Dynamic simulation of the water quality in rivers based on the IWA RWQM1. Application of the new simulator CalHidra 2.0 to the Tajo River

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Abstract This paper presents a new model for the dynamic prediction of water quality in rivers using in-series continuously stirred tank reactors (CSTR) and process transformations based on the IWA RWQM1. The transport model introduces a new parameter *f* (fraction of solids that are not retained in the in-series reactors) that splits hydraulic and solids retention times, regulating the transport of particulate substances along the river stretch. The characterization of the model components is based on elemental mass fractions, and closed mass balance is guaranteed for each process transformation. The resulting model has been implemented in the new simulator CalHidra 2.0 and applied to a branch of the Tajo River in the Madrid area. The spatial profiles of ammonium, nitrates, and dissolved oxygen in different seasonal periods have been used to calibrate the model. The proposed model also has shown its usefulness for exploring the evolution of the water quality in the Tajo River under different scenarios.

Keywords Calibration; hydrodynamic models; river water quality; RWQM1; Tajo River

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Introduction

The basic goal of the new EU Water Framework Directive (EU 2001) is to achieve a 'good status' for both surface and groundwater, with a strong focus on ecological criteria. In agreement with this ambitious objective, research activities are being focused on the development of new tools for the management of integrated water resources. Traditional river water quality models have some limitations when describing river acclimatization to changes in pollutant load or environmental conditions, and when tracking mass continuity if a BOD-based description of model components is used. The IWA River Water Quality Model N°1 (RWQM1) copes with both problems, firstly by incorporating biomass population growth and respiration, and secondly, by describing the composition of organic material as mass fractions of organic compounds (C, H, O, N, and P).

In many cases, the biochemical activity of the river cannot be described properly considering only the transformations occurring in the bulk-liquid (Rauch and Vanrolleghem, 1998) because modelling of the benthic activity is also needed. However, modelling more than one compartment increases the number of state variables, leading to considerably longer calculation times. This paper proposes a new model for the dynamic prediction of water quality in rivers using in-series continuously stirred tank reactors (CSTR) and process transformations based on the IWA RWQM1 model.

Materials and methods

Mathematical model and numerical resolution

The mathematical model developed at CEIT includes three sub-models: the hydrodynamic model, the advection-dispersion model, and the biochemical transformation model.

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Hydrodynamic model. The hydrodynamic model is based on the one-dimensional Saint Venant equations for the description of continuity and momentum conservation (Abbott and Minns, 1998).

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

$$\frac{\partial Q}{\partial t} + \frac{\partial (QU)}{\partial x} + gA\frac{\partial y}{\partial x} + gA(S_f - S_0) = 0 \tag{2}$$

where Q denotes the streamflow (L^3/T), A the cross-sectional area (L^2), q the lateral inflow per unit of length (L^2/T), U the average flow velocity (L/T), g the gravitational acceleration (L/T^2), S_0 bottom slope (−), S_f friction slope (−), y channel depth (L), x longitudinal coordinate (L), and t time coordinate (T). The numerical resolution of the full non-linear hyperbolic partial differential equations is based on a four-point implicit finite difference scheme.

Advection-dispersion model. The advection-dispersion model describes the transport of the model components among the river volumes (Thomann and Mueller, 1987), assuming the river as a series of CSTR (Deksissa *et al.*, 2004). The advection-dispersion model governs the transport of both the solubles and a fraction f of the particulate components (Figure 1). Therefore, this parameter (between 0 and 1) regulates the splitting of the HRT and SRT in the reactors, reproducing the accumulation of particulate substrate and biomass in the river stretch.

$$\begin{aligned}
\frac{\partial Xsol_j}{\partial t}\Big|_{advect-dispers} &= -\frac{1}{A}\frac{\partial (Q{\cdot}Xsol_j)}{\partial x} + \frac{1}{A}\frac{\partial}{\partial x}\left(E{\cdot}A{\cdot}\frac{\partial Xsol_j}{\partial x}\right) \\
\frac{\partial Xpar_j}{\partial t}\Big|_{advect-dispers} &= -\frac{1}{A}\frac{\partial (Q{\cdot}f{\cdot}Xpar_j)}{\partial x} + \frac{1}{A}\frac{\partial}{\partial x}\left(E{\cdot}A{\cdot}\frac{\partial (f{\cdot}Xpar_j)}{\partial x}\right)
\end{aligned} \tag{3}$$

where $Xsol_j$ denotes the concentration of the j^{th} soluble components (M/L^3), $Xpar_j$ stands for the concentration of the j^{th} particulate components (M/L^3), A indicates the cross-sectional area (L^2) and E the dispersion coefficient (L^2/T).

