Sensitivity analysis applied to a water quality model for dissolved oxygen. Application to an irrigation channel in a Valencian community, Spain

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Abstract

This paper presents the sensitivity analysis developed with a mathematical model for Dissolved Oxygen over an irrigation channel in Valencian Community, Spain. This channel transports water from agricultural irrigation, wastewater and industrial discharges, and the processes of dispersion, transport and interaction between the water constituents have been studied.

The Dissolved Oxygen (DO) model, developed in finite differences, integrates the Nitrogen cycle and the BOD study within the DO equations. As a result, we can evaluate the concentration of every constituent in the system. We can make also an estimation of the influence of each parameter in the comparison between the data given by the model and the collected data in the real channel. The results have been contrasted with other mathematical surface water model such as QUAL2E.

The results have been calibrated with data collected in the channel during a measurement campaign, and in the process of calibration, the sensitivity analysis has been used as a tool for optimising this verification process. The study has pointed out the more influencing parameters in the concentrations over the whole system, and the optimum methodology for calibrating the model, which can be used also in unsteady state pollution situations and in branched systems. As a conclusion we show the results of the sensitivity analysis comparing the more important factors influencing the concentration of DO, BOD, Organic Nitrogen, Nitrite and Nitrate and the calibration methodology for this case.
1 The DO model

1.1 Fundamentals

Wastewater discharges in receiving systems, having either urban, industrial or agricultural source, causes a wide spectrum of water quality problems. Among them, the dissolved oxygen (DO) consumption in processes such as decomposition of organic matter, nitrification and respiration is especially outstanding. Although DO is recovered through reaeration and photosynthesis processes, the low concentrations observed in receiving waters can cause serious problems to the environment fauna and flora.

For a one-dimensional receiving system with uniform and steady state flow rate, the water quality model for DO can be formulated through the turbulent diffusion equation (O’Connor, 1967):

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = K_I \frac{\partial^2 C}{\partial x^2} + T_f - T_s$$

where $C = C(x,t)$ represents the concentration of DO at the point of abscissa $x$ at time $t$, and $K_I$ is the longitudinal diffusion coefficient of the system.

In expression (1), $T_f$ and $T_s$ represent the DO source and sink terms, which account for the oxygen load of the discharge, reaeration and photosynthesis, oxygen consumption due to degradation of the suspended and settled carbon organic matter and processes of nitrification and respiration.

The evolution of the different substances in the system consuming DO are modelled by expressions like:

$$\frac{\partial C_k}{\partial t} + U \frac{\partial C_k}{\partial x} = K_I \frac{\partial^2 C_k}{\partial x^2} - k_i C_k + T_{f_c}$$

assumed a first-order decay for the substance $k$, being $k_i$ the decay rate.

Thus, expression (1) takes the form

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = K_I \frac{\partial^2 C}{\partial x^2} - \sum_k r_k k_i C_k + T_{f_c}$$

where $r_k$ is an stoichiometric constant and subscript $k$ ranges through all the substances consuming DO.

Expressions (2) and (3) form a system of partial differential equations (PDE) with a number of equations and unknowns depending on the number of substances with DO consumption in the receiving water. The solution of this system gives the spatial and time evolution of the concentrations of DO and the substances involved in the DO processes. In this case, the complete nitrogen cycle and sediments oxidation integrate the whole system of equations.

1.2 Numerical integration of the PDE system

To perform the numerical integration of this system the Finite Difference Method (FDM) can be applied. In an explicit scheme, in order to avoid numerical dispersion, use can be made, for instance, of the prediction-correction
method by MacCormack. This method requires that the numerical stability condition should be satisfied by all equations (Chapra, 1997).

Taking into account that $\Delta x$, $U$, $K$, and $k$ are different for the different lines, the stability condition requires that the time increment to use satisfies the condition

$$\Delta t \leq \text{MIN} \left[ \frac{(\Delta x_j)^2}{U_j \Delta x_j + 2K_{i,j} + k_{k,j} (\Delta x_j)^2} \right]$$

(subscript $j$ ranging through all the system lines and subscript $k$ through all the considered substances, including DO. In figure 1 we can see the derivatives scheme used in this method.

