

## Article (refereed) - postprint

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Voss, Anja; Alcamo, Joseph; Barlund, Ilona; Voss, Frank; Kynast, Ellen; Williams, Richard; Malve, Olli. 2012 Continental scale modelling of in-stream river water quality: a report on methodology, test runs, and scenario application. *Hydrological Processes*, 26 (16). 2370-2384. [10.1002/hyp.9445](https://doi.org/10.1002/hyp.9445)

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# Continental scale modeling of in-stream river water quality: A report on methodology, test runs, and scenario application

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## Abstract:

To address the continental and large scale aspects of water quality assessments new modelling approaches are required. This paper describes the development of a continental-scale model of river water quality - WorldQual. Simple equations, consistent with the availability of data on the continental-scale, are used to simulate the response of biochemical oxygen demand (BOD<sub>5</sub>) and total dissolved solids (TDS) to anthropogenic loadings and flow dilution. A methodology is developed that is appropriate for scenario analysis on the continental and global scale. Average monthly river water quality is modeled on a 5 arc-minute grid covering all Europe. Loadings are derived from assumptions about water use, return flows and other variables. The model WorldQual is tested against measured longitudinal gradients and time series data at specific river locations. The model performance on European scale shows that a good fit can be reached when using concentration classifications as a measure: For BOD<sub>5</sub>, 51 % of the simulated data is in the same quality class as the measurements and 30 % differ only by one water quality class; for TDS the respective values are 35 % and 41%. WorldQual was applied to investigate the impact of climate change on resulting changes of in-stream concentrations. The results for Europe show that future climate changes only have a small impact on European in-stream concentration levels of BOD<sub>5</sub>, except for the Eastern part and the Black Sea region. This effect is stronger for the IPCM4-A2 scenario than for the MIMR-A2 scenario.

## Nomenclature

BOD<sub>5</sub> = Five-day biochemical oxygen demand (mg l<sup>-1</sup>)

TDS = Total dissolved solids (mg l<sup>-1</sup>)

## INTRODUCTION

Over the past two decades the idea that water research and policy have not only local and regional aspects but also important continental and global scale dimensions has gained credence (e.g. Alcamo et al. 2008). But this new global view of water has focused mostly on the quantity of water rather than its quality. The state of global water quality was assessed twenty years ago (Meybeck et al. 1989) but such an effort has not been repeated since. The reasons for this are not clear, but perhaps it has to do with the difficulty in evaluating water quality on the large scale. In comparison to the relative ease in estimating water availability

through mass balances of precipitation and other measured parameters, estimating the large scale patterns of water quality is usually a more complicated task, requiring more detailed data about sources and sinks of water quality parameters. Also, the spatial distribution of water quality is frequently more heterogeneous and locally determined than water quantity, also increasing data requirements. Furthermore, it is often possible to characterize water quantity with simple metrics such as volume of water per unit drainage area, whereas water quality can only be described by many different biogeochemical quantities, as wide-ranging as the content of dissolved solids, or the consumption of oxygen. The sum of these considerations makes continental or global assessments of water quality a great challenge.

Although catchment scale modelling of water and solute transport and transformations is a widely used technique to study pollution pathways and effects of policies and mitigation measures (e.g. Schob et al. 2006, Bärlund et al. 2007, Hesse et al. 2008, Krause et al. 2008, Volk et al. 2008) there are only a few examples of continental water quality modelling approaches (Seitzinger et al. 2002, Green et al. 2004, Grizzetti and Bouraoui 2006). On global scale, models developed so far focus on pollution pathways and loadings within a river catchment or into a river stream (e.g. Siebert 2005, Van Drecht et al. 2005, Vörösmarty et al. 2010).

Yet these challenges need to be met, first of all, because the lack of understanding of large scale water quality patterns is a major gap in our understanding of the state of the environment. Second, the assessments of the state of worldwide aquatic biodiversity and threats to biodiversity require knowledge of ambient water quality and their trends. Third, poor quality surface waters and groundwater pose a health hazard over large areas that need to be evaluated. Finally, global drivers such as climate change are likely to have a far-reaching continental and global impact on water quality. The Intergovernmental Panel on Climate Change has pointed out that many of the changes expected in water quality may be negative, including reduced dilution capacity of some rivers because of more frequent droughts, or increased bacterial loadings to other rivers due to changes in rainfall patterns (Bates et al., 2008).

To address the continental and large scale aspects of water quality assessments, we present here a continental-scale model of river water quality - WorldQual. The model is generally intended to address the following questions:

- What is the current state of water quality over large areas? (Filling in large gaps in spatial and temporal observations).
- What percentage of river systems will have degraded water quality due to driving forces such as population change and economic growth?
- How will climate change affect water quality over large river areas?
- How will changes in water use and wastewater discharges affect water quality over large continental areas?

The first application of the WorldQual model is to river systems of Europe. The model itself has been developed as part of the EU-funded SCENES Project ("Water Scenarios for Europe and for Neighbouring States" 2006-2011) which has had the principal goal of developing new scenarios of the future of water resources in Europe (Kämäri et al. 2008). Estimates of future water quality are needed for two major reasons: to assess the future state of aquatic ecosystems and to determine the suitability of surface water supply for different water users such as industries, agriculture and the domestic sector. The aim of this paper is to describe a modeling methodology to tackle some of these questions and to present results of applying this methodology. For this, the paper addresses the future of Europe's water resources as

impacted by climate change under natural flow conditions. Biochemical oxygen demand (BOD<sub>5</sub>) is used as a representative measure for scenario calculation but the framework is generic and thus applicable to any other substance e.g. salts or total nutrients.

## MATERIAL AND METHODS

### *Modeling Strategy*

Before explaining the modeling strategy, it should be noted that modeling water quality on the continental scale is only now becoming feasible because of new developments in large scale modeling of water resources. These developments include the availability of “fine” scale continental hydrologic models (5 arc-minute resolution) which allows the tracking of the pathways of rivers on a continental scale grid and enables the matching of river quality monitoring stations with modeled river coordinates. Another new development is the computation of stream velocity which permits time of travel computations in streams on the continental scale. Time of travel is a key variable in computing the longitudinal gradients of non-conservative substances such as BOD<sub>5</sub>. Finally, the development of spatially-explicit water use models makes it possible to locate return flows and wastewater discharges more accurately on the continental-scale.

The design of the WorldQual model is determined by its goals which are:

- To fill in for gaps in observational data over large areas.
- To characterize average and extreme conditions in water quality in the absence of observational data.
- To assess the impact of climate change on water quality over large regions
- To develop scenarios of changing water quality under changing water use and wastewater discharges.

These goals influence the design criteria for the model which can be divided into:

- Spatial and temporal resolution of calculations,
- Water quality constituents,
- Model equations.

### *Spatial and Temporal Resolution*

The first decision regarding the design of WorldQual has to do with selecting the spatial and temporal resolutions of the model. Since water quality can be altered very significantly and quickly in the vicinity of large wastewater sources, we select a model that can compute the continuous spatial change in water quality along each river reach within a 5 arc-minute grid cell. Each river is divided into “reaches”, the size of a grid cell, and within each reach, the model computes continuous spatial changes in water quality from the beginning to the end of the reach. Only “smooth” changes are computed within the river reach since the model cannot take into account every wastewater point source.

With regards to temporal resolution, we select a monthly averaging period for computing water quality. This is a compromise between two cases. On one hand, it would be preferable to compute water quality at daily or hourly intervals, because the model would then simulate temporarily high levels of contamination. However, modeling at this time scale is not realistic because it requires modeling inputs that are not available on the continental basis. On the other hand, it would be preferable to compute annual average water quality because the

database of water quality measurements at this time scale is relatively large, at least in many industrialized countries. However, averaging water quality constituents over a year is too crude a resolution to capture the important seasonal variability of water quality caused by the seasonal variations in flow and other conditions. Hence we select a monthly averaging period as a compromise between daily and annual averages.

### *Water Quality Constituents*

The next decision is to select the water quality constituents to be computed by the WorldQual model. At first we select the following substances to calculate with the model, but other substances will be included into the model calculations later:

- Biochemical oxygen demand (BOD<sub>5</sub>) which is an indicator of the level of organic pollution and its oxygen-depleting potential, and serves as a metric for the overall health of aquatic ecosystems.
- Total dissolved solids (TDS) which is a measure of the suitability of water for household, industrial and agricultural use. Since TDS does not decompose or otherwise decay in a waterway, it is a useful tracer of flow inputs and outputs in a river reach and can be used for validating the flow balance of a river.

These substances are also relevant indicators for studying compliance with the general ecological requirements for European waters specified in the Water Framework Directive of the European Union (Anon 2000). They can contribute to (but are not sufficient for) determining "good ecological status" and "good chemical status" of river systems, as called for by the Directive. We note again that these constituents are only the first parameters to be modeled, and they will be followed by total phosphorus and total nitrogen as indicators of the ecological health and level of eutrophication in rivers.