Biochemical transformation model. The implemented biochemical model is a reduced version of the IWA RWQM1 model (Reichert *et al.*, 2001) that does not include the chemical equilibrium equations for pH prediction. The resulting model includes 16 components (Table 1) and 24 transformations (Table 2). All the model components and process stoichiometry have been characterized by means of their elemental mass composition in C, H, O, N, and P, and the mass continuity has been balanced for all the process transformations (de Gracia *et al.*, 2006). The elemental mass fractions for the model components and the resulting Petersen stoichiometric matrix are presented in Tables 2 and 3 for default values of the main stoichiometric parameters.

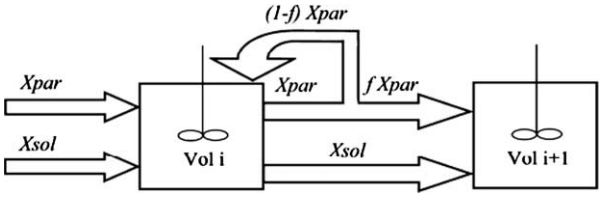


Figure 1 Schematic description of the CSTR conceptual approach

Table 1 Model components of the biochemical model

Model components			Model components		
N°	Name	Description	N°	Name	Description
1	S_S	Easily biodegr. substrate	9	X_H	Heterotrophic organisms
2	S_I	Inert dissolved organic	10	X_{N1}	Organism oxidizers
3	SNH_4	Ammonium	11	X_{N2}	Nitrite oxidizers
4	SNO_2	Nitrite	12	X_{ALG}	Algae and macrophytes
5	SNO_3	Nitrate	13	X_{CON}	Consumers
6	$SHPO_4$	Inorganic dissolved P	14	X_S	Particulate organic material
7	SO_2	Dissolved oxygen (DO)	15	X_I	Inert particulates
8	$SHCO_3$	Bicarbonate	16	X_P	Phosphate adsorbed

The simulation program CalHidra 2.0

The mathematical models and the numerical resolution algorithms have been implemented into a software application developed at CEIT for the Spanish Engineering firm, EPTISA (Salterain *et al.*, 2003). The resulting simulation tool, called CalHidra 2.0, is an object-oriented software with friendly interfaces where the user can define easily the river basin, the boundary and initial conditions, the environmental conditions (temperature and light), and the model parameter values (Reichert *et al.*, 2001). The data interchange option can use ASCII, binary, or Excel files and output results can be visualized graphically or numerically.

Methodology proposed for the application of the water quality model

In dry weather conditions, pollutant removal and water quality in the river is the result of a complex equilibrium between the pollutant load and the biodegradation carried out by the river biomass, including, in a general case, the bacterial activity in the bulk liquid and in the sediments. So, the RWQM1 model includes as model components the concentration of the microorganism populations, making it possible to close mass balances in the whole system. This fact reduces the uncertainty significantly because substrates, nutrients, and biomass concentration cannot vary arbitrarily, but all are closely related by the kinetic and stoichiometric relationships and by the transport equations.

The key parameters for the initial calibration of the proposed model are the fraction of solids that are not retained in each reactor (parameter *f*) and the transfer of oxygen to the liquid phase (parameter K_La). The parameter *f* splits HRT and SRT and enables the model to describe the accumulation of biomass when a high self-depuration activity due to the microorganisms attached to the river bed is observed. Additionally, the parameter K_La allows the model to reproduce the dissolved oxygen measured experimentally. Therefore, the experimental information about the biochemical activity in the river (for example, the spatial and temporal profiles for dissolved oxygen, ammonia, nitrites, nitrates, etc.) should enable the calibration of both parameters *f* and K_La and, as a consequence, the estimation of the active biomass in the different river stretches. Once this initial calibration is made, a finer estimate of the most relevant kinetic and stoichiometric parameters can be carried out.

