INSTRUMENTATION CONTROL AND AUTOMATION

21 NOVEMBER 2022

10:30 CET

IWA Specialist Group on Modelling and Integrated Assessment Webinar Series

Modelling greenhouse gas emissions from urban wastewater systems: State-of-the-art and beyond

Speakers

Ulf Jeppsson Lund University	Liu Ye University of Queensland	Keshab Sharma University of Queensland	Mathieu Sperandio INSA Toulouse	Wim Audenaert AM-Team	Xavier Flores Alsina Technical University of Denmark	Jose Porro Cobalt Water Global

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

A JOINT MIA AND ICA SG WEBINAR

This webinar is a joint venture between:

IWA SG on Modelling and Integrated Assessment

and

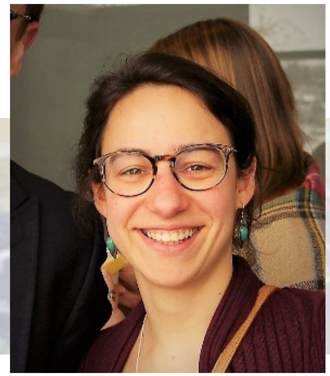
IWA SG on Instrumentation, Control and Automation

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)



inspiring change

LUND UNIVERSITY

GHENT UNIVERSITY

IWA INSTRUMENTATION CONTROL AND AUTOMATION
the international water association

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

INSTRUMENTATION CONTROL AND AUTOMATION
the international water association

Task Groups (TGs)

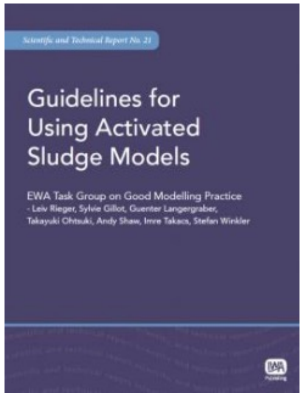
- Benchmarking of Control Strategies for WWTPs (BSM) AND Good Modelling Practice (GMP) AND Design and Operations Uncertainty (DOUT) AND Use of Modelling for Minimizing GHG Emissions from Wastewater Systems (GHG) (all four finished)
- Generalised Physicochemical Modelling (PCM) (in press)
- Membrane Bioreactor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

Working Groups (WGs)

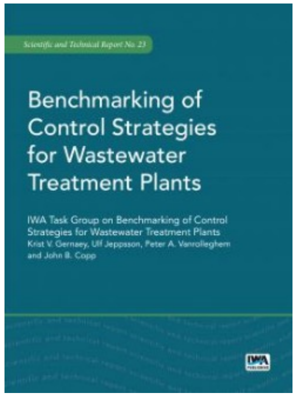
- Integrated Urban Water Systems (IUWS)
- Computational Fluid Dynamics (CFD)
- Good Modelling Practice (GMP)

Conferences / Events

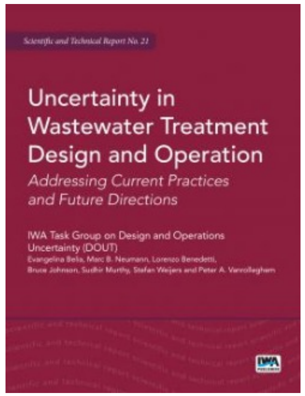
- WRRmod
- Watermatex



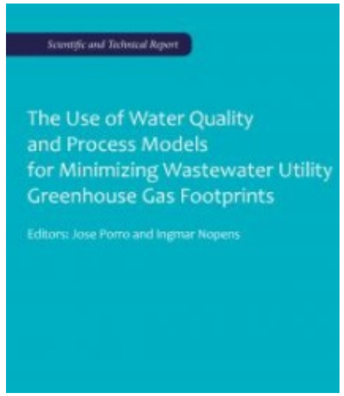
STR
(Sept. 2012)



STR
(Sept. 2014, open access)



STR
(2021, now open access)



STR
(2022, open access)

MIA SG: UPCOMING CONFERENCES

INSTRUMENTATION CONTROL AND AUTOMATION
the international water association

8th Water Resource Recovery Modelling seminar (WRRmod2022+)

- Location: Stellenbosch, South Africa, 18-21 January (NOTE: new dates) 2023
- Chair: Dr. David Ikumi (Univ. Cape Town)

11th Symposium on Modelling and Integrated Assessment (Watermatex2023)

- Location: Québec City, Canada, 23-27 Sept. 2023
- Chair/vice-chair: Prof. Peter Vanrolleghem (Univ. Laval)/Dr. Elena Torfs (Univ. Ghent)

9th Water Resource Recovery Modelling seminar (WRRmod2024), PROBABLY in Stowe, Vermont, USA

FIND MIA SG ON SOCIAL MEDIA

Follow the Modelling and Integrated Assessment Specialist Group on:

- 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!

Newsletter, push messages, webinars, YouTube channel, digital archive

IWA INSTRUMENTATION, CONTROL AND AUTOMATION – ICA SG

INSTRUMENTATION CONTROL AND AUTOMATION
the international water association

- International discussion forum to:
  - Collect & exchange methodologies and experiences, in all aspects of ICA for water systems
  - Collect, summarize and publish practical experience to support and promote the use if ICA in practice
  - Highlight socio-economic and sustainability aspects of ICA. e.g. management problems, operator aspects…

Knowledge

Dissemination

Application






IWA INSTRUMENTATION, CONTROL AND AUTOMATION – ICA SG

ICA SG ACTIVITIES

- Updating social media with relevant information
- Group newsletters

- Organising and supporting conferences & workshops

- Supporting Task Groups, Working Groups & Clusters
- Organising webinars

- Encouraging publications of ICA related papers at conferences and scientific journals

- Leveraging partnerships and relationships with industry organization (e.g. Smart Water Network Forum)

IWA INSTRUMENTATION, CONTROL AND AUTOMATION – ICA SG

INSTRUMENTATION CONTROL AND AUTOMATION

the international water association

ICA SG ACTIVITIES

Current Task Group on MetaData

- Aim: Metadata collection and organization
- Outcome: STR in preparation (2023)

Webinars in preparation

- Advanced nitrogen removal control
- Advanced biological nutrient removal control

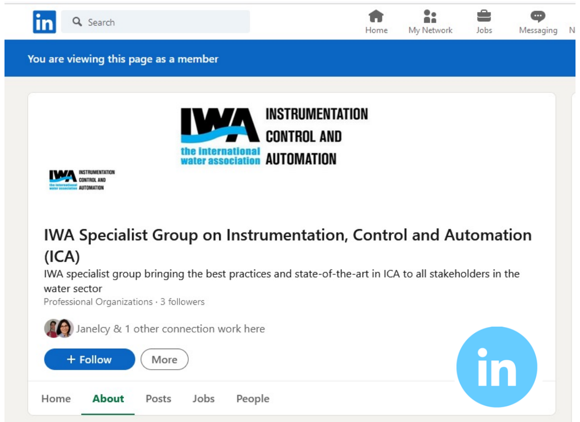
Next 14th Instrumentation, Control and Automation Conference (ICA2025)

- Location: Oslo, Norway, June 2025 (to be confirmed)
- Chair: Harsha Ratnaweera (Norwegian University of Life Sciences)

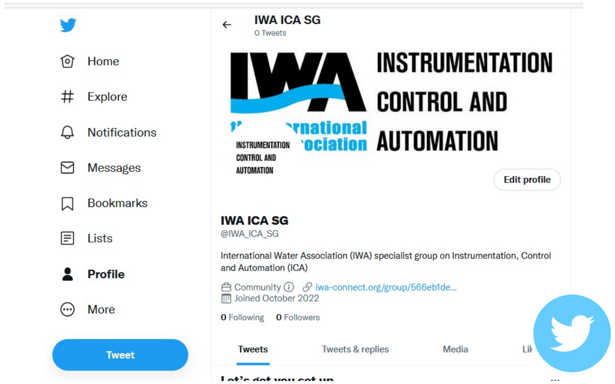
IWA INSTRUMENTATION, CONTROL AND AUTOMATION – ICA SG

SOCIAL MEDIA AND CONTACT

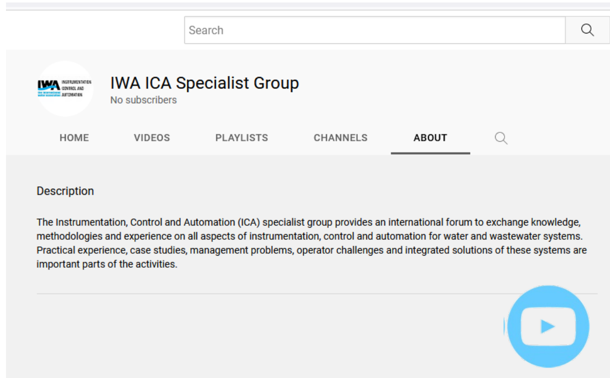
IWA Connect https://iwa-connect.org/#/group/instrumentation-control-and-automation



https://www.linkedin.com/company/iwa-ica-sg/



https://twitter.com/IWA_ICA_SG



https://www.youtube.com/channel/UCqAnJWfqiLJtVSIJSD6BwZw

Chair: Janelcy Alferes (Janelcy.alferescastano@vito.be)

Vice-Chair: Yanchen Liu (liuyc@tsinghua.edu.cn)

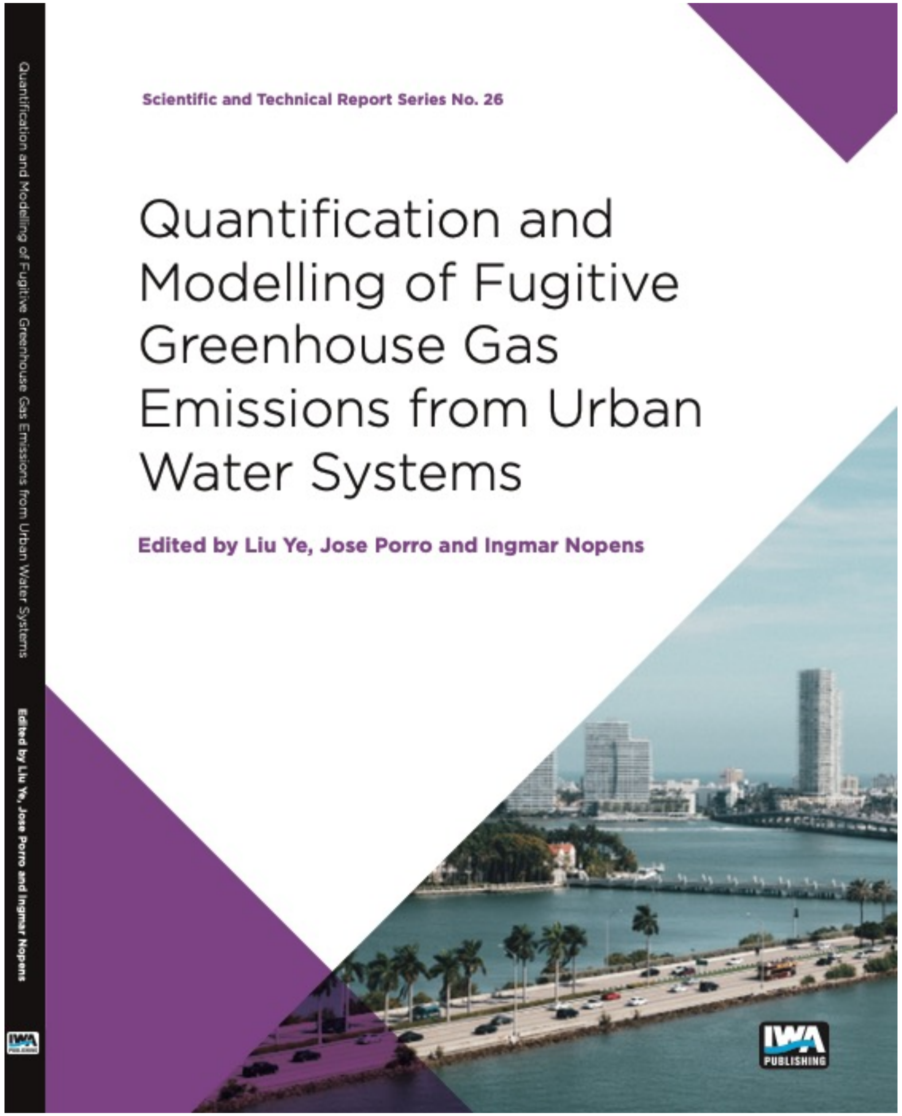
INTRODUCTION TO THE WEBINAR

INSTRUMENTATION
CONTROL AND
AUTOMATION

LAUNCH OF THE IWA BOOK

INSTRUMENTATION CONTROL AND AUTOMATION

Open access, FREE download: **DOI:** https://doi.org/10.2166/9781789060461



Liu Ye (Lead Editor, The University of Queensland)

Jose Porro (Co-Lead Editor, Cobalt Water Global)

Ingmar Nopens (Editor, Ghent University)

Link: https://iwaponline.com/ebooks/book/844/Quantification-and-Modelling-of-Fugitive

THE GHG WEBINAR SERIES

AGENDA AND HOUSEKEEPING

Speaker 1
Keshab Sharma (Univ. of Queensland, Australia)

Speaker 2
Mathieu Sperandio (INSA, France)

Speaker 3
Wim Audenaert (AM Team, Belgium)

Speaker 4
Xavier Flores-Alsina (Technical University of Denmark)

Speaker 5
Jose Porro (Cobalt Water Global, USA)

Q&A Session Moderator: *Liu Ye (Univ. of Queensland, Australia)*

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MODELLING OF CH_4 EMISSION FROM SEWERS: DEVELOPMENT AND APPLICATION

Keshab Sharma (k.sharma@uq.edu.au)
Australian Centre for Water and Environmental Biotechnology (ACWEB)
The University of Queensland, Australia

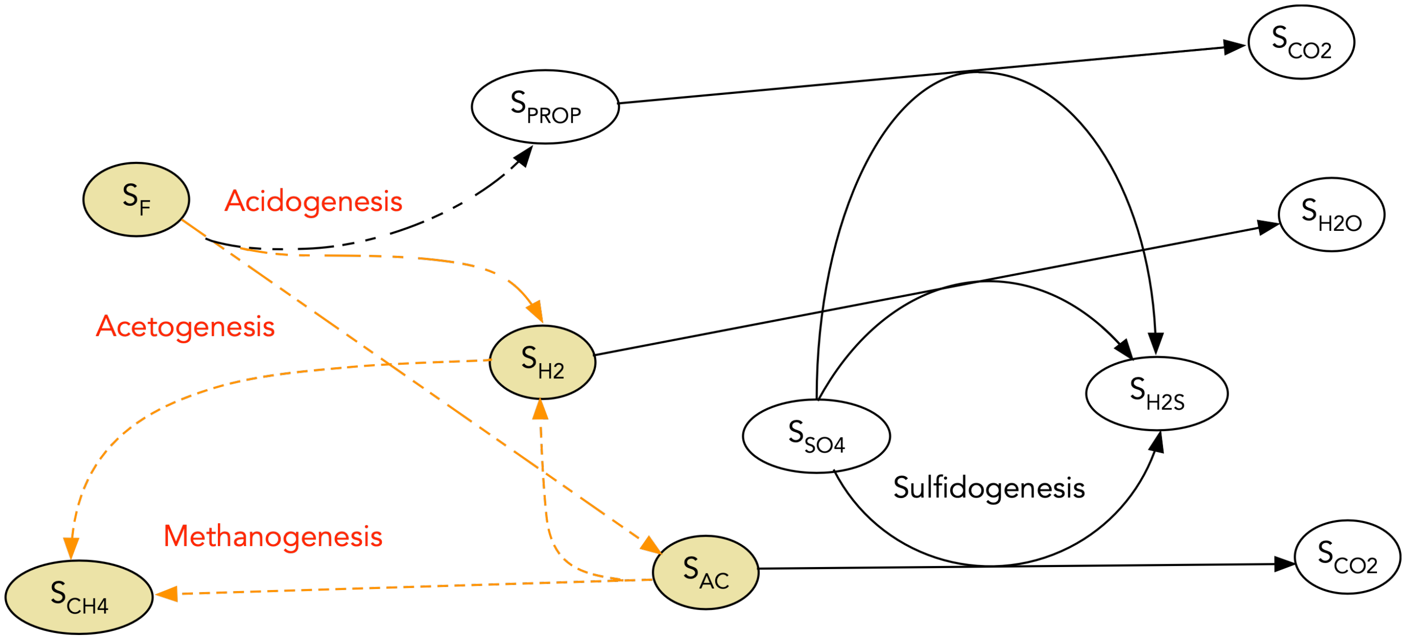
BACKGROUND

- "...wastewater in closed underground sewers is not believed to be a significant source of methane" - IPCC
- Data collected from the field has shown high CH_4 levels in some sewers - up to 20–25 mg/L of dissolved CH_4 in rising main sewers, up to 50,000 ppm in sewer headspace
- Sewers are distributed system – it is difficult to quantify the CH_4 emissions through direct measurements as in the case of the wastewater treatment plant
- Mathematical modelling for CH_4 emission in sewer system is key for GHG inventory for wastewater system

BACKGROUND

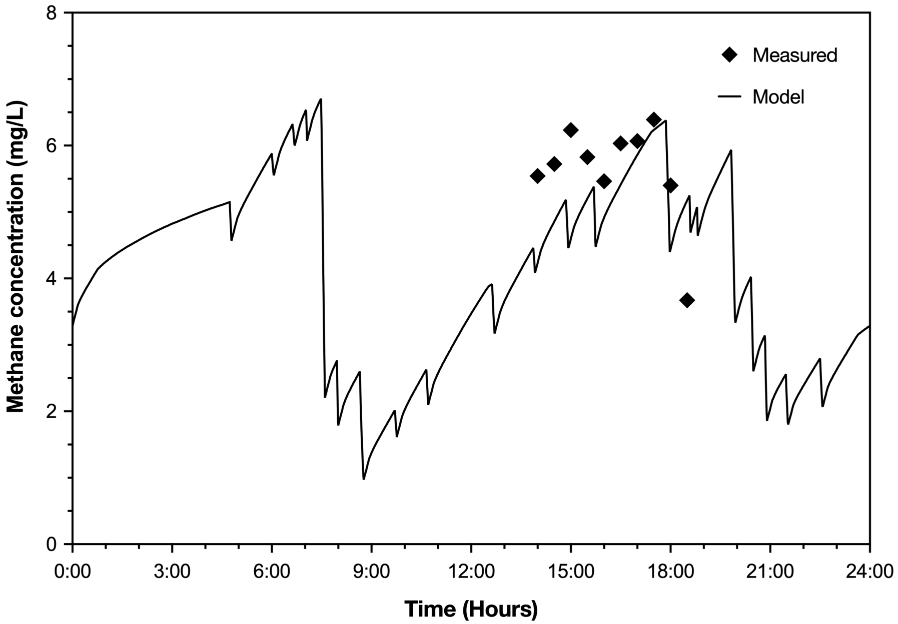
- SeweX model – dynamic sewer process model for predicting hydrogen sulfide production (Sharma et al., 2008)
- Components for CH_4 production in sewer biofilm added (Guisasola et al., 2009)
- Model initially developed based on ADM1 model components and parameters were calibrated using the laboratory data
- Model was later validated using the field data

MODEL DEVELOPMENT



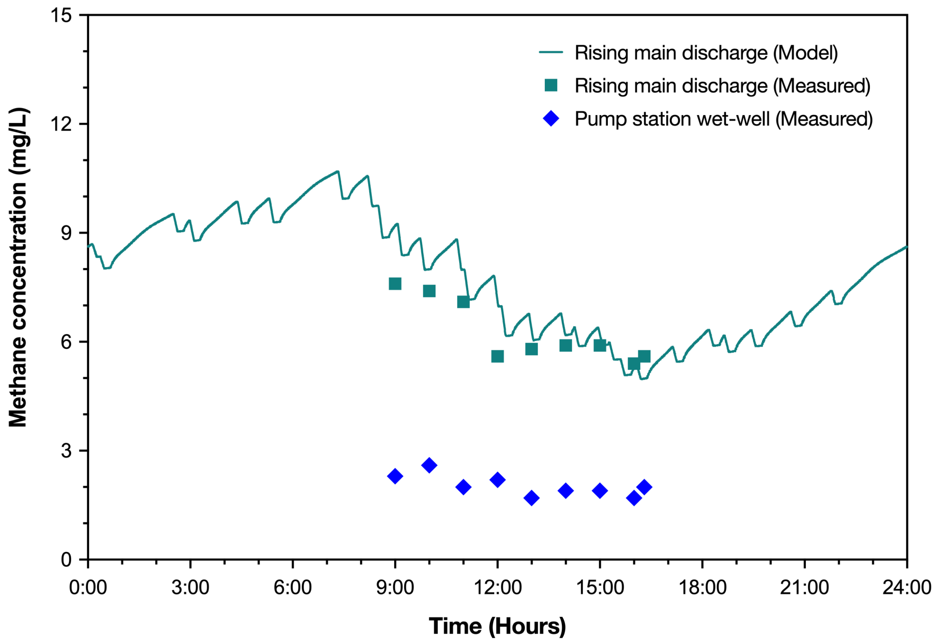
- The model considers the competition for common substrates among the methanogens and sulfate reducing bacteria
- Processes included in the model are:
  - Acetogenesis, Acidogenesis
  - Hydrogenotrophic methanogenesis, Acetoclastic methanogenesis
  - Hydrogenotrophic sulfidogenesis, Acetate-based sulfidogenesis, Propionate-based sulfidogenesis

MODEL VALIDATION

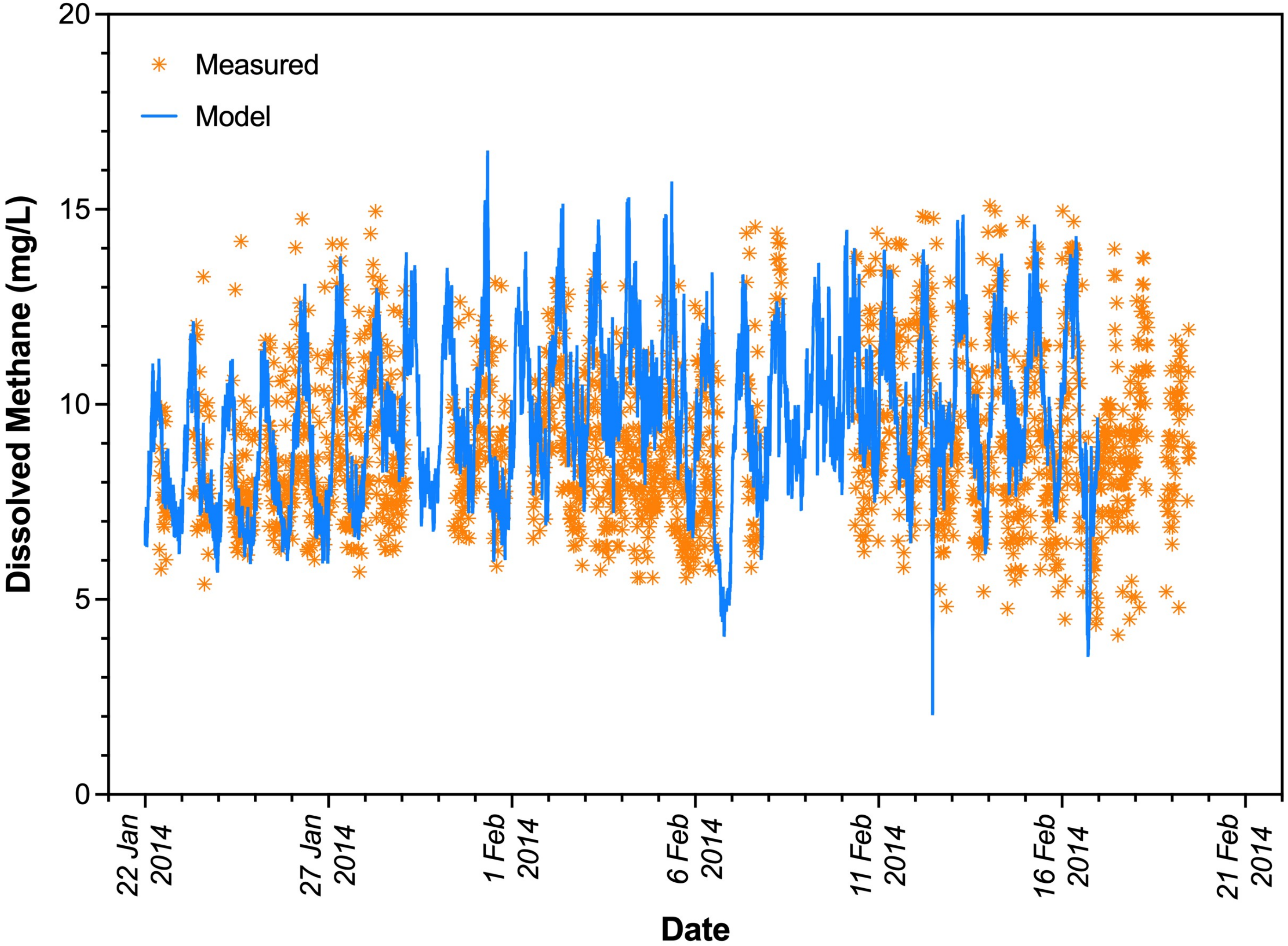


SeweX model predictions vs offline CH_4 data collected from a sewer system in Australia (Guisasola et al., 2009)

SeweX model predictions vs measured CH_4 data (off-line) for a sewer system in Spain



MODEL VALIDATION



Measurements vs. SeweX Predicted CH_4 Concentrations for Gold Coast Sewer System

CHALLENGES

- Mechanistic model to complex for its application to large sewer systems
- A large quantity of data is required which are not readily available
- The entire process would be time consuming and resources intensive
- Simplified approach is therefore required
  - Empirical models

EMPIRICAL MODELS

- **Methane production in pressure main (Foley et al., 2009)**

$$C_{CH_4} = 5.24 \times 10^{-5} \times \left(\frac{A}{V} \times HRT\right) + 0.0015$$

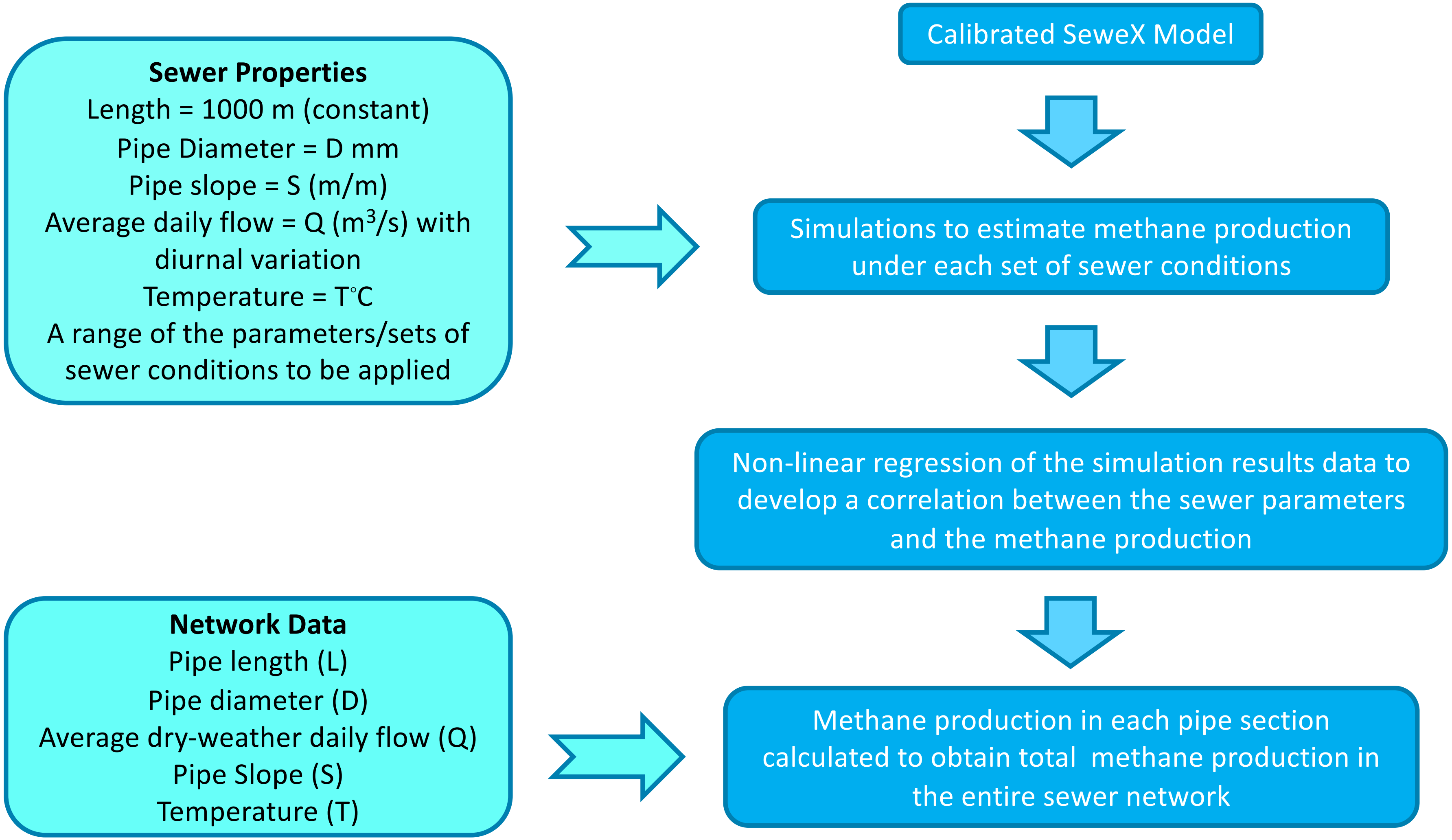
- **Methane production in gravity sewer (Chaosakul et al., 2014)**

$$C_{CH_4} = 6.0 \times 10^{-5} \times \left(\frac{A}{V} \times HRT\right) \times 1.05^{(T-20)} + 0.0015$$

- **Methane production in gravity sewer (Xu et al., 2018)**

$$Q_{CH_4} = Y_{CH_4/x} \cdot X \cdot HRT \cdot 1.05^{(T-20)}$$

EMPIRICAL MODEL DEVELOPMENT AND APPLICATION (GRAVITY SEWER)



GS-MODEL DEVELOPMENT FOR GRAVITY SEWER

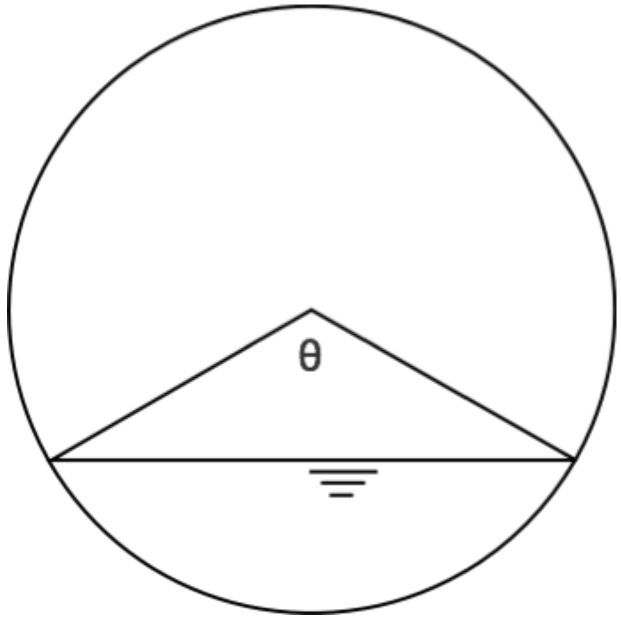
$$\theta = \frac{3\pi}{2}\sqrt{1-\sqrt{1-\sqrt{\frac{\pi Q n}{D^{\frac{8}{3}} S^{\frac{1}{2}}}}}}$$

$$\theta = k \cdot Q^{\alpha} \cdot D^{\beta} \cdot S^{\gamma}$$

$$A_{bf} = \theta \cdot \frac{D}{2} \cdot L = k \cdot Q^{\alpha} \cdot D^{\beta} \cdot S^{\gamma} \cdot \frac{D}{2} \cdot L$$

$$r_{CH_4} = k' \cdot A_{bf} = k \cdot Q^{\alpha} \cdot D^{\beta} \cdot S^{\gamma} \cdot L$$

$$r_{CH_4,20} = k \cdot Q^{\alpha} \cdot D^{\beta} \cdot S^{\gamma}$$



METHANE GENERATION IN GRAVITY SEWER

$$r_{CH_4} = 0.419 \times 1.06^{(T-20)} \times Q^{0.26} \times D^{0.28} \times S^{-0.138}$$

Where,

r_{CH_4} = Methane production rate (kg/km-day)

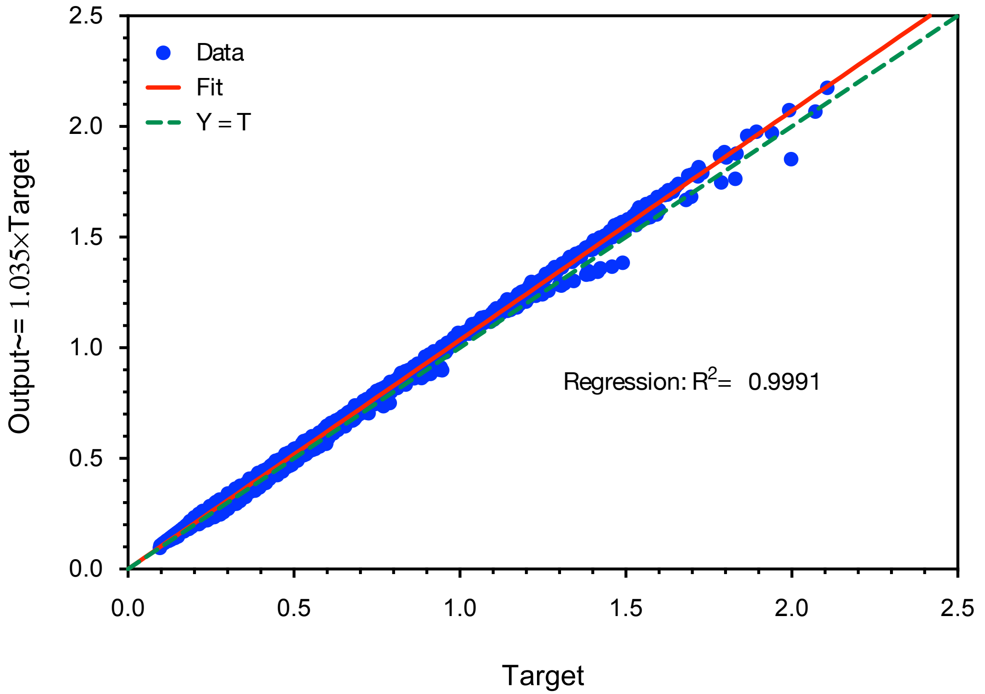
Q = Average flow over a day (m^3/s)

D = Pipe diameter (m)

S = Pipe slope (m/m)

Parameter Correlation Matrix

	k	α	β	γ
k	1.000	0.430	0.714	0.825
α	0.430	1.000	-0.938	-0.156
β	0.714	-0.938	1.000	-0.193
γ	0.825	-0.156	-0.193	1.000



EMPIRICAL MODEL DEVELOPMENT AND APPLICATION (PRESSURE MAIN)

Sewer Properties
Length = 1000 m (constant)
Pipe Diameter = D mm
Pump run time = P (min/day)
Average daily flow = Q (m3/s) with diurnal variation
Temperature = T°C
A range of the parameters/sets of sewer conditions to be applied

Calibrated SeweX Model

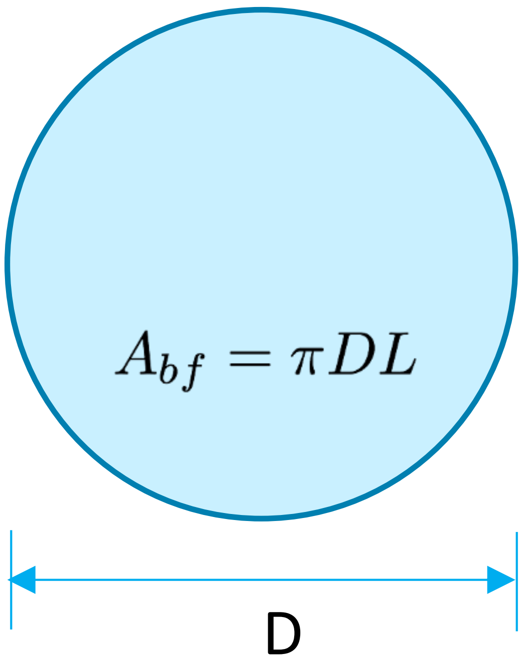
Simulations to estimate methane production under each set of sewer conditions

Non-linear regression of the simulation results data to develop a correlation between the sewer parameters and the methane production

Network Data
Pipe length (L)
Pipe diameter (D)
Average daily flow
Pump run time (hours/day)
Temperature

Methane production in each pipe section to obtain total methane production in the entire sewer network

EMPIRICAL MODEL DEVELOPMENT FOR FORCE MAIN SEWER

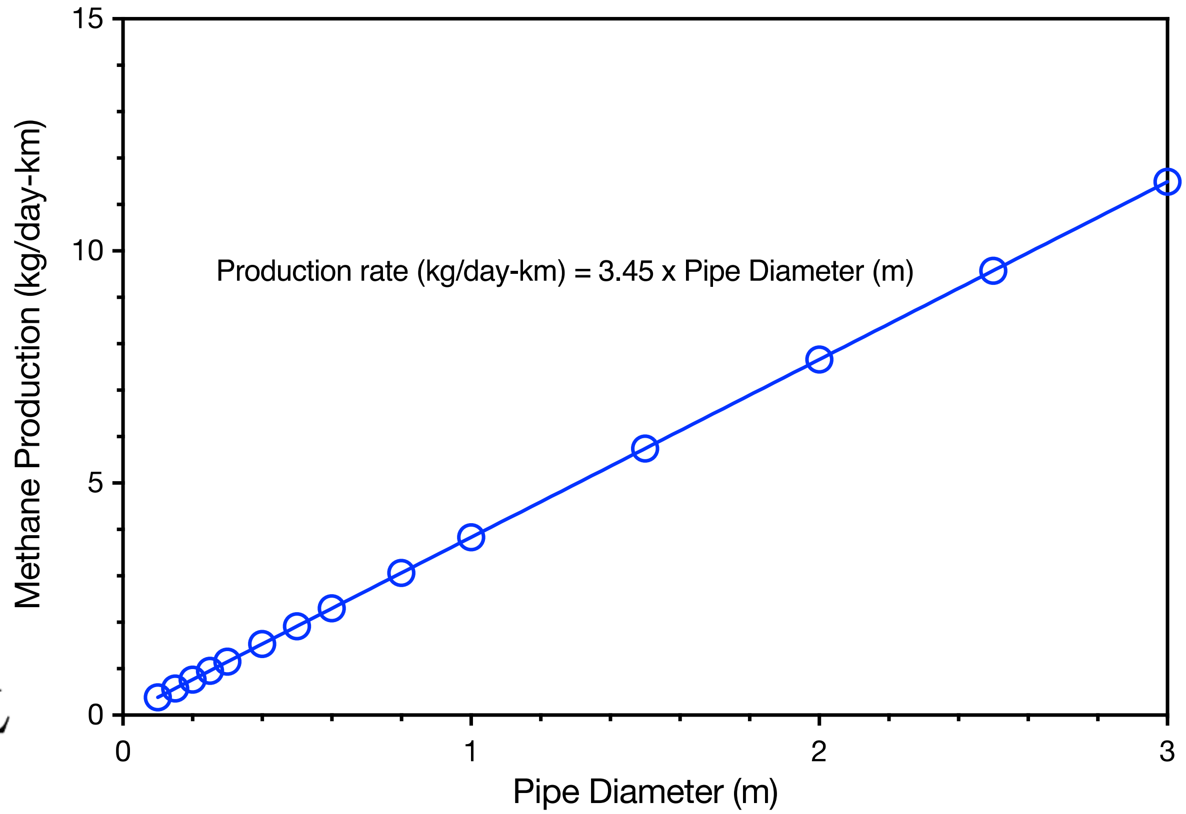


$$r_{CH_4} = k' \cdot A_{bf} = k \cdot D \cdot L$$

Production rate per unit length

$$r_{CH_4} = k \cdot D$$

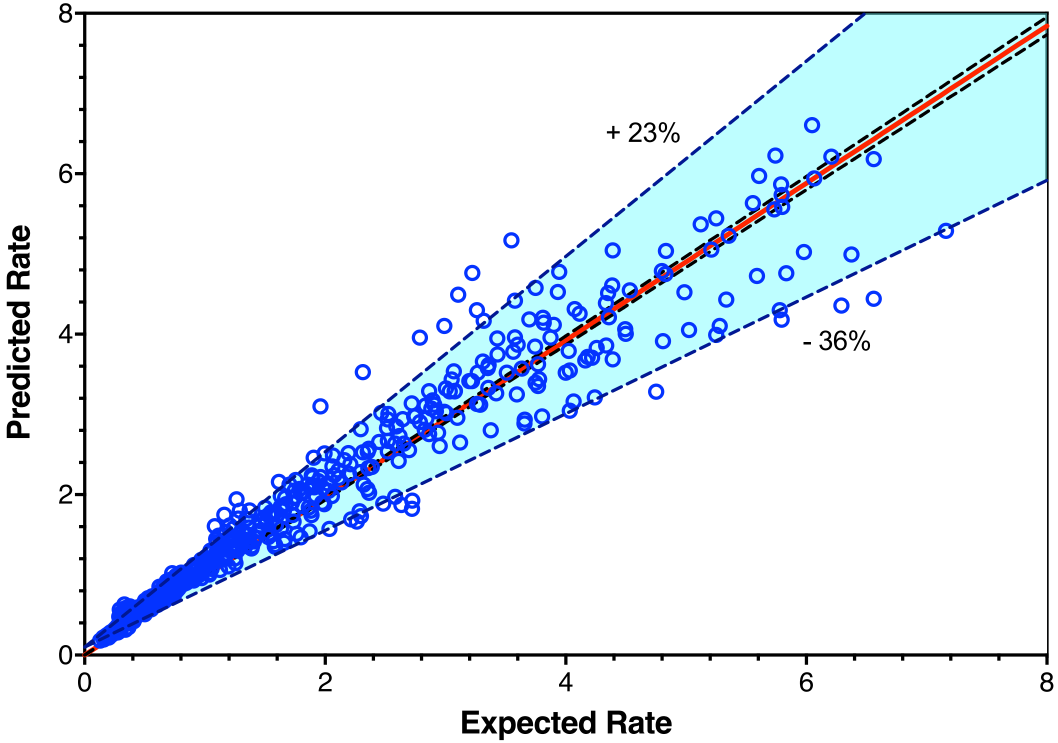
$$k_T = k_{20} \cdot 1.05^{(T-20)}$$



$$r_{CH_4,20} = 3.45 \cdot D$$

EMPIRICAL MODEL DEVELOPMENT FOR FORCE MAIN SEWER

Methane Production Rate (kg/day-km)



Estimated Values for Parameters

Parameter	Estimated value	SE
α	0.202	0.0054
β	0.396	0.0087

$$r_{CH_4,20} = 3.45 \cdot D.N_P^{\alpha}.\beta^{(1-N_P \times P_I/1440)}$$

Where,

r_{CH_4} = Methane production rate (kg/km-day)

T = Temperature(°C)

D = Pipe diameter (m)

N_P= Number of pumping events per day

P_I= Average pumping interval (min)

MODEL APPLICATION – PRESSURE MAIN

Calculation of methane production rate for C27 rising main (Summer)

Pipe No.	Pipe Length (km)	Pipe Diameter (m)	Temperature (°C)	No of pumping events/day	Average Pumping Interval (min)	Methane Production (kg/day)
1	2.04	0.525	28	43	6.37	5.94
2	0.09	0.225	28	19	6.76	0.08
3	0.47	0.525	28	62	5.90	1.56
4	0.06	0.100	28	16	3.92	0.02
5	1.10	0.525	28	75	5.45	3.91
6	0.01	0.150	28	21	2.07	0.00
7	0.20	0.525	28	94	4.61	0.76
8	1.22	0.330	28	41	2.17	1.96
9	0.20	0.525	28	126	3.91	0.83
10	0.54	0.150	28	43	15.44	0.57
11	0.40	0.525	28	164	5.55	2.30
					Total:	17.95

Data Series	No of days of measurement	Total measured methane (kg)	Total methane predicted by the model (kg)	Difference
Summer	27	23.46	17.95	-23.49%
Winter	26	15.18	15.07	-0.73%

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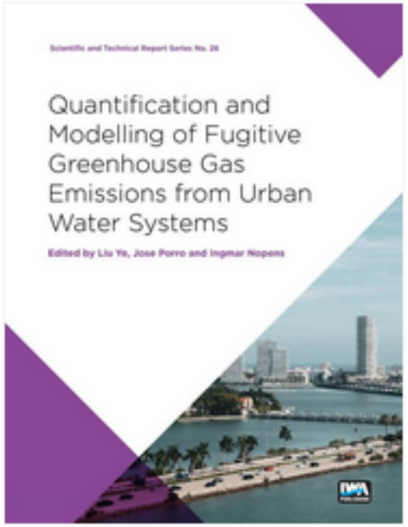
MODELLING N_2O EMISSIONS

-STATE OF THE ART –
-MODELLING OF FULL SCALE NITRIFYING BIOFILM REACTOR

Mathieu Sperandio
(sperandio@insa-toulouse.fr)
INSA, France
Toulouse Biotechnology Institute

DETERMINISTIC MODELS FOR N_2O EMISSION STATE OF THE ART



Quantification and Modelling of Fugitive Greenhouse Gas Emissions from Urban Water Systems

Edited by Liu Ye;, Jose Porro;, Ingmar Nopens

IWA Publishing

DOI: https://doi.org/10.2166/9781789060461

Chapter 7

Modelling N_2O production and emissions

Mathieu Spérandio[1], Longqi Lang[1], Fabrizio Sabba[2], Robert Nerenberg[2], Peter Vanrolleghem[3], Carlos Domingo-Félez[4], Barth F. Smets[4], Haoran Duan[5], Bing-Jie Ni[5] and Zhiguo Yuan[5]

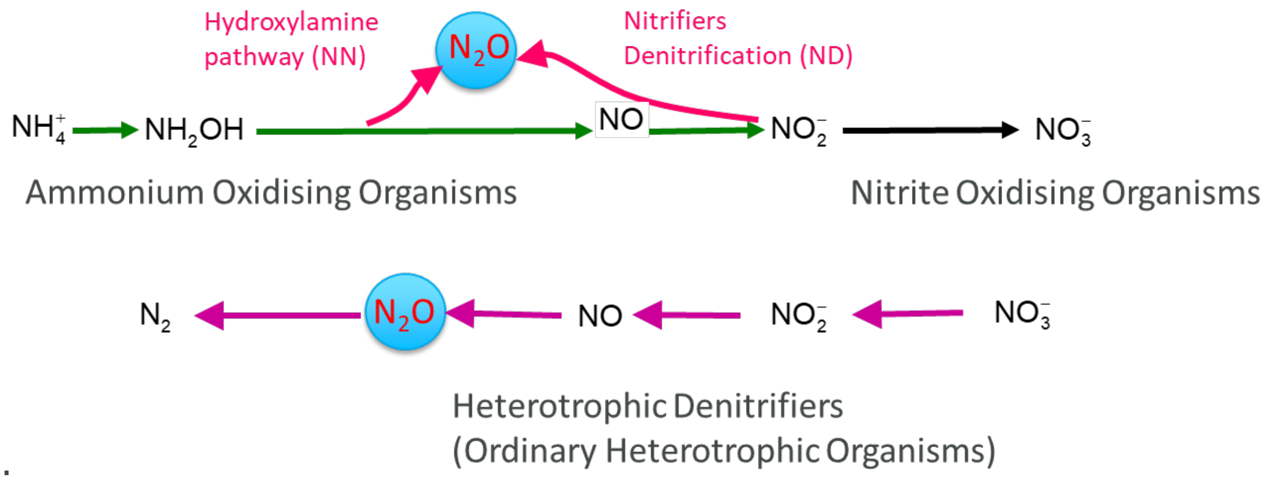
[1]TBI, Université de Toulouse, CNRS, INRAE, INSA, Toulouse, France. E-mail: sperandio@insa-toulouse.fr
[2]Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre Dame, IN 46556, USA
[3]Modeleau, Département de génie civil et de génie des eaux, Université Laval, 1065 av. de la Médecine, Québec, QC G1V 0A6, Canada
[4]Department of Environmental Engineering, Technical University of Denmark, 2800 Kongens Lyngby, Denmark
[5]Advanced Water Management Centre, The University of Queensland, St Lucia, QLD 4072, Australia. E-mail: z.yuan@awmc.uq.edu.au

SUMMARY

Mathematical modelling of N_2O emissions is of great importance for the understanding and reduction of the environmental impact of wastewater treatment systems. This chapter reviews the current status of the modelling of N_2O emissions from wastewater treatment. The existing mathematical models describing all known microbial pathways for N_2O production are reviewed and discussed. These include N_2O production and consumption by heterotrophic denitrifiers, N_2O production by ammonia-oxidizing bacteria (AOB) through the hydroxylamine oxidation pathway and the AOB denitrification pathway and the integration of these pathways in single-pathway N_2O models. The two-pathway models are compared to single-pathway models. The calibration and validation of these models using lab-scale and full-scale experimental data is also reviewed. The mathematical modelling of N_2O production, while still being enhanced by new knowledge development, has reached a maturity that facilitates the estimation of site-specific N_2O emissions and the development of mitigation strategies for wastewater treatment plants taking into account the specific design and operational conditions of the plant.

