Qualitative Modelling of N_2O Production from WWTPs: A Knowledge-Based Approach for Decision Support

Jose Porro[1,4], Joaquim Comas[1], Ignasi Rodriguez-Roda[1,2], Peter Vanrollghem[3], Ingmar Nopens[4]

Universitat de Girona[1], ICRA[2], *modelEAU* Université Laval[3], Ghent University[4]

4th IWA/WEF Wastewater Treatment Modelling Seminar
Spa, Belgium March 30 – April 2, 2014

Agenda

- Intro to Qualitative Modelling
- Qualitative N_2O Risk Model for WWTP Control Benchmarking
- Validation Cases
- Concluding Remarks

Why use Qualitative Modelling?

- When phenomena of biological nature cannot be predicted adequately by general and validated deterministic models due to **lack of sufficient mechanistic understanding** of the underlying kinetics and population dynamics (Comas et al., 2008)

- When understanding of complex mechanism is not needed to answer questions or provide **decision support**

Qualitative Modelling Techniques

Artificial Intelligence (AI) or Knowledge-based systems

mimic human perception, learning and reasoning to solve complex problems (Chen et al., 2008)

- Rule-based reasoning
- Case-based reasoning Black Box
  - Statistical / Data Mining
  - Machine learning / Data mining
- Agent technology
- Neural networks

Differences of AI with Numerical or Deterministic Methods

ARTIFICIAL INTELLIGENCE	NUMERICAL METHODS
Symbolic processes	Numerical processes
Complex processes	“Normal” processes
Heuristic resolution	Mathematical resolution
Approximate solutions	“exact” solutions
Approximate information	Exact information
QUALITATIVE	QUANTITATIVE

Rule-based System Development

Knowledge Aquisition

↓

Knowledge Representation in a graphical way

↓

Codification of the branches by means of production rules:

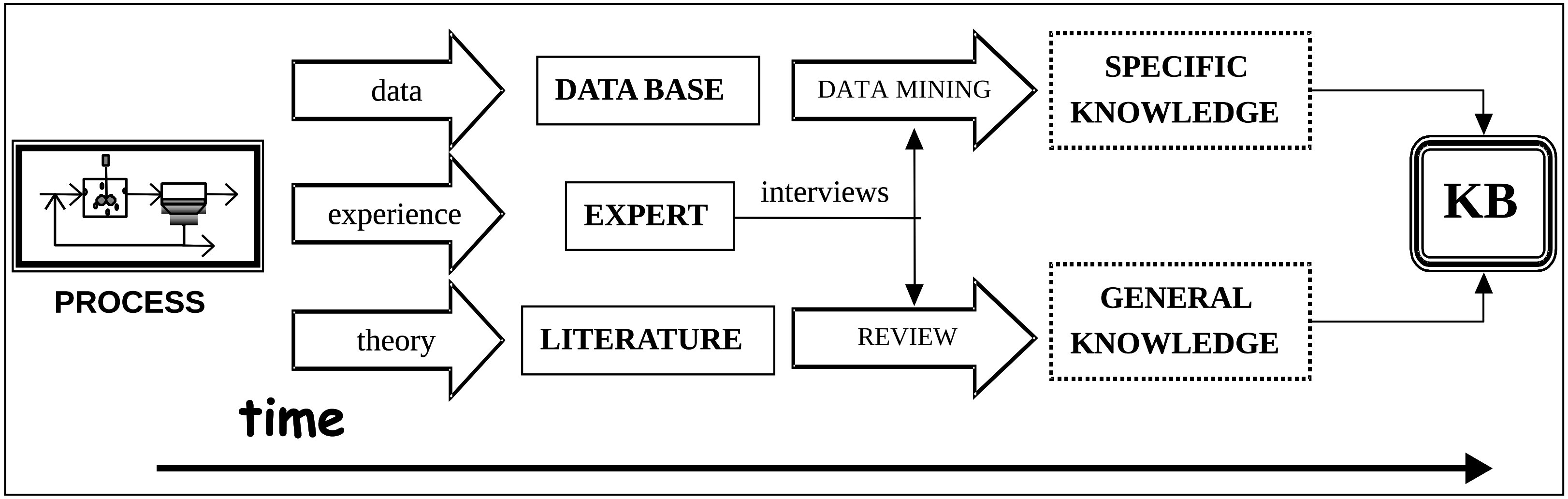
IF <conditions> THEN <conclusions>

↓

Knowledge Base

Rule-based System: knowledge acquisition

Knowledge acquisition : Sources and methods



Environmental Decision Support Systems (EDSS)