Results

Description of the case study: the Tajo River in the Madrid area

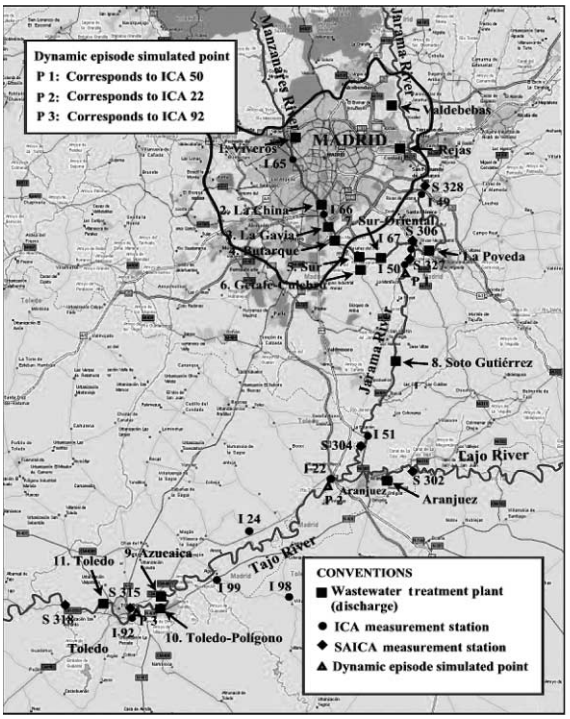
The Tajo River originates in the centre of Spain (Sierra de Albarracín) and flows to Lisbon, where it joins the Atlantic Ocean. The studied area covers a 125 km length of river including branches of the Tajo, Jarama, and Manzanares rivers, where the latter receives the main effluents of Madrid WWTPs. Figure 2 shows the main river branches,

Table 2 Elemental mass fraction of the model components

Mass fractions	1 S_S	2 S_I	3 SNH_4	4 SNO_2	5 SNO_3	6 $SHPO_4$	7 SO_2	8 $SHCO_3$	9 X_H	10 X_{N1}	11 X_{N2}	12 X_{ALG}	13 X_{CON}	14 X_S	15 X_I	16 X_P
α_C	0.57	0.61	0.00	0.00	0.00	0.00	0.00	0.20	0.52	0.52	0.52	0.36	0.36	0.57	0.61	0.00
α_H	0.08	0.07	0.22	0.00	0.00	0.01	0.00	0.02	0.08	0.08	0.08	0.07	0.07	0.08	0.07	0.01
α_O	0.28	0.28	0.00	0.70	0.77	0.67	1.00	0.79	0.25	0.25	0.25	0.50	0.50	0.28	0.28	0.67
α_N	0.06	0.03	0.78	0.30	0.23	0.00	0.00	0.00	0.12	0.12	0.12	0.06	0.06	0.06	0.03	0.00
α_P	0.01	0.01	0.00	0.00	0.00	0.32	0.00	0.00	0.03	0.03	0.03	0.01	0.01	0.01	0.01	0.32
α_C	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
gCOD/gOM	1.79	1.87							1.61	1.61	1.61	0.93	0.93	1.79	1.87	