Keywords: AOB pathways, calibration, heterotrophic denitrification, modelling, N_2O

DETERMINISTIC N_2O MODELLING
STATE OF THE ART

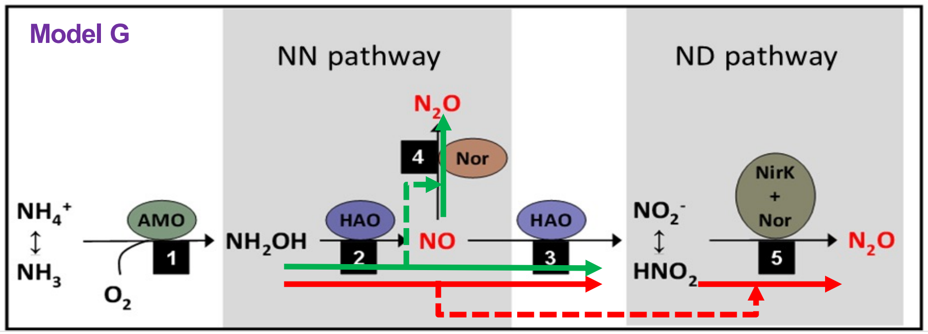


- N_2O models related to denitrification
  - **Multistep denitrification (N_2O, NO), ASMN:** Hiatt and Grady 2008
  - **Other concepts, electrons carriers :** Pan et al., 2013 ; Domingo-Félez and Smets 2020
- N_2O models related to nitrification
  - **Single pathway (Nitrifier denitrification – ND):** 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
- N_2O models related to chemical pathways
  - Harper *et al.*, 2015 ; Su *et al.*, 2019

COUPLING MICROBIAL REDUCTION AND OXIDATION PROCESS

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

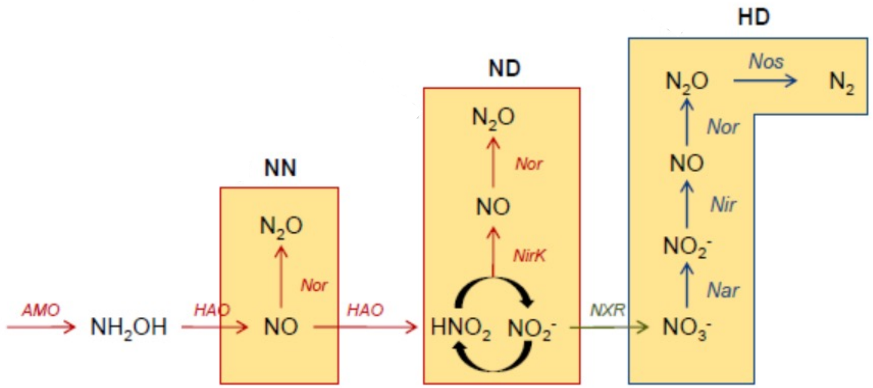
Nitrification: 2-pathway model (Pocquet et al., 2016)



Stoichiometry of the 2 pathway model (Gujer matrix).

Process	S_{NH}	S_{NH2OH}	S_{NO}	$S_{NO_2^-}$	S_{N2O}	S_{O2}	X_{AOB}
1	-1	1				$-8/7$	
2	$-i_{N,BM}$	$-1/Y_{AOB}$	$1/Y_{AOB}$			$-(12/7 - Y_{AOB})/Y_{AOB}$	1
3			-1	1		$-4/7$	
NN 4		-1	-4	1	4		
ND 5		-1		-1	2		

Nitrification + denitrification



Pocquet et al., 2016

Hiatt and Grady, 2008

Model-based evaluation of strategies to mitigate N_2O emissions from a full-scale nitrifying biofilm reactor

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the international water association

- Nitrifying biological active filters (BAFs) (~1 kg NH_4-N m^{-3} d^{-1})
- In Seine Aval WRRF, N_2O emission = 2% to 4% of NH_4-N removed
- ~80% of the carbon footprint

Full-scale quantification of N2O emissions

Seine-Aval WRRF

Justine Fiat, Beatriz Gonzalez Vazquez
Ahlem Filali, Sylvie Gillot, Yannick Fayolle
Jean Bernier, Sam Azimi, Vincent Rocher
Mathieu Spérandio

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NITRIFYING BIOFILTERS: IMPORTANCE OF PHYSICAL DESCRIPTION

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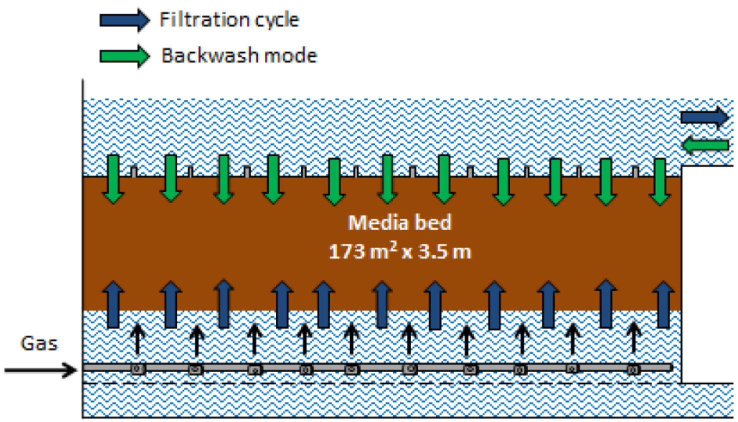
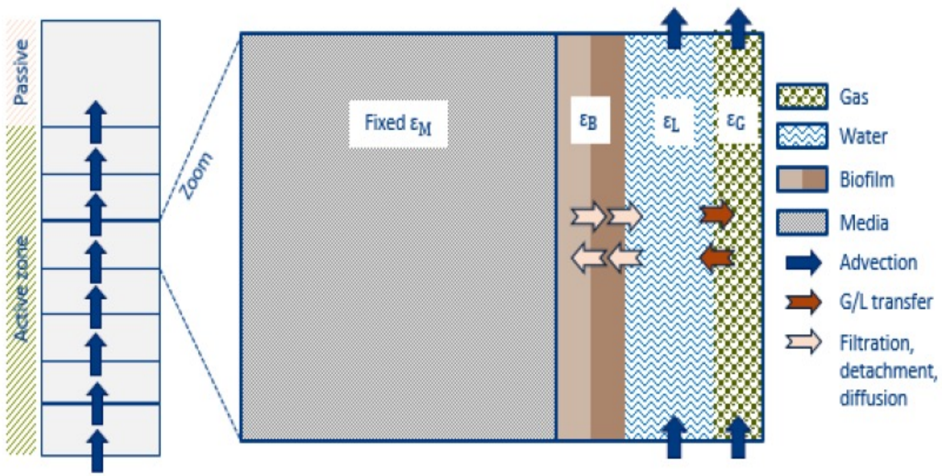
Considering the plug-flow behavior of the gas phase in nitrifying BAF models significantly improves the prediction of N_2O emissions

Justine Fiat [a], Ahlem Filali [a], Yannick Fayolle [a], Jean Bernier [b], Vincent Rocher [b], Mathieu Spérandio [c], Sylvie Gillot [d]

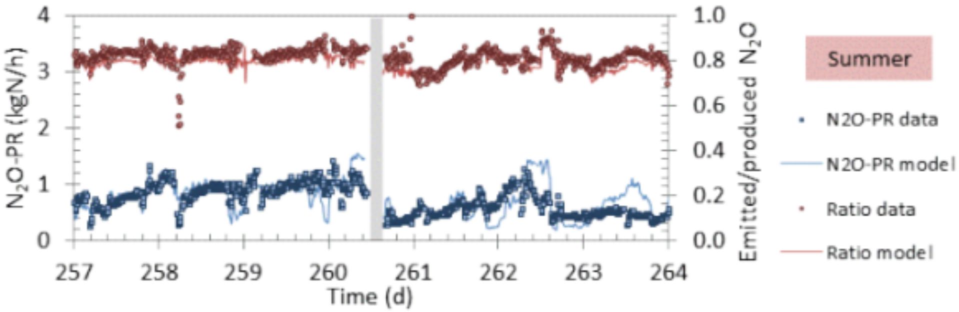


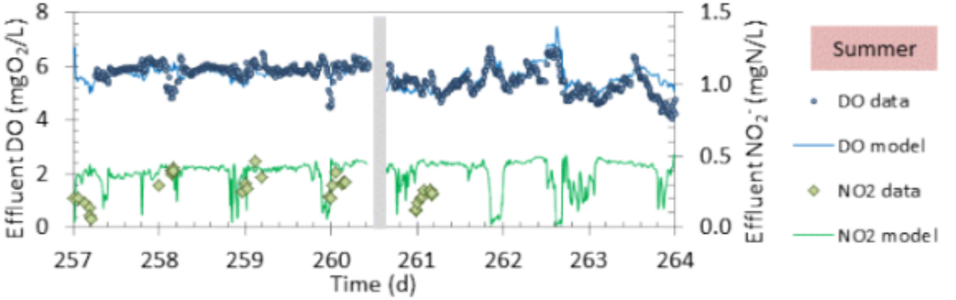
Physical description

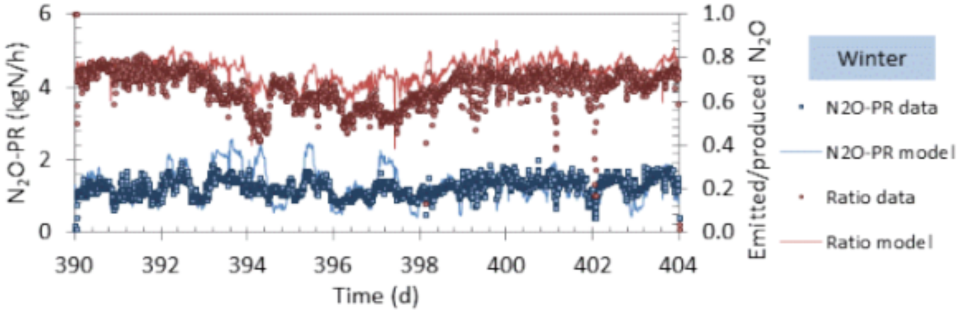
Compartments for gas and liquids

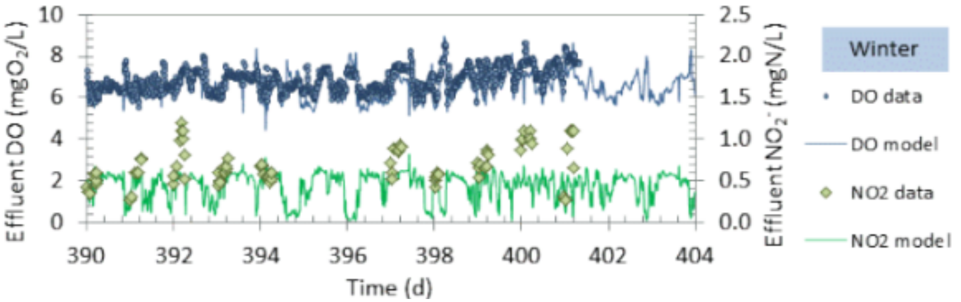


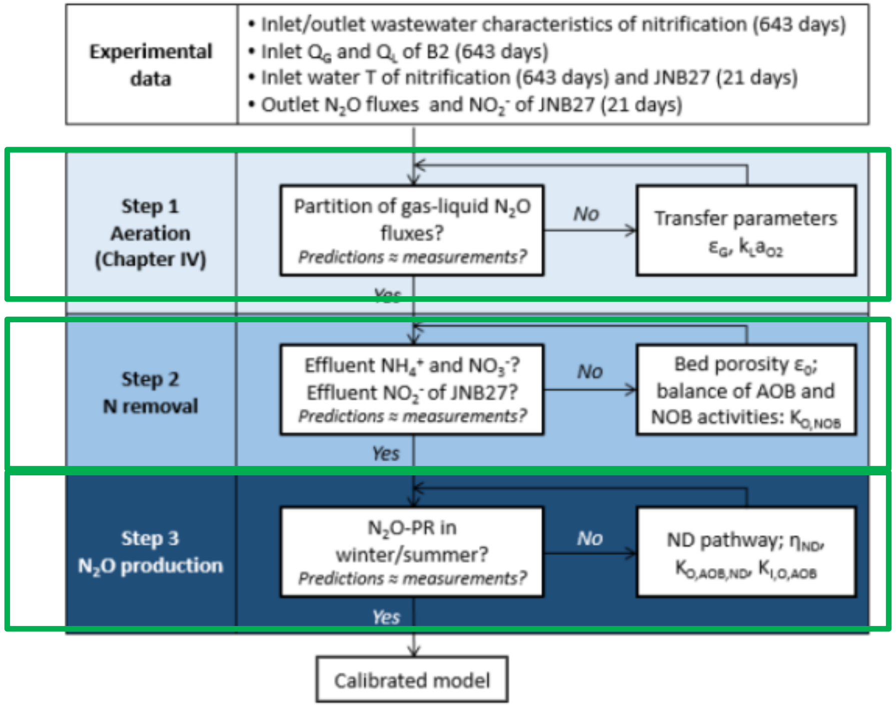
Nitrifying model calibration (Fiat et al., 2019)

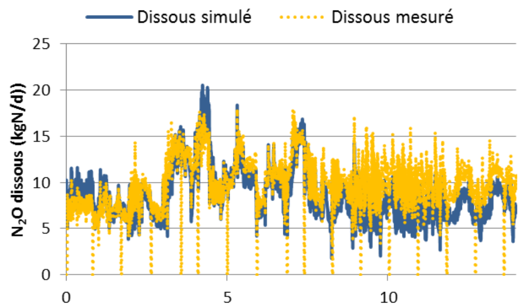




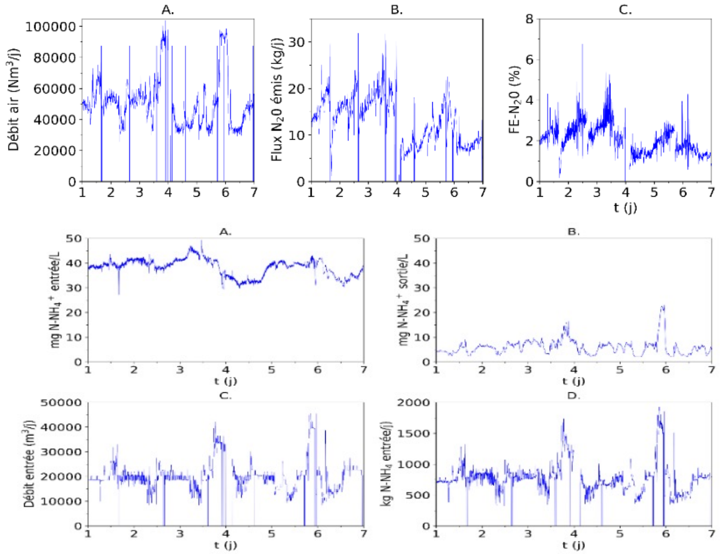


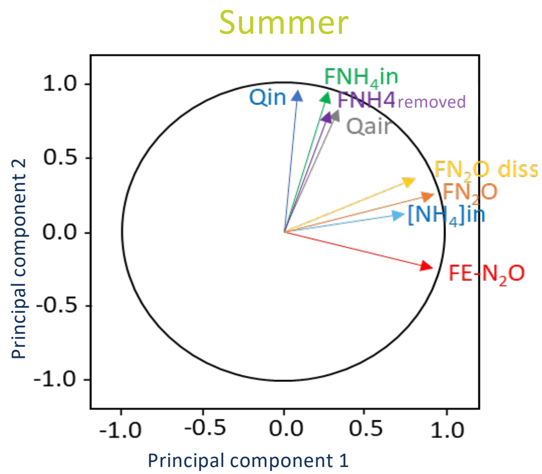


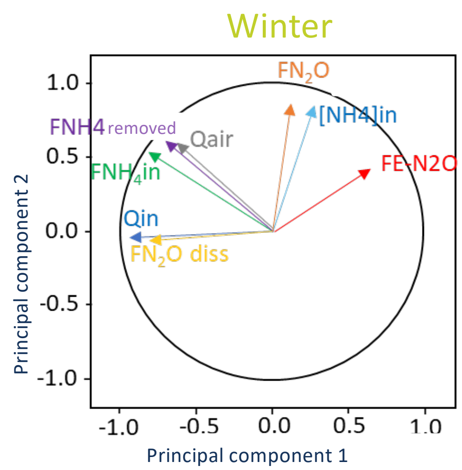




Statistical data analysis: sources of variability?







Major sources of variability: rain (flow, dilution), seasons (temperature, flow, concentration)

- N_2O emission factor correlated to NH_4 concentration (Summer and Winter)
- N_2O emission rate (F-N_2O) correlated to NH_4 concentration and NH_4 loading rate (Winter)
- N_2O emission factor (EF) inversely correlated to Qin (Winter) and flux of dissolved N_2O

Simulation based on long term operational data (2 years) (Fiat et al., 2019)

N_2O emission *vs* NH_4 load

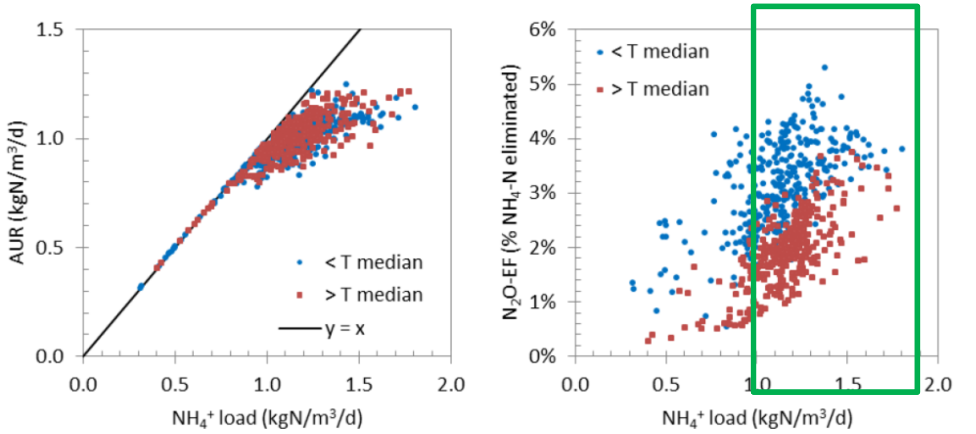


Figure VI.3-4. Evolution of the AUR and N₂O-PR predicted by the model in 2014-2015 with the applied NH₄⁺ load (n = 643).

Concentration in the biofilm

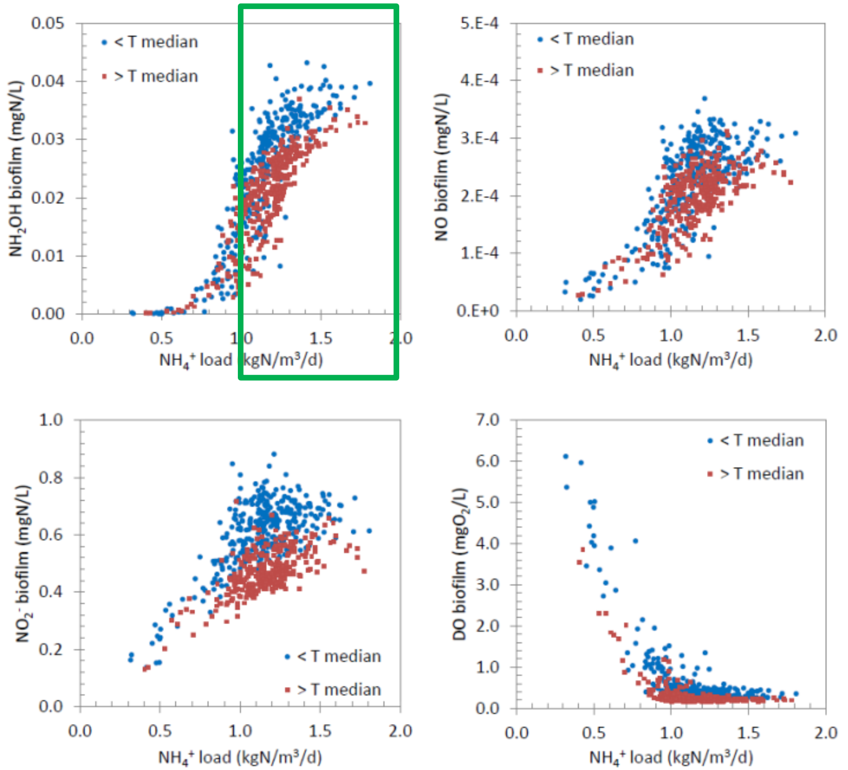
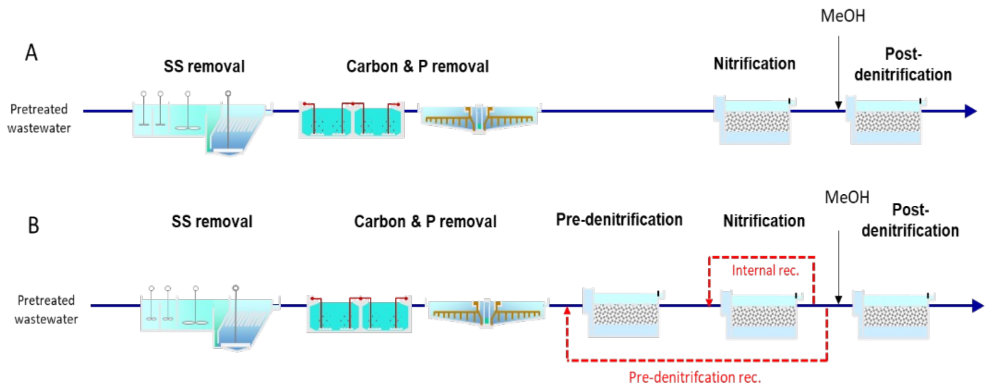


Figure VI.3-6. Evolution of average concentrations in the biofilm predicted by the model in 2014-2015 with the applied NH₄⁺ load (n = 643).