### *Model Equations*

In selecting model equations the challenge is the same as with all river modeling, namely that a compromise must be found between the desire to simulate conditions precisely, and the reality that data limitations will hinder the running and testing of the model. These data limitations are especially crucial for modeling water quality on the continental basis. Aim of this paper is to show, that the model is generally able to work on global scale with simple types of equations and with a limited amount of data input. Therefore the model presented here was fed with standard values from literature or with results from other model calculations as described in the next section. Therefore also, the model is not calibrated.

Solute transport in open water channels is an important topic in water quality studies. In addition to any biological and biochemical reactions that may occur in river streams, polluting solutes that enter water courses are transported and dispersed downstream. The ability to describe and predict the effects of the transport processes on the distribution of solute concentration is of great importance. In applications on such a large scale only very simple approaches can be considered, such as was introduced by Chapra (1977). Based on this work different formulations for conservative and non-conservative substances were derived.

For non-conservative substances (e.g. BOD<sub>5</sub>) the equation from Thomann and Mueller (1987) was used, which describes the change in concentration of a substance  $c$  within a river reach as a function of an initial concentration and of a distributed load that enters at an equal rate along the river reach within a grid cell (Fig.1). The advantage of this approach is that it calls for a

distributed wastewater load along the river reach within a grid cell rather than requiring information on the location of all point sources within the reach. We note that it is feasible to estimate the total load within a 5 arc-minute grid using available information (see below) but it is not possible to estimate the location and magnitude of every point source along every river reach over an entire continent. The mathematical formulation for non-conservative substances is given in equation (1) assuming a temperature dependent decay rate  $dec(T)$ :

$$C(x) = C_0 * e^{-dec(T) \cdot x / u} + C_d * (1 - e^{-dec(T) \cdot x / u}) \quad (1)$$

with

$$C_0 = \frac{\sum_{i=1}^8 (Q_{in,i} * C_{in,i})}{Q_1} \quad (2)$$

$$C_d = \frac{S_{input}}{L * A_c * dec(T)} \quad (3)$$

and

$$A_c = \frac{Q}{u} = \frac{Q_0 + Q_1}{2 \cdot u} \quad (4)$$

and

$$dec(T) = dec(20) * \Theta^{T-20} \quad (5)$$

where

$C_1$	=	downstream concentration	$[t / km^3]$
$C_0$	=	initial upstream concentration	$[t / km^3]$
$C_{in,i}$	=	concentration in inflow	$[t / km^3]$
$C_d$	=	concentration in distributed inflow	$[t / km^3]$
$x$	=	position in river stretch	$[km]$
$L$	=	total flow length in grid cell	$[km]$
$S_{input}$	=	substance loading	$[t / month]$
$A_c$	=	cross - sectional area	$[km^2]$
$u$	=	river flow velocity	$[km / month]$
$T$	=	water temperature	$[^{\circ}C]$
$dec(20)$	=	decay rate at 20 °C	$[1 / month]$
$dec(T)$	=	decay rate at water temperature $T$	$[1 / month]$
$\Theta$	=	temperature correction coefficient	$[-]$
$Q_1$	=	outflow from grid cell	$[km^3 / month]$
$Q_0$	=	inflow from upstream (incl. tributaries)	$[km^3 / month]$
$Q_{in,i}$	=	inflow from each upstream grid cell	$[km^3 / month]$

Temperature dependent decay rates for BOD<sub>5</sub> follow equation (5) (Benham et al. 2006, Bowie et al. 1985). The decay rate at 20 °C is 0.23 1/month and the temperature correction coefficient is 1.047 (Paliwal et al. (2007), Bowie et al. (1985), Thomann and Mueller (1987), Chapra (1997)).

For conservative substances the equation from Thomann and Mueller (1987) was selected. It simulates the change in an initial concentration and distributed source as it is diluted by increasing flow input along the river reach. The concentration is expressed in equation (6):

$$C(x) = C_0 * e^{-q_d x} + C_d * (1 - e^{-q_d x}) \quad (6)$$

with

$$q_d = \ln\left(\frac{Q_1}{Q_0}\right) * \frac{1}{x} \quad (7)$$

and

$$C_d = \frac{S_{input}}{Q_1} \quad (8)$$

where

$$q_d = \text{coefficient for distributed inflow} \quad [1/km]$$

Other variables are the same as in (1). Conversion factors are also used here to obtain a consistent result.

Note that the equations are different mainly in that in Equation 1 the decay rate of the substance is the mechanism of decrease in concentration, whereas flow dilution is the cause in Equation 6. The flow dilution effect is not included in (1) because an analytical solution is not available for the case where concentration is affected by both a decay coefficient and flow dilution. However, the lack of a dilution term only affects calculations within a grid cell. The mass balance carried out at the beginning of each grid cell ensures that the dilution effect is properly taken into account for both equations.

#### *Data input*

Data input into the model equations can be divided into hydrological components and pollution loadings. Here the strategy for modeling water quality on the European-scale takes into account the large gaps in data at different locations and over time.

Hydrological variables like river discharge, cell runoff, and flow velocity will be fed by output from the global model WaterGAP (Water – Global Assessment and Prognosis, Fig. 2). WaterGAP is developed at the Center for Environmental Systems Research of the University of Kassel, Germany. It comprises two main components, a global hydrology model and a Global Water Use Model (Alcamo et al. 2003, Döll et al. 2003, Flörke and Alcamo 2004, Verzano 2009). The Global Hydrology Model simulates the macro scale behaviour of the terrestrial water cycle to estimate water resources. All calculations are performed on 5' grid cell level to ensure that the most detailed input information available on that level can be used. The Global Water Use Model of WaterGAP (Aus der Beek et al. 2010, Flörke et al. 2011) consists of five sub-models to determine the water withdrawals and water consumption in the household, electricity, manufacturing, irrigation, and livestock sectors. In this context, water withdrawals depict the total amount of water used in each sector while the consumptive water use indicates the part of withdrawn water. The water use sectors only consume a part of the water withdrawals and the remaining water returns into the river system. These return flows are used to calculate input loadings in WorldQual.

Pollution loadings in WorldQual are distinguished between point sources and diffuse sources. Point sources are divided into manufacturing, domestic and urban loadings, whereas diffuse loadings come from scattered settlements, agricultural input (for instance livestock farming and irrigated agriculture), and also from natural background sources. Detailed information about the development of point and diffuse loading calculations are described in Williams et al. (this issue) and Malve et al. (this issue). The country-scale estimates of water use and pollution loadings are downscaled by the model within the respective countries using demographic and socio-economic data. Water temperature used in the WorldQual model to calculate decay rates of non-conservative substances is calculated by a non linear function (Voß et al. 2009).

#### *Baseline climate and scenario selection*

Climate forcing data used for the baseline in this study has been compiled and regionalised by the Climate Research Unit (CRU) of the University of East Anglia, Norwich, UK (version TS 2.1, Mitchell and Jones, 2005). CRU data covers Europe in 10' resolution and monthly time steps. In order to use it for the water quality modelling the dataset have simply been disaggregated to a spatial resolution of 5'.

The climate scenarios chosen for this work were based on two global circulation model - IPCC SRES A2 emission scenario combinations essentially comparing the effect of different future rainfall patterns.

- IPCM-A2: IPSL-CM4, Institute Pierre Simon Laplace, France + A2 scenario (Denvil, 2005): high temperature increase with low precipitation increase or precipitation decrease
- MIMR-A2: MIRCO3.2, Center for Climate System Research, University of Tokyo, Japan + A2 scenario (Nozawa, 2005): high temperature increase, high precipitation increase or low decrease.

The original spatial resolution (IPCM4-A2: lat 2.5° x lon 3.75°, MIMR-A2: lat 2.8° x lon 2.8°) was re-sampled by bilinear interpolation to 5' minutes grid cells.

The time frame of the climate scenarios used in the model calculations are the 2050s (2040 – 2069). As base year 2005 is used as it is the reference year for water use calculations in the SCENES project. Scenario development in SCENES was a stakeholder driven process (Kämäri et al. 2008). A characteristic feature in all storylines developed in this process was the focus on climate change impacts as a major trigger to changes in human and thus societal awareness and behaviour (Kok et al. 2009, Kok et al. 2011). Thus the SCENES stakeholders who participated in the storyline development also played a key role in choosing an appropriate IPCC SRES scenario to relate the modelling work within SCENES to the storylines. Their recommendation was to concentrate on the A2 scenario only in order to emphasise the trigger role of climate change in all storylines.

