Postdoc / Research engineer - 12 months
Modeling and data assimilation for wastewater treatment (PHOSTWIN project)

Objectives ans scientific context

The aim is to propose and calibrate a simplified deterministic model that describes the operation of an activated sludge wastewater treatment plant. The calibration algorithm will rely on a data assimilation strategy based on on-line measured data, and will allow to reconstruct the variables that are not measured. The modeling will specifically describe the biological and chemical phosphate removal phenomena, and other main processes in the basin.

This precise modeling will lead in a second time to propose piloting strategies allowing to optimize the respective contributions of biological and physico-chemical phosphate removal. The goal being to operate with as small as possible residual concentration in phosphorus, while keeping an efficient nitrogen treatment.

Administrative context

The CRITT GPTE (Toulouse Biotechnology Institute, INSA Toulouse) and Institut Mathématiques de Toulouse (IMT) have a 4 years-long colaboration. They have successfully developed a control algorithm that optimizes the nitrogen treatment and proposes a daily diagnosis of the plant. This solution combines an innovative automate that pilots the aeration of the basin (AERATION module, Inflex automate developed at INSA and operating since 10+ years in tens of waste-water plants) together with a computation software (DIAGNOSTIC module). The approach relies on the detection of singular points on the oxygen and redox signals, together with a correlation library that links the oxygen and redox profiles with the progression of the biological reactions. A license was obtained for this software, which is now distributed by a company in the Toulouse region.

The PHOSTWIN project aims to propose a piloting strategy that removes efficiently the phosphorus, while preserving an acceptable nitrogen treatment. This project is co-funded by Agence de l'Eau Adour-Garonne (Toulouse) and AMIES (Agence pour les Mathématiques en Interaction avec l'Entreprise et la Société). The postdoc contract must be endorsed before the end of 2024.

Main steps

The approach is divided in 5 steps.

Step 1 : Model simplification

The biological operation of an activated sludge can be described rather accurately by the ASM model, which is internationally acknowledged as a reference model. The complete model describes the evolution of numerous chemical and biological species, and its expression requires several tens of Ordinary Differential Equations (ODEs), that are coupled and nonlinear. However, depending on the objective and the context, accounting for all the equations may not be relevant. Our approach will consist in selecting the equations that are necessary, and reduce the number of parameters.

We will consider 3 possible states for the basin:

- aerobic: presence of O_2 due to the aeration,
- anoxic: absence of O_2 and presence of NO_3,
- anaerobic: absence of O_2 and NO_3.

The mechanisms related to these 3 states are linked with nitrogen treatment (nitrification and denitrification) and phosphorus treatment (biological absorption and chemical adsorption on Fe hydroxyles). In each of these states, we will propose a simplification of the mechanisms that operate, which amounts to fix some constants instead of making them depend on the concentrations. Moreover some quantities vary on a time scale of weeks (like water temperature, that influences the reactions rates, and biomass content) and can be considered as constant. The simplified model will be composed of linear ODEs (or at least ODEs with less nonlinearities) in each of the identified regimes. The direct simulations of this simplified model will be qualitatively confronted to available measurements. This will allow to be more precise on the mechanisms that can be simplified or not.

Step 2: Model calibration using experimental data

In this second step, we will use available data in order to calibrate the model parameters. We will use complete data obtained on an experimentally over-instrumented station during more than 3 years. The phosphate measurements are not available in routine operation, but will be used here for the model development. If the model does not reproduce the data, we will resume the simplification (step 1) in order to obtain satisfying results. The data assimilation procedure will follow a variational framework, with a L2 minimization of the misfit between the model and the data. Some sensors are not perfectly calibrated and their calibration deviates with time. Therefore some precaution will be used and maybe we will add some calibration parameters in the set of unknowns. A preliminary study showed that the numerous parameters are delicate to estimate as a whole, and maybe some other constants measured on the signals will be incorporated in the objective function.

Step 3: Identifiability of NH4, NO3, PO4 concentrations
In routine operation, the NH4, NO3 and PO4 concentrations are not measured. The available data are: inflow rate, dissolved oxygen and redox potential. However, regarding NH4 and NO3, one can identify some instants when these chemicals have disappeared in the basin since O2 and redox profiles show respectively detectable singular points. This provides a reliable initial value. Regarding phosphorus, the situation is more complex since the dephosphating bacteria absorb phosphate during aerobic condition, reject a small amount during anaerobic phase, and reject a large amount during anoxic phase. There are thus 3 constants associated to PO4: aerobic dephosphatation speed, anoxic rephosphatation and anaerobic rephosphatation. We will study to what extent the PO4 concentration can be reconstructed, at least qualitatively and ideally quantitatively. These reconstructed variables provide potential orders for the aeration of the basin.

Step 4: Theoretical piloting strategy
We will propose an optimal strategy for the piloting of the aeration of the basin. In a first step, we will assume the source term is known (in volume and concentration) and constant along time. The optimal piloting will consist in proposing a periodic aeration strategy that ensures complete nitrogen removal and a level of phosphorus as low as possible. In a second time we will assume the source term is known but changes along time. It follows from the PhD of Erika Varga (2022) that improving the biological dephosphatation usually requires to increase the total aeration time (and thus increase the power consumption), and a compromise will have to be found between the quality of the treatment and the power expenses.

Step 5: Effective piloting strategy
In real life operation, the source term is not precisely known and the piloting strategy cannot rely on its knowledge. The real time piloting must adapt the aeration orders on the measured O2 and redox signals.

Expected timeline
The steps 1 and 2 will be conducted together – during 4 to 6 months. The model and the corresponding data assimilation code will be developed.
Step 3 will rely on a numerical study based on the software previously developed. In the case the answer is negative (non identifiability of PO4 and associated constants), several scenarios will be considered depending on the relative values of the constants. This will then be conducted in parallel of steps 4 and 5, in order to determine if a piloting strategy can be proposed depending on the reactive constants, or even independently of these constants in the case they are not identifiable. These steps will last for the 4 or 5 last months of the project.

Expected outcomes
- scientific journal articles
- effective simulation software code (operational numerical twin)
- software that implements the effective piloting strategy

Mathematical tools
The proposed project will require: modelling, numerical computation, data assimilation, optimal command.
The software that will be developed will use the Python language.

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