High N_2O emission :

- for high NH_4 load (>1 kg N m^{-3} d^{-1})
  (high NH_4 => high NH_2OH in biofilm)
- in winter (low T, in blue)
  (lower N_2O reduction by heterotrophs)

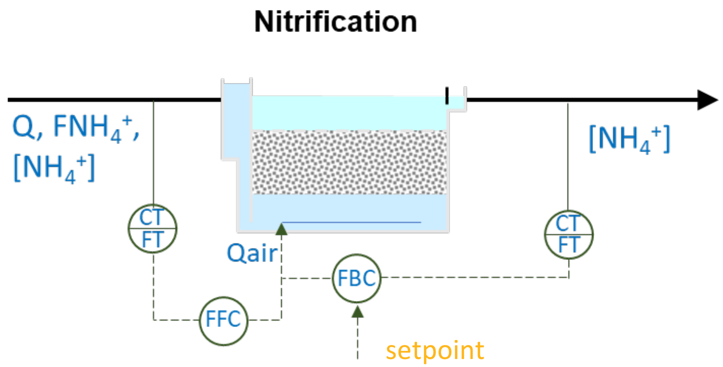
Benchmarking control scenarios (Gonzalez et al., WRRmod 2021)



Air flow control (Q_{air})

expectation: limiting N_2O stripping and DO limitation

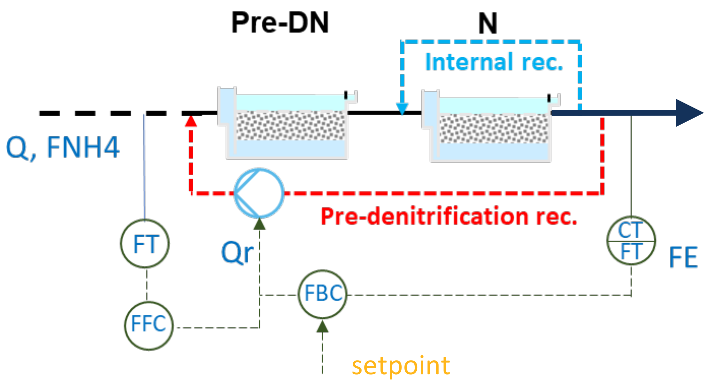
- Feedback with $[NH_4^+]$ out: FB_Air_NH4
- Feedforward with inlet NH_4^+ load: FF_Air_FNH4
- Feedback + feedforward: FF_Air_FNH4 + FB_Air_NH4



Recirculation control (Q_r):

expectation: dilution + liquid circulation, predenitrification of N_2O

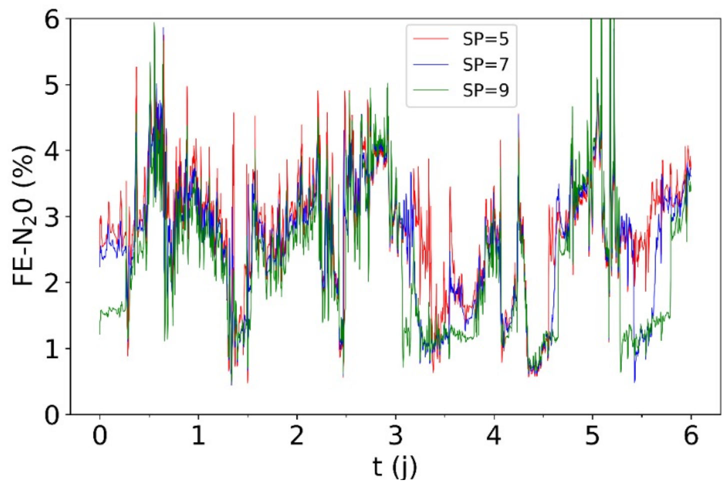
- Feedforward with Qin : FF_Qr_Qin
- Feedforward with Qin and pre-DN
- Feedback with FE N_2O setpoint: FB_QR_N2O



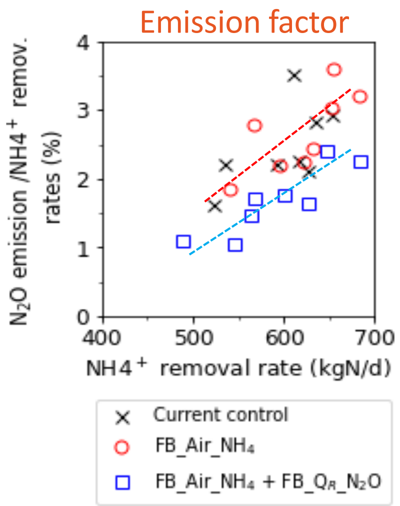
Benchmarking control scenarios

Air flow control

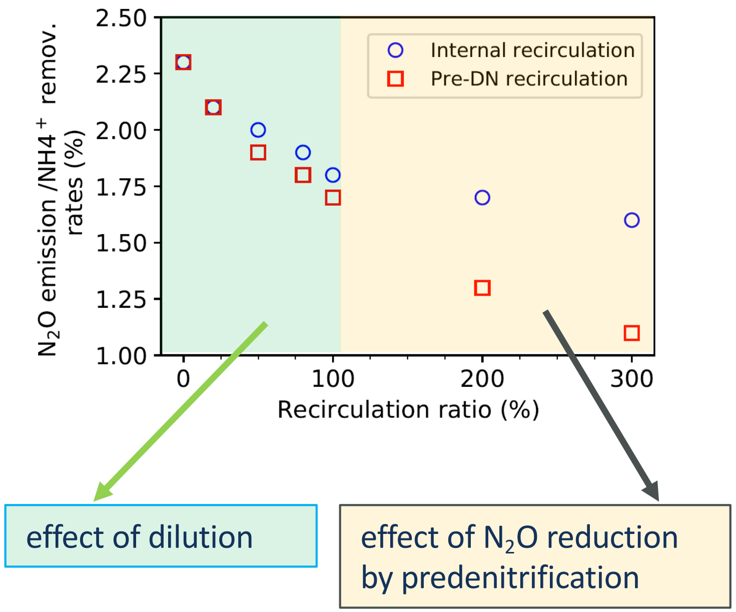
- Emission poorly influenced by the control typology (FF, FB, FF+FB)
- N_2O emission factor (inversely) correlated to $[NH_4]$out setpoint



Recirculation control (Q_r):



- N_2O emission factor reduced by recirculation
- Up to 60 % reduction for recirculation ratio 200%



CONCLUSIONS

- N_2O models reach the age of maturity
  - still perfectible
  - very useful for identifying influencing factors and possible strategies for mitigation
  - … after appropriate calibration

- A major challenge for modelling full-scale systems is to describe appropriately heterogeneities

AGENDA AND HOUSEKEEPING

Speaker 1
Keshab Sharma (Univ. of Queensland, Australia)

Speaker 2
Mathieu Sperandio (INSA, France)

Speaker 3
Wim Audenaert (AM Team, Belgium)

Speaker 4
Xavier Flores-Alsina (Technical University of Denmark)

Speaker 5
Jose Porro (Cobalt Water Global, USA)

Q&A Session Moderator: *Liu Ye (Univ. of Queensland, Australia)*

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FULL 3D SIMULATION FOR ROOT CAUSE ANALYSIS, ENHANCEMENT OF MEASUREMENT CAMPAIGNS AND VIRTUAL MITIGATION STRATEGY TESTING

Wim Audenaert
(Wim.Audenaert@AM-Team.com)

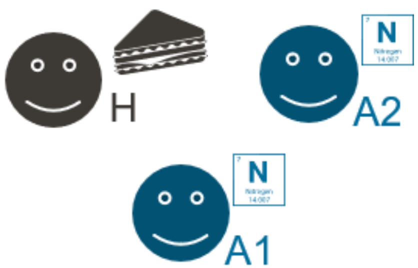
AM TEAM
Advanced Modelling for process optimisation

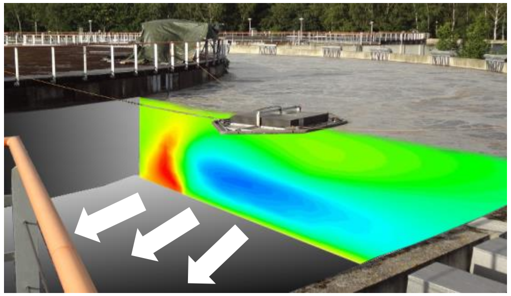
N2O EMISSION IS A 3-STEP PROCESS

Step 1:
N_2O gets **produced** somewhere in your bioreactor (just explained)

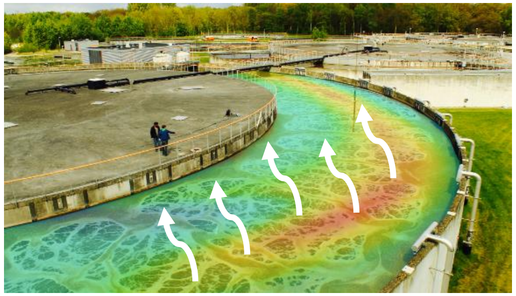
Step 2:
N_2O gets **transported** through the water flow in your bioreactor

Step 3:
N_2O gets **emitted** from your bioreactor





Liquid sensors



Gas measurements

This is the root cause of the problem

This is what we measure

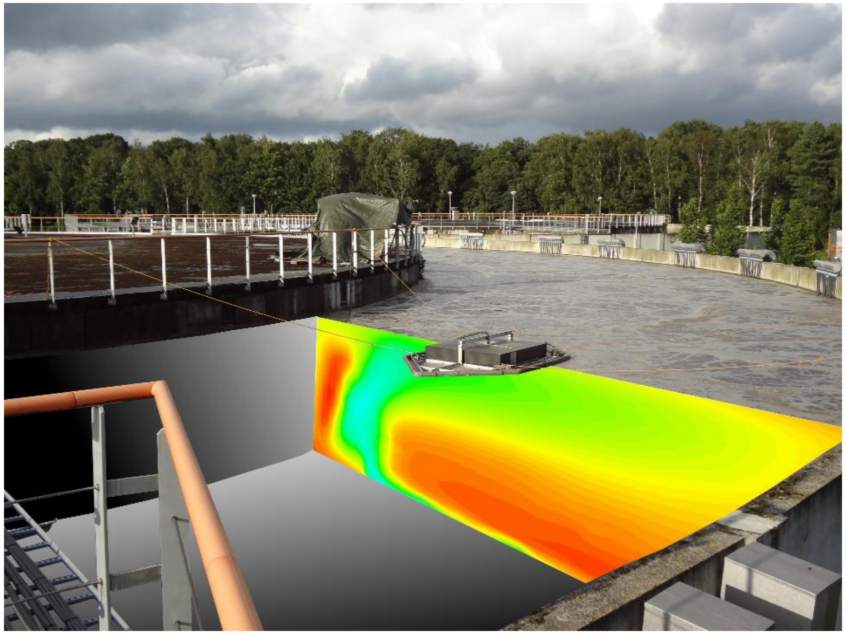
This has climate impact

HOW MODELLING CAN HELP PRACTITIONERS OVERCOMING THE N2O CHALLENGE

- Assessment stage
  - Quantification of N_2O emissions
  - Comparison and prioritization of WWTPs
  - Enhance, reduce or replace onsite measurements
- Mitigation stage
  - Virtual testing of mitigation strategies
  - Comparison and selection of strategies
  - Mitigation + optimisation of effluent quality
  - Obtaining generic learnings every utility can apply

3D PROCESS SIMULATION: COMPUTATIONAL FLUID DYNAMICS (CFD) + BIOKINETICS

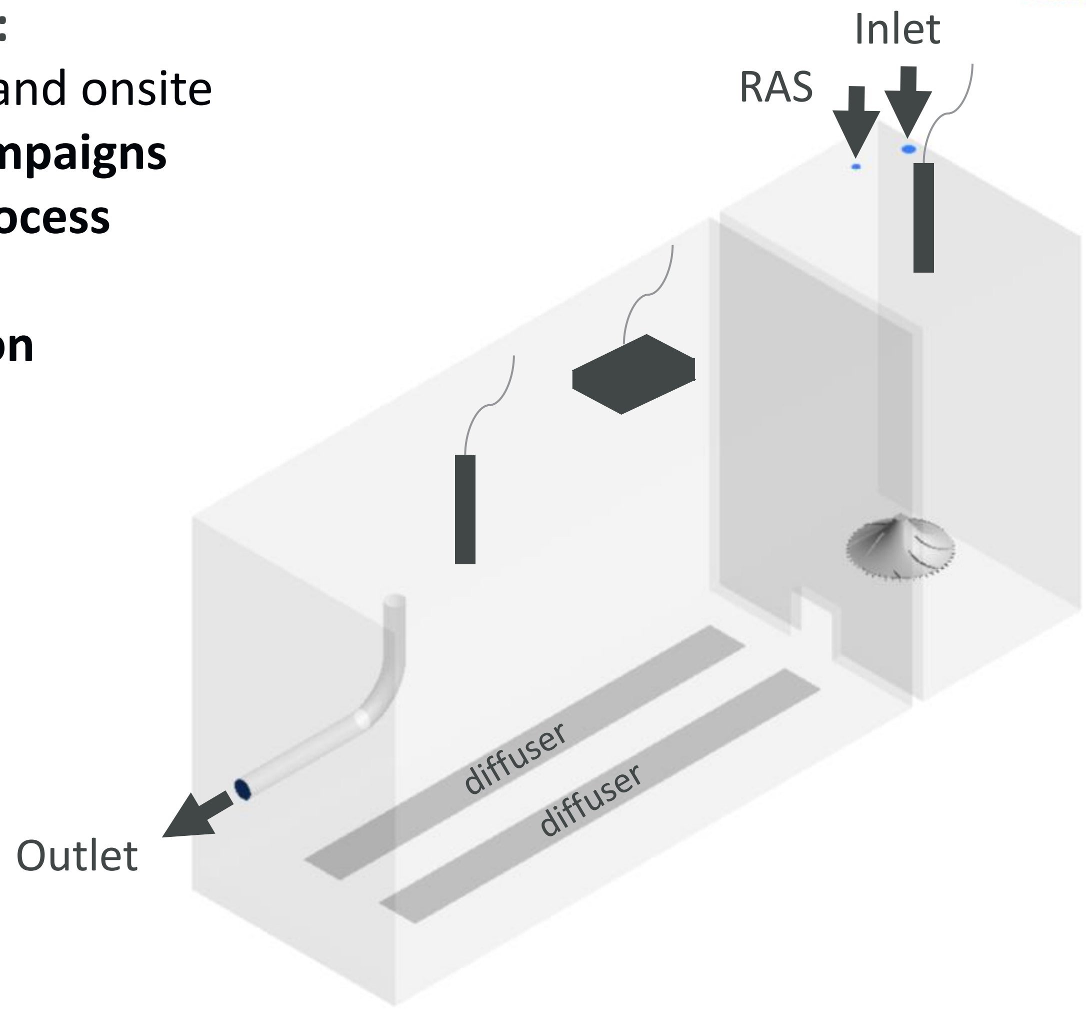
- Physics
  - N2O transport, diffusion, stripping
- Biology
  - ASM models with extended N_2O pathways



CASE FROM NEW ZEALAND

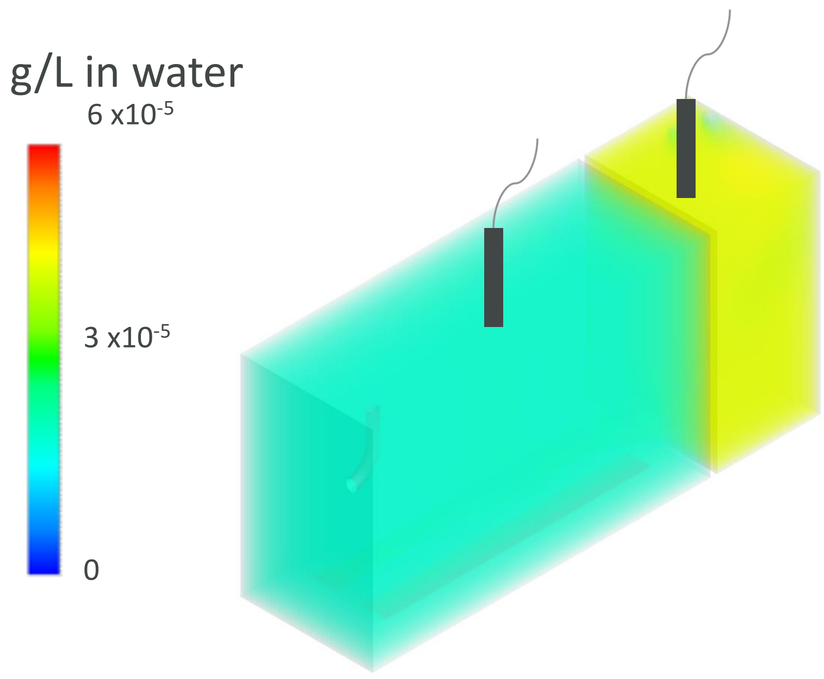
Goals of this project:

- **Enhance** piloting and onsite **measurement campaigns**
- Obtain **generic process understanding**
- Effective **mitigation**

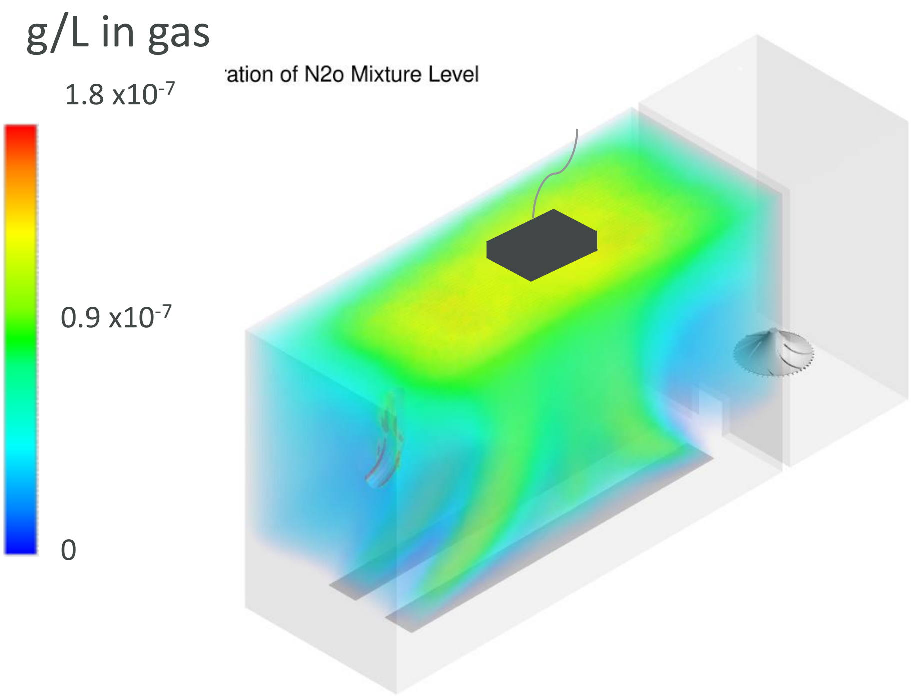


3D SIMULATION RESULTS N2O

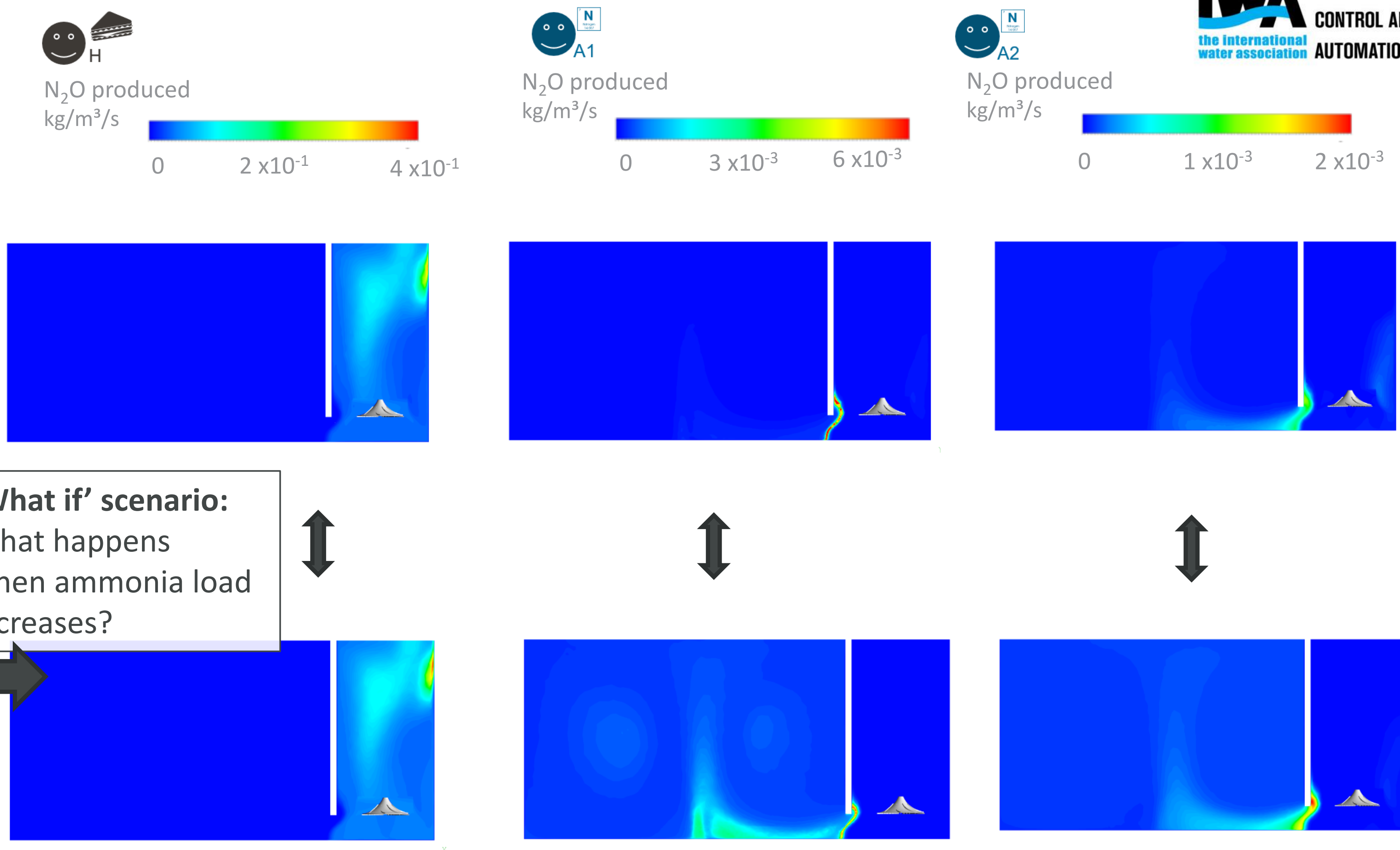
Liquid N_2O concentration



Off gas N_2O concentration



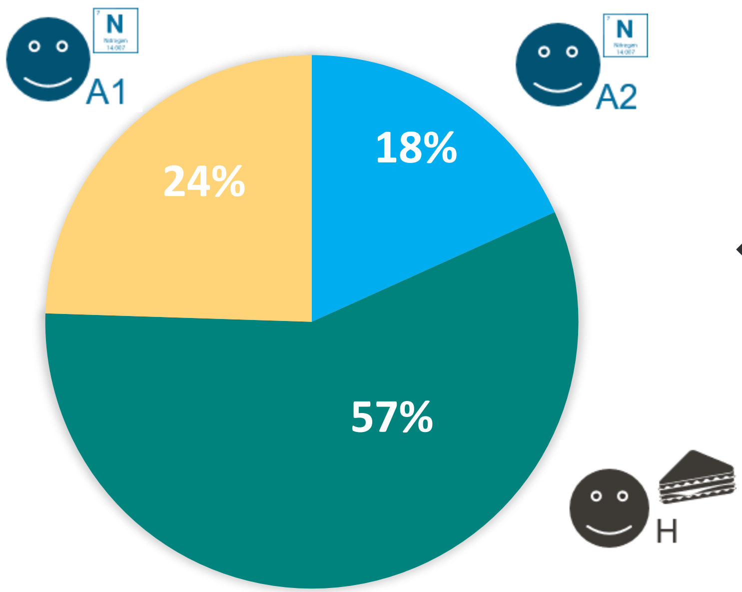
COMPARISON OF PATHWAYS



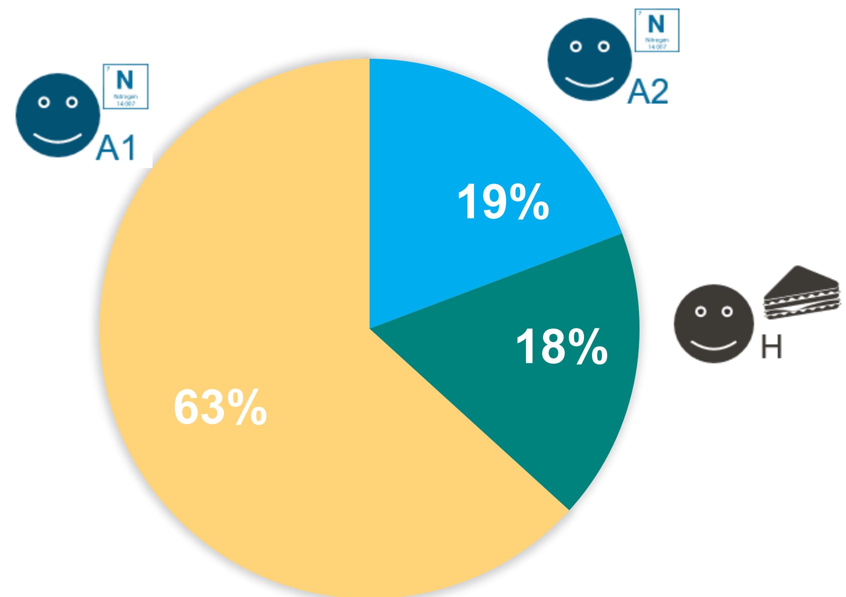
'What if' scenario: What happens when ammonia load increases?

