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A robust calibration methodology of wastewater treatment models based on Markov Chain Monte Carlo (MCMC) algorithms

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Summary of key findings

The use of mathematical models and simulation of wastewater treatment plants (WWTPs) have become very important for optimising their design and operation. However, there are innovative processes, especially those related to biofilm like IFAS and MBBR, for water and sludge lines, which performance description requires complex models that include biofilm interactions. These complex environmental models are usually over-parameterized and identifiability issues have to be faced. This abstract presents the usefulness of the calibration procedure of complex mathematical models. For this, a two phase's calibration procedure base on Markov Chain Monte Carlo (MCMC) algorithms is proposed. In the first phase a comprehensive sensitivity and identifiability analysis is performed and in the second phase a step-wise Monte Carlo algorithm is carried out.

Background and relevance

Nowadays, the use of mathematical models and simulation of wastewater treatment plants (WWTPs) have become very important for optimising their design and operation. In the last decades, several models that dynamically describe the biochemical transformations taken place in the biological processes have been developed (Henze et al., 2000). One of the main advantages of mathematical modelling and computer simulation is the capacity to analyse many different scenarios in a very little time. This is a vital property for the optimisation algorithms since a lot of simulations need to be carried out to locate the optimal points and, in real life, this would be unfeasible in terms of time and budget.

In general, models of urban wastewater processes need a calibration procedure in order to fit the experimental data. Companies usually use default values for all model parameters as they have been highly studied in the literature. However, there are innovative processes, especially those related to biofilm like IFAS and MBBR, for water and sludge lines, which performance description requires complex models that include biofilm interactions.

Actually, companies that commercialize these specific technologies use spreadsheets to design them. Nevertheless, the objective of recent studies is to promote the development of these models as was done with ASMs in order to dispose universal models. The main problem is that these models are characterized by a large amount of parameters with uncertain values to be assessed (there are not default values) and also several model outputs to be fitted with the measured data. Further, generally limited experimental data is available due to the large human and economic requirements. Owning to these aspects, complex environmental models are usually over-parameterized and identifiability issues have to be faced (Freni et al., 2011). It is for that reason that each company needs a specific model validated for its technology with their own parameter estimations. For their determination, a robust and advanced calibration/validation procedure able to reproduce experimental data for different operational conditions is highly required.

In this work, a model calibration methodology is proposed. The methodology consists of different steps that can be classified into two major phases. The objective of the first phase is to select the parameters to be calibrated. For this, a comprehensive sensitivity analysis and a correlation study are carried out with the aim of assessing the identifiability of the parameters and reducing the number of estimated parameters by fixing the value of the non-identifiable ones. A novel feature is that, rather than generating a single subset containing the most sensitive parameters, different subsets are selected based on their identifiability. On another note, in the second phase the model calibration is performed by means of a group-wise Monte Carlo methodology, specifically SCEM-UA algorithm (Vrugt et al, 2003) was carried out.

As a result of this phase, the probability distributions of the estimated parameters are obtained. Figure 1 shows the detailed flow-chart of the proposed calibration procedure.