- ✓ **Complex management of environmental systems**
- ✓ **Single AI techniques could not succeeded** →
  - **advantages but limitations**
  - **all knowledge could not be captured in one reliable model**

- ✓ **Link control algorithms and mathematical models to AI techniques**
- ✓ **Environmental Decision Support Systems, which integrate**
  - **numerical control**
  - **mathematical modelling,**
  - **heuristic knowledge (literature, experts),**
  - **experiences**

"a new tool INTEGRATING different reasoning models (mahemtical, AI, GIS, et.) complementing each other and thus increasign the overall potentialities. This tool helps to reduce the time in which decisions are made, and improves the consistency and quality of those decisions"

Qualitative Modelling Examples

- **Poch et al., 2004 – KBS EDSS for WWTP Supervision and Technology Selection**
    - **Garrido et al. 2012 – KBS EDSS for WWTP Technology Selection**
        - **NOVEDAR_EDSS**
- **Rodriguez-Roda et al., 2002 – Hybrid KBS/CBS DSS for WWTP microbial operational problems**
- **Comas et al., 2003 – KBS for assessing risk of WWTP settling problems of microbial origins**

Integrating Mathematical and Qualitative Modelling

UWS Deterministic Modelling tools have done well to address complexity and dynamics of urban water systems for:

- Effluent Quality
- Operational Cost

Idea is to build on the previous success and **extend** capabilities and **decision support** by leveraging Deterministic model output data for Qualitative Assessment

- Microbial operational problems
- GHG emissions potential

Qualitative Model for Assessing Risk of Solids Separation (AS Risk Model)

- WWTP population imbalances can lead to filamentous **bulking**, filamentous **foaming** and **deflocculation**; but dynamics still not well understood.
- Combining heuristic **knowledge** from the WWTP operators with specific data streams can identify these problems; however, these data tend to appear only after the onset of the problem.
- Attempts have been made to explain the development of filamentous bacteria by means of **mathematical modelling**, however, none have led to a general and experimentally validated model.
- As an alternative, a **qualitative risk assessment model**, which integrates empirical knowledge with the mechanisms of standard deterministic models, has been reported to infer **solids separation problems** of microbiological origin, as a function of **influent composition** and **operational conditions** (**Comas *et al.*, 2008**).

Qualitative Model for Assessing Risk of WWTP N_2O Production

N_2O Risk Knowledge Parallels AS Risk Knowledge

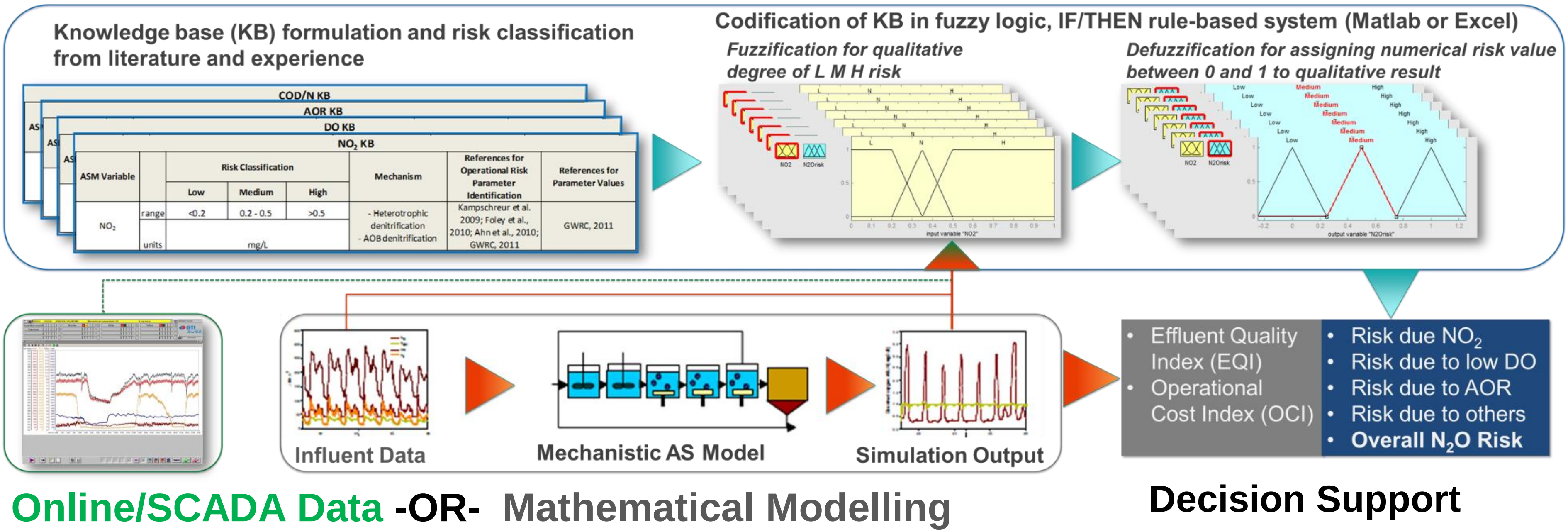
- Complex microbial phenomena
- No widely validated and accepted **mathematical models**
- Significant amount of **knowledge** from literature
- Clear **operational parameters** already associated with **¨risk¨** (Kampschruer et al., 2009; Foley et al., 2010; Ahn et al., 2010; Chandran et al.; GWRC, 2011)
- Therefore, a **qualitative N_2O production risk assessment modelling** approach has been proposed (**Porro *et al.*, 2014**).