COMPARISON OF ROOT CAUSES

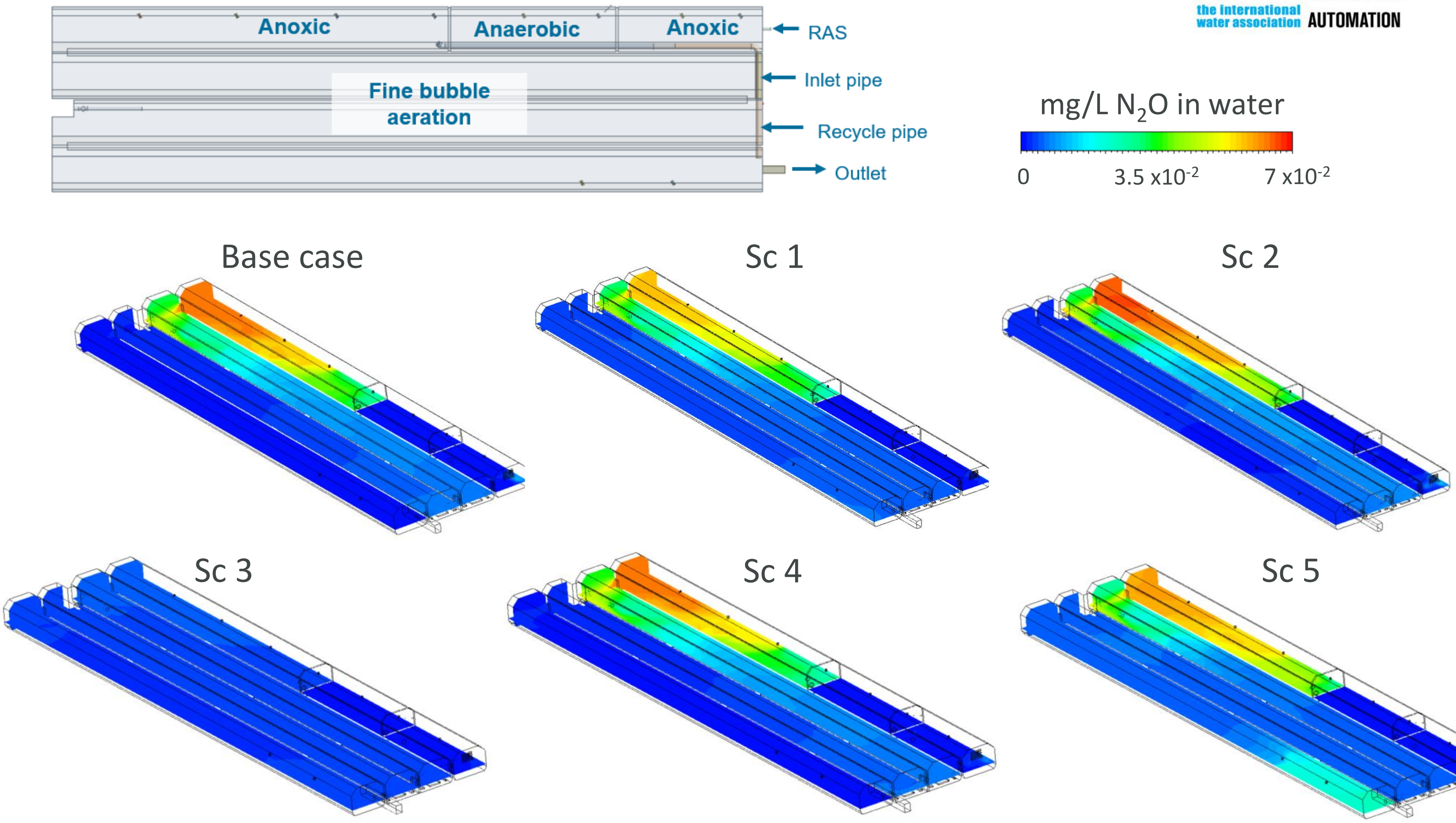
Low ammonia scenario



High ammonia scenario

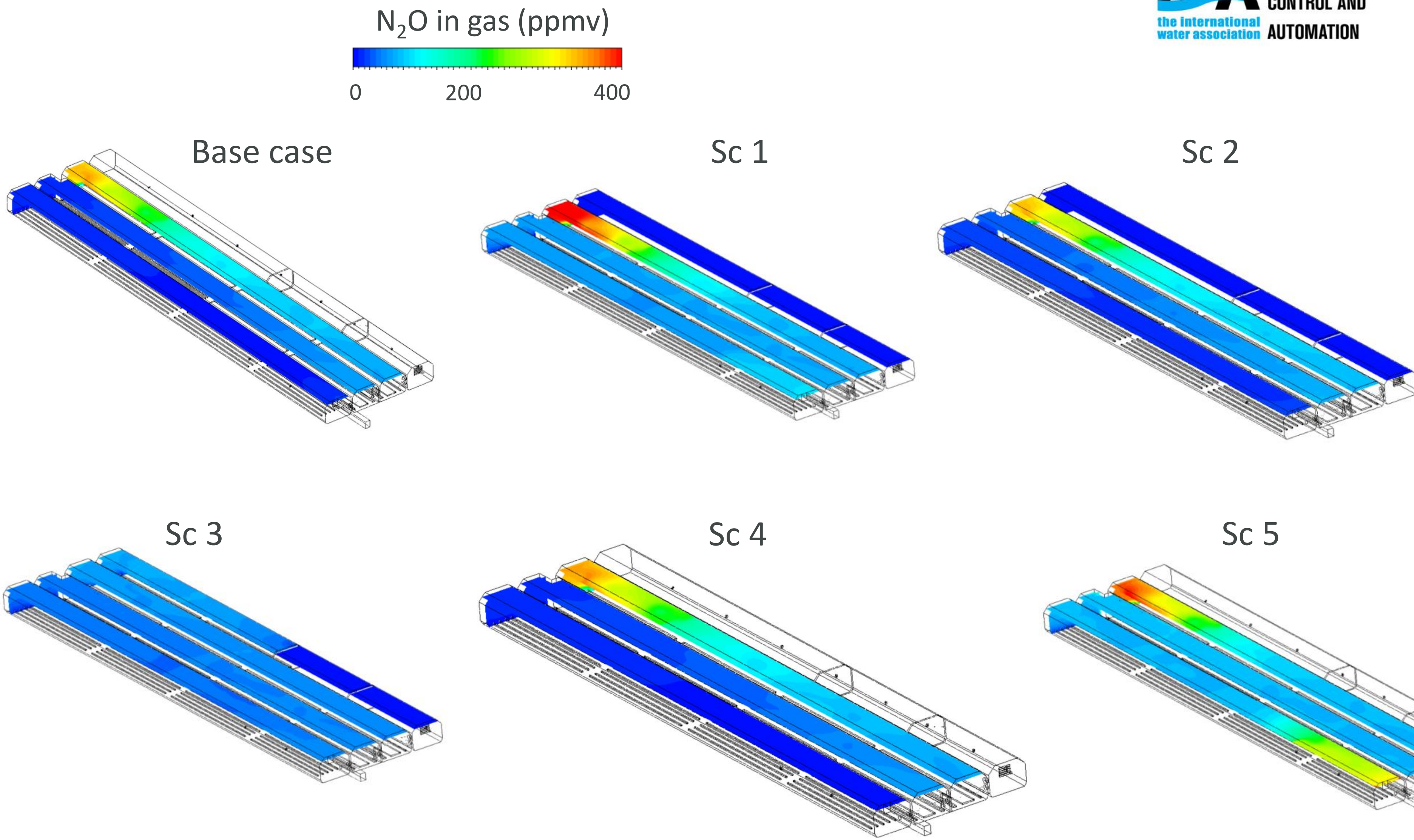


LIQUID N2O CONCENTRATION – FULL-SCALE



LIQUID N2O CONCENTRATION – FULL-SCALE

INSTRUMENTATION CONTROL AND AUTOMATION

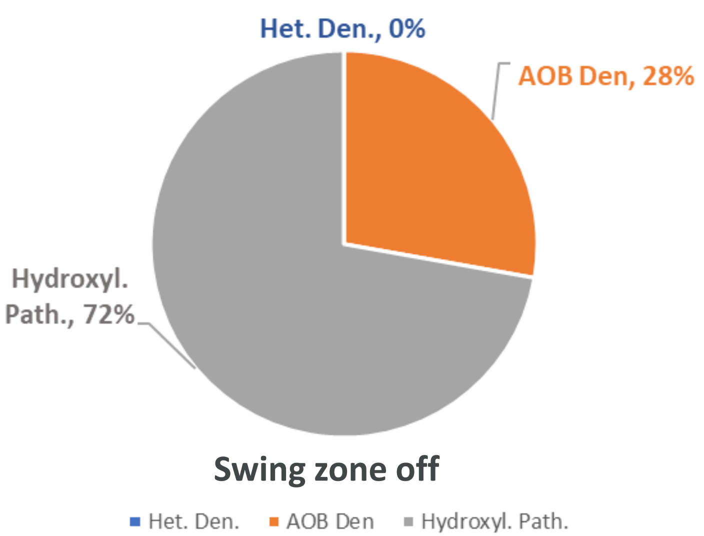


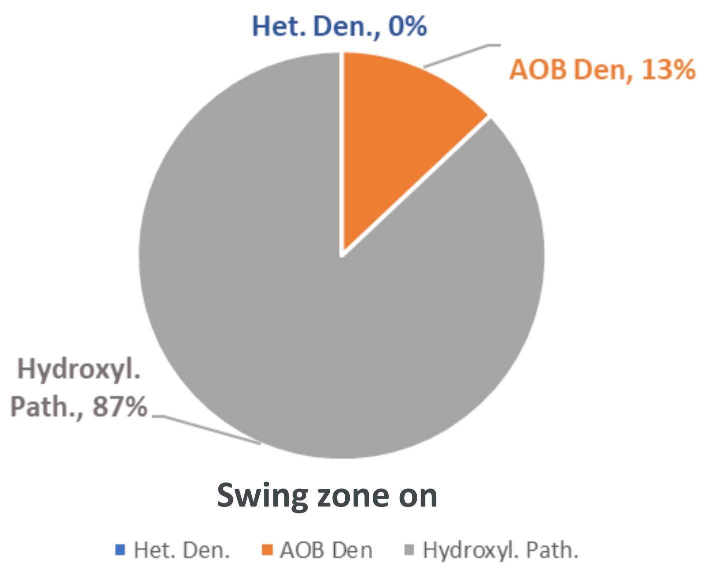
COMPARISON OF 2 SCENARIOS: SWING ZONE

Mass balance

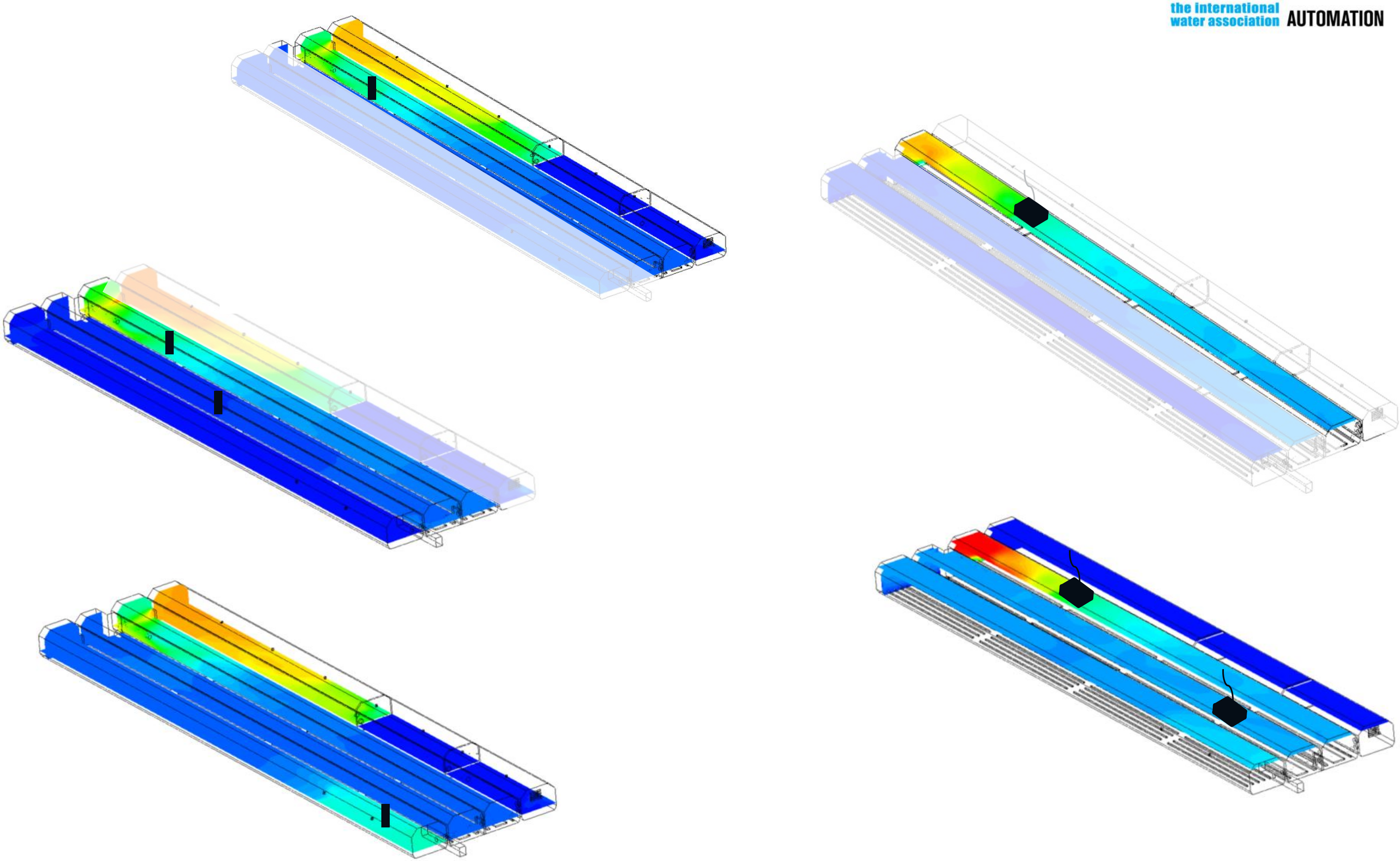
Units: kgN/s	**Swing zone off**	**Swing zone on**
Net production	1.26e-5	6.25e-6
Effluent	2.34e-6	6.83e-7
Off gas	1.03e-5	5.57e-6

Swing zone on:
- 45.9% of emissions
- 50.4% of net N_2O production





GUIDING OF MEASUREMENT CAMPAIGNS



CONCLUSIONS

- The Pareto principle applies to N_2O: 80% of your N_2O can be produced in 20% of your bioreactor
- Onsite N_2O measurements reveal the symptoms. Curing the patient lies in addressing the root causes
- CFD-N_2O simulation acts like an ‘x-ray’
- Many strategies are possible, but the ‘perfect one’ likely does not exist
- CFD-N_2O allows ‘what-if’ testing for N_2O root cause analysis, regulatory reporting, and mitigation

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am-team.com/n2o

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DTU

Benchmarking GHG emissions in water treatment systems: past, present and future prespectives

Xavier Flores-Alsina

Process and Systems Engineering Centre (PROSYS), Department of Chemical and Biochemical Engineering, Technical University of Denmark.

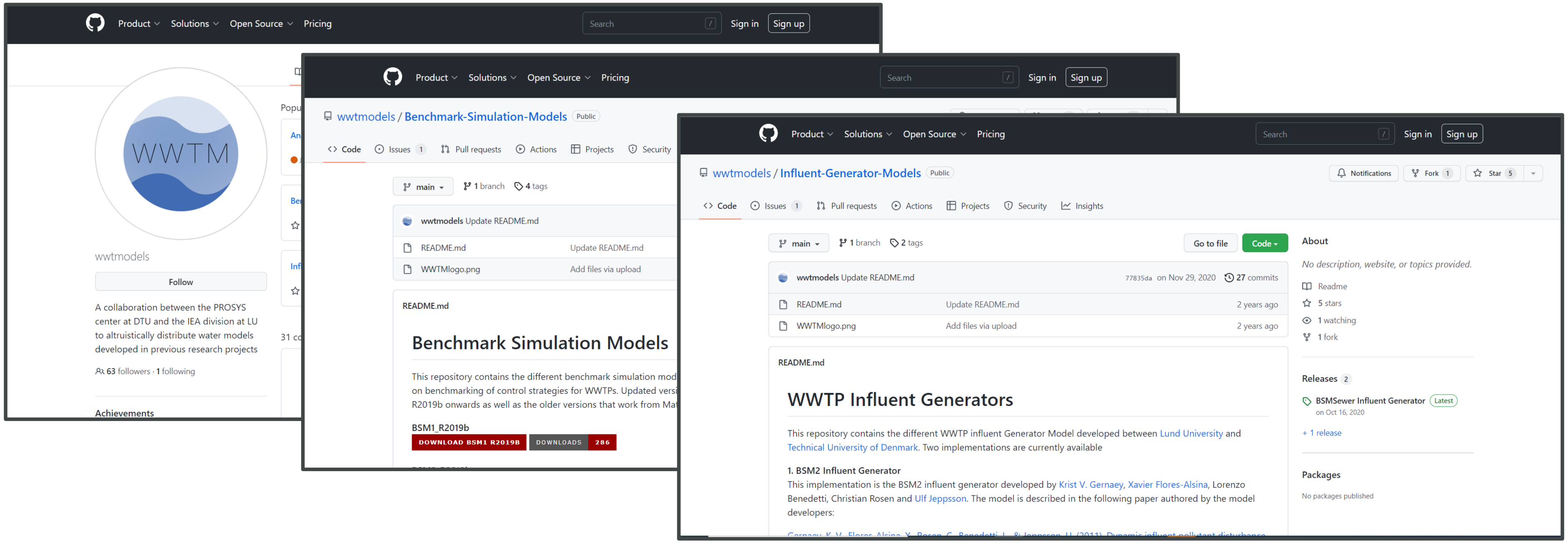
Background information

- BSM development – ongoing effort since 1997
- Work started as part of an EU COST action
- IWA Task Group on *Benchmarking of Control Strategies for WWTPs* initiated in 2005
- Scientific and Technical Report published in 2014
- Now is open access

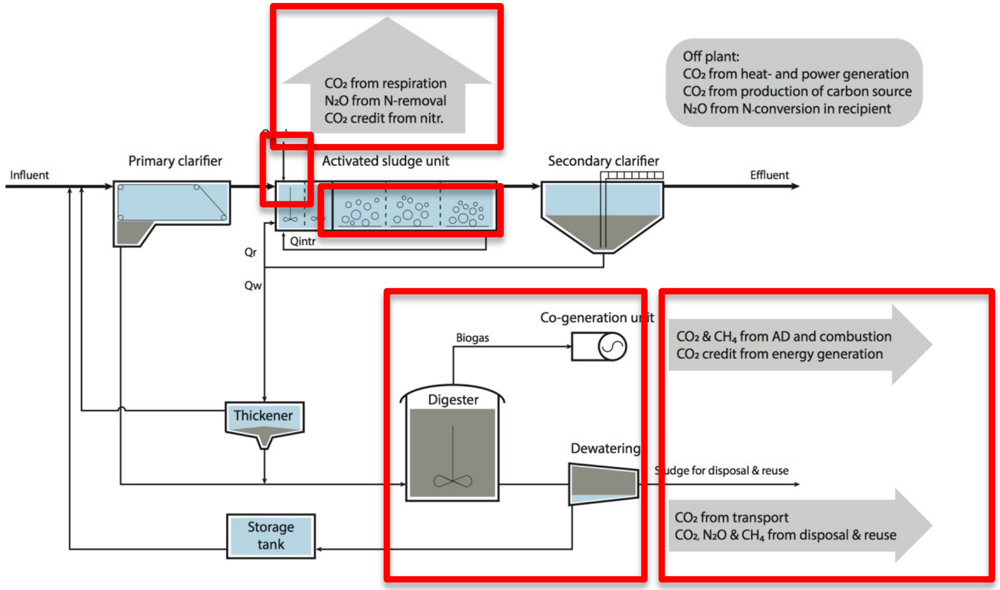
Objective: provide a 'realistic' simulation benchmark protocol for objective comparisons of control and monitoring strategies for WWT systems

Background information

Finalised versions of BSM1, BSM1_LT, BSM2, the influent wastewater generator model and more available for free



Past: How did we include GHG emissions within the BSM platform?



- **Mathematical models**

ASM1 extended with N2O production

ADM1

- **Evaluation criteria**

EQI

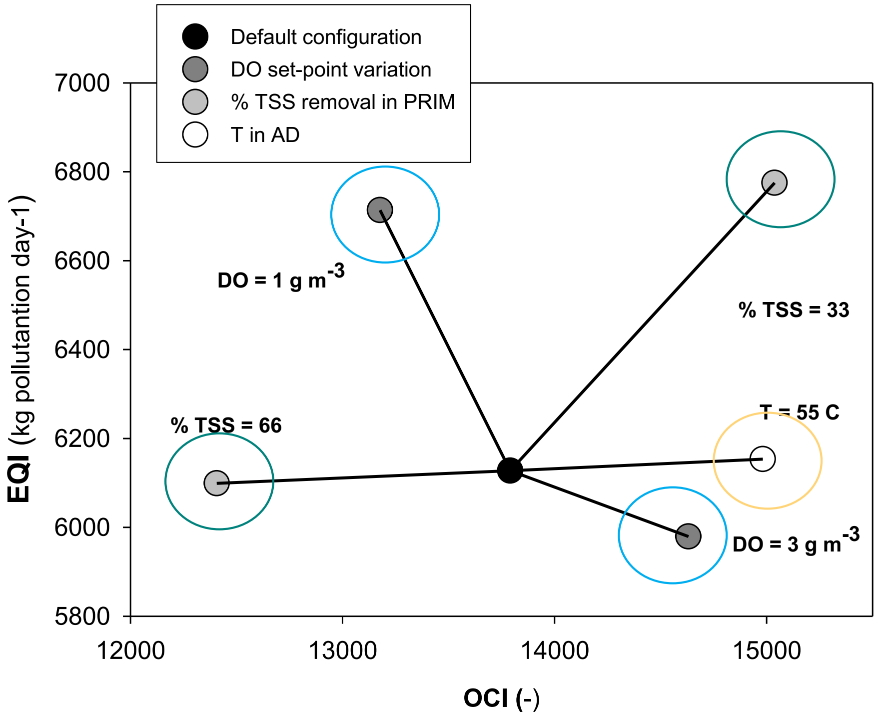
OCI

GHG emissions

  - 1) Direct secondary treatment emissions
  - 2) Sludge Processing
  - 3) Net power GHG
  - 4) Chemicals
  - 5) Sludge disposal & reuse

- **Plant layout, influent disturbances & simulation procedure remain the same**

Simulation results (I)