![Scheme of the Mac-Cormack method](image1)

1.3 Boundary conditions

MacCormack's formulation can be directly applied to calculate the concentrations at the inner calculation points within every line of the network for time $t$, based on the values at every point and at the contiguous ones in the previous time step. Nevertheless, in order to obtain the solution boundary conditions must be forced at both ends of a line.

**Outlet node.** It is assumed the concentration profile to be horizontal at any time. This is based on the fact that the real concentration slope, as a function of distance $x$ is unknown. This hypothesis is acceptable if the line is long enough.

![Outlet node of the system](image2)

**Inlet nodes.** At inlet nodes, inlet flowrate $Q$ and concentration $C_k = C_k(t)$ of the different substances carried by this flowrate must be known. At any time step this concentration will be assigned to the first calculation point of the line connecting with the inlet node.
Inner nodes receiving outer flowrate. These are internal system nodes in which one or more tributary lines discharge some flowrate (for example, lines a and b) that is received by a line transporting the received flowrate (for example, line c). In addition, an external inlet of constant flowrate, $Q_e$, with known concentration of the substances under study, $C_{ke} = C_{ke}(t)$, can be considered. Assuming a complete mixing in the node, the concentration of substance k in the initial point of the line c at time step $n$ can be evaluated using the mass balance equation

$$C_{k1,c}^n = \frac{Q_a C_{k,f,a}^n + Q_b C_{k,f,b}^n + Q_e C_{ke}^n}{Q_a + Q_b + Q_e}$$

where subscript f stands for the final point of the tributary lines. Of course, if no flowrate enters through this node, magnitudes $Q_e$ and $C_{ke}$ will vanish.

Concentration profiles at inner nodes of the system. At the end point of a line conveying flowrate to an inner node of the system, the FDM cannot be directly applied since in this line an additional downstream point does not exist. As a consequence, a suitable hypothesis about the concentration profiles must be made. In some models the adopted solution considers horizontal profiles, as in the case of the outlet node of the system. This solution would be right if the line were long enough. With this solution the model treats the system lines individually, only mathematically connected by the mass balance equation (5).

Nevertheless, in order to treat the receiving system in a global way trying to look for a closer mathematical relationship among the lines meeting at an internal node, a different approach based on slope continuity must be used. Thus, assumption is made considering that the slope of the concentration profile at the final point of every line discharging at the inner point to be the same as the slope of the concentration profile at the initial point of the line transporting the received flowrate. This property will be independent of the concentration jump between every tributary line and the receiving line connected at the node.
Referring to Figure 5, given the concentration profile obtained at the lines a and c at time step n, this hypothesis forces a vertical displacement for the concentration profile on line c, with value $C_{k,c}^n - C_{k,a}^n$, avoiding discontinuity at this node in a fictitious way and producing a continuous profile. The evaluation of the spatial concentration gradients when applying the MacCormack scheme at the final point of the line a is based on this continuous profile. The same procedure should be used for the line b and for any other line discharging on the considered node.

Figure 5. Concentration profile at an inner node of the system.

2. Model sensibility analysis as a tool for calibration.

It is necessary to assess the model performance in terms of calibration, to make sure that the obtained data are sufficiently representative of reality. It is important to understand the general behaviour of the water quality model: one way to do so is the sensitivity analysis.

There are several sorts of sensitivity analysis formulation, (Chapra, 1997) but in this work we will be using the parameter perturbation analysis. The objective of this technique is to vary each one of the model parameters while holding the other terms constants. The corresponding variations of the state variables reflect the sensitivity of the solution to the varied parameter. Thus, if we need to quantify the sensitivity of one equation to a parameter, such as the concentration of DO to a parameter $k$, we would merely calculate this equation for $(x+\Delta x)$ and $(x-\Delta x)$ and estimate the variation in the concentration. This variation in the output variable is called the relative effect (figure 6). The formulation for the relative effect ($RE$) used is shown in equation (6) in which the mean values of function are used, considering that this function depends on the variable $time$.

$$RE = \frac{f(x+\Delta x) - f(x-\Delta x)}{\frac{2 f(x)}{\Delta x}}$$  (6)

This relative effect provides a transfer function to propagate the relative error of the input parameter into the relative error of the prediction.
This sensibility analysis must be found in the frame of a whole calibration process. This process of calibration is the “tuning” of the model to fit a data set, i.e.: the model parameters needs to be varied in order to obtain an optimal agreement between the model calculations and this data set.