N_2O Risk Model Knowledge Base Formulation

Process/ Condition	Operational Parameter / Condition	ASM Variable		Risk Classification Low	Medium	High	Mechanism	References for Operational Risk Parameter Identification	References for Parameter Values
Denitrification	high NO_2	NO_2	range	<0.2	0.2 - 0.5	>0.5	- Heterotrophic denitrification - AOB denitrification	Kampschreur et al. 2009; Foley et al., 2010; Ahn et al., 2010; GWRC, 2011	GWRC, 2011
			units		mg/L				
Nitrification	high NO_2	NO2	range	<0.2	0.2 - 0.5	>0.5	AOB denitrification	Kampschreur et al. 2009; Foley et al., 2010; Ahn et al., 2010; GWRC, 2011	GWRC, 2011
			units		mg/L				
	low DO	DO	range	> 1.5	0.4 - 1.5	< 0.4	AOB denitrification	Kampschreur et al. 2010	Tallec et al., 2008
			units		mg/L				
	Non-limiting DO, NH4, AOR	DO	range	< 1.8	2.15	> 2.5	AOB nitrification	Ahn et al., 2010, Chandran et al., 2011, Law et al., 2012	Law et al., 2012
			units		O2 mg/L				
Internal Recycle	Internal Recycle Rate	XQ	range	>10	5 -10	<5	AOB denitrification	Foley et al., 2010	Foley et al., 2010
			units		XQ				
Anoxic/Oxic transitions	Anoxic/Oxic transitions	Delta DO between reactors	range	≤0.5	1.25	≥2	AOB nitrification	Yu et al., 2010; Chandran et al., 2011	Yu et al., 2010 (transition form 0 to 4 mg/L created sharp spike)
			units		delta mg/L				
Rapid Process Changes	Spikes in NH4, flow, swings in COD:N	Delta	range	<20	30	>50	- Heterotrophic denitrification - AOB denitrification - AOB nitrification	Kampschreur et al. 2009; Foley et al., 2010	arbitrary
			units		%				

