Mathematical models of wastewater treatment processes are important tools for process design and optimization. To obtain reliable predictions, it is necessary to calibrate dynamic models on the basis of dedicated experiments and measurements. When direct measurements of certain compounds are not possible, a soft sensing approach may be used instead, for which a reliable process model is essential. Common to the biological wastewater treatment models are the growth rate functions that describe the speed of bacterial growth with respect to a given substrate [1]. The Monod growth rate function is the default choice in wastewater treatment modeling. However, when the Monod function does not capture the behavior of a certain group of bacteria, its extrapolation for purposes of process design and optimization can be detrimental [2].

In almost every microbial growth process, one can describe substrate affinity as a monotonically increasing rate function with a concave shape. This qualitative feature is used in the construction of shape constrained spline (SCS) functions, which are flexible enough to reproduce the behavior of substrate affinity effects of the considered shape. As such, an SCS function serves as a single biokinetic growth model, which replaces the classic yet incomplete library of candidate growth rate functions. Thanks to the enforced shape, it is interpretable in the same way as any of the classically considered alternatives and in spite of its increased parametric flexibility. In this paper, SCS functions are evaluated as valuable alternatives to classic growth rate functions for biokinetic process modeling. As a proof of concept, initial experiments were performed on simulated microbial growth rate measurements by fitting both a classic library of rate functions and the proposed SCS function. All computations were performed with Matlab and the SCS toolbox [3]. The growth rate was first simulated as a Monod function and subsequently as a hyperbolic tangent function, creating two scenarios that serve as examples of a “typical” microbial growth rate and of a more “exotic” growth rate.

Initial results show that there is an excellent fit for both the library functions and the SCS function in the first scenario. In the second scenario, where the “exotic” function maintains the same qualitative behavior but is not present in the library, the SCS function is easily able to fit the function, while the fit for the best library function is significantly worse.

The consequences can be visualized through the use of the optimized growth rate functions in a mathematical model based on ordinary differential equations (ODEs), such as the activated sludge model. In a simple example, the ODE describes the substrate concentration in a biological treatment reactor. For the second scenario, the substrate concentration differs over time between the growth rate obtained as an SCS function and the growth rate found among the best library candidates. The difference could potentially have a strong impact on the reliability and usefulness of the model, for example leading to false predictions when the library approach is used.
The SCS functions can fit all functions and require less computational efforts than searching through a library of functions. They are black-box models in essence, but are still very interpretable, thus giving them a “white-box” feature. When faced with an exotic growth rate that is not already part of the library, it is still possible to find the growth rate with the SCS approach if the overall shape remains the same. Continued work aims at the use of the SCS approach for diagnosis, that is, for determining whether a given growth rate belongs to the known growth rates based on its shape. Furthermore, the computational benefits are demonstrated through a more complex ODE example that requires additional nonlinear, indirect parameter optimization.

References:

