Sensitivity analysis and calibration of the parameters of ESWAT: application to the River Dender

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Abstract. The paper deals with the sensitivity analysis and parameter calibration of a complex river water quality model, implemented in ESWAT. The Extended SWAT includes a QUALIIIE-based river quality simulator, in view of an integrated analysis of water quantity and quality management practices. The sensitivity analysis uses Latin Hypercube Sampling and criteria related to the duration of low concentrations of dissolved oxygen and the occurrence of high algae concentrations. The analysis on the river Dender shows that parameters related to the growth and die-off of the algae have the largest impact, while also the BOD decay constant and the benthic oxygen demand are important. A subsequent calibration of these most important parameters shows however that the optimal values of the parameters related to the activity of the algae are statistically not significant. This apparent contradiction is due to the poor information content of the measurements. It is concluded that the application illustrates the complementarity of the sensitivity analysis and the parameter calibration.

Keywords: Algae bloom; calibration; dissolved oxygen; modelling; rivers; river water quality; sensitivity analysis; water quality

Introduction

The SWAT simulator (Soil Water and Assessment Tool) was developed by the USDA and the Blackland Research Center (Arnold, 1996). It aims at the analysis of water quantity and quality management and includes features for studying the impact of climate change, agricultural practices and economic issues. ESWAT is an extended version of SWAT, whereby an in-stream water quality model has been implemented. Moreover, the processes are represented on a sub-daily time step, to allow for applications on smaller river basins and for the simulation of the impacts of eutrophication (van Griensven and Bauwens, 2001).

For models with many parameters, such as ESWAT, a trial and error calibration is very tedious, if not impossible. Automatic calibration procedures also pose problems, mainly due to the high correlation that often exists between the many parameters. A two step, semi-automated procedure is therefore suggested in this paper. In the first step, a sensitivity analysis for the model parameters is performed. An automated calibration is then performed in a second step, including only those parameters that have a significant effect on the model output.

The procedure is applied to the Dender river basin (Belgium), using ESWAT.

The Dender basin

The Dender river, a tributary of the river Scheldt, drains an area of 1384 km². The Dender rises at Ath, at a height of 40 m amsl. At the mouth, about 60 km downstream, the height is less than 10 m amsl. The main channel is partly canalised and contains 14 sluices are constructed. The river is heavily polluted by domestic, industrial and agricultural pollution (Demuynck et al., 1997).

Methods

While SWAT allows for the simulation of runoff and diffuse pollution from the watersheds to the river and the further transport along the river, it does not represent the river quality.
processes. In ESWAT, an in-stream water quality model was implemented, based on the approach used in QUAL2E (Brown and Barnell, 1987). For more details about the model, refer to van Griensven and Bauwens (2001).

The sensitivity analysis presented here focuses on the parameters of the in-stream quality model only, which includes 30 parameters.

Sensitivity analysis of models with a large numbers of parameters has become feasible through the Latin Hypercube Sampling technique (McKay, 1988), whereby the number of model runs can be limited to ca. 4/3 times the number of parameters. The LHS technique was implemented, using the UNCSAM software package, which also allows for the calculation of the different sensitivity measures (Janssen et al., 1992).

For the subsequent calibration of the most sensitive parameters, the Shuffled Complex Method is used (Duan et al., 1992). In contrast to the classical gradient search methods, this method is able to consistently find the global optimum as it searches for the best solution over the entire parameter space. The search technique is based on the simplex method but uses statistical techniques to find the global optimum very fast. The method does however not allow for the calculation of the variance and covariance matrices. As the latter are essential for the calculation of confidence bands and correlation, a final search is performed, starting from within the neighbourhood of the optimum, using a Gauss-Marquard-Levenberg algorithm. To this purpose, the PEST program is being used (Anonymous, 1998).

The sensitivity criteria
Because most of the biological life in the river depends on the amount of dissolved oxygen (DO), this variable is of great interest. For basic water quality, the standard in the EU is set to 5 mg/l. The time during which values of DO are less than 5 mg/l is therefore taken as a first criterion. On Figure 1 it can be seen that simulation values of dissolved oxygen are often beneath this standard.

The variable chlorophyll-a is considered to be 2% of the total concentration of phytoplankton in the river (Bowie et al., 1985). As algae blooms cause sharp drops in the oxygen concentration at night, high chl-a concentrations are also an indication of potentially harmful conditions. The time during which chl-a concentrations exceed a certain threshold value can therefore also be considered as a criterion. The value was set to 11 µg/l, being the value that was exceeded 10% of the time for the test case, using default parameters of the quality model (Figure 2).

Parameter sampling
For the (pseudo-) random sampling in view of the sensitivity analysis, the parameters are sampled with a given variation around a nominal value. These variations are expressed in terms of probability distributions. Nominal values may usually be found through e.g. default values for the parameters. Ranges of parameters may be available from literature (e.g. Bowie et al., 1985), although the latter may be biased due to the system and model dependence of the parameter values. Most of the time, little is known about the distribution.
The nominal values for the test case consisted of a mixture of literature values and values obtained after a first rough manual calibration of the model on the test data. Uniform distributions were considered for all the parameters, within the ranges specified in Table 1. The ranges are based on literature data and on personal experience.