## RESULTS AND DISCUSSION

To test the model, 15 basins across Europe were selected. These represent a range of large river basins (> 9000 km<sup>2</sup> to 820 000 km<sup>2</sup>), climates (arid and humid), geogenic background conditions (e.g. different salt concentrations) and degrees of anthropogenic influence (e.g.



different population densities and pollution loadings). Another important criterion is that at least monthly measurements were available for different substances in these basins for testing the model. In this paper, results from all catchments are summarised and the BOD<sub>5</sub> results presented more detailed examination of the Ebro, Thames river basins and similarly the TDS results for Ebro and Vistula basins.

Test results are presented in two formats. Firstly, longitudinal profiles show the ability of the model to simulate spatial gradients of river water quality. In Figures 3 to 10 (a, b) model calculations are compared to monthly average observations because this corresponds to the target temporal resolution of the model. The model is tested against data from high river flow periods (Figs. 3 to 10 a) and low flow periods (Figs. 3 to 10 b). The year 2000 is selected for testing because of the good availability of data. The second format for testing the results is to compare model calculations on yearly time series of measurements at specific locations in the rivers (e.g. up- or middle stream) (Figs. 3, 4, 7, 8 c).

Because of the lack of data density the quality of model calculation can not be presented with usual methods like, Nash-Sutcliffe coefficients or coefficients of determination. Concentrations were divided into classes and the difference of these classes between calculated and measured values evaluated. The concentrations were equally distributed into 7 (BOD<sub>5</sub>) or 9 classes (TDS) in order to have comparable data sets. The resolution for BOD<sub>5</sub> is 5 mg/l and for TDS 250 mg/l. Another possibility to test the model quality is the use of the 90-percentile concentration. Here a set of all available data pairs of monthly average concentrations (measured and simulated) for the year 2000 is used (BOD<sub>5</sub>: Ebro (205), Thames (50), Europe (1421), TDS: Ebro (207), Vistula (306), Europe (1468)).

### *BOD<sub>5</sub>*

The results for Europe show that for the complete data set the model gives a satisfactory result since 51% of reaches were predicted in the same water quality class as observed data and 30 % show a difference of only one class between measured and simulated values. 9 % of rivers were modelled with a difference of two classes and only 8 % differ by more than two classes. The 90-percentile (Tab. 2) for the measured data is 7.7 mg/l and for the calculated 11.0 mg/l. The modelled results generally overestimate the observed values. This is an encouraging result given that the model has not been calibrated for water quality (only for river flows) and is driven by national level data that has largely been reported through European level databases. There will be regions where the model poorly reproduces observed data due to local conditions that are not captured in European scale data. Two examples for the Ebro and the Thames river basins will serve to illustrate this point.

For the Ebro, the model shows a clear underestimation of BOD<sub>5</sub> concentrations in comparison to longitudinal measurements for high and low flow conditions as well as in the monthly time series. (Figs. 3a to 3c); 20 % of the measured and calculated values belong to the same water quality class, 40 % differ by one class and 13 % by two classes. 27 % show a difference of more than three classes. Underestimation in the Ebro is mainly due to the estimation of pollution loading of livestock. In WorldQual the loading input from livestock production is generally treated as a diffuse source, but according to European Pollutant Emission Register database (2010), many animal production facilities within the Ebro basin (poultry and pork) discharge their wastewater directly into the river water and are thus point source inputs. This phenomenon can be found mainly in the down stream region. If the inputs are modified to treat the animal waste like inputs from a manufacturing point source, the modified input loadings show an increase of the manufacturing loads from 1.2 t to 117.9 t, from 1.2 % of

total loadings to 54.7 % respective (Tab. 3). With this modified input the BOD<sub>5</sub> in-stream concentration fit improves considerably when compared to the longitudinal measurements for both high and low flow conditions (Figs. 4a and 4b). However, the BOD<sub>5</sub> concentration is now overestimated in summer between June and September (Fig. 4c). These results are also reflected by the model goodness-of-fit (Tab. 2). The difference of classes between measured and calculated values are not better than with the regular input and the 90-percentile shows an overestimation with 14 and 22.6 mg/l respectively (Tab. 2). More information is probably needed on the timing of the animal production discharges if this aspect of the model is to be improved.

In contrast to Ebro, the Thames shows an overestimation of simulated values against measured along river length especially for low flow conditions (Figs. 5a / b). This result is confirmed by the 90-percentile (Tab. 2). For regular input only 14 % of calculated concentration values belong to the same class as the measured ones, but as can be seen 70 % show only a small difference of one and 16 % of two classes. One source of uncertainty may be the inaccurate estimation of river flows in the Thames, especially in the upper catchment. Another more important uncertainty factor concerns the share of domestic loading that, especially for the middle and down stream Thames, is very high (~80%, Tab. 3). Local information on domestic sewage treatment shows that within the Thames basin removal of BOD is likely to be 97 % rather than 90 % used in the standard load estimation methods for WorldQual (Williams et al., this issue, Butwell et al., 2009). Making this correction, the simulated BOD<sub>5</sub> concentration fit much better to in-stream measurements (Figs. 6a / b). Only the upper part of the catchment shows still an overestimation in concentrations probably due to the underestimation of river flows in this region mentioned above. The 90-percentiles of measured and calculated values are 2 mg/l and 4 mg/l, respectively and there are no differences within the water quality classes (Tab. 2).

#### *TDS*

Of all calculated concentrations of European rivers 35 % belong to the same class as measured values – 41 % and 14 % differ by one and two classes, respectively. Only 7 % show a difference by three or more water quality classes. The calculated TDS concentration for Europe is generally underestimated (Tab. 4). The 90-percentiles differ by about 400 mg/l. Possible reasons can be river flow conditions and uncertainties in loading input, as for the BOD<sub>5</sub> concentration. A third factor can be the geogenic background concentration. As can be seen in Tab. 1, the background calculation is based on the geologic variation considering a median salt concentration of all available non-agricultural water quality measurement points within the rivers of a country (Salminen 2005). In the case that data for a country are not available the drinking water mean value of 250 mg/l was used. As for BOD<sub>5</sub>, taking account of the lack of model calibration and the use of high level European data, these results are encouraging.

As for BOD<sub>5</sub> allowance for local conditions can improve the model performance in specific basins. In the Vistula river basin modelled TDS concentrations underestimate the measured concentrations (Figs. 7a - c) especially in the upper part of the river. For the first 300 km the measured TDS values are very high, up to 4200 mg/l. These upstream levels are due to the contribution of salt effluents from the mining industry (Ericsson & Hallmans 1996, Buszewski et al. 2005, Turek 2004). This input load is not accounted for in the model estimated loads and therefore the 90-percentiles of measured and calculated values differ by ~1600 mg/l (Tab. 4). Only 8 % of the calculated values have the same water quality class as the measured values. 70 % differ by one or two classes and 22 % by three or more classes. In

order to raise the TDS concentrations in the model to these levels an additional input of 12 Mio t salt would be needed, which is about 91 % percent of the total loading amount mentioned in Ericsson & Hallmans (1996) (Tab. 5). Using the modified input the simulated concentration along the river length fits the measured high and low flow conditions very well, and also the monthly dynamics are closely reproduced (Figs. 8a – c). The 90-percentiles differ only by ~300 mg/l (Tab. 4). 47.5 % of calculated values belong to the same class as the calculated ones, 42.6 % differ by one or two classes, and only 10 % show a difference of three or more classes.

With regular loading input the model calculates a concentration for the Ebro River that is too low for low flow conditions, especially in the lower half of the river (Figs. 9a / b). The 90-percentile confirms this result with a measured value of 862 mg/l against a calculated value of 543 mg/l (Tab 4). Main factor of TDS input within the Ebro basin is the irrigation sector (~66 % with regular input, Tab. 5). There is evidence of significantly higher irrigation following a monthly cycle that is clearly different from that used in the WorldQual loading calculations (Causapé et al., 2006, Tedeschi et al. 2001). They report very intensive irrigation practices especially in the downstream part of the Ebro for the effluents of Cinca and Segre Rivers. Using these local data TDS loadings increase from 0.7 Mio t to 12.5 Mio t per year. Furthermore the monthly distribution is changed. With these changes the contribution of loading from the irrigation sector rises up to 97 % (Tab. 5). The results with the modified input show a better result for low flow conditions and a similar one for high flow conditions (Figs. 10a / b). All in all there is more dynamics along the river, but the 90-percentiles in Tab. 4 show a clear overestimation of TDS concentration because of too high concentration values for the months June and July.

