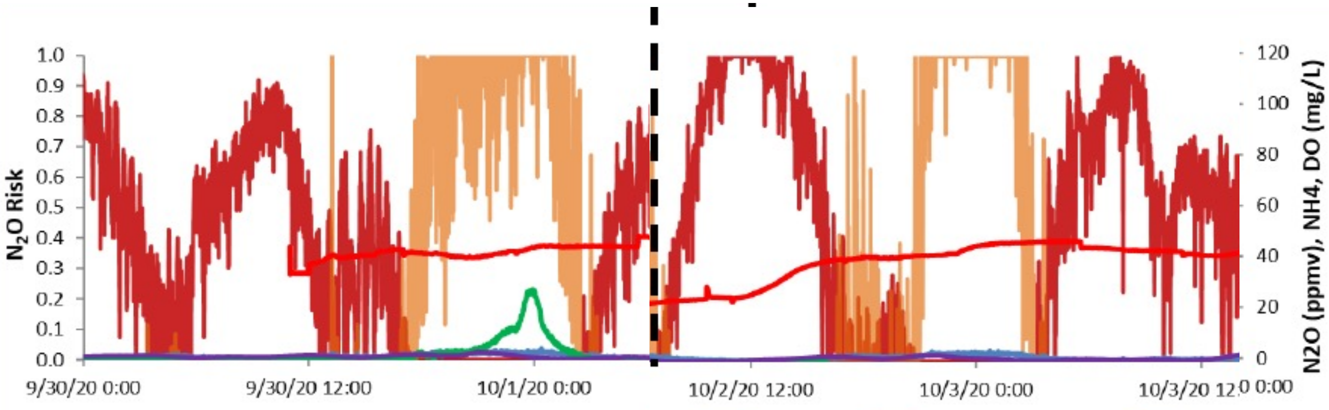
New measurement campaign
lower DO setpoint (testing mitigation strategy)



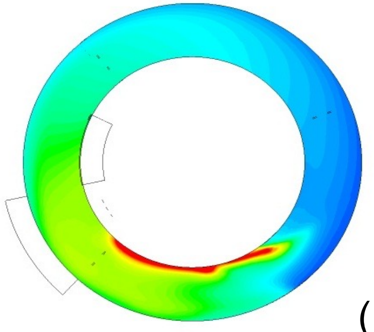


Eindhoven WRRF The Netherlands

N_2O risk assessment model



High variations



(Rehman 2016)

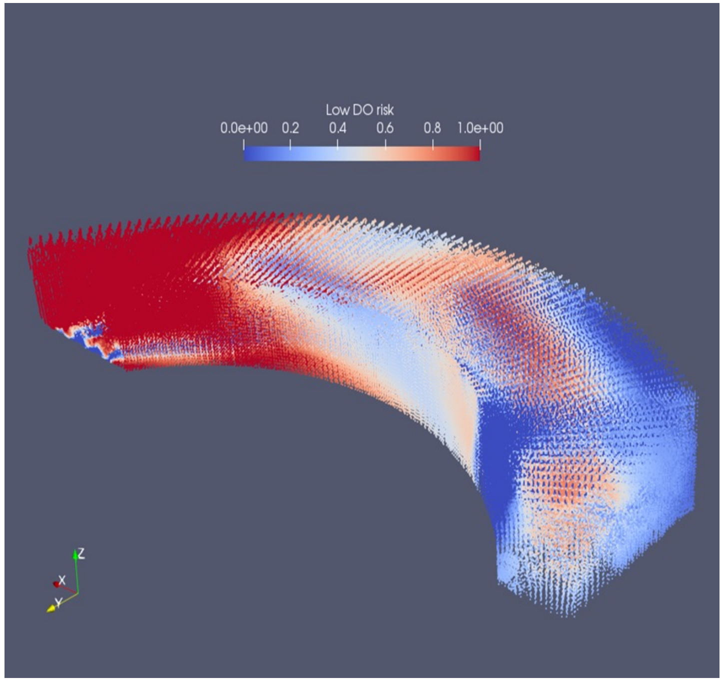
CFD-N_2O risk model

CFD-biokinetic model

DO parcels

N_2O risk model

Low DO risk (**high-load/flow**)



(Porro et al., 2019)