Since the emphasis in a sensitivity analysis lies on the variations, the distribution types are not the major focus. A uniform distribution can therefore be considered as adequate. In UNCSAM, a uniform distribution can be applied for which the variation is specified as a fraction of the nominal value. Like that also a characterising of the variations is made (e.g. small or large for local or global sensitivity analyses). In this study we apply a global sensitivity analysis around the nominal values that gave good results after the first rough calibration (those given in Table 1) and we chose a variation of 90% of the nominal value of the parameters. The ranges are smaller than those given in Table 1. However, sampling with larger ranges would give unreliable results because values that lie far away from the optimum for this model are no reflection of the real parameter values possible for this model.

### Measures of sensitivity

Various statistics can be employed to quantify the sensitivity and uncertainty contribution of the model outputs to model inputs and parameters. Widely used are those based on linear regression and correlation analysis between the inputs and the simulated model outputs. Hereby, the parameters with significant correlation are determined to be important.
The ordinary regression coefficients (ORC), $\beta_0$, $\beta_1$, \ldots, $\beta_p$, are obtained by assuming a linear relation between the model parameters $x_1, \ldots, x_p$ and the model output $Y$:

$$Y(k) = \beta_0 + \beta_1 x_1(k) + \ldots + \beta_p x_p(k) + e(k)$$

with $k = 1, \ldots, N$, where $N$ is the number of model-outcomes. $e(k)$ represents the error due to a non-perfect matching of the linear approximation.

The ORC are obtained by minimising the criterion

$$\sum_{k=1}^{N} \left( Y(k) - \beta_0 - \sum_{i=1}^{p} (\beta_i x_i(k)) \right)^2.$$

The goodness of the linear approximation can be assessed by considering the coefficient of determination ($R^2$) of the regression:

$$R^2 = \frac{S_{\hat{y}}^2}{S_y^2},$$

with $S_{\hat{y}}^2 / S_y^2$ the variation on the expected value and the variation on the approximated value.

Because an extension of the set of regression coefficients with additional variables will invariably lead to an increase of $R^2$, independent of the significance of the added variable, an alternative measure can be introduced: the adjusted coefficient of determination $R^2_{adj}$:

$$R^2_{adj} = 1 - (1 - R^2)(N - 1) / (N - (1 + p)).$$

The closer the value of this coefficient is to 1, the better the regression.

If the parameters are highly correlated, numerical problems may occur when applying a linear regression analysis. The Variance Inflation Factor is a suitable measure for the correlation. It is defined as:

$$VIF_i = [C_x^{-1}]_{ii} \text{ with } [C_x^{-1}]_{ii} \text{ the } i \text{-th element of the inverse of the correlation matrix.}$$

A linear regression can be applied as long as the VIF is smaller than 5.

In this study, the normalised regression coefficients (NRC) are used as sensitivity measures. They represent the relative change of the output, $\Delta Y / Y_{\text{gem}}$, due to a relative change of the parameter values, $\Delta x / x_{\text{gem}}$. The subscript “gem” refers to the average or nominal value.

Results and discussion

Sensitivity analysis

The global Dender model contains 179 parameters and initial conditions that can be changed by the user. The sensitivity analysis presented here, however, only focuses on the parameters related to the in-stream water quality processes (Table 1). Initial conditions that are of no influence after a period of stabilisation are not considered and parameters that were judged not important, based on knowledge of physical, chemical and biological laws, are also left out.

The sensitivity analysis was carried out, based on simulations of the water quality variables at the mouth of the river for the whole year of 1994. The results are given in Table 2.

The largest VIF value for all the cases amounts to 1.68, indicating that the correlation between the parameters is not too high and that a linear regression can be applied. The regression between the parameters and the duration of low oxygen concentration leads to a value for $R^2_{adj}$ of 0.62. If the occurrence of high algae concentrations is considered as a criterion, the value is 0.66. Those values are low because it is a global analysis. The linear relationship becomes smaller when parameters are sampled that differ strongly from the optimum parameter value.

It is seen that when the duration of low DO concentrations is taken as a criterion, the parameters that influence the activities of the algae (the maximum algae growth rate, $u_{\text{max}}$, the algae light self shading coefficient, $\Lambda_1$, and the algae die-off rate, $k_{dd}$), rank among the
most important. Also the benthic oxygen demand, rk4, and the BOD decay constant rank
among the top 5. These results are similar to those found by Manache (1999) for the same
river, but with a different model.

When the high algae concentrations are considered, the parameters that control the algae
activity obviously remain important. However, new parameters appear in the list: the ratio
of chlorophyl to algae biomass, ai0, the algae settling rate, rs1, the oxygen production per
unit algae growth, ai3, the minimum light intensity for algae bloom, A0, and the sediment
shading coefficient, A2.