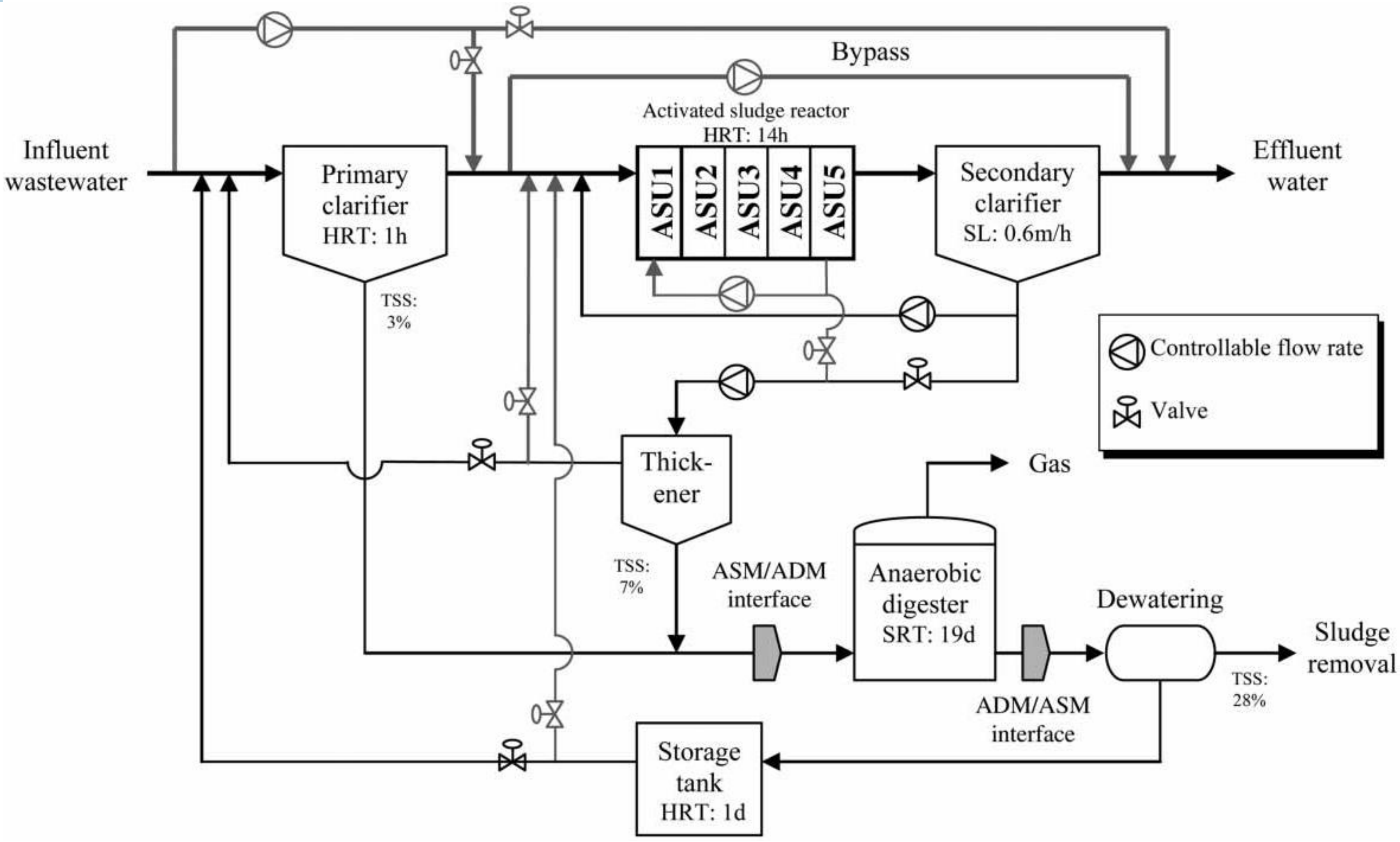
Integrated Mathematical / Knowledge-Based Risk Assessment Modelling Framework

Risk Assessment Modelling



N_2O Risk Model Implementation in BSM2 Platform

BSM2 plant configuration (Nopens et al. 2010)



To prove knowledge-based concept, simulated two scenarios for reactor ASU4 DO: Scenario 1 (*2.0 mg/L*); Scenario 2 (*1.3 mg/L*)

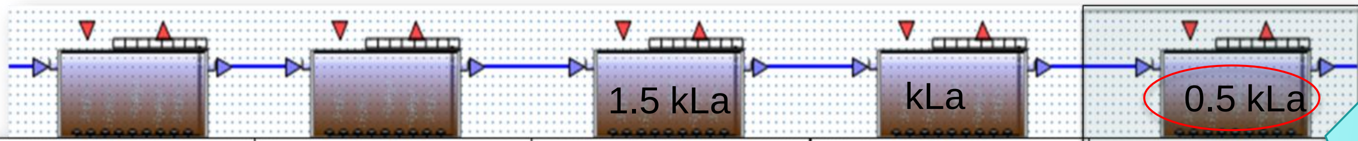
N_2O Risk Model BSM2 Results

Summary of Benchmarking Results (Porro et al., 2014)

	Scenario1 DO 2.0	Scenario2 DO 1.3
Time Under High N_2O Risk (%)	64	98 ↑
Average Overall N_2O Risk Score	0.47	0.54
EQI (kg poll·d^{-1})	5612	5694
OCI (-)	10537	10023 ↓

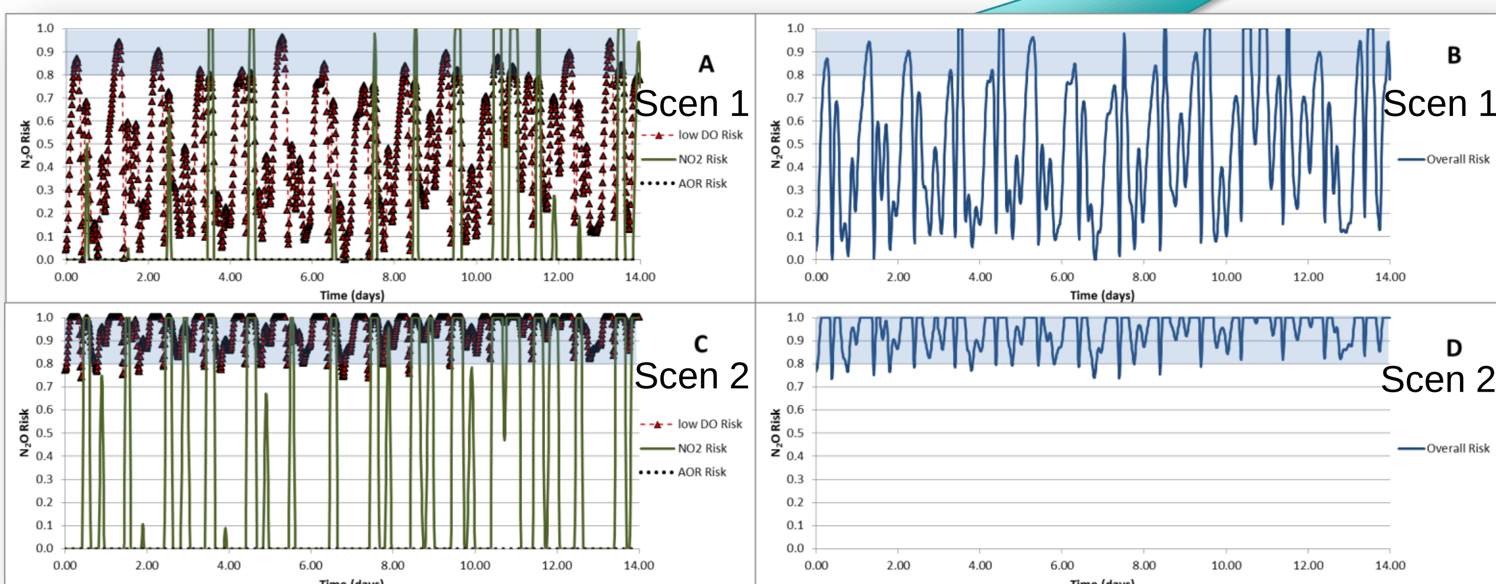
N_2O Risk Model BSM2 Results

Individual and Overall N_2O Risk for two DO strategies

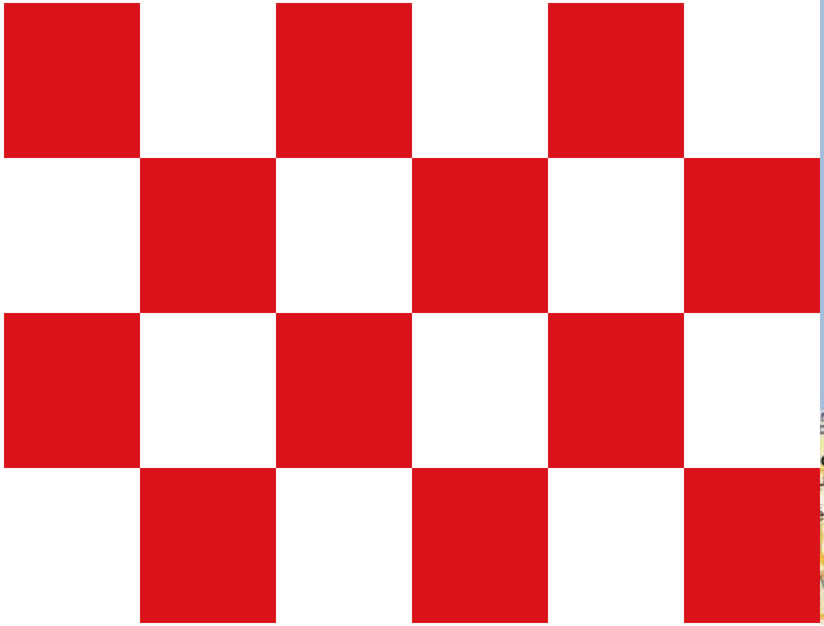


	ASU1		ASU2		ASU3		ASU4		ASU5		Overall	
	Average Overall Risk	% of Time Under High Risk	Average Overall Risk	% of Time Under High Risk	Average Overall Risk	% of Time Under High Risk	Average Overall Risk	