Development and verification of a new simulation tool for water quality prediction in the Ebro River

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Abstract

The implementation of the new EU Water Framework Directive (EU-WFD) is demanding the stakeholders to develop appropriate modelling tools to improve water quality and to optimise ecological resources. Based on these key points and on its experience in mathematical modelling, the research Centre CEIT and EPTISA, in collaboration with the Confederacion Hidrografica del Ebro (CHE), has developed a new water quality simulator as a first step towards the modelling of Integrated River basin Water Quality Management. Some of the main features of the developed simulator are presented in the paper. The hydraulic model is based on the resolution of the complete Saint Venant's equations. The four-point implicit finite difference algorithm solves these well-known equations numerically. The water quality model is based on the latest IWA River Water Quality Model Number 1 and presents some clear differences with respect to other existing models such as consistency, closed mass balances and easy integration with the Waste Water Treatment Plant models.

The experimental validation that includes the calibration in winter time of the main model coefficients from both the hydraulic and the water quality models has been assessed on the basis of the experimental campaign carried out in a 75 Km branch of the Ebro River in Zaragoza (Spain). Some results of this experimental campaign are also presented.
1 Introduction

Nowadays, planning, design and management of river basin systems is a complex task that can be assisted by computer simulation tools. Existing urban drainage systems, new wastewater treatment plants and in many cases, polluted receiving waters are different but related parts of the entire water cycle that should be considered as a single entity in order to achieve sustainable development. Despite the fact that considerable modelling effort has been carried out in recent years, a tool that allows the simulation of integrated river basin system is still under development.

More than ten years ago, the research centre CEIT started a new line of investigation in order to develop simulators based on mathematical modelling in the field of wastewater treatment plants (WWTP) and to explore their application in the optimisation of design and management of the process. Many practical applications of model-based design and operation has been carried out during last years ([1] to [6]). The experience gained during this period of time was the basis for a new research programme, with the objective of developing a new methodology towards the simulation of the whole-integrated urban drainage system, “the river basin” [7]. To attain this objective the investigation has been oriented to three complementary areas: research on WWTP, research on sewer systems and research on river water quality modelling. However, the same approach for modelling quality transformations in the urban drainage system, in the treatment plant and in receiving water bodies is sought and justified by the fact that basically the biochemical processes occurring are essentially the same.

The software architecture that fits best this objective is a collection of components implemented as an object-oriented model. This modular and flexible architecture allows the user the direct online comparison between real data and simulated results, simple building and simulation of different scenarios, easy model calibration and realistic exploration of operational strategies.

2 Description of the simulator

Figure 1 shows the basic model that includes the hydrodynamic component, the water quality component and the components (user interface and Simulator manager), which are necessary for the execution basically: Input/Output and management components. This modular design allows a more comprehensive understanding of the integrated model and also permits the up-to-date of the simulator including the future sediment component. The execution is free of synchronization points since data dependencies control the execution profile. That is, based on the hydrodynamic model, the hydraulic conditions (flow, water level, and velocity) are obtained and then the water quality state variables are computed with the water quality component, including transport processes and biochemical reactions.
The IOmodule is a windows interface that makes the simulator been friendly. It provides Input/Output screens to facilitate both the Input/Output preparation of data and to guide the execution of the model. Figures 2 shows an example of the appearance of the Input/Output screens.

2.1 Hydrodynamic

Several models can describe the flow water behaviour in a river. However, for estimating the effects of point sources, diffuse sources and transformation processes over long river branches, cross sectionally averaged (one dimensional) St. Venant equations [9] or some approximations to these equations are adequate hydrodynamic submodels. Equation (1) denotes continuity (mass conservation) and Equation (2) momentum conservation.

\[
\frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t} = q \tag{1}
\]

\[
\frac{\partial Q}{\partial t} + gA \frac{\partial y}{\partial x} + gA (S_f - S_o) = 0 \tag{2}
\]
where \( Q \) denotes streamflow (\( L^3/T \)), \( A \) cross-sectional area (\( L^2 \)), \( q \) lateral inflow per unit of length (\( L^2/T \)), \( U \) average flow velocity (\( L/T \)), \( g \) gravitational acceleration (\( L/T^2 \)), \( S_0 \) bottom slope (-), \( S_f \) friction slope (-), \( x \) longitudinal coordinate (\( L \)), \( y \) channel depth (\( L \)) and \( t \) time coordinate (\( T \)).