Incomplete mixing
high DO and low DO conditions

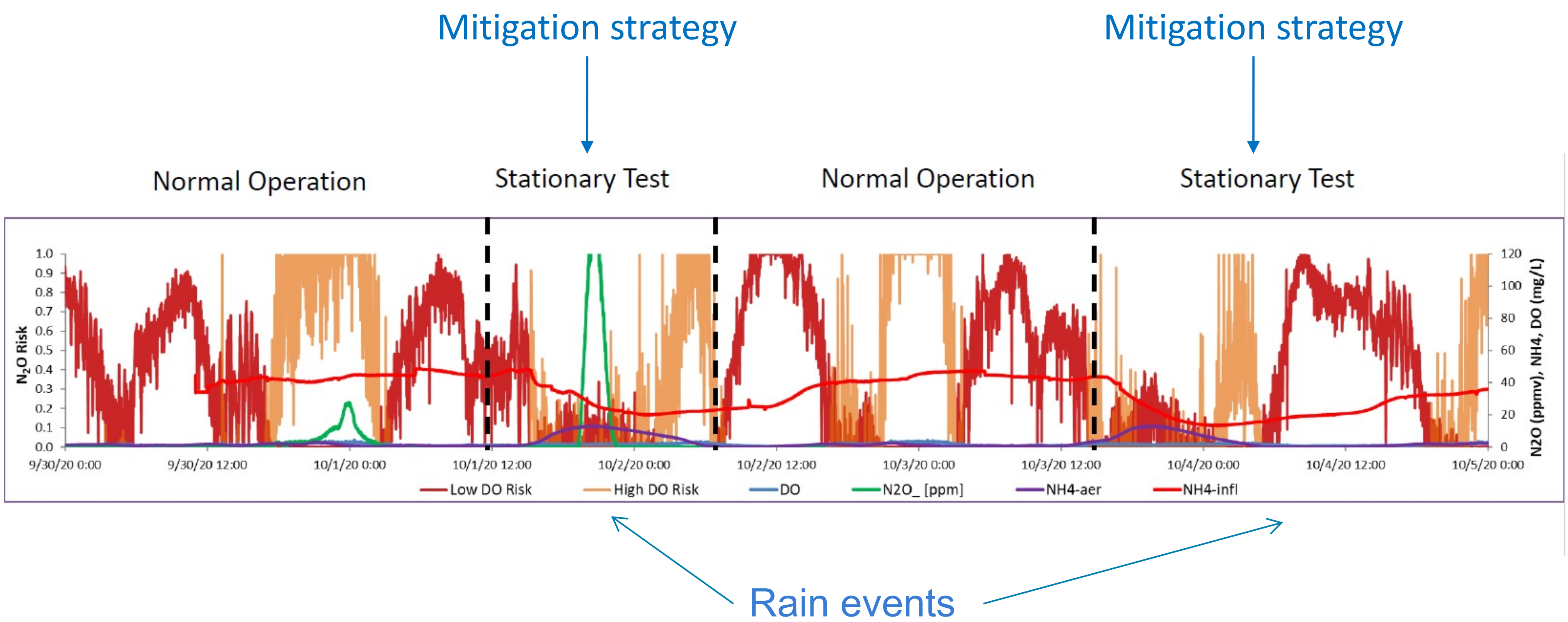
High N_2O emission risk caused by both conditions

Potential mitigation strategy:
decrease max DO setpoint
increase min DO setpoint

Simulating mitigation strategy

Flow sheet model

New measurement campaign lower DO setpoint (testing mitigation strategy)



Take home messages

- LESSWATT: innovative protocol targeting CF reduction in WRRFs
- Use of CFD-biokinetic modeling for detailed hydrodynamic description
- Use of N_2O risk assessment modeling framework for defining high risk operating conditions
- Use of innovative LESSDRONE for collecting high freq data
- Transferable protocol for different WRRFs

Thank you!

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CLOSING REMARKS

Great thanks to all presenters for a great show!

Look out for MIA's NEXT webinar in October/November 2021:

"Modelling Wastewater Treatment Resilience for Improved Decision Making and Resource Recovery" (working title)

If you have ideas for your own future webinar then contact MIA MC and we will help you make it happen!

Find out more at

http://iwa-mia.org/

https://iwa-connect.org