% of Time Under High Risk	Average Overall Risk	% of Time Under High Risk	Average Overall Risk	% of Time Under High Risk
Scenario 1_DO2.0	0.58	21	0.31	21	0.56	33	0.41	10	0.51	19	**0.47**	**64**
Scenario 2_DO1.3	0.44	13	0.11	2.4	0.74	50	0.46	30	0.95	96	**0.54**	**98**

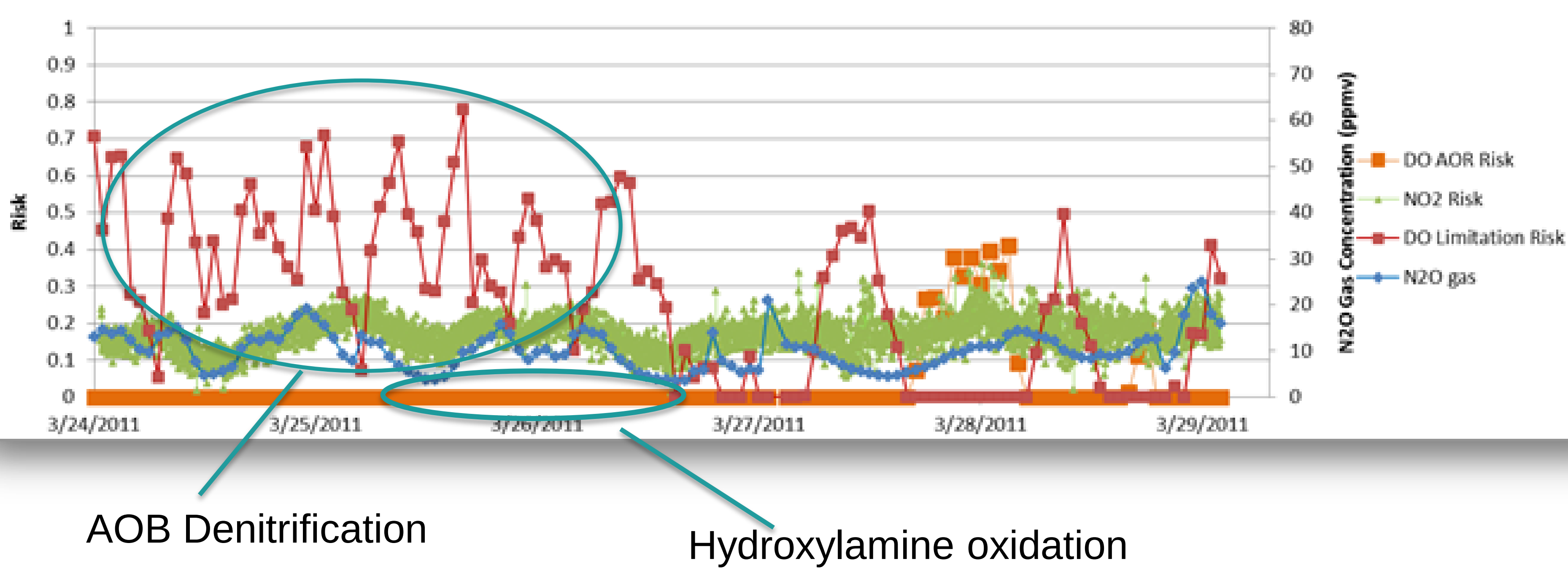
Risk ≥ 0.80 = High Risk
Overall Risk = Max of Individual Risks