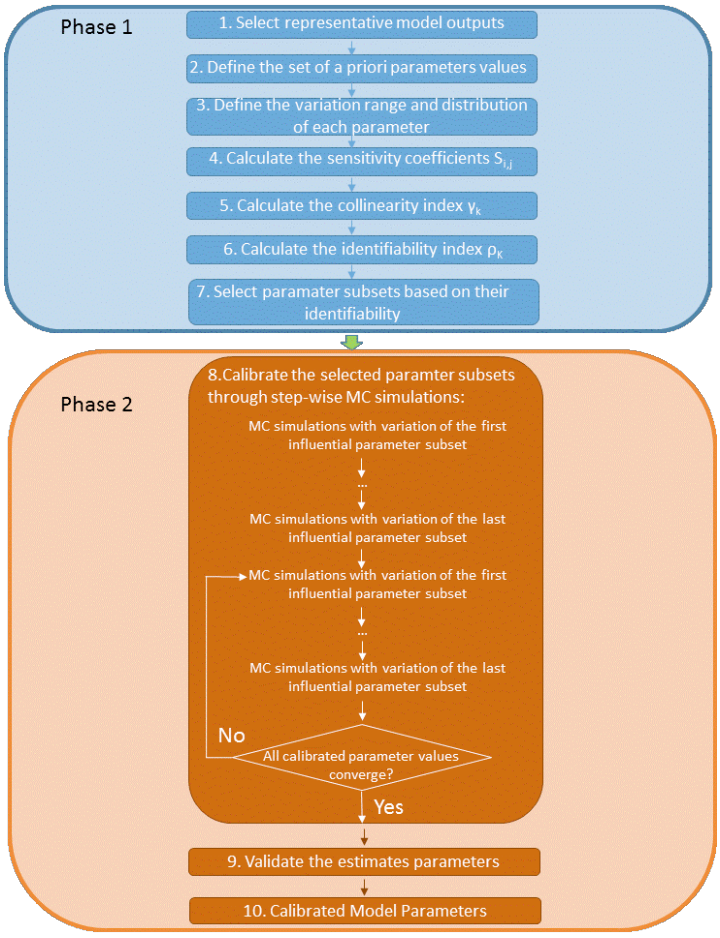

Figure 1. Flow chart of proposed calibration methodology

Results

Once the sensitivity and identifiability analysis was carried out, 4 subsets of two parameters each were selected and formed (except the last group) based on the ranking generated by the identifiability index. The parameters with the highest rate of identifiability, or what is the same, the parameters with higher sensitivity and lower correlation between them, are μ_{NH} -μ_{NO}, then the next ones are $K_{NH3,NH}$ - $K_{IN,NH3,NO}$ and finally the couple formed by $K_{O2,NH}$-$K_{O2,NO}$. Being in the latter subset only formed by δ_0.

By means of the sensitivity and identifiability analysis, the number of model parameters to be identified was reduced from 55 to 7, enabling a better capability for calibrating the model in the second phase of the procedure. Although the number of parameters has been drastically reduced, not all influential parameters can be expected to be identifiable since the LH-OAT and identifiability module have been performed.

The values of the model parameters obtained through MCMC algorithm are consistent with previous studies. The temperature was constant in the simulated periods and set equal to 30ºC. Therefore, the kinetic model parameters refer to that temperature.

The most influential model parameters calibrated are μ_{NH} and μ_{NO}. The calibrated value of the ammonium oxidizers bacteria growth rate, μ_{NH}=1.61d^{-1}, is in agreements with the literature values as well as μ_{NO} with a calibrated value of 1.36d^{-1}.

Figures 2 and 3 show the obtained posterior distributions of μ_{NH} and μ_{NO} parameters. As can be seen, the plots representing the posterior distributions provide an accurate estimate of the optimum parameter values.

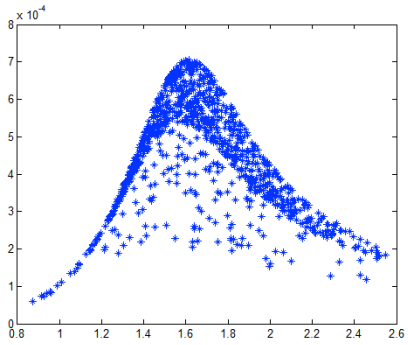

Figure 2. μ_{NH} posterior distribution

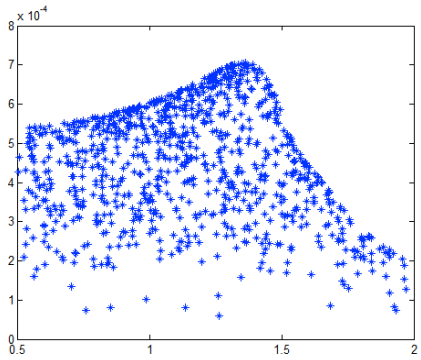

Figure 3. μ_{NO} posterior distribution

Once analysed parameter calibrated values, a dynamic simulation for the entire period were carried out. As can be seen in figure 4, good prediction accuracy with respect to the long term behavior of SNH_4, and SNO_2 was observed in the simulated dynamic period.

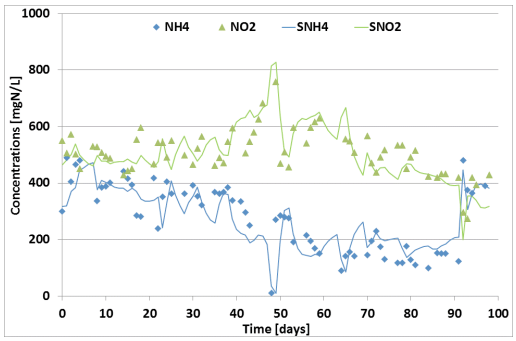

Figure 4. Experimental data vs simulation results

Discussion

In conclusion, a procedure for calibration of a nitritation model based on a comprehensive sensitivity and identifiability analysis and novel step-wise Markov Chain Monte Carlo-based calibration of the subsets of influential parameters has been presented.

The number of parameters to be calibrated was reduced thanks to an accurate sensitivity and identifiability analysis. The model was subsequently calibrated by using SCEM-UA methodology achieving satisfactory estimates of the model parameters.

References

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