#### *Scenario application: Impact of climate change on water quality*

The in-stream concentration of BOD<sub>5</sub> in Europe for the baseline 2005 shows that little influence of loading on water quality is detected for Northern Europe (Fig. 11). In contrast, the highest concentrations can be found for the Iberian Peninsula, Western Asia and Eastern Mediterranean. All other rivers of Europe have low to medium BOD<sub>5</sub> concentrations. The BOD<sub>5</sub> concentration in rivers for the scenario calculation is coupled with water quality classes, which are used in literature and present the natural and chemical status of a river system (Pettine 2004). Thereby <1 mg/l means very good and >50 mg/l means highly polluted river streams. For the baseline as well as for the two scenarios all cells within a river basin belong to one of these seven classes. In order to investigate the in-stream BOD<sub>5</sub> concentrations in more detail, the differences between the classes (scenario minus baseline) were calculated for the IPCM4-A2 and MIMR-A2 scenarios (Figs. 12 a,b). Thereby positive values (degradation of water quality), negative values (improvement of water quality) and zero values (no changes) occur. The climate change scenarios have three potential effects on water quality: first, the changes in precipitation lead to changes in runoff and thus in-stream water availability; second, changes in air temperature affect in-stream degradation of organic substances and thus the BOD<sub>5</sub> concentration; and third, two loading components in WorldQual namely diffuse loading and wash-off from sealed areas is affected by changes in precipitation.

As can be seen for both scenarios there is no change in water quality classes in most rivers of Northern, middle and Western Europe. Following the IPCM4-A2 scenario in Eastern Europe and in the Black Sea region the in-stream concentration will get worse by up to 2 classes compared to the baseline 2005. Different patterns can be found in the MIMR-A2 scenario in which only the Black Sea region will show an increase of BOD<sub>5</sub> concentrations.

Analyses concerning the impact of climate change on the BOD<sub>5</sub> decay rate and on the affected loadings have shown, that they are very small and do not considerably influence the in-stream concentration. The main effect for the results is the change in water availability due the different climate conditions. IPCM4-A2 is drier than MIMR-A2 and therefore there will be smaller river flow for IPCM4-A2. If you have no changes in loadings the effect of less river availability will be an increase of concentration and a decrease of water quality.

## CONCLUSIONS

This paper has presented a new global scale water quality model – WorldQual and illustrated its performance through its application to modelling BOD<sub>5</sub> and TDS across Europe. The use of such a model at the European scale has also been illustrated by considering the effects of climate change on future BOD<sub>5</sub> concentrations.

With reference to the European rivers it has been shown that the model is robust and works in the expected way. Overall of Europe, comparisons between observed and modelled concentrations were encouraging given that the models were only calibrated for water flow and not water quality. The aim of the model is to provide a mechanism for investigation trends in water quality which might occur in response to continental scale drivers such as climate change, European policy or changing populations. Global models are no substitute for detailed models of individual catchments if the focus of management is at that local scale. However, it has been shown that local information can improve the simulations of individual river basins within the WorldQual model framework.

Because of the acceptable model performance in targeting water quality classes the modeling methodology described here can be applied to scenario analysis pointing out potential water quality hotspots.

The results for Europe show that future climate changes are likely to have only a small impact on European in-stream concentration levels of BOD<sub>5</sub>, except for the Eastern part and the Black Sea region. In these regions, the impact on flow conditions seems to be more pronounced than in other parts in Europe, leading to a potential degradation of water quality. This effect is expected to be larger for the IPCM4-A2 scenario than for the MIMR-A2 scenario.

As a next step the model will be tested with further substances like total nitrogen and total phosphorus and other scenario calculations including changing socioeconomic drivers, such as treatment levels and population, which are expected to have a bigger effect on in-stream water quality.

## Acknowledgements

The authors thank the European Commission for funding the research that resulted in this paper (SCENES project, FP6 contract 036822). We also gratefully acknowledge the Environment Agency England and Wales (prov. by R. Williams, NERC-CEH Wallingford), the General Inspectorate of Environmental Protection (prov. by I. Kardel, Warsaw University of Life Sciences) and the Confederación Hidrográfica del Ebro, Zaragoza (prov. by M. Fry, NERC-CEH Wallingford) for providing the in-stream water quality data for Thames, Vistula and Ebro respectively used to test the model as presented in this paper. Data for calibration of the modelled river discharge were acquired from Global Runoff Data Centre (GRDC).

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700 Table 1. Assigned background concentrations of total dissolved solids  
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COUNTRY	CONCENTRATION [mg l <sup>-1</sup> ]	COUNTRY	CONCENTRATION [mg l <sup>-1</sup> ]
ALBANIA	250	JORDAN	250
ANDORRA	250	KUWAIT	250
AZERBAIJAN	250	LEBANON	250
AUSTRIA	186	LATVIA	278
ARMENIA	250	LIECHTENSTEIN	250
BELGIUM	247	LITHUANIA	640
BOSNIA AND HERZEGOVINA	250	LUXEMBOURG	250
BULGARIA	250	MALTA	250
BELARUS	250	MOLDOVA	250
CROATIA	250	NETHERLANDS	293
CYPRUS	250	NORWAY	17
CZECH REPUBLIC	109	POLAND	263
DENMARK	99	PORTUGAL	74
ESTONIA	250	ROMANIA	250
FAROE ISLANDS	250	RUSSIAN FEDERATION	250
FINLAND	25	SAUDI ARABIA	250
FRANCE	127	SLOVAKIA	206
GEORGIA	250	SLOVENIA	250
GERMANY	135	SPAIN	288
GREECE	229	SWEDEN	24
HUNGARY	606	SWITZERLAND	250
ICELAND	250	SYRIAN ARAB REPUBLIC	250
IRAN	250	TURKEY	250
IRAQ	250	UKRAINE	250
IRELAND	105	MACEDONIA	250
ISRAEL	250	EGYPT	250
ITALY	201	UNITED KINGDOM	78
		SERBIA AND MONTENEGRO	250

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Table 2. Difference of 90-percentiles of calculated values against measured values for BOD<sub>5</sub> in-stream concentration with regular and modified input loading [mg/l].

	regular		modified	
	measured	calculated	measured	calculated
Europe	7.73	10.97	-	-
Thames	2.01	11.57	2.01	4.03
Ebro	14.00	7.86	14.00	22.60

Table 3. BOD<sub>5</sub> loadings and loading fractions 2000 for Ebro and Thames for different sectors with regular and with modified input loading.

	manufacturing		domestic		scattered settlements		urban runoff		diffuse		total
	[t/a]	[%]	[t/a]	[%]	[t/a]	[%]	[t/a]	[%]	[t/a]	[%]	[t/a]
Ebro - regular	1 201	1.2	15 075	15.2	16	0.02	2	0.002	82 734	83.5	99 029
Ebro - modified	117 906	54.7	15 075	7.0	16	0.01	2	0.001	82 734	38.4	215 734
Thames - regular	1 013	1.3	62 871	80.0	430	0.55	1 323	1.683	12 977	16.5	78 613
Thames - modified	304	1.4	7 960	37.1	27	0.13	167	0.779	12 977	60.5	21 435

Table 4. Difference of 90-percentiles of calculated values against measured values for TDS in-stream concentration with regular and modified input loading [mg/l].

	regular		modified	
	measured	calculated	measured	calculated
Europe	776.23	370.83	-	-
Vistula	1970.74	297.73	1970.74	1669.36
Ebro	861.62	543.24	861.62	1546.23

Table 5. TDS loadings and loading fractions 2000 for Ebro and Thames for different sectors with regular and with modified input loading.

		industry	domestic	scattered settlements	urban runoff	diffuse	total
Ebro - regular	[t/a]	1 201	15 075	16	2	82 734	99 029
	[%]	1.2	15.2	0.02	0.002	83.5	100.0
Ebro - modified	[t/a]	117 906	15 075	16	2	82 734	215 734
	[%]	54.7	7.0	0.01	0.001	38.4	100.0
Thames - regular	[t/a]	1 013	62 871	430	1 323	12 977	78 613
	[%]	1.3	80.0	0.55	1.683	16.5	100.0
Thames - modified	[t/a]	304	7 960	27	167	12 977	21 435
	[%]	1.4	37.1	0.13	0.779	60.5	100.0