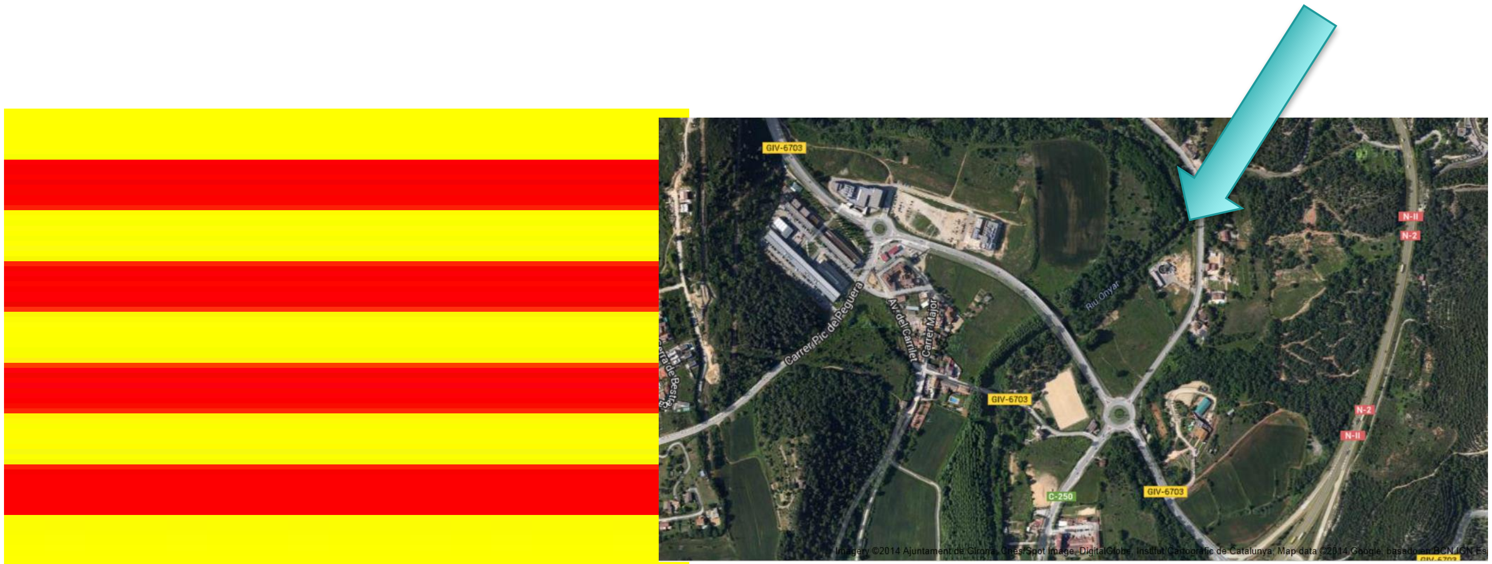
Validation Case: Aarle-Rixtel WWTP The Netherlands



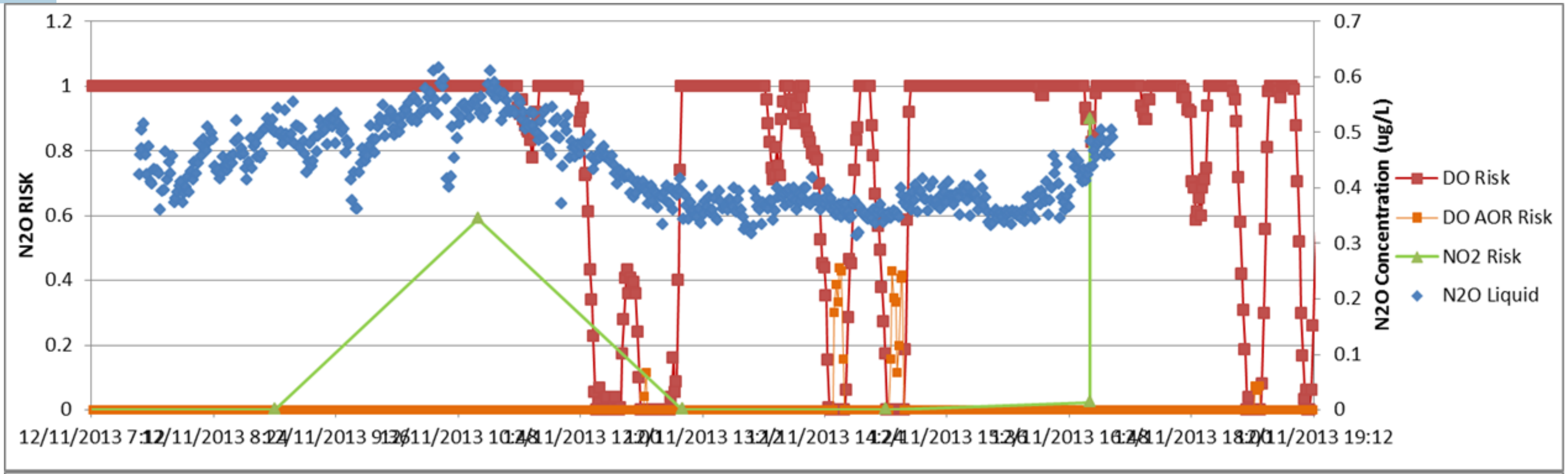
Validation Case: Aarle-Rixtel WWTP (Aarle-Rixtel, The Netherlands)



