ICA2025OSLO
14th IWA Specialised Conference on Instrumentation, Control and Automation

# The dissolved oxygen ramp is immoral, but there is hope

M.Y. Schneider*, E. Torfs**, J.P. Carbajal

* BIOMATH, Department of Data Analysis and Mathematical Modelling, Ghent University, Coupure Links 653, Ghent 9000, Belgium, mariane.schneider@ugent.be

** modelEAU, Département de génie civil et de génie des eaux, Université Laval, pavillon Adrien-Pouliot, 1065, av. de la Médecine, Québec, G1V 0A6, Canada, elena.torfs@gci.ulaval.ca

*** Juan Pablo Carbajal, Institute for Energy Technology, OST Eastern Switzerland University of Applied Sciences, Oberseestrasse 10, 8640 Rapperswil, Switzerland, juanpablo.carbajal@ost.ch

**Abstract:** At the last ICA conference, we asked if machine learning has made mechanistic models obsolete. Now we can show an approach to soft-sensor design based on a mechanistic model that is complementary to and addresses some of the challenges of heavily data-driven approaches. The approach is dynamical systems analysis (DSA), which is often used in research on robotics, large climate models, or for stellarator design. We show how DSA can be used to systematically analyse the model structure of mechanistic models for features of interest without the need to numerically solve the underlying equations. Moreover, the proposed approach allows testing the uniqueness of the selected features and at the same time increases the understanding of the system. To exemplify DSA, we used activated sludge models (ASM) to design a soft sensor that takes a ramp in the dissolved oxygen signal to predict the ammonium effluent concentration for an on-site wastewater treatment scenario. The DSA exposed the ramp as highly immoral, which means nearly all other states in the model besides a low ammonium concentration can lead to a ramp, making the ramp a very spurious, hence suboptimal, predictor. However, DSA also allows us to identify that a further restriction of the ramp with a minimal slope significantly reduces the false predictions. The DSA additionally, gives a basis for discussion on which next sensors and experiments to conduct and can be used for model structure verification.

**Keywords**: dynamical systems design; on-site reuse; soft sensors;

On-site recovery and reuse plants are a potential game-changer when it comes to water and resource shortages. However, monitoring on-site recovery and reuse plants is challenging because instrumentation investments need to be kept low and sensor maintenance is often not feasible for many, spatially distributed plants without permanent, trained staff. Hence, soft sensors with features that are robust to sensor wearing such as drifts are required to deal with the specific conditions of on-site recovery and reuse plants. Another challenge of small plants is that very high inflow concentrations might occur and the inflow tends to undergo large fluctuations. Therefore, it can be hard to train a data-driven soft sensor for all eventualities.

## Methods

We use dynamical systems analysis (DSA), a fundamental mathematical approach to analyse the equations of mechanistic models. As such, the approach can identify and display all mathematically possible occurrences of a feature in the phase space without the need to simulate the entire time series first, making it very robust and generic while also being computationally efficient. The model we used as a basis for the analysis is the activated sludge model (ASM) number 1 (Henze et al., 2000).

As a feature, we selected a ramp in the dissolved oxygen signal ($S_{O2}$). The ramp feature occurs where the following two conditions are fulfilled:

$$\dot{S}_{O2} > 0 \quad (1)$$

$$\ddot{S}_{O2} = 0 \quad (2)$$

The ramp is used for a classification of the effluent ammonium concentration.

The code and examples are open-access and can be found here: https://gitlab.com/sbrml/dsa-signal-features.

**Results**

Figure 1 shows the ramp feature when the time series is simulated. We show this figure to illustrate the feature, however, it is not part of the DSA. The DSA directly identifies the states at the point where a ramp occurs (marked with a vertical line) based on conditions (1) and (2) without generating the entire time series.