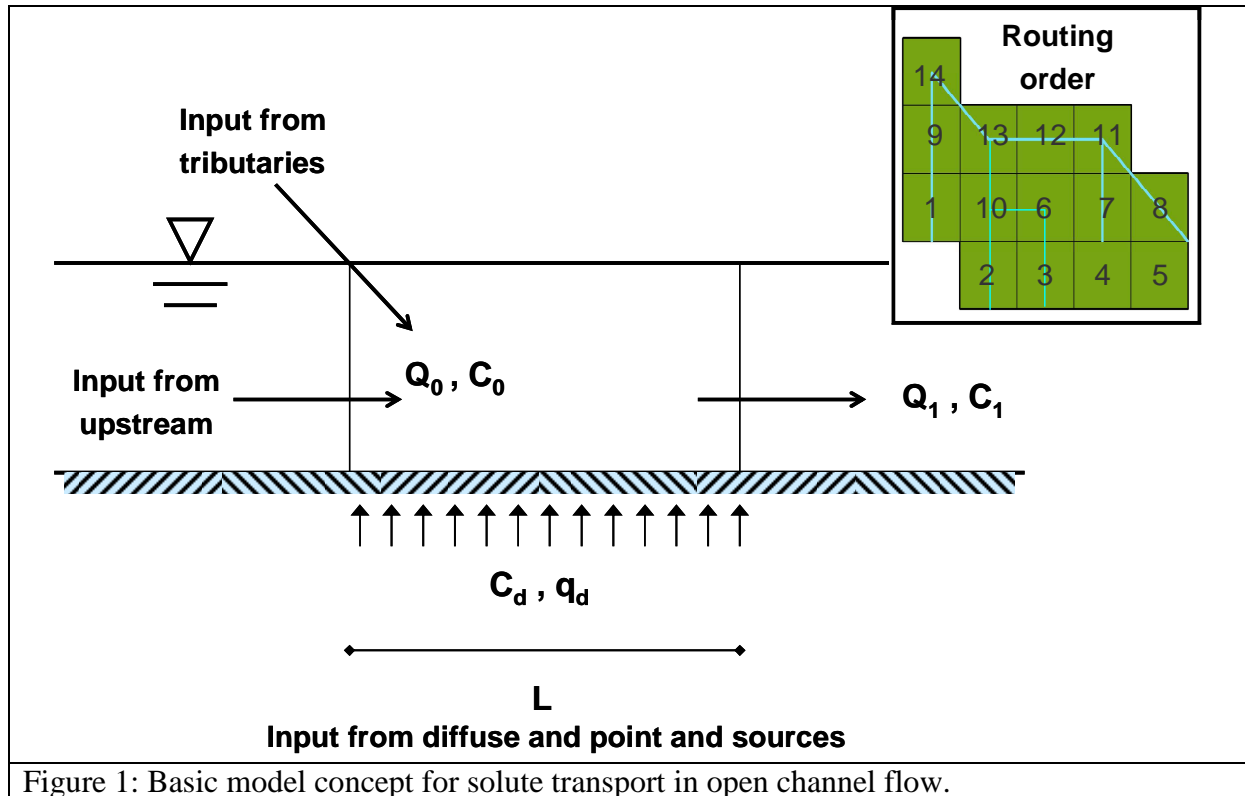


Figure 1: Basic model concept for solute transport in open channel flow.

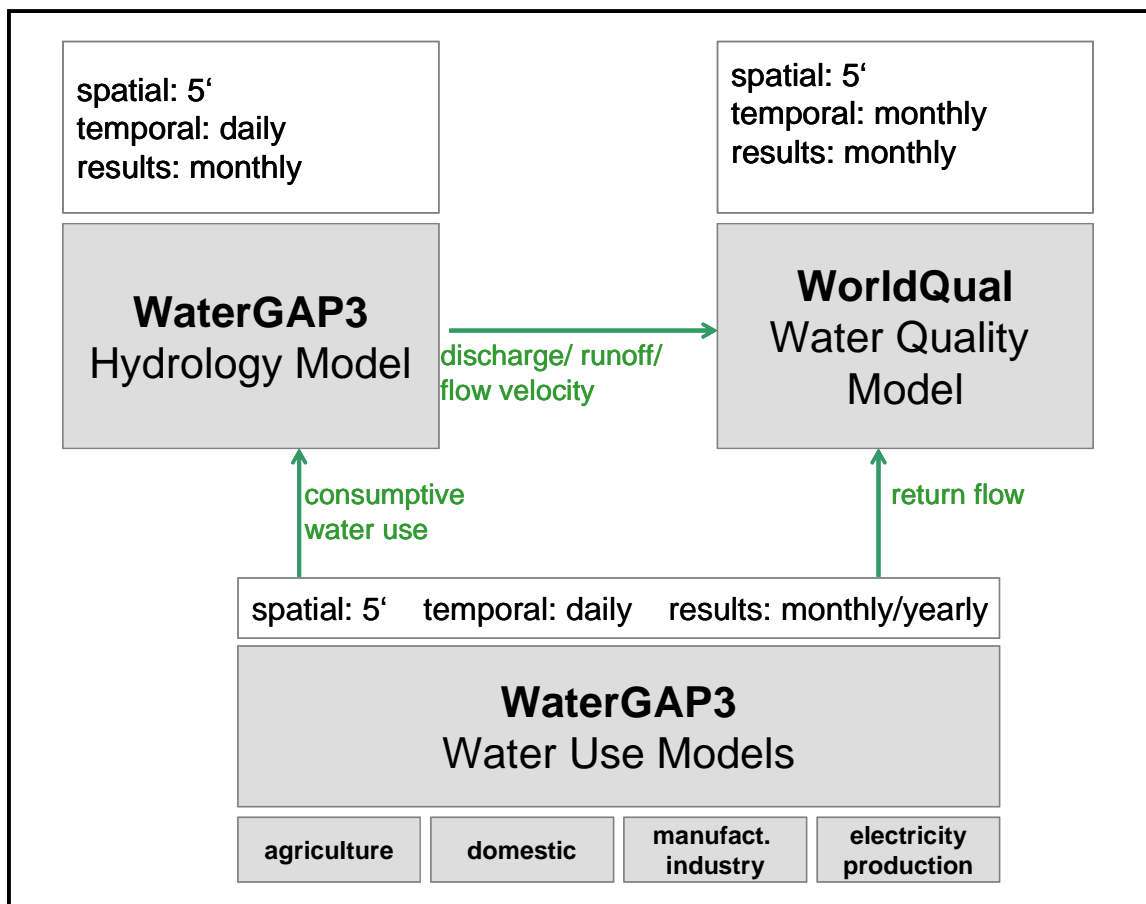
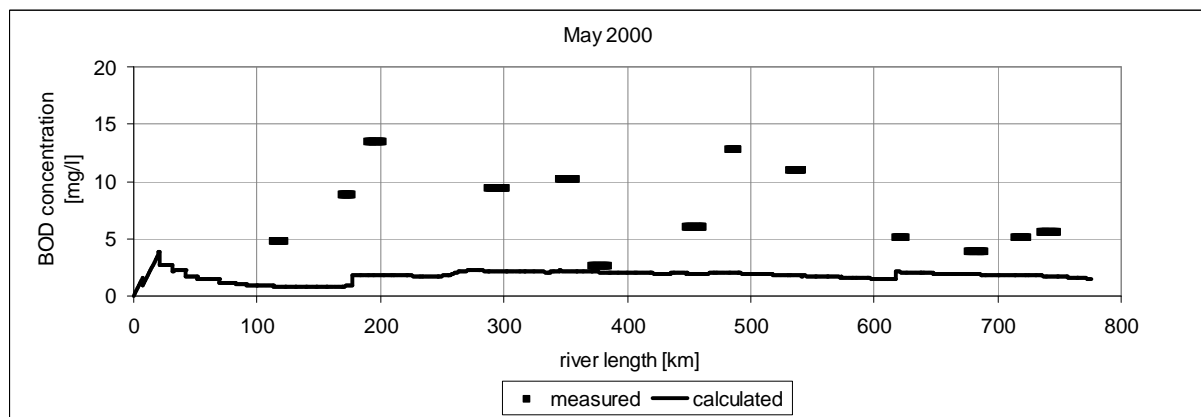
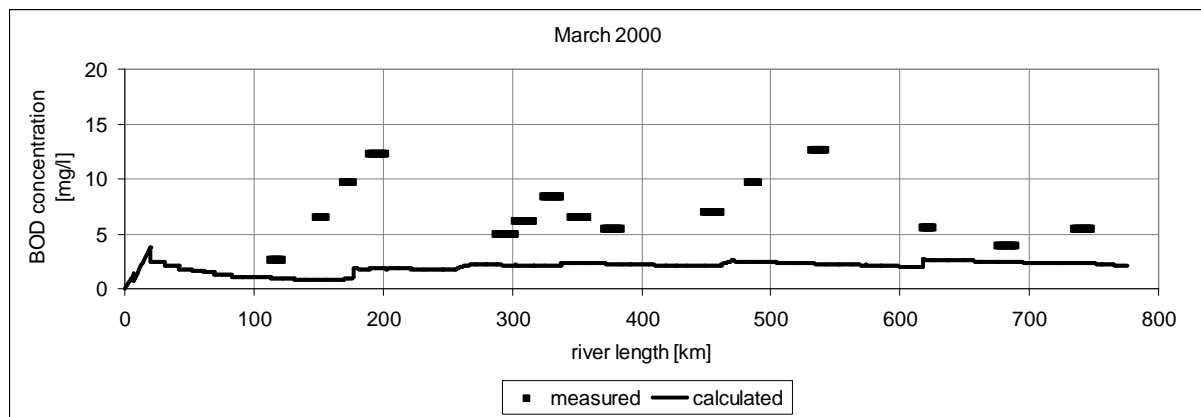


Figure 2: Linkage between WaterGAP (Hydrology Model and Water Use Models) and WorldQual.

