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Calibration and sensitivity analysis of a one-dimensional model of pollutant transport and degradation in maturation ponds.

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The following hyperbolic system of conservation laws is used as a model of pollution dynamic in maturation ponds:

$$\frac{\partial AC(x,t)}{\partial t} + \frac{\partial QC(x,t)}{\partial x} = -k(t)AC(x,t) \quad (1)$$

$$\frac{\partial A(x,t)}{\partial t} + \frac{\partial Q(x,t)}{\partial x} = 0 \quad (2)$$

where A is the flow cross-section, C the contaminant concentration, Q the flow discharge, k the contaminant degradation coefficient. In maturation ponds, the water elevation is generally maintained to a given level so that the section A can be considered independent of time, leading to a discharge Q independent of space, according to the continuity equation (2). This model is discretized using an explicit finite volume approach and a Godunov scheme, that enables the flux QC to be computed by solving a Riemann problem.

In this study, the model is applied on a waste water system composed of three consecutive waste stabilization ponds, with a residence time of approximately five weeks. The system is considered uni-dimensional but with three different widths, so that $A(x)$ is piecewise constant with two discontinuities. Several measurements of the input and output discharge and concentration of chemical oxygen demand (COD) are available, approximatively each 15 days during one year. The model gives an estimation of the concentration in space and time, but will be calibrated according to the concentration at the system output as a function of time.

The only parameter to calibrate in this model is the degradation coefficient. However, since it is time dependent, a piecewise linear function is defined with N values of k, leading to a N-criteria calibration. The model calibration is classically performed by minimizing an error function. However, in this study, it appeared that the classical Root Mean Squared Difference (RMSD) failed in finding a global optimum of the k_n, since the convergence was rarely reached. Another kind of objective functions can be used for model calibration, that are based on a weak formulation of the distance between model outputs and measurements:

$$J_p = \sum_i \left(C_i(k) - C_i^m\right) \left|C_i(k) - C_i^m\right|^{p-1} \quad (3)$$

were $C_i(k)$ and C_i^m are the output concentrations respectively given by the model and observed and where p is a real value, that will give more weight to the high differences between outputs and observations when it is high whereas a small value of p will lead the model to fit the observations in average. Because these functions are monotone, the model calibration is transformed from a global optimization problem to a local root finding problem, that can be solved using a simple gradient-based method such as Newton's algorithm. Dealing with multi-criteria calibration, the N optimum parameters can be found by the intersection of N objective functions.

The gradient-based algorithms require the derivative of the function J_p, which depends on the derivative of C with respect to k i.e. the sensitivity of C with respect to k. An equation-based approach is used to compute the sensitivity. It consists in differentiating the model equation (1) with respect to the parameter of interest (here k). The sensitivity equation is then solved using the same framework as the model. The sensitivity analysis is also performed with respect to boundary conditions (here the input concentration and discharge) or to geometrical data such as the cross-section. However, the sensitivity equation can be solved only when the model equation is differentiable. In this study, the discontinuity in cross-sections leads to locally infinite values of the sensitivity. It has been shown in previous studies that this problem can be eliminated by introducing an additional source term in the sensitivity equation, that is applied only in case of discontinuity.

This calibration process, involving weak form-based objective functions and sensitivity solution, has shown good performance in this first study, despite the lack of accurate observation data. Its application to a more instrumented system (with more data and less uncertainties) is thus planed.