

# Advancing toward net-zero: Deploying explainable machine learning techniques to reduce N<sub>2</sub>O emissions from wastewater

Keywords: Net-zero, N<sub>2</sub>O emissions, full-scale wastewater treatment, explainable machine learning (XAI)

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## Background

The global temperature increase should be limited to 1.5°C pre-industrial levels to significantly reduce the risks and impacts of climate change (Paris Agreement, 2015). Therefore, greenhouse gas (GHG) emissions need to be reduced by 45% by 2030 and reach net-zero by 2050 (IPCC, 2018). More than 140 countries, including Switzerland, have set a net-zero target by 2050. Recent results indicate that the potent GHG and ozone depleting substance N<sub>2</sub>O (265 kgCO<sub>2</sub>-eq) dominates GHG emissions of wastewater treatment and accounts for around 20% of N<sub>2</sub>O emissions in Switzerland (Gruber et al., 2021). The development of efficient, cost-effective and sustainable reduction measures requires in-depth understanding of microbial pathways, controlling parameters, process engineering, plant operation and a holistic perspective on GHG emissions from wastewater treatment including energy use. However, a N<sub>2</sub>O mechanistic model which is able to come up with those cross-plant reduction measures is lacking (Duan et al., 2021; Ye et al., 2022). On the other hand, multi-year N<sub>2</sub>O monitoring campaigns across different full-scale plants are available, yet their potential to reveal hidden relationships and mechanisms remains unexplored. The aim of this thesis is to combine insights from explainable machine learning (XAI) to build a mechanistic model which is able to reduce N<sub>2</sub>O emissions across different wastewater treatment plants in Switzerland and beyond.

### **Objectives of the suggested topic**

The main objective is to make use of machine-learning (ML) techniques to support mechanistic N<sub>2</sub>O-model building. Two long-term full-scale datasets, including DNA-data, are available for advanced analysis using ML models. The specific tasks to reach the objective are

- Screening analysis of different ML models
- Optimization and training of the two best ML models
- Understand predictions of the ML models through XAI tools and if possible translate into mechanistic building blocks

### **Approach**

At the start of your master thesis, there will be a clear overview of existing full-scale data including N<sub>2</sub>O off-gas concentrations and the related operating conditions for a specific wastewater treatment plant.

The master thesis will involve following steps

- Literature review: Get insights in (1) the topic of N<sub>2</sub>O emissions from full-scale biological wastewater treatment, (2) different types of ML models to predict N<sub>2</sub>O emissions and (3) possible XAI tools to understand predictions of the ML models.
- Research questions: Define clear research questions related to the research gaps found in literature.
- Data: Get familiar with the available data.
- Methodology: (1) Create a benchmark model (able to predict average N<sub>2</sub>O emissions), (2) generate different ML models, (3) benchmark models based on predictive accuracy, (4) keep two most promising models and (4) optimize them. (5) Employ XAI tools and if possible (6) translate into mechanistic building blocks.
- Results: Visualize and describe the outcomes of each part of the methodology.
- Discussion: Describe the findings in the broader context of the existing literature.
- Conclusion: Answer the research questions.

### **Specific information and requirements**

The thesis will be conducted in the Department of Process Engineering at Eawag. A workplace with a computer will be provided in Dübendorf.

Requirements are:

- Excellent programming skills
- Nice to have: basic knowledge of biological wastewater treatment, experience with machine learning

### **Advisors and Supervisors**

Advisor: Prof. Dr. Eberhard Morgenroth and Dr. Andreas Frömelt

Supervisor: Dr. Laurence Strubbe

### **Contact information**

Name: Laurence Strubbe

Email: Laurence.strubbe@eawag.ch

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