(a)



(b)



(c)

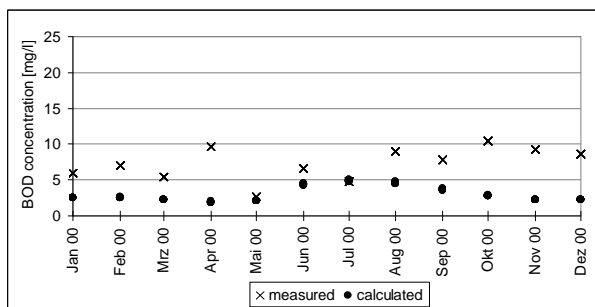


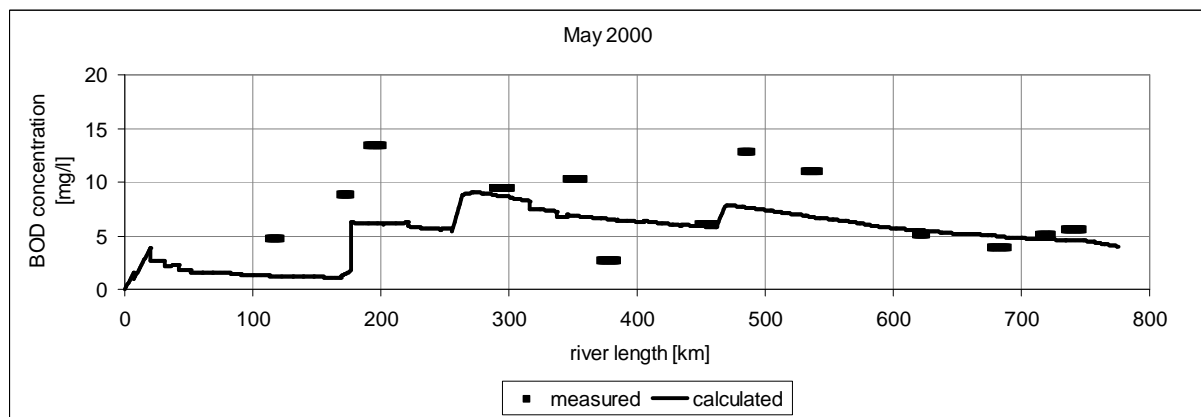
Figure 3. BOD<sub>5</sub> results for Ebro River with regular input.

(a) Longitudinal profile, high flow, May 2000

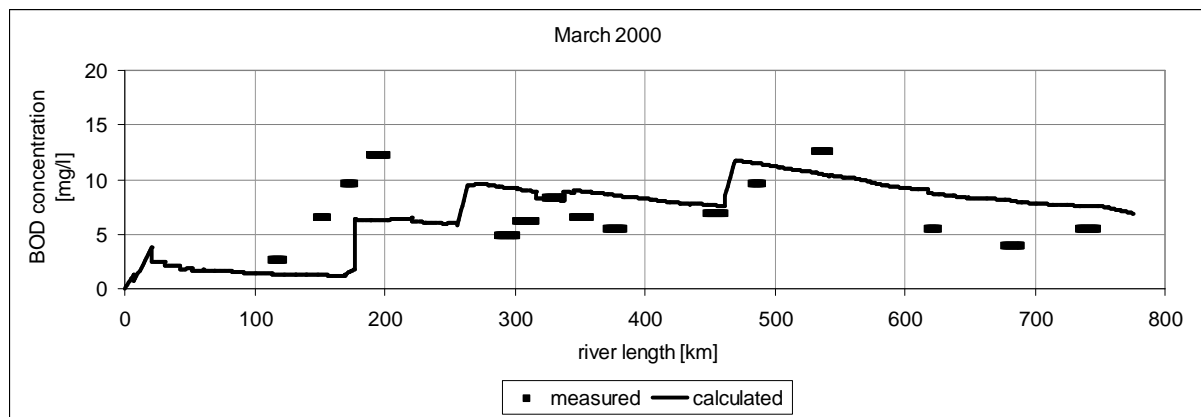
(b) Longitudinal profile, low flow, March 2000

(c) Time series – middlestream

(a)



(b)



(c)

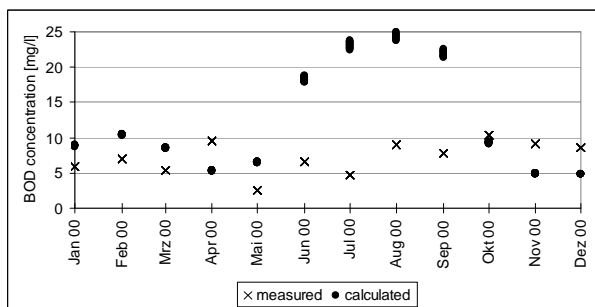


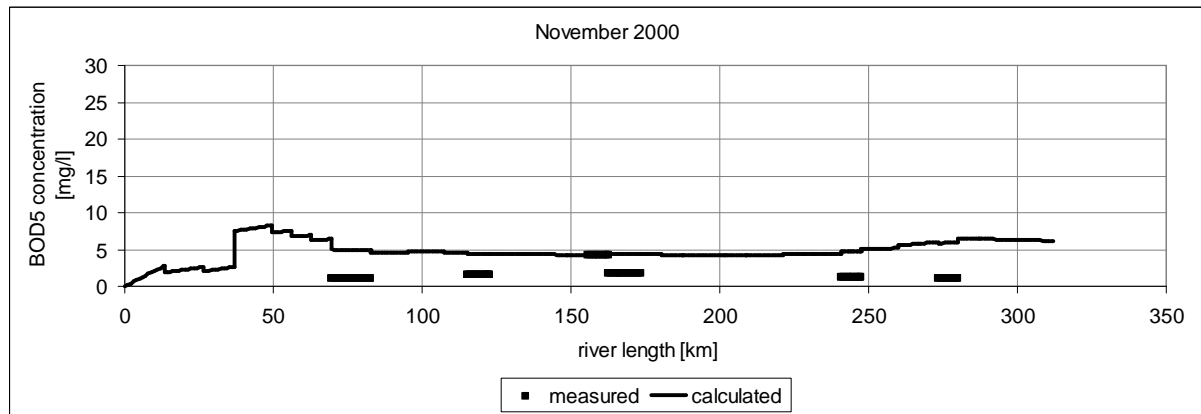
Figure 4. BOD<sub>5</sub> results for Ebro River with modified input.

(a) Longitudinal profile, high flow, May 2000

(b) Longitudinal profile, low flow, March 2000

(c) Time series – middlestream

(a)



(b)

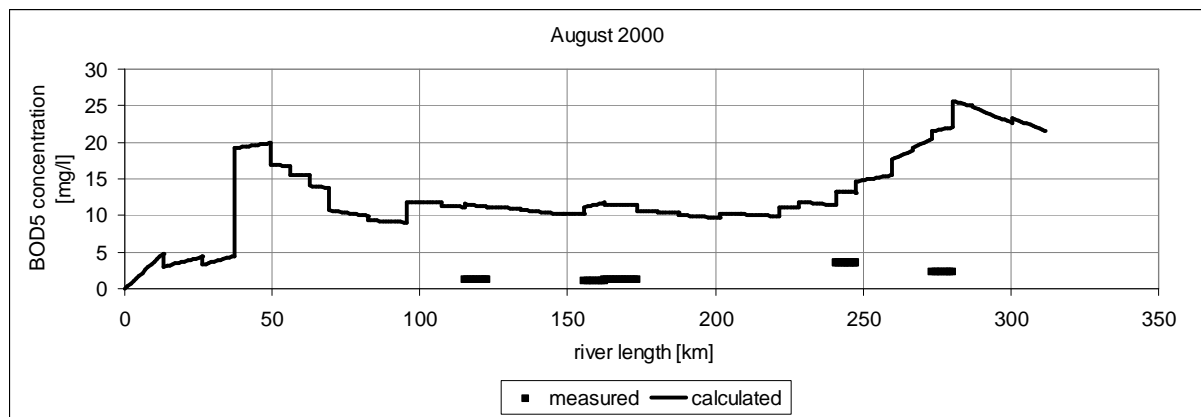
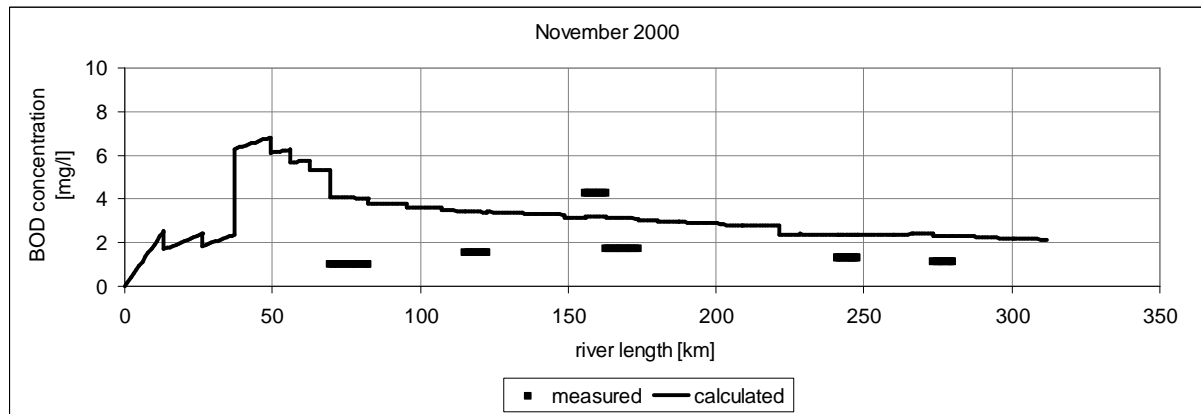