In our case the domain of the Ebro River is discretized into linear slices and the model computes the flow and water levels for each slice using the full nonlinear hyperbolic partial differential equations. The numerical resolution is based on a four-point implicit finite difference scheme. The method is straightforward in the sense that it formulates a sparse matrix based on the discretized St. Venant flow equations and the network connectivity.

![Example of an Input/Output screen.](Figure 2)

2.2 Water quality module

The aim of the water quality component is to separate the effect of transport of pollutants in the variations of their concentrations, from those due to transformation processes during their transport through the system. As shown in Figure 1, the Water Quality Model (WQModel) is divided into two groups of processes: the Transport Model (TModel) and the Biochemical model (Bmodel).

2.2.1 Transport Model (TModel)

To characterize the transport effects, the model incorporates advection/dispersion diffusion equations. Basically the TModel component is based on the one-dimensional pollutant continuity (advection-dispersion) equation solved by the
control-volume approach. The equations of TModel are assuming that substance is completely mixed over the water column, that is the substance is considered to be conservative and therefore Fick’s diffusion law can be applied. Once the equation is discretized the Crank-Nicolson method is for its numerical implementation.

$$\frac{\partial C}{\partial t} = -U \frac{\partial C}{\partial x} + \frac{\partial}{\partial x} E \frac{\partial C}{\partial x}$$

(3)

Where C denotes concentration (kg/L^3), U average flow velocity (L/T) and E the dispersion coefficient (L^2/T).

### 2.2.2 Biochemical Model (BModel)

The biochemical model introduced in the simulator is a reduced version of the River Water Quality Model No. 1 proposed by the IWA Task group on River Water Quality Modelling [8]. Its general formalism (Petersen matrix with process stoichiometry and kinetics) is identical to the formalism used in activated sludge models. However, the description of the composition of organic material and process stoichiometry is based on elemental mass fractions of organic compounds instead of chemical oxygen demand (COD) and content of nitrogen and phosphorous per unit of COD a distinguishing feature from others models. Although the elemental mass balance approach has the disadvantage of introducing model parameters that may not be identifiable in typical applications, it clarifies model assumptions and can be the basis for a thorough identifiability analysis. The implemented version includes the components shown in Table 1.

<table>
<thead>
<tr>
<th>NAME</th>
<th>COMPONENT</th>
<th>UNITS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ss</td>
<td>Biodegradable dissolved organic substances</td>
<td>[grOM/m³]</td>
</tr>
<tr>
<td>S_l</td>
<td>Inert dissolved organic substances</td>
<td>[grOM/m³]</td>
</tr>
<tr>
<td>S_NH4</td>
<td>Ammonium: NH₄⁺</td>
<td>[grN/m³]</td>
</tr>
<tr>
<td>S_NH3</td>
<td>Ammonia: NH₃</td>
<td>[grN/m³]</td>
</tr>
<tr>
<td>S_NO2</td>
<td>Nitrite: NO₂⁻</td>
<td>[grN/m³]</td>
</tr>
<tr>
<td>S_NO3</td>
<td>Nitrate: NO₃⁻</td>
<td>[grN/m³]</td>
</tr>
<tr>
<td>S_HPO4</td>
<td>Part of inorganic dissolved phosphorous: HPO₄²⁻</td>
<td>[grP/m³]</td>
</tr>
<tr>
<td>S_H2PO4</td>
<td>Part of inorganic dissolved phosphorous: H₂PO₄⁻</td>
<td>[grP/m³]</td>
</tr>
<tr>
<td>S_O2</td>
<td>Dissolved oxygen: O₂</td>
<td>[grO/m³]</td>
</tr>
<tr>
<td>X_H</td>
<td>Heterotrophic organisms</td>
<td>[grOM/m³]</td>
</tr>
<tr>
<td>X_N1</td>
<td>Organisms oxidising ammonia to nitrite</td>
<td>[grOM/m³]</td>
</tr>
<tr>
<td>X_N2</td>
<td>Organisms oxidising ammonia to nitrate</td>
<td>[grOM/m³]</td>
</tr>
<tr>
<td>X_ALG</td>
<td>Algae and macrophytes</td>
<td>[grOM/m³]</td>
</tr>
<tr>
<td>X_CON</td>
<td>Consumers</td>
<td>[grOM/m³]</td>
</tr>
<tr>
<td>X_S</td>
<td>Biodegradable particulate organic material</td>
<td>[grOM/m³]</td>
</tr>
<tr>
<td>X_I</td>
<td>Inert particulate organic material</td>
<td>[grOM/m³]</td>
</tr>
<tr>
<td>X_P</td>
<td>Phosphate adsorbed to particles: HPO₄²⁻</td>
<td>[grP/m³]</td>
</tr>
<tr>
<td>X_H</td>
<td>Particulate inorganic material</td>
<td>[grMI/m³]</td>
</tr>
</tbody>
</table>
3 Experimental verification