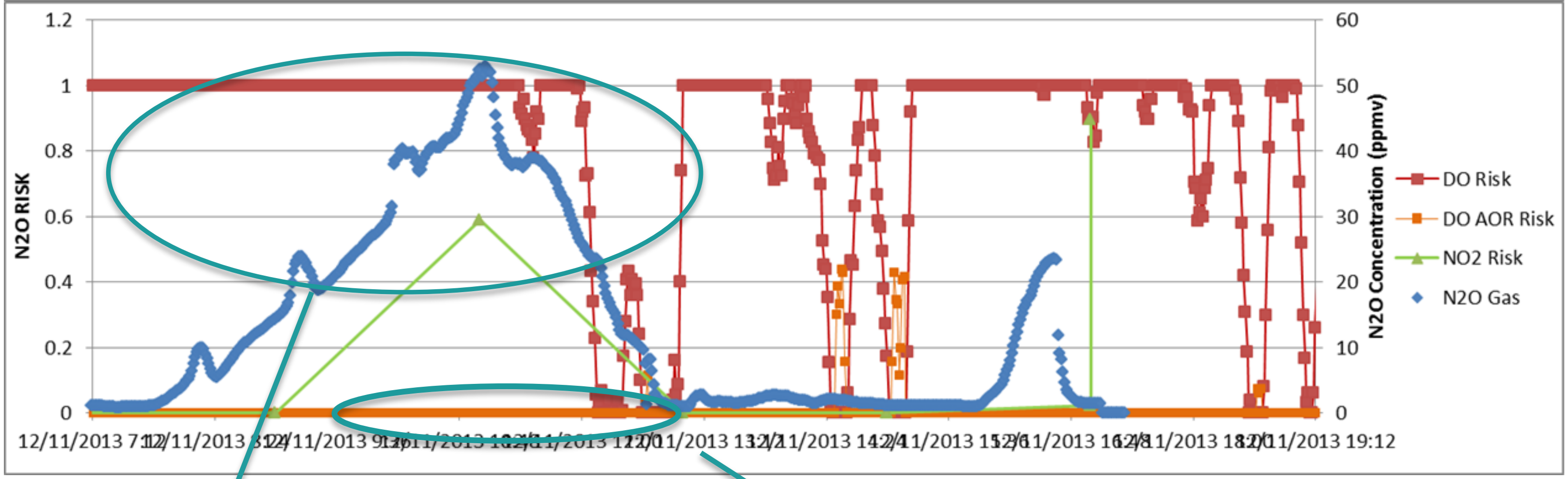
Validation Case: Catalonia



Validation Case: Catalonia, Spain)



Per N_2O Líquid



Per N_2O Gas

AOB Denitrification

Hydroxylamine oxidation

Concluding Remarks

- N_2O Risk Model **adds value** and **decision support** to Energy Optimization Control Strategy Benchmarking with third dimension added to Water Quality and Costs
- Proved it can be an effective for assessing N_2O production risk from a plant-wide and reactor level
- Diagnosing specific risks allows for identification of **mitigation opportunities**
- It can be used for hypothesizing mechanisms and **selecting** appropriate N_2O **mechanistic models**
- N_2O Risk model validation proves risk model answers N_2O risk questions correctly
- Helps provide more **holistic** accounting of N in modelling

Acknowledgements:
Waterboard Aa en Maas

www.sanitas-itn.eu

The research leading to these results has received funding from the People Program (Marie Curie Actions) of the European Union's Seventh Framework Programme FP7/2007-2013 under REA agreement 289193.

This presentation reflects only the author's views and the European Union is not liable for any use that may be made of the information contained therein.