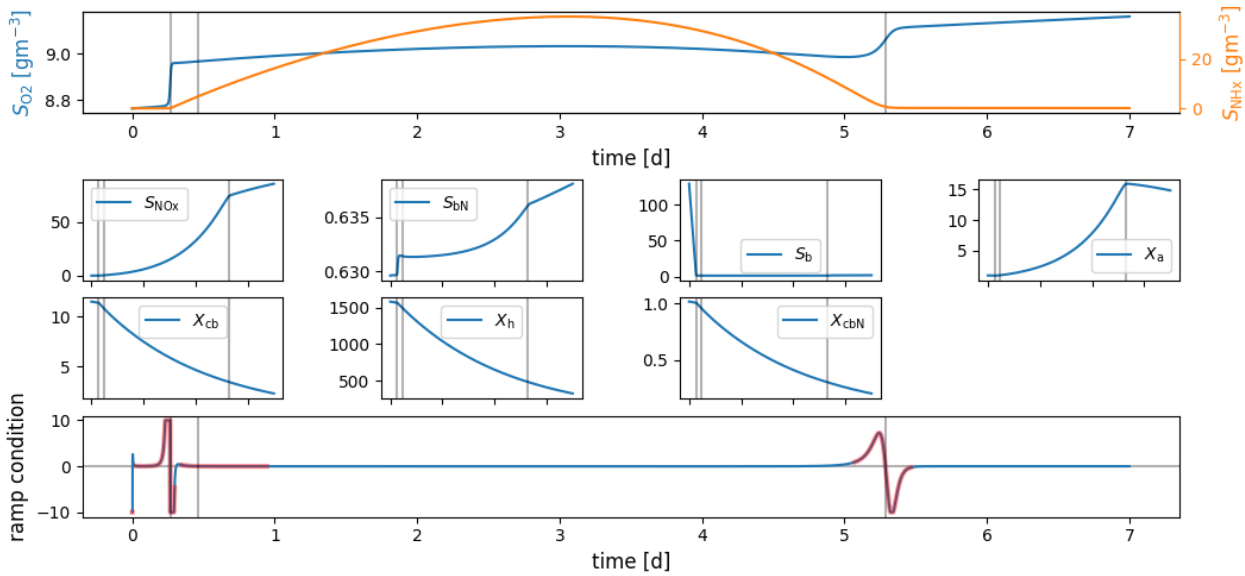


*Figure 1: The top panel shows the dissolved oxygen (SO2) and the ammonium (SNHx) concentrations representing the measured signals. The ramp time instances are marked on all panels as vertical lines and the time intervals on the x-axes are the same. The second ramp is a false positive for the effluent ammonium concentration estimation, the third one is a true positive feature, and the first one is a true positive that is not caused by the ammonium reaching a concentration below the threshold at the ramp-occurrence time, but the ammonium is already low before. By looking at the other panels, potential causes for the ramp features can be visually detected. The plots are for one single set of initial conditions. Each of these three ramp observations corresponds with one point on an inflection point curve. The time series are displayed here to display the ramp features. However, these time series will not be simulated in the DSA to obtain the inflection point curves. The units of all state variables are g m$^{-3}$ (Schneider et al., 2024).*

Figure 2 shows the results of the DSA. Every point is a ramp for the combination of ASM1 state variables indicated on the x and y-axis and the other not displayed states that vary as well. The blue colour indicates an effluent ammonium concentration below an arbitrary threshold T, orange above, hence the blue dots are true positive occurrences of the ramp feature, and the orange dots are false positive occurrences. This shows the tendency of the ramp feature to false positive predictions. Furthermore, the DSA shows several interesting patterns. Some of which we can explain, others we cannot. These are patterns that might best be exploited by data-driven methods if they also exist in the real world. For example, the bottom left panel shows that if the slope of the dissolved oxygen signal at the location of the occurrence of the ramp is high, there will be no false positive predictions any more. However, this comes at the cost of some false negative predictions. The top right panel shows a possibility to reduce these false negative predictions by adding the autotrophic nitrifying organisms' concentration ($X_a$) as a further restriction. This can be used for future soft-sensor design.