Table 3 Stoichiometric matrix at the transformation processes

Transformations	S_S gCOD	S_I gCOD	SNH_4 gN	SNO_2 gN	SNO_3 gN	$SHPO_4$ gP	SO_2 gO	$SHCO_3$ gCOD	X_H gCOD	X_{N1} gCOD	X_{N2} gCOD	X_{ALG} gCOD	X_{CON} gCOD	X_S gCOD	X_I gCOD	X_P gP
Aerobic growth X_H (NH_4)	−1.85		−0.01			−0.01	−0.85	0.27	1.00							
Aerobic growth X_H (NO_3)	−1.85				−0.01	−0.01	−0.80	0.27	1.00							
Aerobic respiration of X_H			0.07			0.02	−0.77	0.25	−1.00						0.23	
Anoxic growth X_H (NO_3)	−2.22			1.07	−1.07	−0.01		0.39	1.00							
Anoxic growth X_H (NO_2)	−3.71			−1.63		0.00		0.86	1.00							
Anoxic respiration of X_H			0.07		−0.27	0.02		0.25	−1.00						0.23	
Growth of X_{N1}			−4.78	4.70		−0.02	−15.13	−0.32		1.00						
Aerobic respiration of X_{N1}			0.07			0.02	−0.77	0.25		−1.00					0.23	
Growth of X_{N2}				−20.71	20.63	−0.02	−22.33	−0.32			1.00					
Aerobic respiration of X_{N2}			0.07			0.02	−0.77	0.25			−1.00				0.23	
Growth of X_{ALG} (NH_4)			−0.06			−0.01	1.00	−0.39				1.00				
Growth of X_{ALG} (NO_3)					−0.06	−0.01	1.29	−0.39				1.00				
Aerobic respiration X_{ALG}			0.06			0.01	−0.60	0.26				−1.00			0.40	
Death of X_{ALG}			0.03			0.00	0.20	0.00				−1.00		0.95	0.25	
Growth of X_{CON} (X_{ALG})			0.13			0.02	−0.15	0.32				−5.00	1.00	3.85		
Growth of X_{CON} (X_S)			0.13			0.02	−4.77	1.45					1.00	−5.77		
Growth of X_{CON} (X_H)			0.45			0.13	−3.80	1.18	−8.65				1.00	3.85		
Growth of X_{CON} (X_{N1})			0.45			0.13	−3.80	1.18		−8.65			1.00	3.85		
Growth of X_{CON} (X_{N2})			0.45			0.13	−3.80	1.18			−8.65		1.00	3.85		
Aerobic respiration X_{CON}			0.06			0.01	−0.60	0.26					−1.00		0.40	
Death of X_{CON}			0.03			0.00	0.20	0.00					−1.00	0.95	0.25	
Hydrolysis	1.00		0.00			0.00	0.00	0.00						−1.00		
Adsorption of HPO_4						−1.00										1.00
Desorption of HPO_4						1.00										−1.00



WWTP LIST

1. Viveros
2. La China
3. La Gavia
4. Butarque
5. Sur
6. Getafe-Culebro
7. Sur Oriental
8. Soto Gutiérrez
9. Azucaica
10. Toledo-Polígono
11. Toledo

Figure 2 Case study Manzanares, Jarama, and Tajo river branches, ICA and SAICA measurement stations and the main WWTP discharges

measurement stations, and WWTP discharges (numbered in the studied branch). Since most of the WWTPs in the area were designed for C removal, the main objective of the simulation studies has been the investigation of a new scenario where the main WWTPs are updated for C and N removal.

Simulation results

Steady-state simulation of ammonium, nitrates, and oxygen concentration profiles along the river branches for different seasonal periods of 2003 are used for the first calibration of the parameters f and K_La (trial and error procedure is used). As an example, Figure 3 shows NH_4, NO_3, and DO calibrated spatial profiles of February and August. The three River branches and the location of the WWTP discharges (arrows) are indicated in the top of the figure to aid the interpretation of the results. The WWTPs' discharges lead to high NH_4, concentration in the Manzanares River, which will be greatly nitrified along the Jarama stretch. Comparing February to August, it can be shown that higher summer temperatures prompt a faster biodegradation of NH_4, leading to a faster increase in NO_3. Additionally, DO in-river concentration becomes lower in August in the discharge zone. This should be specifically analysed using smaller discretization step size of in-series tank volumes in order to detect possible low-oxygen zones and denitrification episodes. Nevertheless, parameters $f = 0.08$ and $K_La = 35$ day^{-1} were reasonably able to reproduce different month's experimental profiles. For this initial calibration, the rest of the parameters had default values (Reichert *et al.*, 2001).