Figure 5. BOD<sub>5</sub> results for Thames River with regular input.

(a) Longitudinal profile, high flow, November 2000

(b) Longitudinal profile, low flow, August 2000

(a)



(b)

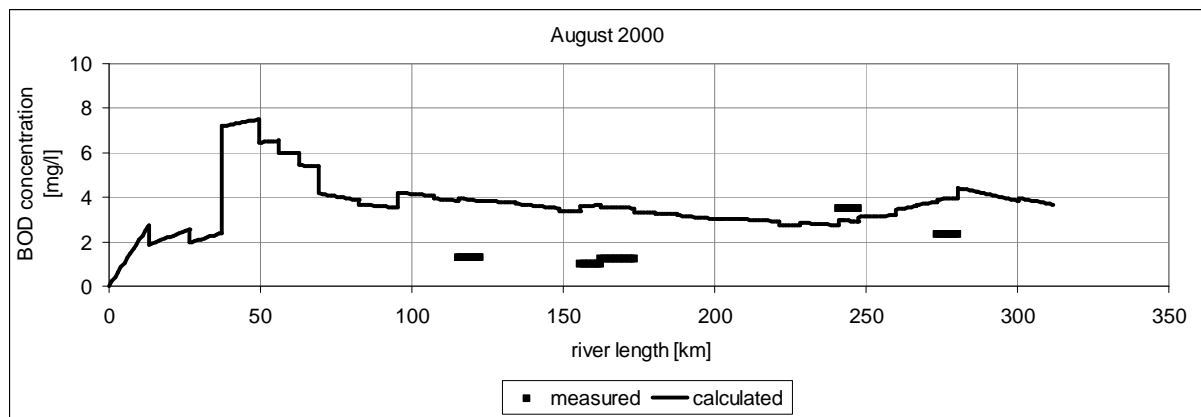
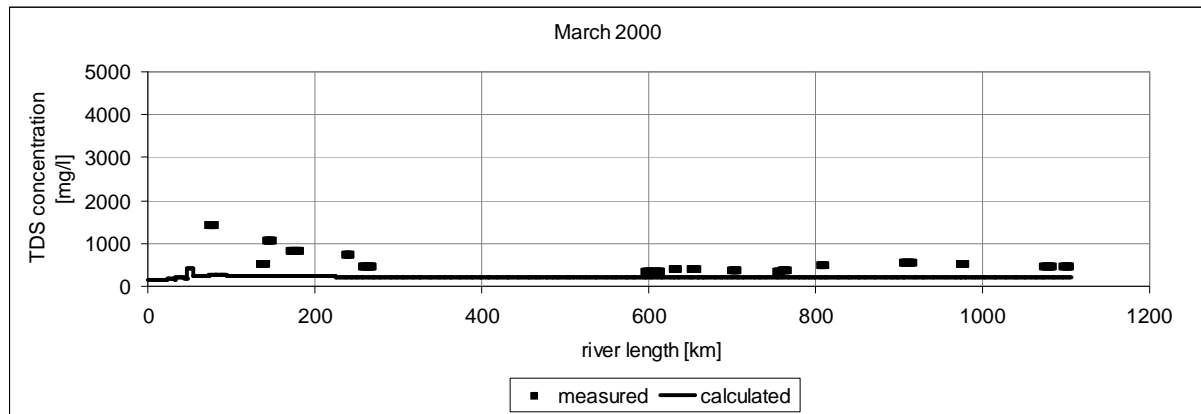


Figure 6. BOD<sub>5</sub> results for Thames River with modified input.

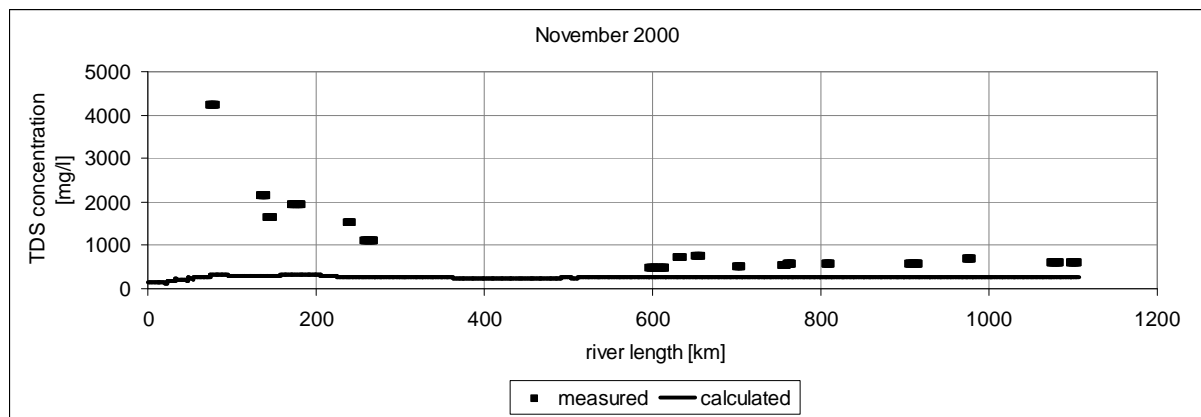
(a) Longitudinal profile, high flow, November 2000

(b) Longitudinal profile, low flow, August 2000

(a)



(b)



(c)

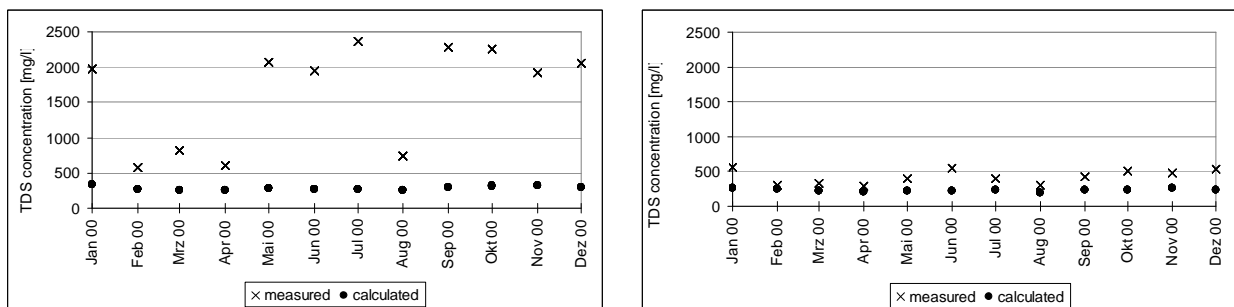


Figure 7. TDS results for Vistula River with regular input.