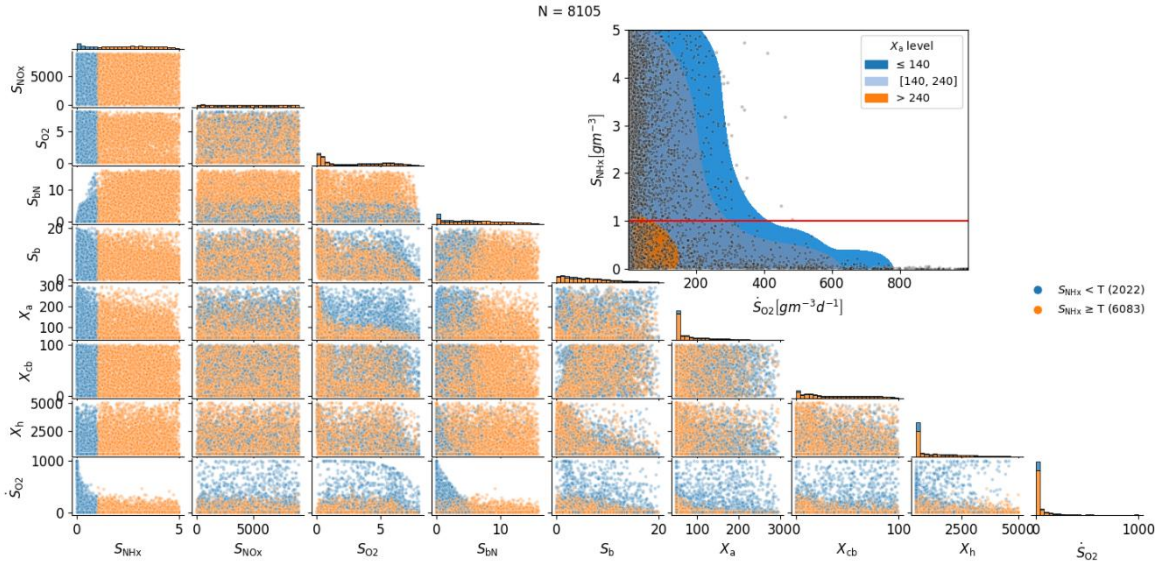


*Figure 2: Ramp feature hypersurface for the ASM1 states for a total of 8105 ramps each. $S_{NOx}$: Nitrite and Nitrate, $S_{O2}$: dissolved oxygen, $S_{bN}$: soluble biodegradable organic nitrogen, $S_b$: soluble biodegradable organics, $X_a$: autotrophic nitrifying organisms, $X_{cb}$: particulate and colloidal biodegradable organics, $X_h$: ordinary heterotrophic organisms, dotO2: first derivative w.r.t. time of the dissolved oxygen. All units are $gm^{-3}$ except for dotO2 which is $gm^{-3}d^{-1}$.*

One example that we explored with DSA is whether a turbidity sensor would be useful to further restrict the false negative soft-sensor predictions. The results of the DSA displayed for the sum of the autotrophic and heterotrophic organisms (Figure 3) show that the pattern for the autotrophic organisms alone (Figure 2) cannot be reproduced. The heterotrophic organisms create ramps at high dissolved oxygen slopes even for high organism concentration, which would cover the pattern of the autotrophic organisms. Hence high turbidity values, would not allow to reduce the false negative soft sensor predictions. This shows that we do not need to design experiments with a turbidity sensor to reduce the slope tolerance for the soft-sensor prediction. This example demonstrates that and how DSA can be used to systematically explore potential features and sensors for monitoring and experimental design of complex systems with a natural component.