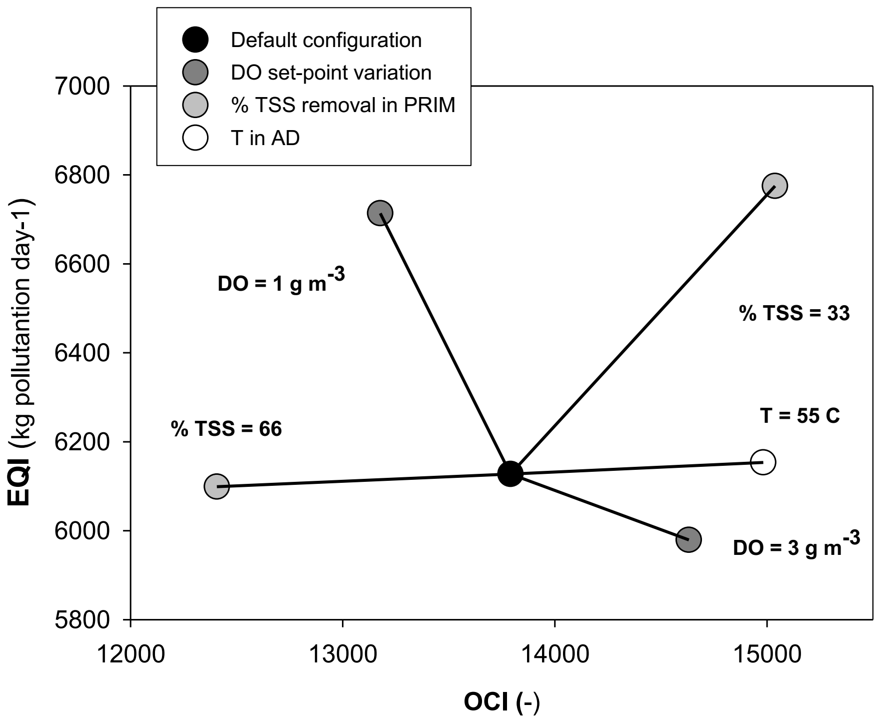


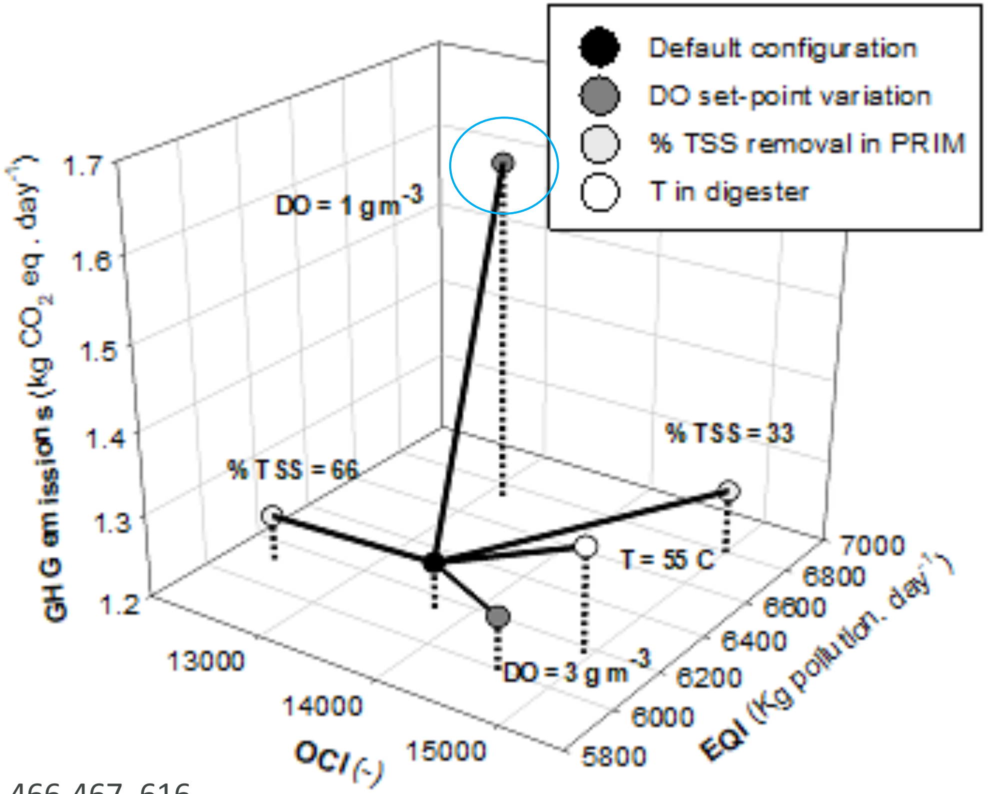
- Higher DO set-points improve EQ but also increase OCI
- Increase TSS efficiency in the primary gives more revenues due to higher energy recovery, but the change in the COD / N ratio damages DN
- Operate in termophilic conditions it is just a more expensive way to operate the plant

Flores-Alsina et al., 2014. Sci. Tot. Env. 466-467, 616

Simulation results (II)

Low DO values, decrease OCI, off-site CO_2 emissions (energy related) but increase N_2O production





Flores-Alsina et al., 2014. Sci. Tot. Env. 466-467, 616

Present : Plant-wide model describing GHG emissions and nutrient recovery options

Water Research 215 (2022) 118223

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journal homepage: www.elsevier.com/locate/watres

A plant-wide model describing GHG emissions and nutrient recovery options for water resource recovery facilities

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Control strategies
EBPR
GHG emissions
BSM2

ABSTRACT

In this study, a plant-wide model describing the fate of C, N and P compounds, upgraded to account for (on-site/off-site) greenhouse gas (GHG) emissions, was implemented within the International Water Association (IWA) Benchmarking Simulation Model No. 2 (BSM2) framework. The proposed approach includes the main biological N_2O production pathways and mechanistically describes CO_2 (biogenic/non-biogenic) emissions in the activated sludge reactors as well as the biogas production (CO_2/CH_4) from the anaerobic digester. Indirect GHG emissions for power generation, chemical usage, effluent disposal and sludge storage and reuse are also included using static factors for CO_2, CH_4 and N_2O. Global and individual mass balances were quantified to investigate the fluxes of the different components. Novel strategies, such as the combination of different cascade controllers in the biological reactors and struvite precipitation in the sludge line, were proposed in order to obtain high plant performance as well as nutrient recovery and mitigation of the GHG emissions in a plant-wide context. The implemented control strategies led to an overall more sustainable and efficient plant performance in terms of better effluent quality, reduced operational cost and lower GHG emissions. The lowest N_2O and overall GHG emissions were achieved when ammonium and soluble nitrous oxide in the aerobic reactors were controlled and struvite was recovered in the reject water stream, achieving a reduction of 27% for N_2O and 9% for total GHG, compared to the open loop configuration.

1. Introduction

In recent years, the scarcity of natural resources and the concern about climate change have shifted the water sector paradigm. Therefore, wastewater treatment plants (WWTPs) are becoming water resource recovery facilities (WRRFs). This fact has promoted both the chemical and environmental engineering community and the water industry to widen the scope of these utilities. To better understand and to design these new facilities, plant-wide modelling tools have become essential (Jeppsson et al., 2013). Wastewater treatment modelling researchers have integrated the main unit operations of a WRRF (primary clarifier, biological reactor, secondary settler, thickeners, anaerobic digester, dewatering unit, etc.) to account for all the interactions amongst processes (Barat et al., 2013; Gernaey et al., 2014; Grau et al., 2007; Hauduc et al., 2019; Solon et al., 2017; Vaneeckhaute et al., 2018) in view of simulating WRRF under different scenarios and of designing novel control strategies for a better performance.

Plant-wide WRRF modelling comprises chemical and physico-chemical models to assess the new challenges of the wastewater treatment. Particularly, precipitation models of common chemical compounds in wastewater (Hauduc et al., 2015; Kazadi Mbamba et al., 2016, 2015b), aqueous phase chemistry models (Flores-Alsina et al., 2015; Solon et al., 2015) and mass transfer models (Amaral et al., 2019; Lizarralde et al., 2015) have been proposed and calibrated to study different subprocesses of a WWRF in addition to the traditional activated sludge models (ASM) based on biological processes (Batstone et al., 2002; Henze et al., 2015). Recently, Solon and co-workers (Solon et al., 2017) proposed a novel plant-wide model capable of predicting the fate of phosphorus (P) in both water and sludge lines as well as the interactions with sulphur (S) and iron (Fe) thanks to the implementation of comprehensive physico-chemical process models. This work combined a

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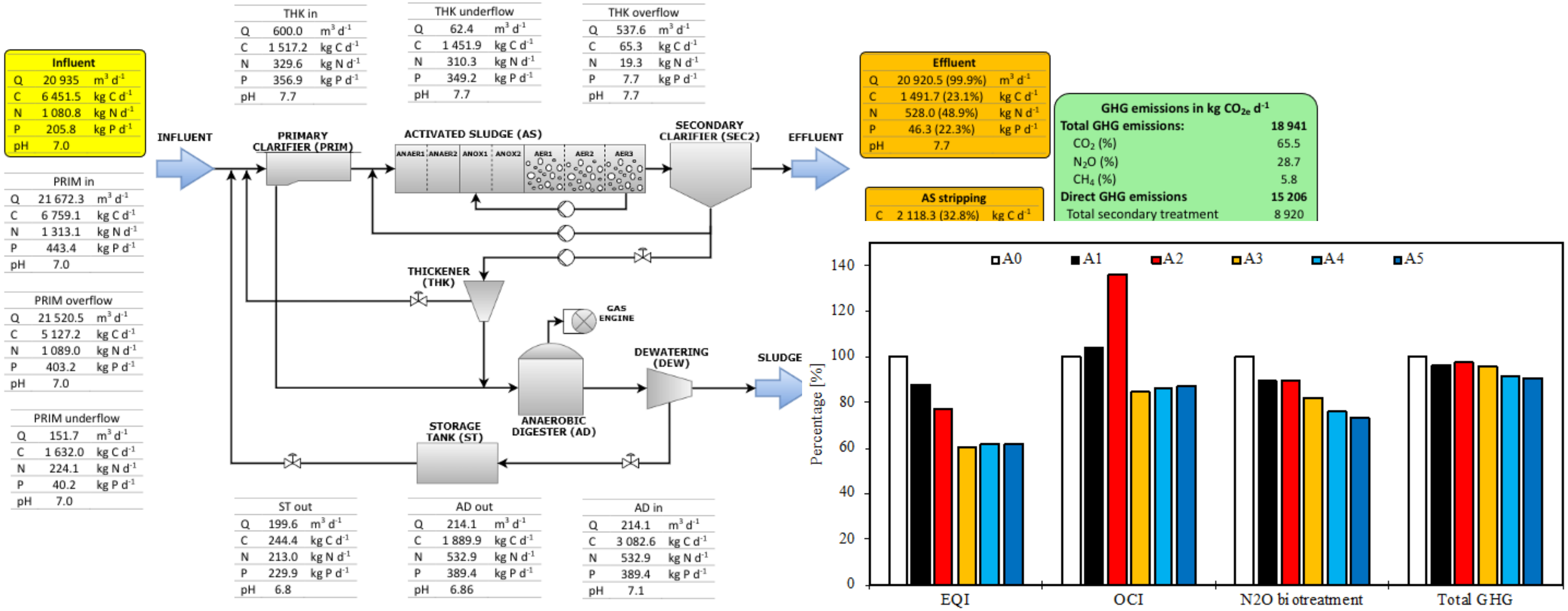
Solis et al., 2022. Water Research. 215, 118223

- **Expanded the scope**

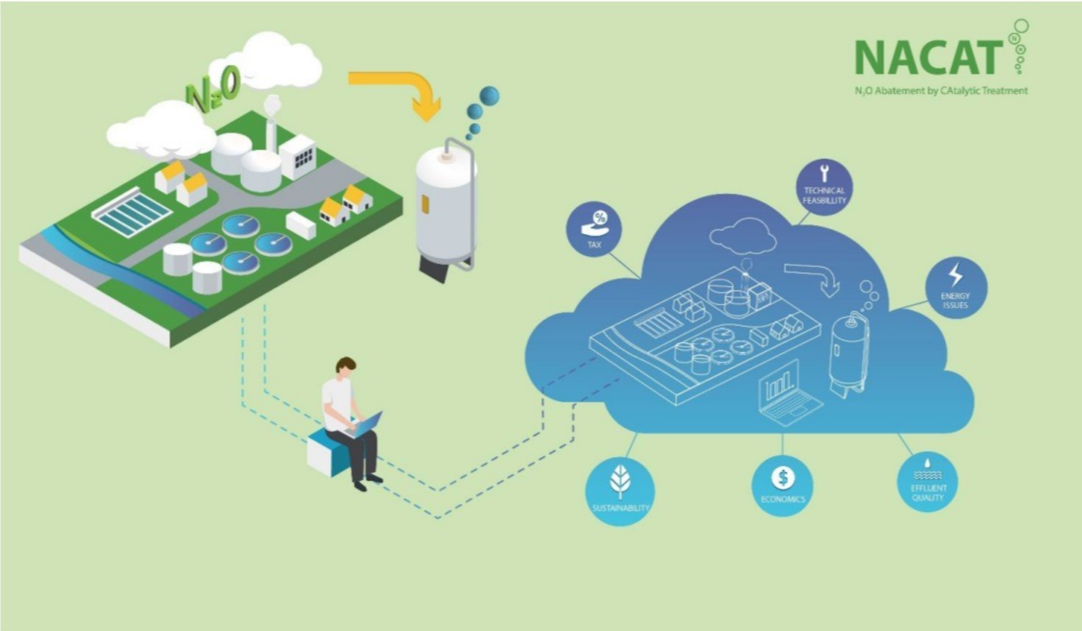
- Modified influent disturbances
- Modified plant layout
- Modified mathematical models (and model interfaces)
- Modified evaluation criteria
- Expanded the potential strategies

Results



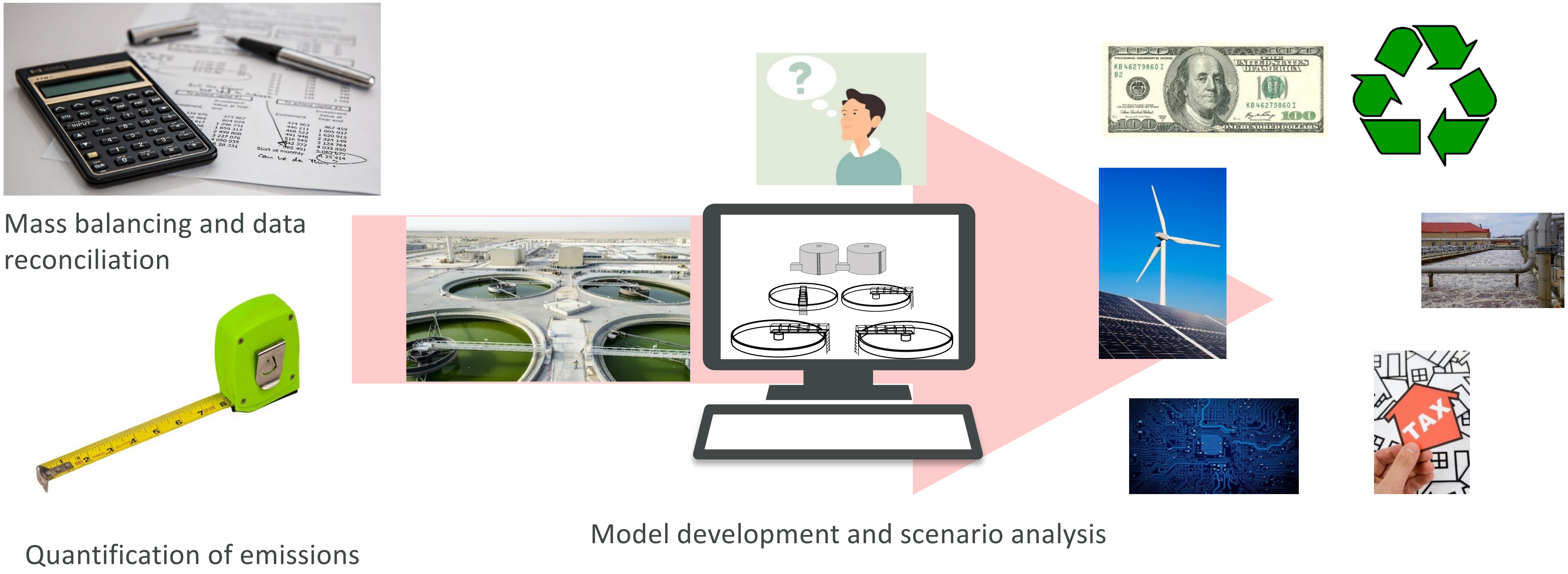
Solis et al., 2022. Water Research. 215, 118223

Future : Virtual replicas to assess catalytic treatment



mudp
TOPSOE
TÅRNBYFORSYNING
EnviDan
DTU
VandCenterSyd
Hillerød Forsyning

Future : Virtual replicas to assess catalytic treatment



Conclusions and take home messages

- The inclusion of GHG emissions provides an additional criterion when evaluating control/operational strategies in a WWTP, offering a better idea about the overall “sustainability” of plant control/operational strategies.

- Simulation results show the risk of energy-related (aeration energy in AS/energy recovery from AD) optimization procedures, and the opposite effect that N_2O and its 300-fold stronger GHG effect (compared to CO_2) might have on the overall GWP of the WWTP.

- The importance of considering the water and sludge lines together and their impact on the total quantity of GHG emissions are shown when the temperature regime is modified and the anaerobic digester supernatants return flows controlled.

- While these observations are WWTP specific, the use of the developed tools is demonstrated and can be applied to other systems

AGENDA AND HOUSEKEEPING

Speaker 1
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Q&A Session Moderator: *Liu Ye (Univ. of Queensland, Australia)*

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Using AI and machine learning for accounting of, reducing, and monitoring wastewater N2O process emissions

Jose Porro and Mickaël Tessier, Cobalt Water Global

IWA Specialist Group on Modelling and Integrated Assessment Webinar Series

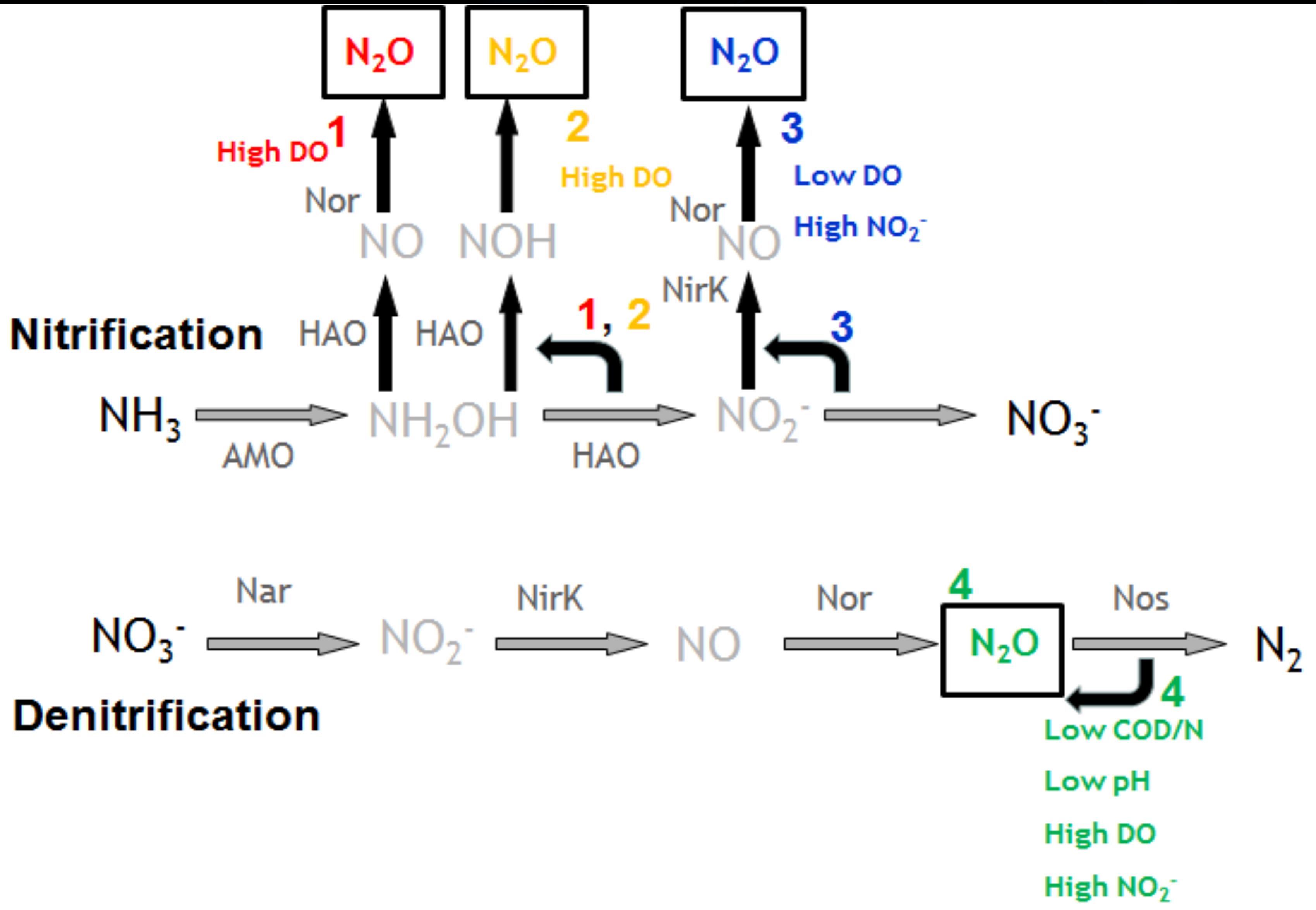
Modelling greenhouse gas emissions from urban wastewater systems: State-of-the-art and beyond

21.November.2022

The N2O Reduction Journey

- *Accounting/screening/prioritizing N2O action*
- *Measuring and reducing N2O*
- *Monitoring the process and N2O after reducing N2O*

KNOWLEDGE OF N_2O PATHWAYS AND INFLUENCING (RISK) FACTORS



AI / MACHINE LEARNING (ML) APPROACH FOR MITIGATING WRRF N_2O EMISSIONS

Knowledge Base

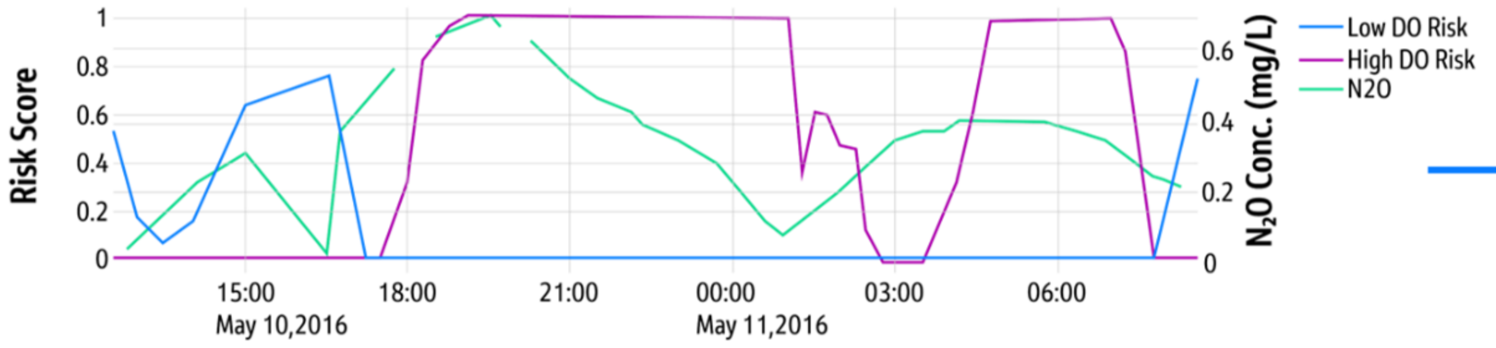
Process/ Condition	Operational Parametr/ Condition	Variable	References linking operational conditio to N_2O risk
Nitrification	High No_2	No_2	Kampschreur et al. 2009; Foley et al., 2010; Ahn et al., 2010; GWRC, 2011
	Low DO	DO	Kampschreur et al. 2008; Kampschreur et al. 2009;
	High DO	DO	Ahn et al., 2010, Chandran et al., 2011, Law et al., 2012, Peng et al., 2014

Peer reviewed literature

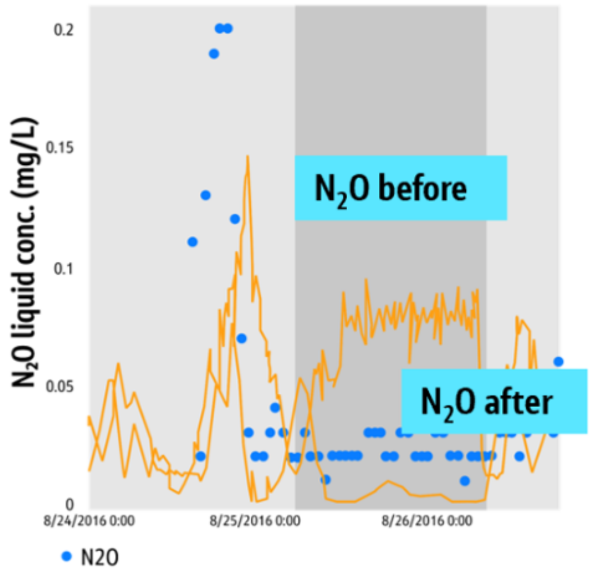
Can be coupled with mechanistic and CFD models