Once the initial model calibration is made, the model predictions can be used to explore the biochemical behaviour of the river under different plant discharge scenarios. In this sense, the future upgrading of the existing plants to nitrogen removal and their consequences on the river water quality have been analysed carefully using model-based

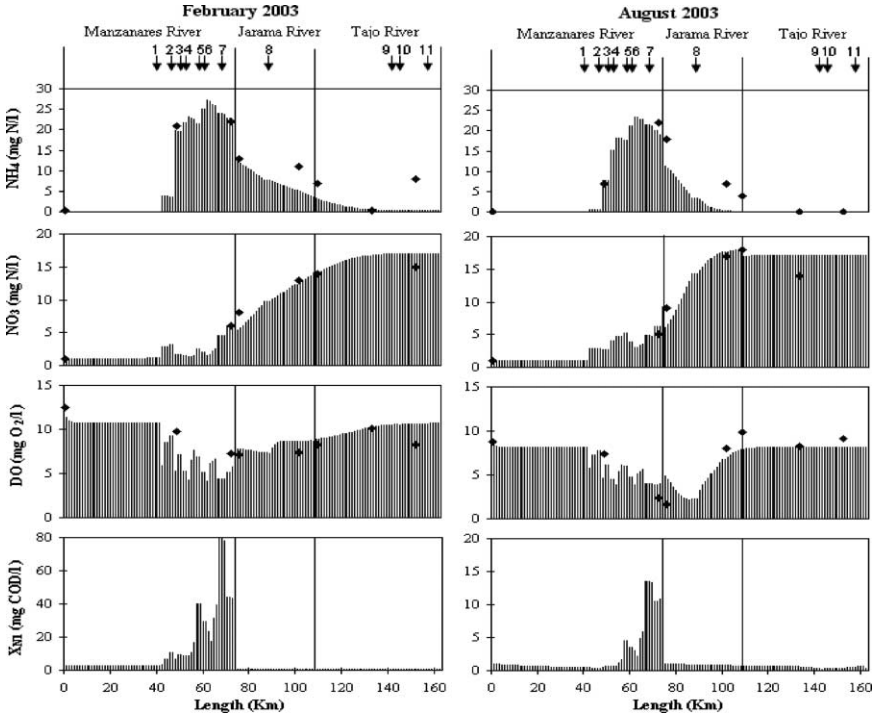


Figure 3 Spatial profiles of NH_4, NO_3, DO, and X_{N1} concentration in the river branches

dynamic simulations. Figure 4 shows a typical example of the river water temperature and the nitrogen discharge concentrations predicted by the ASM1 model (Henze *et al.*, 2000) for a WWTP with limited nitrification at low temperatures. These simulations have been used as input data in the calibrated river water quality model.

Figure 5 shows the yearly evolution of ammonium, nitrates, dissolved oxygen, and nitrifying biomass in the river. As shown in Figure 2, the point P1 is located in the Manzanares River just downstream of the city of Madrid, P2 is located shortly after the Jarama and Tajo rivers come together and finally, P3 is near Toledo. The simulation results show a significant increase in the ammonium concentration in winter, due to the loss of nitrification expected in the plants and the limited self-purification of the river at low temperatures. However, for higher temperatures, nitrification appears simultaneously in the WWTPs and in the river, affecting the ammonium and nitrate concentrations. In this exploratory example, the DO concentration seems to be high enough during the whole year. However, the increment of nitrates in this summer scenario should be analysed carefully since it can prompt algae growth and possible eutrophication problems.