Therefore, after the data set is collected there will be many parameters that can be varied (EPA, 1985). However, rather than arbitrarily trying to vary all of these, we should look for a systematic way to attain the best fit. With the aid of the proposed analysis, we can evaluate which are the most influencing parameters in the system as a whole, or in each one of the different parts of the same, therefore the adjust can be made in the quickest way. In the next figure 7 the proposed calibration process is scheduled.

As we can see, the establishment of the relative error is important in the calibration process to adjust the parameters. This error is related to the accuracy of the whole model. This accuracy is referenced to the purpose or the objectives determined at the start of the simulation model and it must be taken into account that there is an intrinsic error that can not be avoided and this is the lower limit of this value. The quantification of this error is shown in equation (7).

\[ S_r = \sum_{i=1}^{n} (c_{cal,i} - c_{m,i})^2 \]  

(7)

where \( c_{cal,i} \) and \( c_{m,i} \) are the calculated and measured concentrations respectively, (Mac Berthouex, 1994).

The objective of calibration (parameter optimisation) of any model of a physical system is to identify values of some parameters in a model which are not known a priori. In fact, in this case, the value of these parameters are not known but included inside accepted intervals (Saffi and Ouazar, 1999). This optimisation process is achieved by inputting data into the model and subsequent comparison of the computed values of output variables and the values as measured in the real system. In the trial-and-error calibration, the model parameters are adjusted according to a model judgement in order to provide a better match, minimising the error as the sum mentioned in equation 7. There are some other methods of optimisation that can be used in this task, we can even use the aid of some optimisation model, not concerned with the model in use.

In the next point, the example developed for a Valencian Community Channel will illustrate this methodology, shown in figure 7.
3 Application to an Irrigation Channel in Valencian Community Spain.

This methodology has been applied to a particular Valencian Community Irrigation Channel. This channel receives sewer and exceeding irrigation waters. In figure 8 the geographical situation of the channel is described.

The output solutions given by this model are DO, BOD, Ammonia, Nitrite and Nitrate concentrations. In order to obtain these concentrations, the equations defining the previously presented DO model, have been solved. To calibrate the model, we have measured these concentrations all along the channel, through over six kilometres along the same, and these values accomplish the data set used for the calibration.

There have been done multiple sets of measures in order to represent different situations. Now, we will use the steady state concentrations collected on July the 28th, 1999 in order to work with one data set.
In the next figure 9, are represented the DO concentrations calculated with the model and the measured ones, prior to the adjustment process.

The next step in the calibration process, is the establishment of the sensitivity analysis applied to this case (with an initial mean error about 37%). The matrix shown in Table 1 determines the table of influences, as relative effect.

As it can be seen, we can establish which are the more influencing input parameters over the output concentrations. For instance, if the objective is the DO, the more influencing input is the temperature parameter over reaction, which can be slightly modified and causes a big relative effect, followed by the oxygen saturation concentration.
Table 1. Relative effect with 15% variation in input parameters.

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<th>OUTPUT PARAMETER</th>
<th>DO</th>
<th>BOD</th>
<th>N as Ammonia</th>
<th>N as Nitrite</th>
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The calibration process will continue with the estimation of all the input parameters in order to minimise the error and adjust the measured and the predicted concentrations along the line. The relative effect will be considered until the estimation of the parameters is finished, avoiding to waste time in those parameters having little influence, such as the longitudinal dispersion coefficient. After calibration of the model, the mean error of the predictions improved until about 13% as a mean value.

In figure 10 we can see the comparison with the measured and predicted values, and also the concentrations obtained with other model: QUAL2 from USEPA, it can be shown the better adjust between them (USEPA, 1996). We can see that the calibration process has given good results when the parameters are well adjusted, and referring to figure 7, comparison with other models is very useful for validation.
Conclusion

In this paper we have presented the methodology for calibration a DO model, developed in finite differences, and the main characteristics of this model.

The main numerical procedures have been pointed out, and also the importance of a sensitivity analysis for the quick calibration with sufficient accuracy.

In order to illustrate such methodology, the equations have been solved for a real case study in Valencian Community and it can be observed, in the relative effect table, the influences over the solutions of the internal parameters.

Acknowledgements

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