Decision Support Tools for Urban Wastewater Treatment: The Development of a Hybrid Model for the Optimization of a Biofilter Mechanistic Model for Nitrogen Removal

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In the water sector, mechanistic models describing wastewater treatment by activated sludge processes are recognized as important decision support tools. The models contain a large number of parameters that require a complex preliminary calibration phase. In the case of wastewater treatment by biofiltration, which is a compact, reactive process largely applied in the urbanized region of Paris, the bio-physical-chemical processes taking place within a biofilm, makes for complex equations. These biofilter mechanistic models require relatively high computing power and have not yet been well established within the scientific community. On the other hand, data-driven Machine Learning (ML) models describe a system only based on the information extracted from the data. These models have strong interpolation strengths and are much faster in computation, which makes them very attractive for real-time control applications. Moreover, model-hybridization is a process that combines a mechanistic model, which integrates relevant knowledge about processes, with a ML-model that increases the accuracy of estimates by including information about poorly described sub-processes. In literature, hybrid models have been successfully applied to activated sludge models in experimental and small-scale set-ups.

This thesis aims to optimize wastewater modelling for nitrogen removal by biofiltration using operational data. The objectives are first to calibrate a previously developed mechanistic biofilter model (Zhu, 2020); secondly, to develop a ML-model to identify the residual error of the mechanistic model; thirdly, to integrate these two components into a hybrid model that will increase performance; and fourthly to demonstrate a hybrid approach in an operational process control.

The work began with pre-processing and cleaning of operational data acquired on the industrial site during the 2019-2020 period (Seine aval WWTP, 6,000,000 eq.hab., near Paris, managed by SIAAP). A global sensitivity analysis identified the most influential parameters on the model's response as those characterizing the composition, filtration and the biological reactions. The simulation results using the calibrated parameters show that the model predicts the high-frequency variations of NO_3-N, COD and TSS effluent concentrations reasonably well during calibration. The model performance with the NO_3-N validation dataset is however of less satisfaction.

Next, a cooperative parallel hybrid model was developed in which the recalibrated mechanistic model is supported by a ML-model in order to improve the accuracy of effluent quality prediction. Different ML models were trained to predict the residual error of the mechanistic model for NO_3-N, TSS and COD effluent concentrations. They were given the effluent concentrations simulated by the mechanistic model, as well as information on the influent water quality and the treatment parameters (such as the set points). The best results were obtained with a neural network consisting of three layers. The performance of the hybrid model is significantly better than that of the mechanistic model during the calibration period (RMSE: 0.9 mgNO_3-N/L vs 2.5 mgNO_3-N/L) and the validation period (RMSE: 1.0 mgNO_3-N/L vs 3.8 mgNO_3-N/L), where the hybrid model error is of the same order as the measurement error (around 1 mgN/L). Finally, the development of a Hybrid Model Predictive Controller for methanol dosage in a denitrification filter has promising first results.

This thesis affirms that a hybrid model simulating a complex and reactive wastewater treatment process, such as nitrogen removal by biofiltration, is more accurate than a mechanistic model alone in describing the denitrification behaviour in a biofilter, thus significantly improving the performance quality. Hybridization is therefore an important instrument in building confidence in process modelling and its development here constitutes a key step towards the application of digital twins.

Research Framework

Bruno Tassin (LEESU, ENPC) and Peter Vanrolleghem (model*EAU*, ULaval) are the Director and Co-Director respectively. The work is further supervised by Vincent Jauzein, Sam Azimi and Vincent Rocher (SIAAP), as well as by Ilan Juran (W-SMART).

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