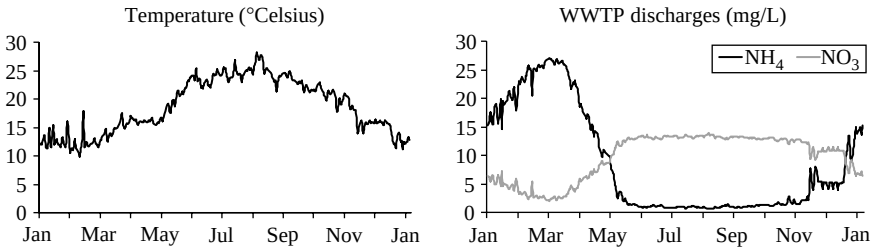


Figure 4 Description of input data to simulate the yearly perturbation of the river water quality: water temperature and WWTP effluent discharges of ammonium and nitrates

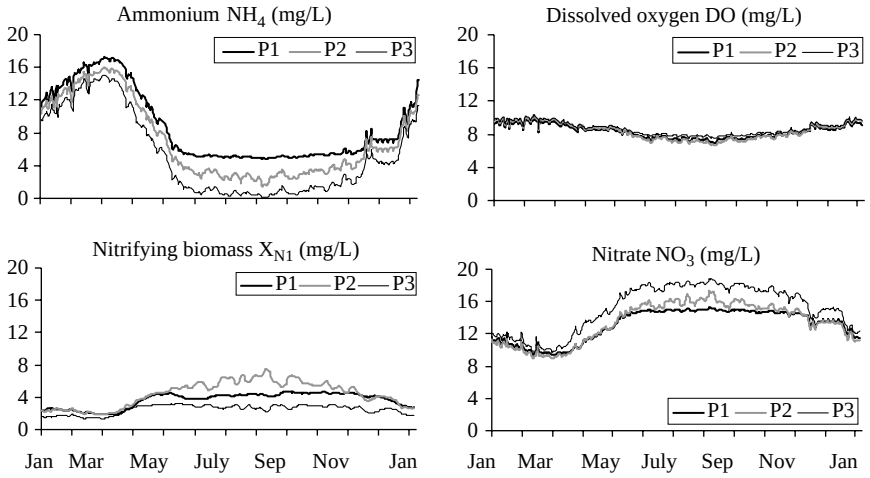


Figure 5 Dynamic simulation of the water quality evolution predicted in the river at three different measuring points as a consequence of discharges from the WWTP

It is important to remark the significance of the value of the parameter *f*, since it determines the accumulation, or 'wash-out', of microorganisms along the river, and therefore the river water quality scenario. In this sense, a more sophisticated calibration procedure that evaluates the uncertainty in the estimation of the parameter *f* (for example Monte Carlo techniques) would be very useful to predict the probability of different river scenarios, characterized by the presence or not of significant biochemical activity (Martin *et al.*, 2006).

Other sets of simulations also can be carried out to explore different scenarios in the integrated system, including plants and receptors. Typical examples are the selection of the most appropriate quality requirements in the WWTP effluent (Rauch and Vanrolleghem, 1998), the required dilution rate (or minimum ecological flow) to maintain the biochemical quality in the river, or the spatial and temporal impact of possible uncontrolled discharges.

Conclusions and further research

A new mathematical model for the dynamic prediction of water quality in rivers using in-series CSTR and process transformations based on the RWQM1 has been developed and implemented in the CalHidra 2.0 simulation tool. The model uses a new parameter *f,* which splits HRT and SRT, allowing solids retention in the in-series reactors. Therefore, the new model is able to predict the biomass accumulation and the biochemical activity experimentally observed in many high-loaded rivers.

The proposed model has been applied successfully to the analysis of the nitrogen removal in a branch of the Tajo River in the Madrid area. The spatial profiles of ammonium, nitrates, and dissolved oxygen at different seasonal periods have been used for the calibration of both the solids retention time and oxygenation along the selected case-study.

Once calibrated, the proposed model has been used to explore the water quality in the Tajo River under different scenarios. As an illustrative example, the impact of the future upgrading of several WWTPs for nitrogen removal was studied. The model structure's closed mass balance has facilitated the prediction of the biomass acclimatization to changes in water temperature or load conditions. Moreover, the similarities between

the RWQM1 and the conventional WWTP models facilitate an integrated exploration of the whole system.

Further research is being carried out into the modelling of the relationship between the parameters f and K_La and the hydrodynamic conditions of the river. Besides, an uncertainty-based model analysis would improve model predictive capability understanding and allow a quantitative risk analysis of different river scenarios.

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