Risk Assessment

ML Predictions



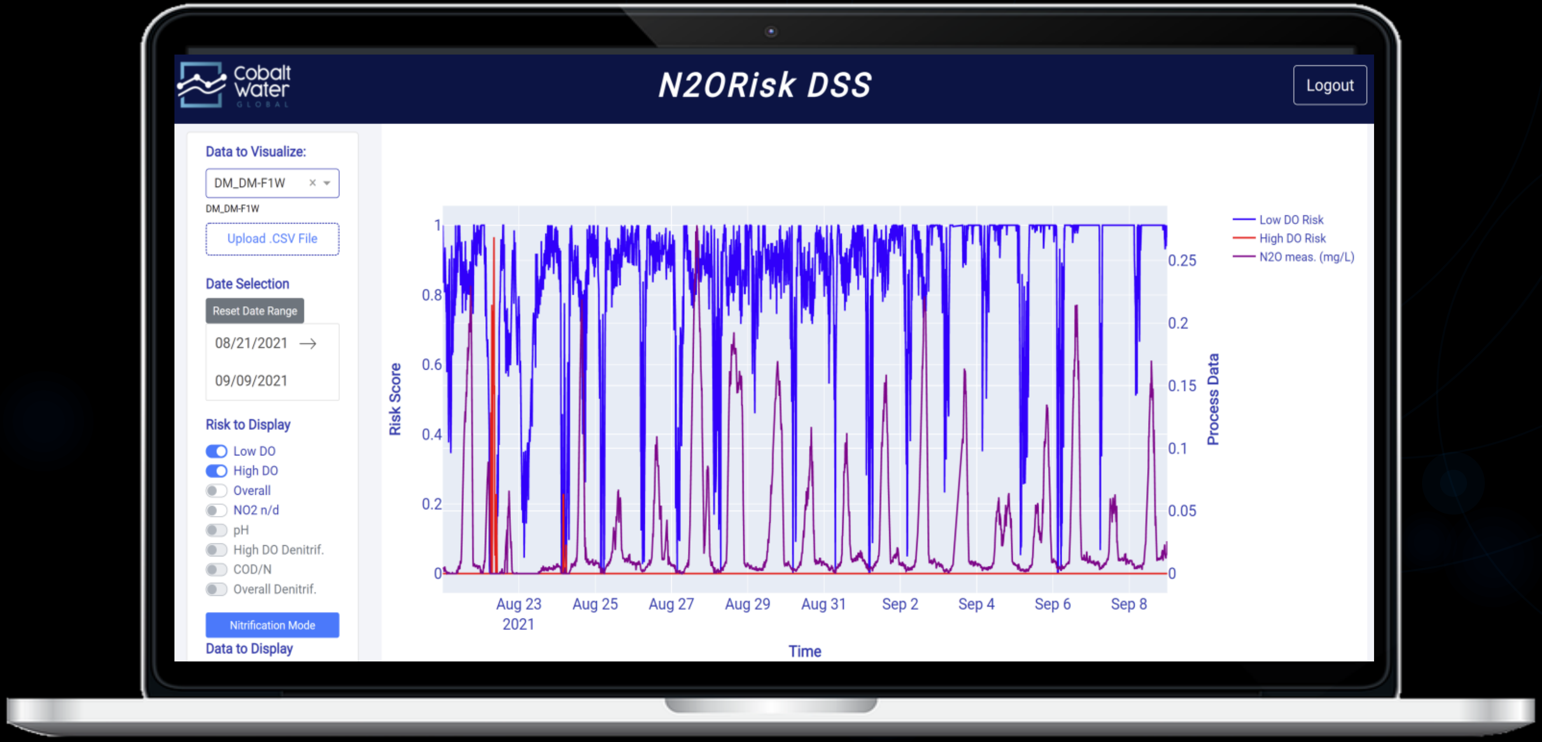
Mitigation



*The **N2ORisk DSS** is the first AI/ML platform to:*

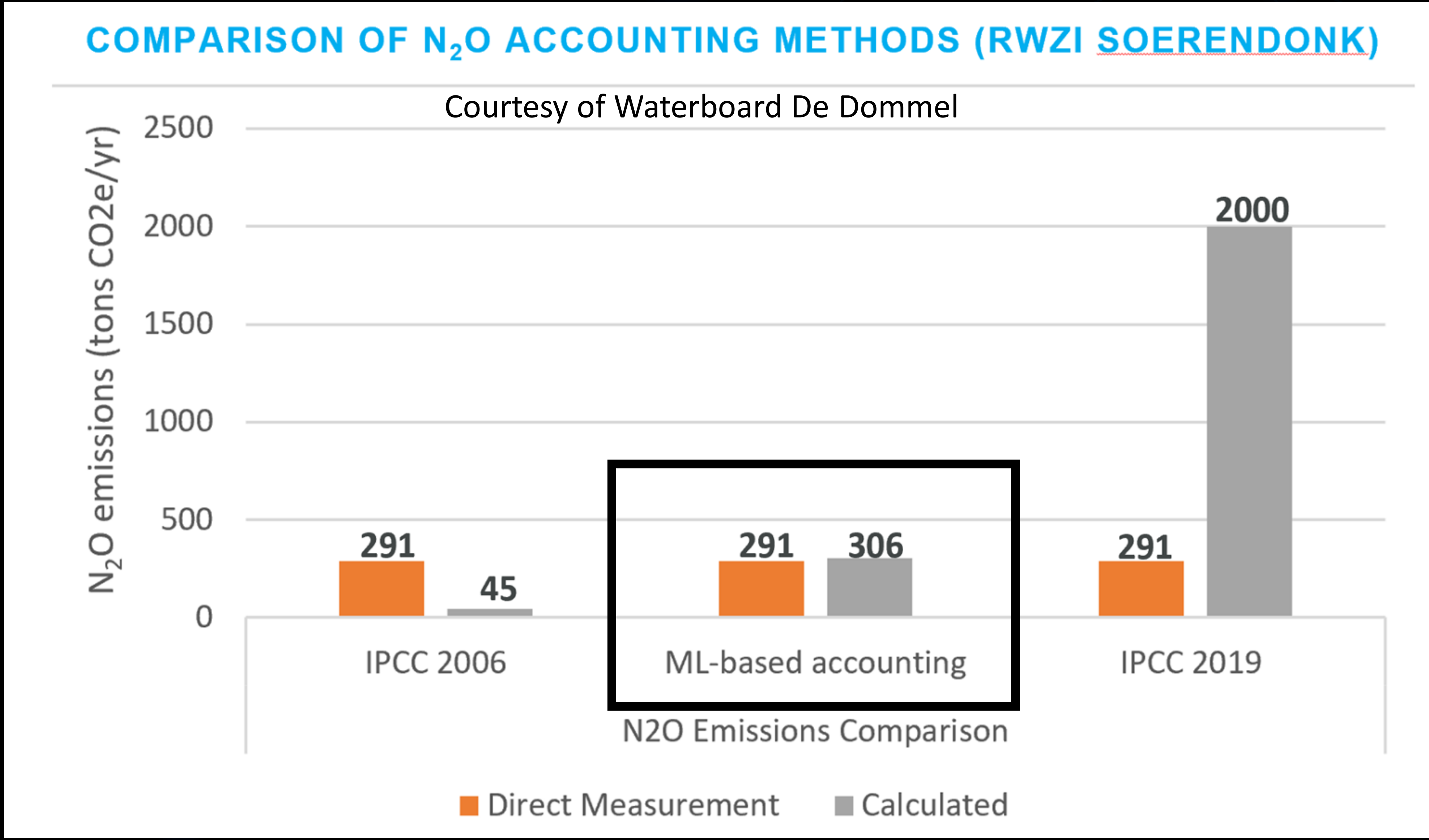
*1) **Account for**; 2) **Reduce**; and 3) **Monitor***

wastewater N_2O process emissions



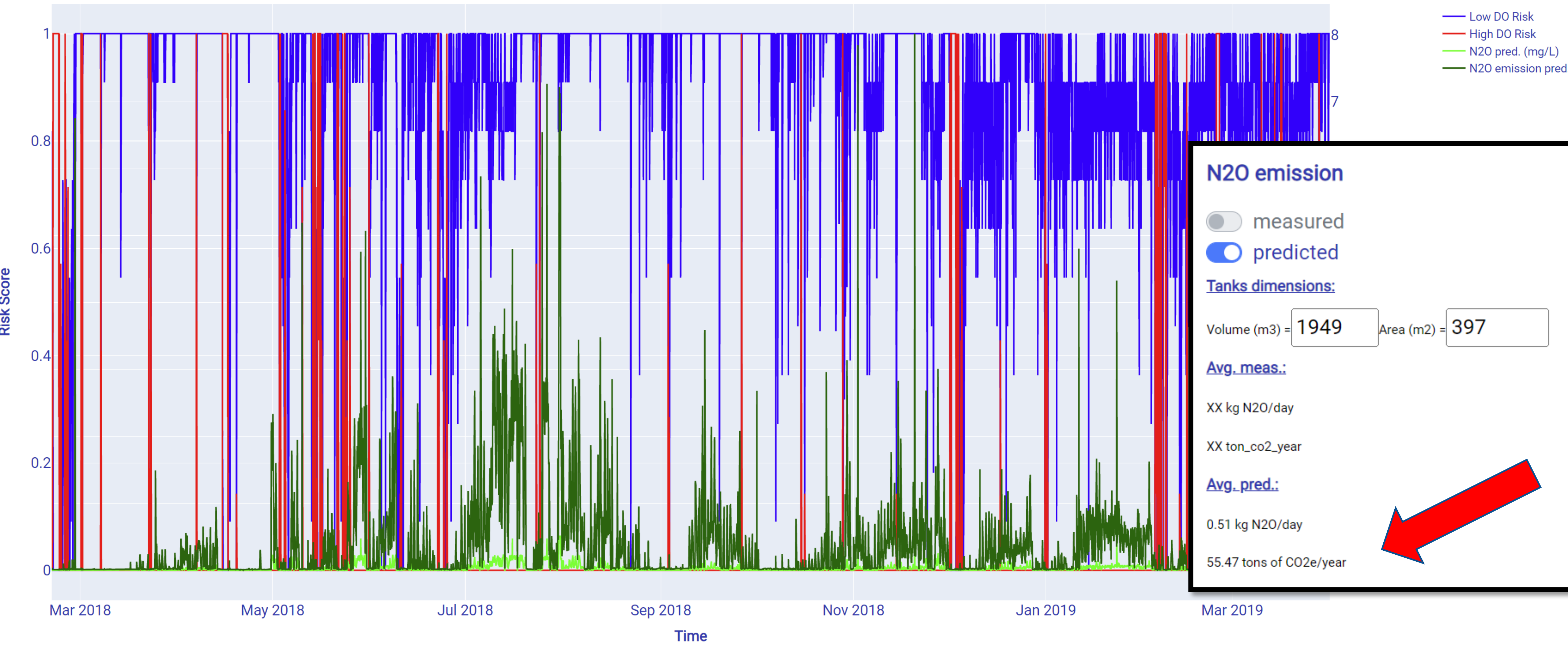
Accounting of N_2O emissions, screening/prioritizing sites

The Emission Factor Problem



Using available plant data for accounting of N2O process emissions
Northeast Illinois, USA

Tank Pass 1 Predicted N_2O Risk and Emissions



N2O emission

measured

predicted

Tanks dimensions:

Volume (m3) = 1949 Area (m2) = 397

Avg. meas.:

XX kg N2O/day

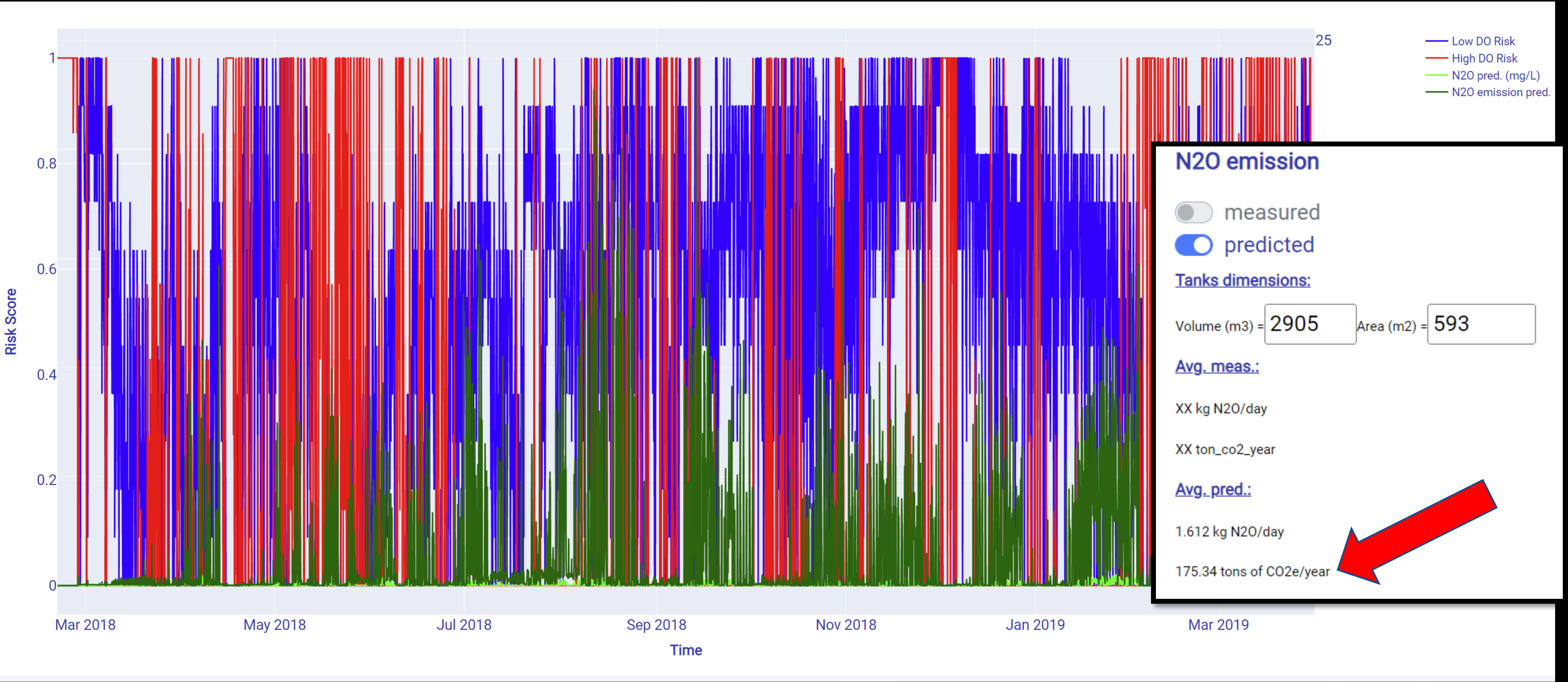
XX ton_co2_year

Avg. pred.:

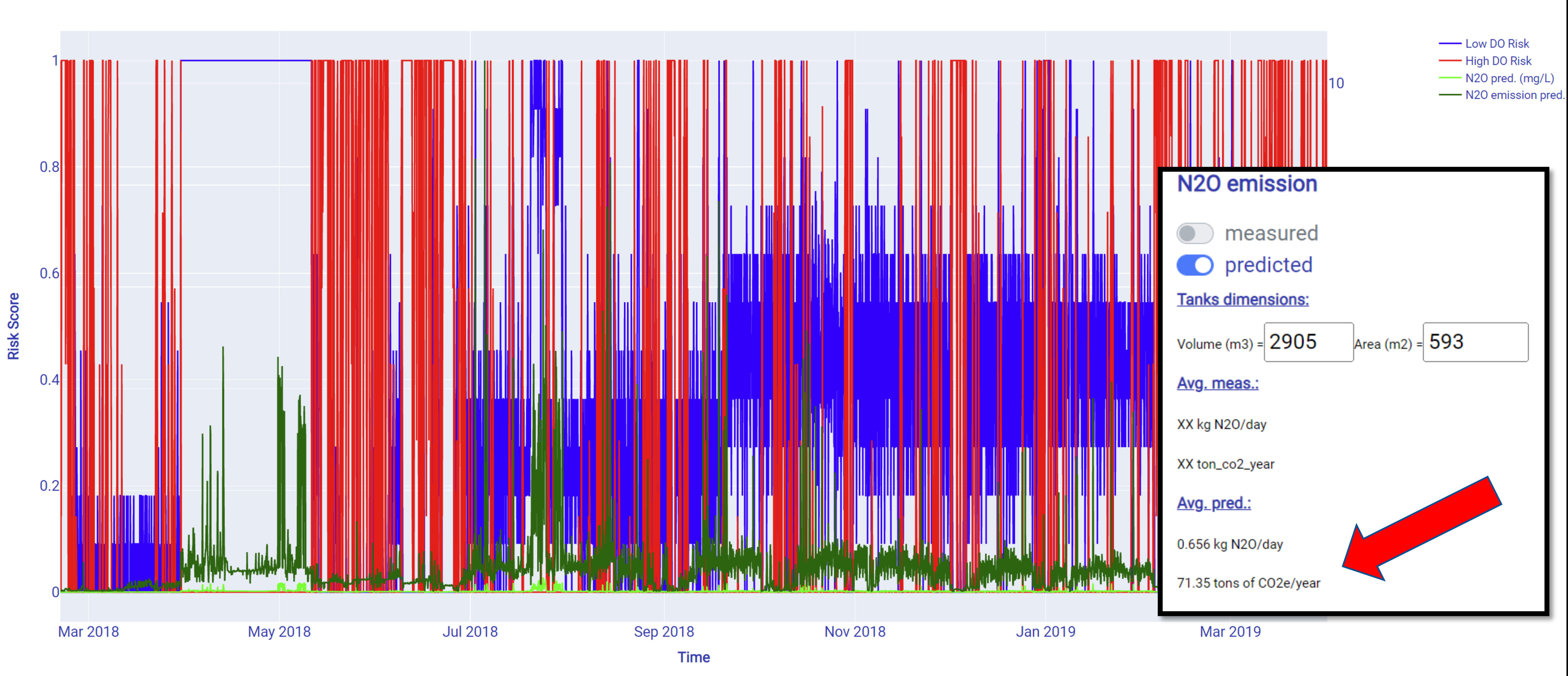
0.51 kg N2O/day

55.47 tons of CO2e/year

Tank Pass 2 Predicted N_2O Risk and Emissions

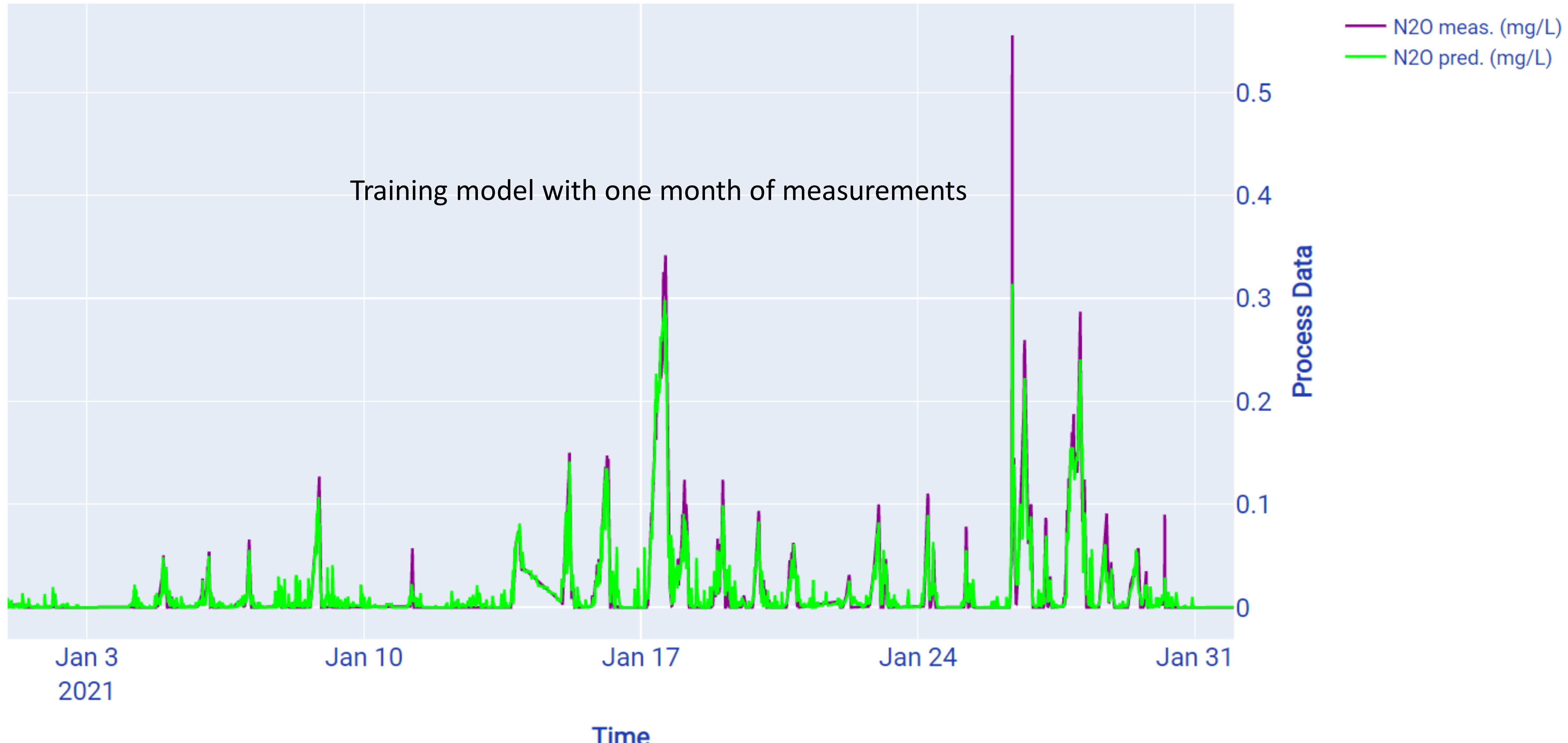


Tank Pass 3 Predicted N_2O Risk and Emissions

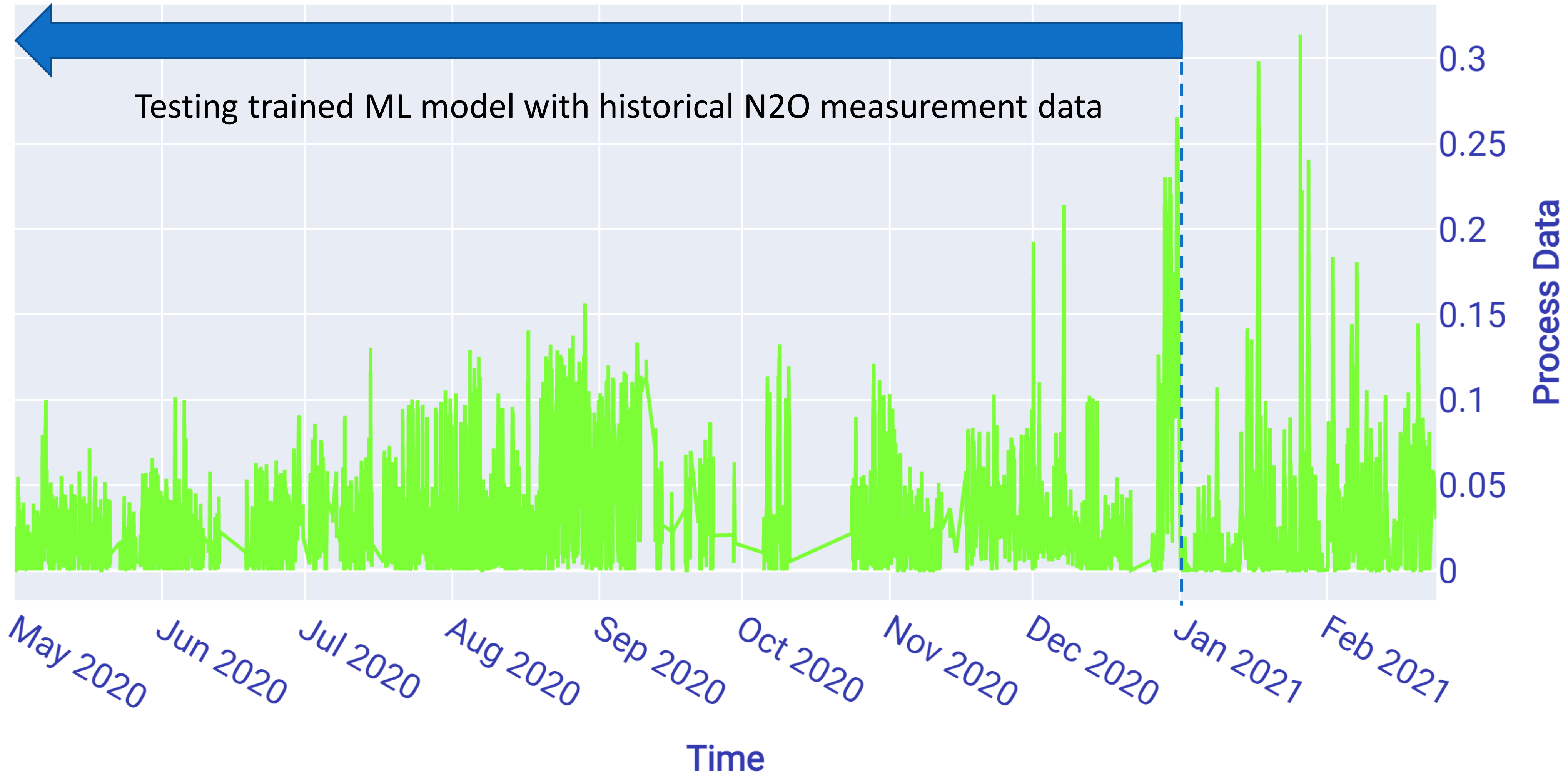


Measuring and reducing N2O

Monitoring the process and N2O

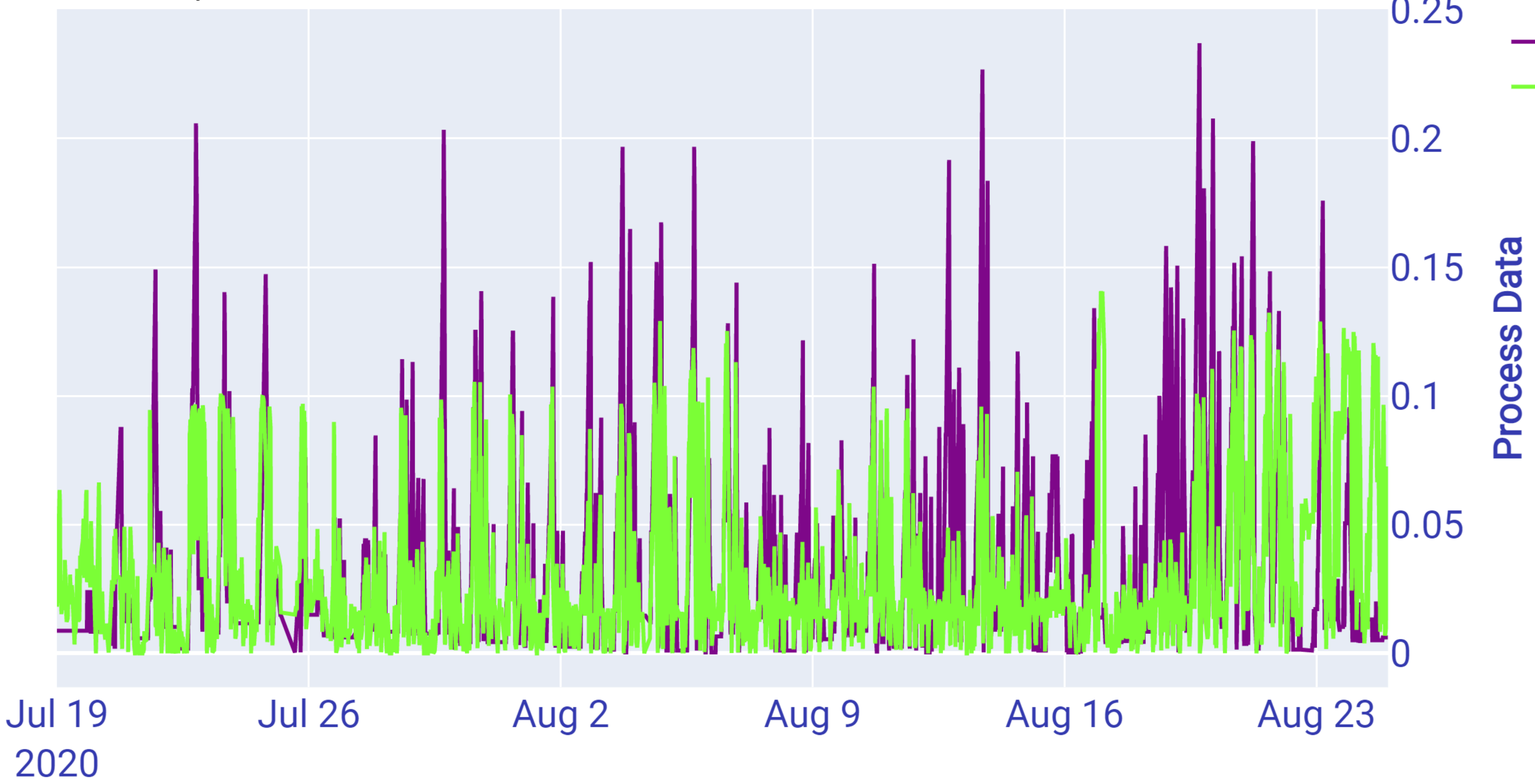


How long to measure



How long to measure

Zooming into roughly one-month in July/August 2020 to test trained January 2021 ML model with historical N2O measurement data



Avg. meas.:

2.684 kg N2O/day

291.94 tons of CO2e/year

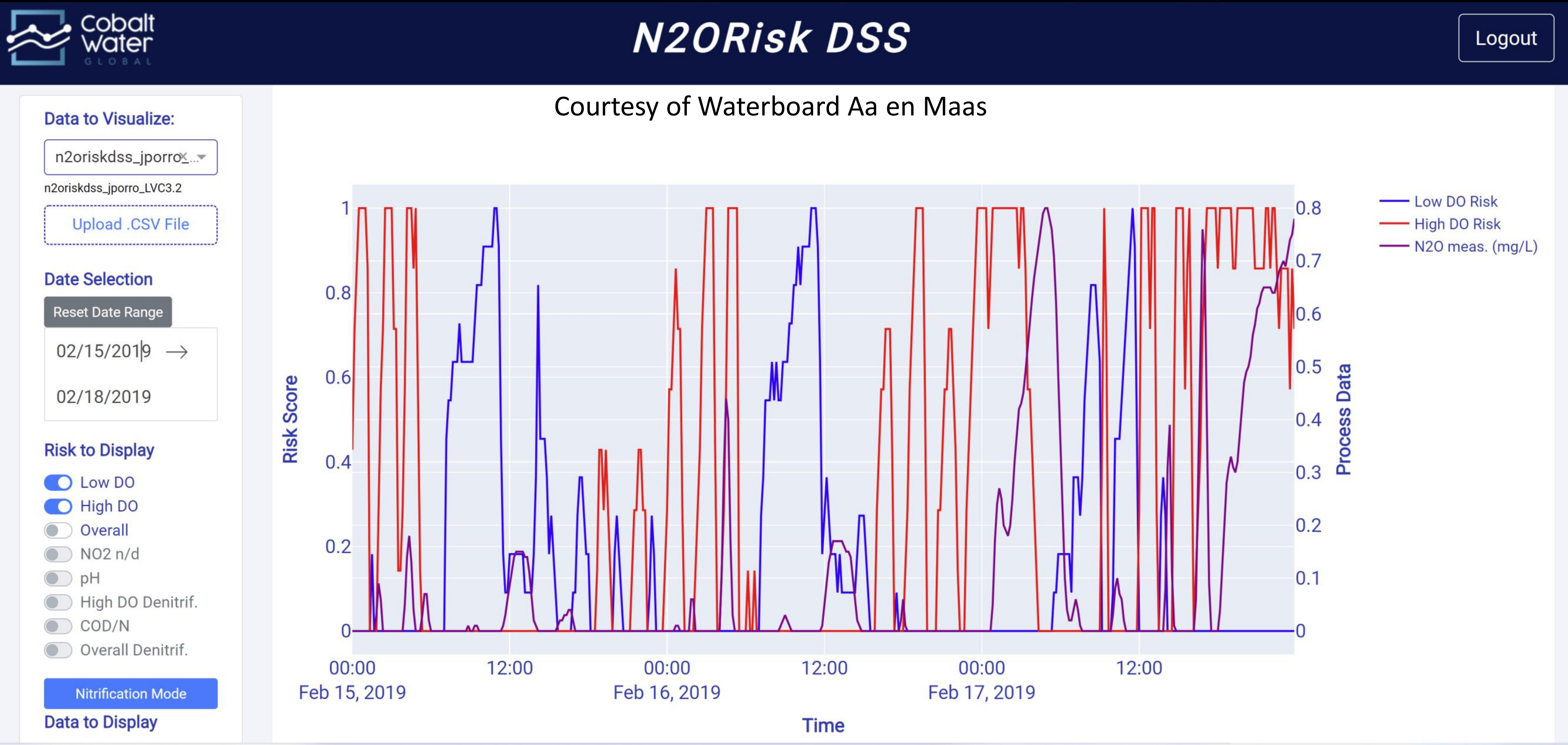
Avg. pred.:

2.653 kg N2O/day

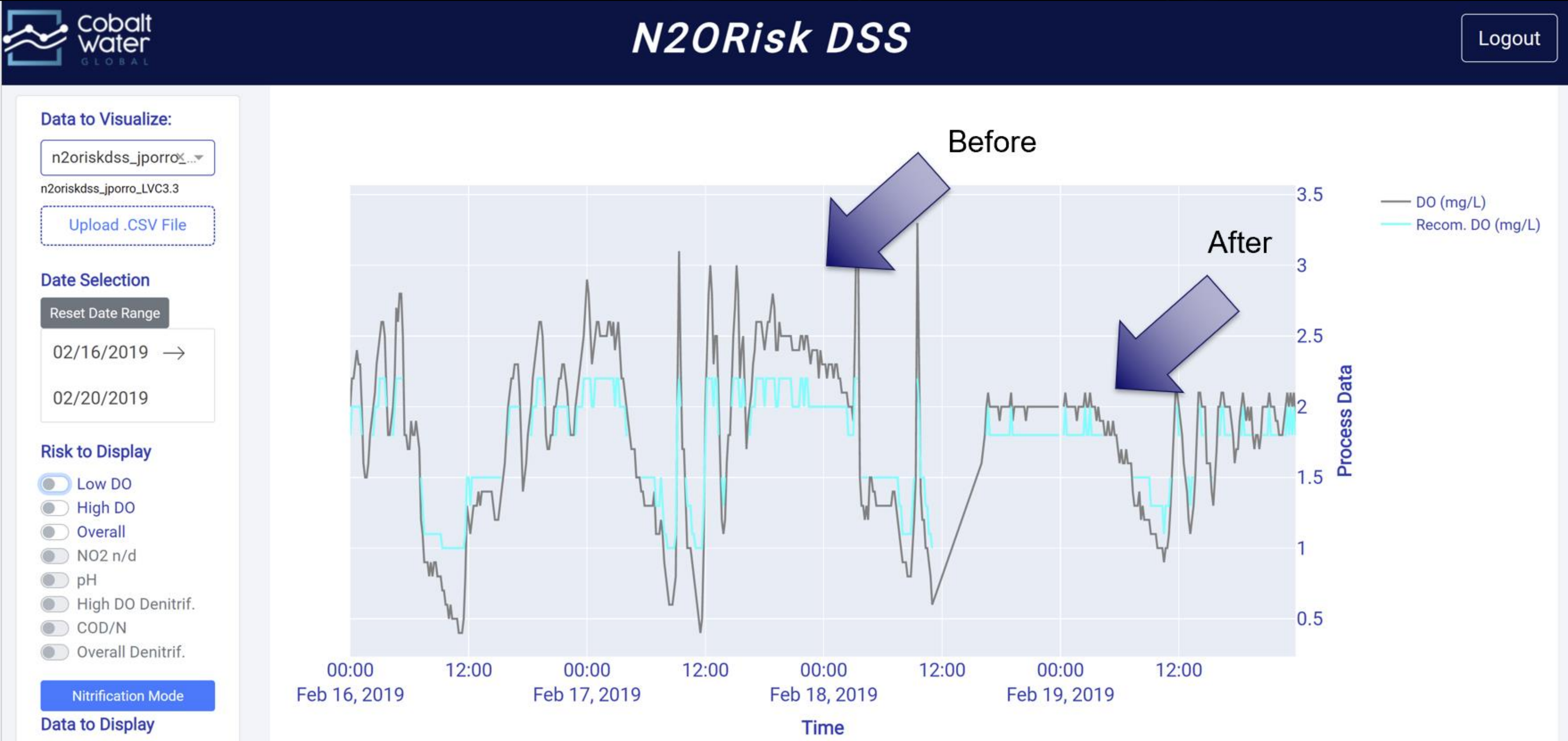
288.57 tons of CO2e/year

Confirms we can use historical data for baselining purposes and do not need to measure for a full year to understand season/operational variability and accurately estimate N_2O emissions

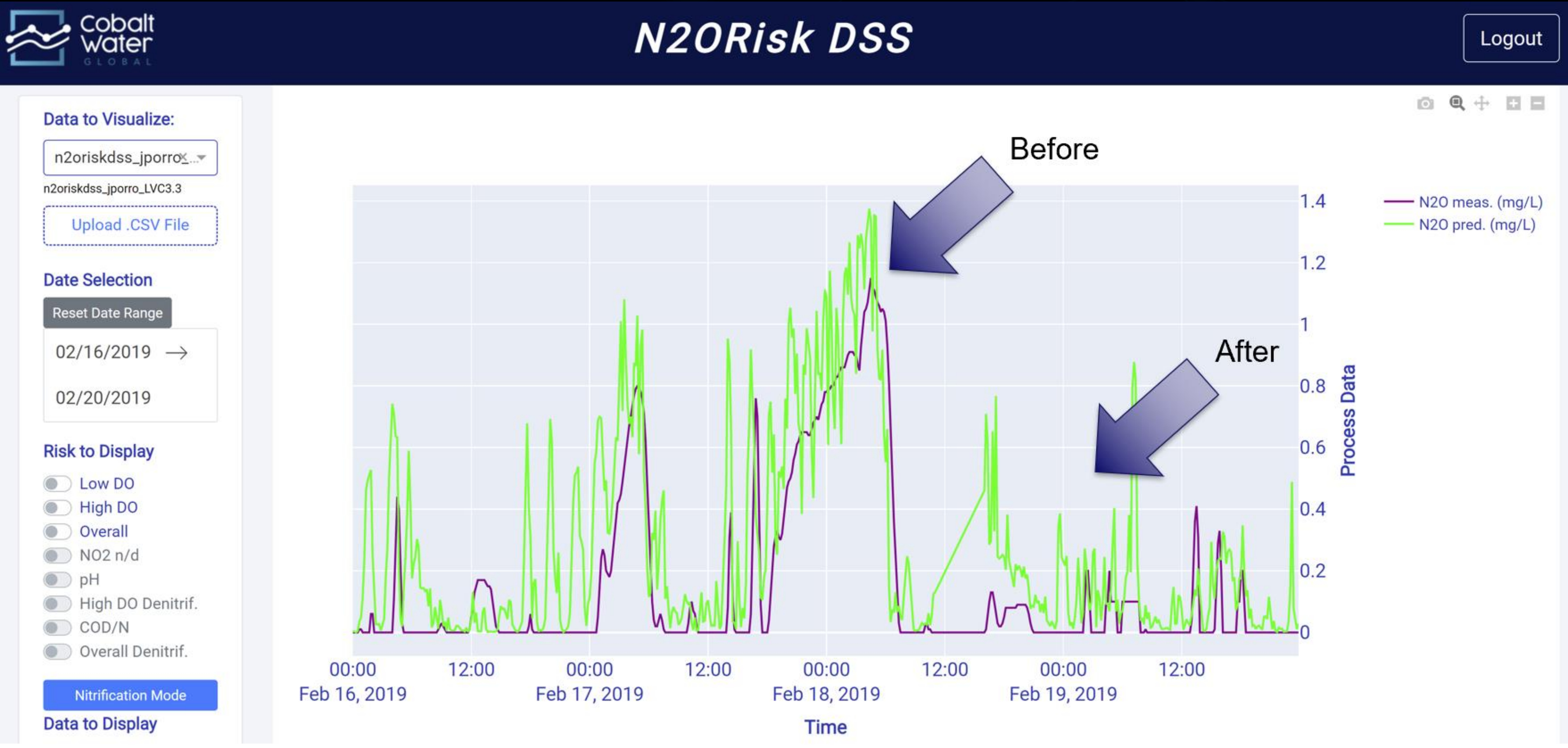
Land van Cuijk RWZI Knowledge-based AI/ML Insights



Reducing N_2O with Knowledge-based AI/ML Insights

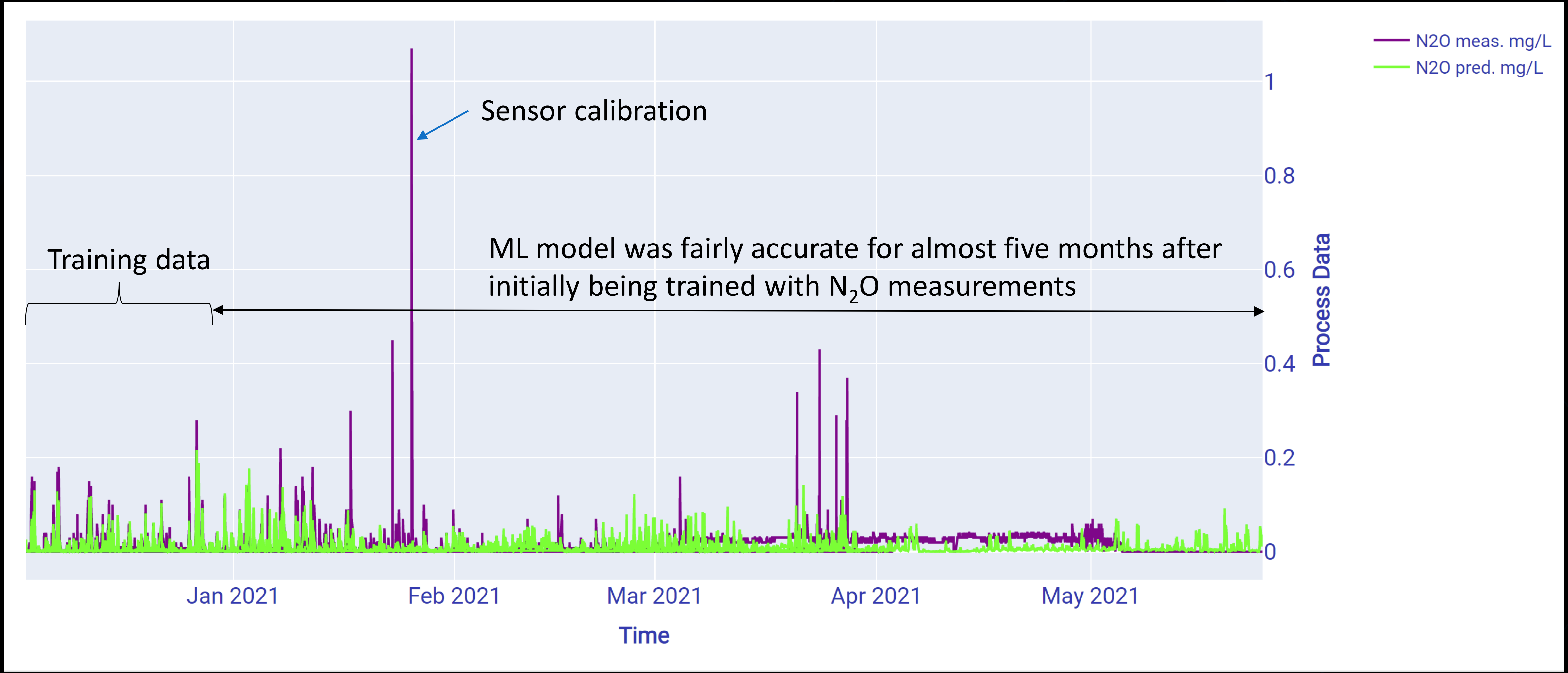


Reducing N_2O with Knowledge-based AI/ML Insights



Monitoring process and N_2O after reducing

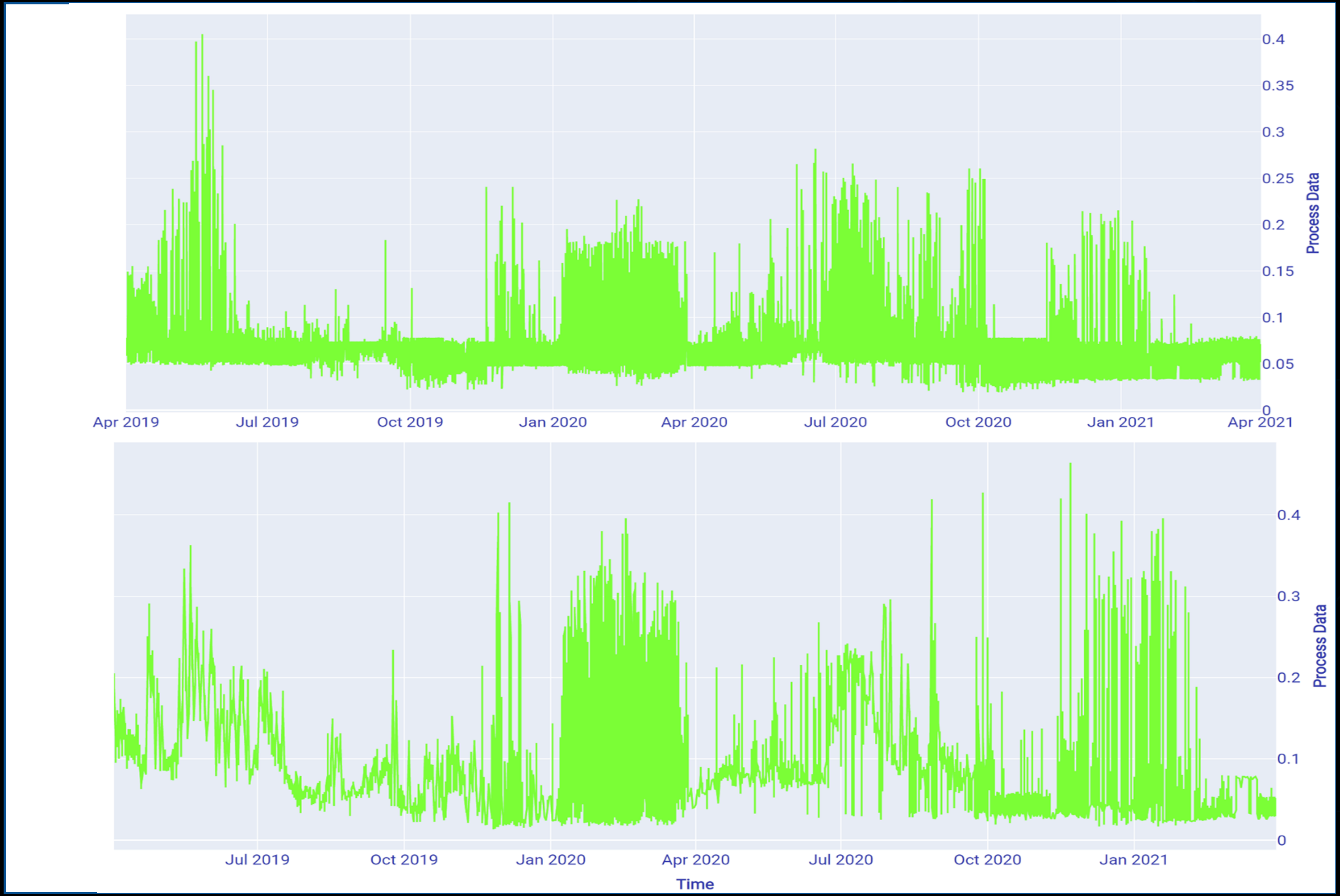
Testing of ML model based on first month of measurements against measured N_2O for several months after at site in NL



Getting more out of your measurements and monitoring N2O in other lanes w/ ML

Lane 1

Lane 2



Integrating N20Risk DSS with other tools

- *ASM mechanistic models*
- *CFD/Biokinetic models*
- *Digital twins*
- *Advanced control solutions*

N2O Reduction Journey

- *Journey can start now!*
- *AI/ML can take you through this journey*

Thank you

Jose.Porro@cobaltwater-global.com

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CLOSING REMARKS

Great thanks to all presenters for a wonderful event!

Make sure to follow MIA's NEXT webinar on December 21, 2022, at 15:00 (CET):

"MODELLING PHOTOTROPHIC SYSTEMS"

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

IWA the international water association

INSTRUMENTATION CONTROL AND AUTOMATION

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