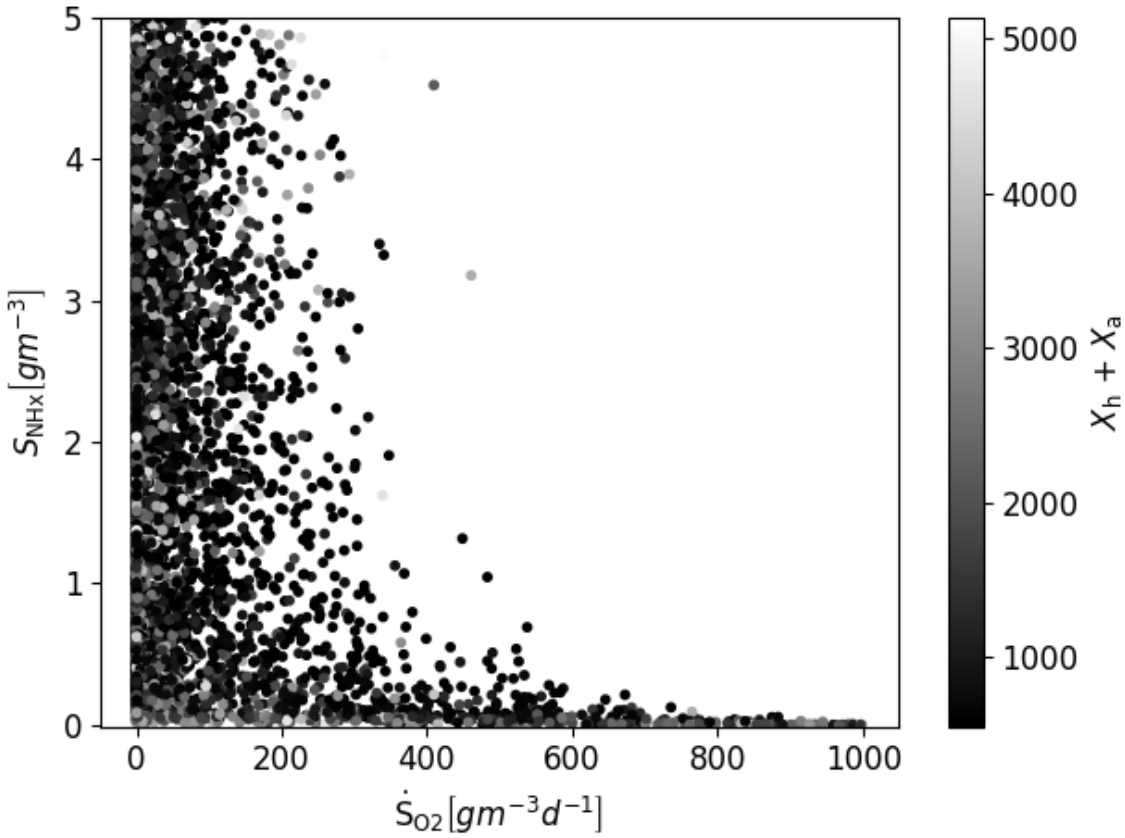


*Figure 3: Result of the DSA displayed for the heterotrophic organisms. There is no clear pattern visible where a high or a low heterotrophic organism concentration would allow a separation based on the slope of the $S_{O2}$.*

**Conclusions**

We exemplarily showed that and how DSA can be used as a systematic approach for feature analysis for soft-sensor and experimental design. Thanks to the very wide range of the phase space that can be covered with DSA, the robustness of soft sensors and the understanding of the system's dynamics can be increased. However, DSA is limited to the underlying mechanistic model it is analysing, hence we will further explore the results not just for ASM1, but also add a comparison with ASM3.

**REFERENCES**

Henze, M., Gujer, W., Mino, T., van Loosdrecht, M.C.M., 2000. Activated sludge models ASM1, ASM2, ASM2d and ASM3, IWA publishing. IWA, Londen, UK.

Schneider, M., Torfs, E., Carbajal, J.P., 2024. The dissolved oxygen ramp is immoral. https://doi.org/10.31224/4184