The first experimental campaign to assess the simulation model took place during the last month of November 2001 and lasted 15 days with the objective of analyzing its dynamic behaviour under winter conditions. Figure 3 shows the characteristics of the sampling sites where several chemical parameters were measured.

3.1 Case study

The simulator has been applied to a 75Km branch of the Ebro River located near Zaragoza (Spain) (Figure 3). The branch is divided into 30 segments (of approximately 2500m in length) of varying slope from 0.00032 to 0.0022 and each segment is partitioned into slices of 500m.

Figure 3: Test Application: Ebro River.
3.2 Hydrodynamic simulation
Figure 4 shows a classical output of the model. The execution profile shows a dynamic flow behaviour based on a given hydrograph. The used data were obtained from the experimental campaign.

Figure 4: Dynamic simulation of flow during the experimental verification

3.3 Experimental data calibration
Figure 5 shows the predicting capability of the model in three sampling points P1, P5 and P6 (see Figure 3) based on measured parameters (TSS, VSS, N-NO₃ and P-PO₄). It can be seen that during the low flow period, the experimental values remain relatively stable. Under these conditions the measured values obtained by model simulation including different inflows into the Ebro River are comparable to the experimental ones.

As flow increases motivated by a rain event, the solid content of TSS and VSS increases rapidly and the concentration of the dissolved parameters (N-NO₃ and P-PO₄) decreases by dilution. These two facts have been well described by model simulation as is shown in Figure 5.

3.4 Dynamic behaviour of the state variables
Figure 6 shows the dynamic behaviour of four state variables, two dissolved (Sₛ and Sᵢ) and two particulate (Xₕ and Xᵢ) at measuring points P1, P2, P3, P4, P5 and P6 (Figure 3).

The profile shows the effect of organic accumulation from point P1 to P6 produced by wastewater discharges. This organic accumulation reflects the mass conservation principle: an increase in biodegradable substrate (Sₛ and Xₛ) must be followed by an increase in the resulting heterotrophic biomass (Xₕ). Also the different parameters show a cycle on a daily basis due to daily temperature fluctuations. After the rain event, the concentration of particulate materials decreases by dilution while the concentration of dissolved materials increases. In the case of inert soluble substrate (Sᵢ) this increase is due to a higher content in
sampling location P1. Thus this increase of $S_1$ in location P1 is added to the next sampling locations. The moderate increase in $S_0$, is mainly because of a lower biodegrading biomass ($X_H$) in the river by dilution after the rain event.

![Graphs showing VSS, TSS, NO3, and PO4 concentrations over time.](image)

**Figure 5:** Some results of the experimental model verification.
Figure 6: Simulated state variables during the experimental verification

Summary and conclusions

The behaviour of a new Water Quality Model for River simulation, based on the RWQM1 model proposed by the IWA, has been assessed on the basis of an experimental campaign carried out in a branch of 75 Km of the Ebro River in Zaragoza (Spain). This assessment has included the calibration of the hydraulic
component, both the transport and biological processes, and the achievement of a methodology for future measurement campaigns. Further improvements are being explored including sediment transport.

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References