Parameter calibration
For the calibration of the model parameters, 79 4-hourly observations of DO, spread over ca. 5
weeks during the period September – December 1994, were available. The calibration is per-
formed by minimising the sum of squared differences between model outputs and the observa-
tions, considering the 8 most important parameters, as based on the low DO concentration
criterion. A variance-covariance analysis allows for the calculation of the confidence intervals
of the parameters. The results of the optimisation are represented in Table 3 and Figure 3.

It can be seen that the parameters related to the algae activity are found to be statistically
not different from zero (0 is included in the confidence interval) and that only the classical
parameters, such as those related to BOD decay and reaeration, are statistically significant.

This may seem to be in conflict with the results of the sensitivity analysis, as it may be con-
cluded from the calibration results that the algae processes can be ignored. The problem that is
observed here is, however, a problem of parameter identifiability. As the measurements took

Table 2 The normalised regression coefficient and the rank
of importance in the sensitivity analysis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>NRC</th>
<th>Rank</th>
<th>Parameter</th>
<th>NRC</th>
<th>Rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>umax</td>
<td>-0.3144</td>
<td>1</td>
<td>umax</td>
<td>1.3861</td>
<td>1</td>
</tr>
<tr>
<td>rk4</td>
<td>0.1998</td>
<td>2</td>
<td>kdd</td>
<td>-0.8208</td>
<td>2</td>
</tr>
<tr>
<td>A1</td>
<td>-0.1923</td>
<td>3</td>
<td>ai0</td>
<td>0.6110</td>
<td>3</td>
</tr>
<tr>
<td>rk1</td>
<td>0.1791</td>
<td>4</td>
<td>A2</td>
<td>0.5071</td>
<td>4</td>
</tr>
<tr>
<td>kdd</td>
<td>0.1766</td>
<td>5</td>
<td>rs1</td>
<td>-0.4796</td>
<td>5</td>
</tr>
<tr>
<td>rk2</td>
<td>-0.1361</td>
<td>6</td>
<td>A1</td>
<td>0.4322</td>
<td>6</td>
</tr>
<tr>
<td>A2</td>
<td>-0.1306</td>
<td>7</td>
<td>ai3</td>
<td>-0.4062</td>
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</tr>
<tr>
<td>bc1</td>
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<td>A0</td>
<td>-0.3856</td>
<td>8</td>
</tr>
<tr>
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</tr>
<tr>
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<td>10</td>
<td>rk2</td>
<td>-0.2933</td>
<td>10</td>
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</table>

Table 3 The calibration results

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Starting value</th>
<th>Calibrated value</th>
<th>95% lower limit</th>
<th>95% upper limit</th>
</tr>
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<tbody>
<tr>
<td>umax</td>
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<td>2.33</td>
<td>-1.75</td>
<td>6.43</td>
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<tr>
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<td>5</td>
<td>4.59</td>
<td>-3.20</td>
<td>12.4</td>
</tr>
<tr>
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<td>0.08</td>
<td>-3.99</td>
<td>4.15</td>
</tr>
<tr>
<td>kdd</td>
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<td>-0.24</td>
<td>1.2</td>
</tr>
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<td>0.42</td>
<td>0.03</td>
<td>0.81</td>
</tr>
<tr>
<td>rk2</td>
<td>0.3</td>
<td>0.59</td>
<td>0.20</td>
<td>0.98</td>
</tr>
<tr>
<td>A2</td>
<td>100</td>
<td>99</td>
<td>45</td>
<td>154</td>
</tr>
<tr>
<td>bc1</td>
<td>0.1</td>
<td>0.39</td>
<td>0.34</td>
<td>0.43</td>
</tr>
</tbody>
</table>
place during the fall and winter – a period with reduced or no algae activity – they do not contain sufficient information to derive the algae-related parameters.

The application illustrates very well the complementarity of the sensitivity analysis and the parameter calibration. While it might be concluded from the latter that the algae cycle might be neglected, the sensitivity analysis tells otherwise and indicates that additional measurements are necessary for a good calibration of the model.

Conclusions
A sensitivity analysis for the parameters of the in-stream water quality component of ESWAT on the river Dender showed that the parameters related to the algae activity rank among the most important, together with the parameters that control the BOD decay, the reaeration and the sediment oxygen demand. A subsequent automated calibration of the most important parameters resulted however in parameters for the algae cycle, which are not statistically significant. These results are not necessarily contradictory, as there is evidence that the information content of the measurements was too limited to allow for a determination of the algae-related parameters.

The paper therefore not only shows that a sensitivity analysis can be useful as a means for reducing the number of parameters that need to be optimised, but also that it adds value to a model calibration and that it can provide valuable information for the planning of a measurement campaign, in view of the calibration.

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Environmental Protection Agency, Athens, Georgia.