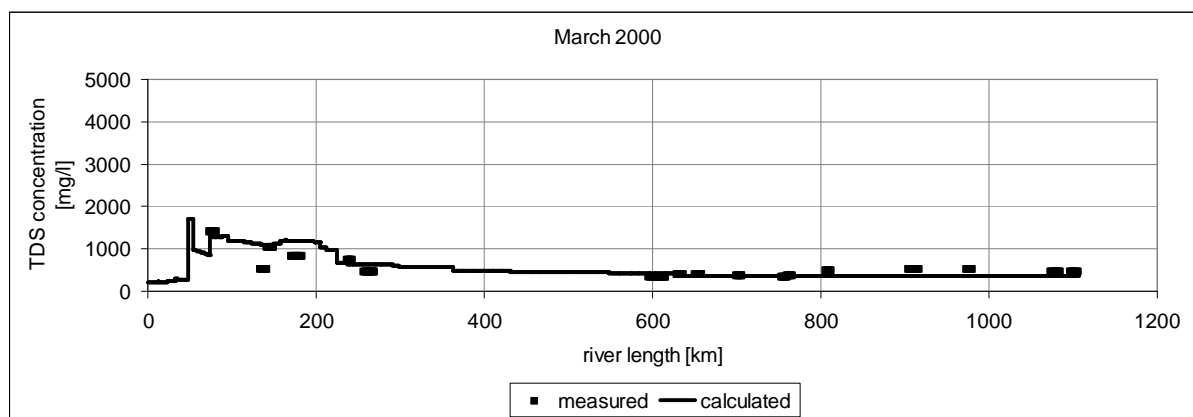
(a) Longitudinal profile, high flow, March 2000

(b) Longitudinal profile, low flow, November 2000

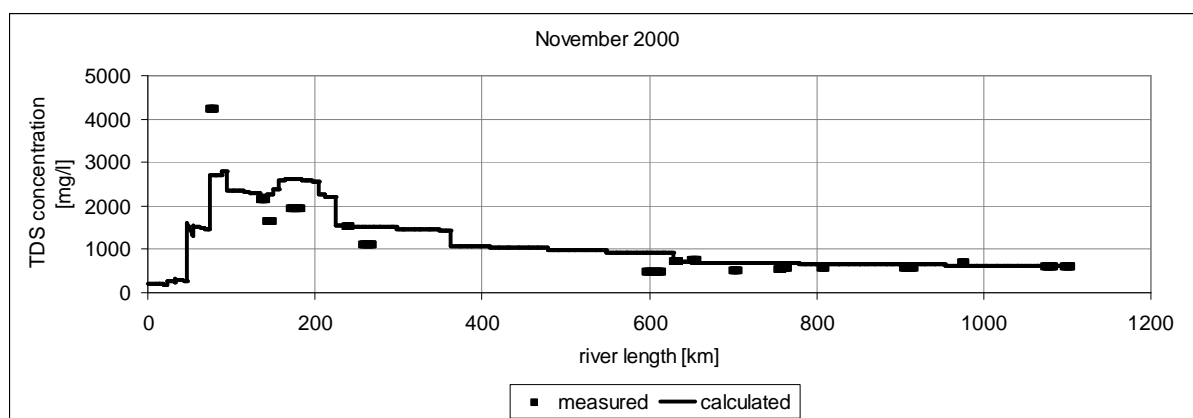
(c) Time series – upper- and middlestream



(a)



(b)



(c)

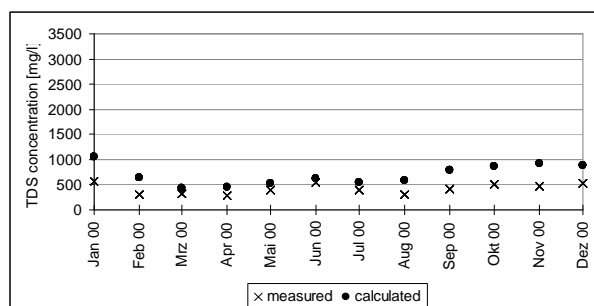
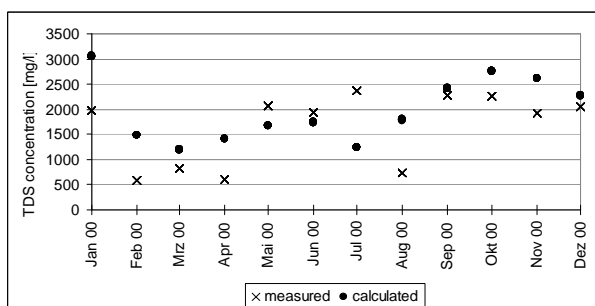


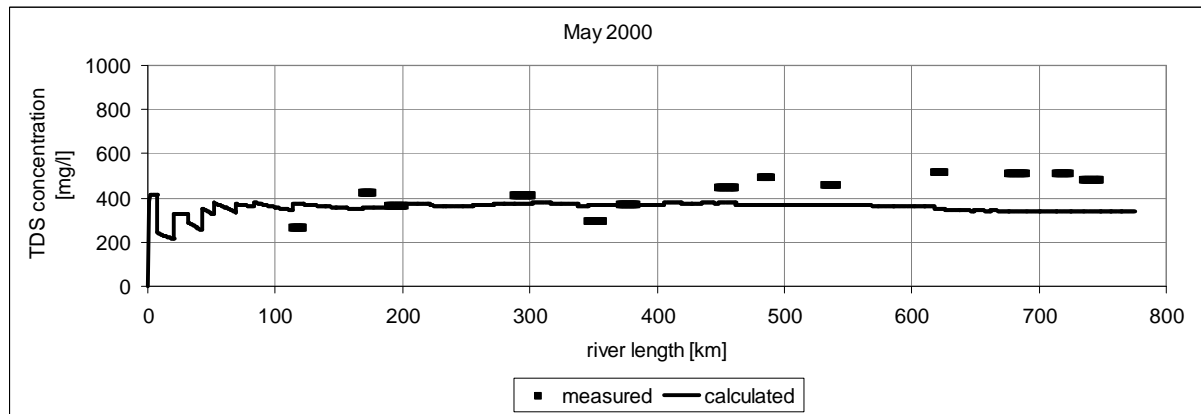
Figure 8. TDS results for Vistula River with modified input.

(a) Longitudinal profile, high flow, March 2000

(b) Longitudinal profile, low flow, November 2000

(c) Time series – upper- and middlestream

(a)



(b)

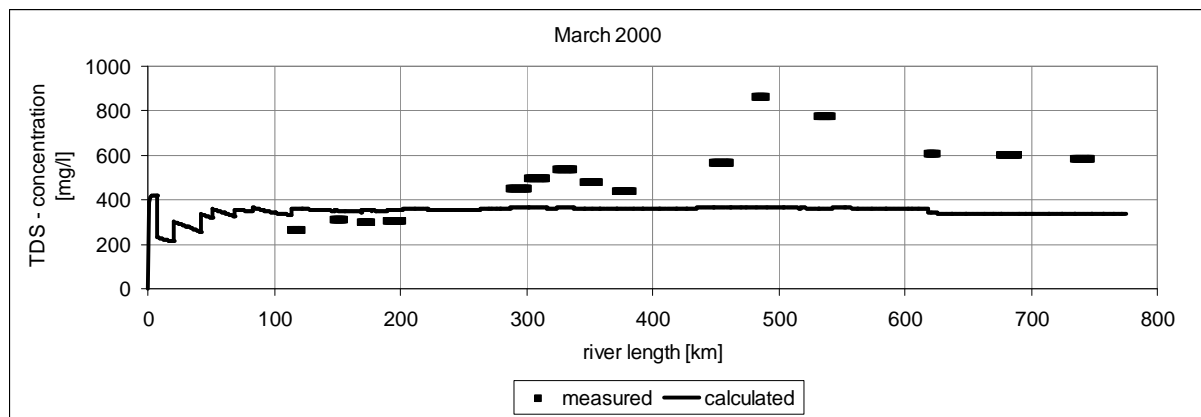
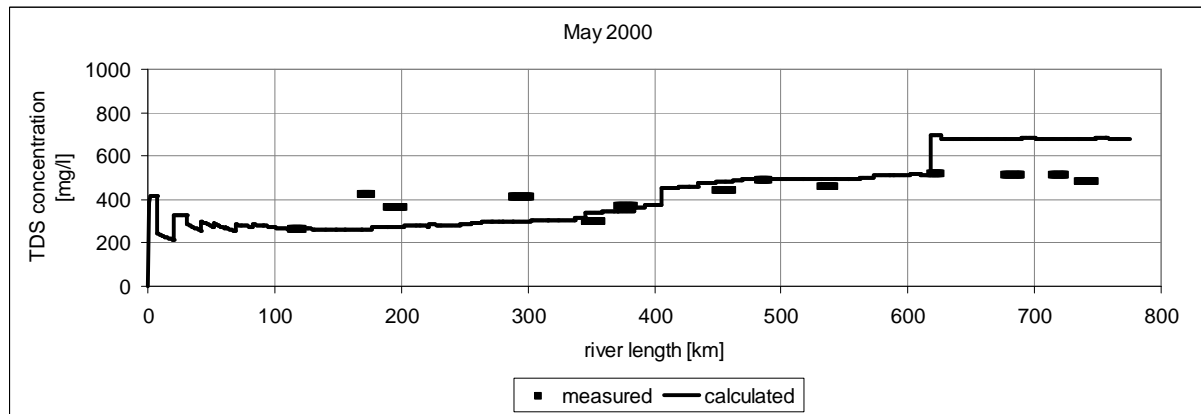


Figure 9. TDS results for Ebro River with regular input.

(a) Longitudinal profile, high flow, May 2000

(b) Longitudinal profile, low flow, March 2000

(a)



(b)

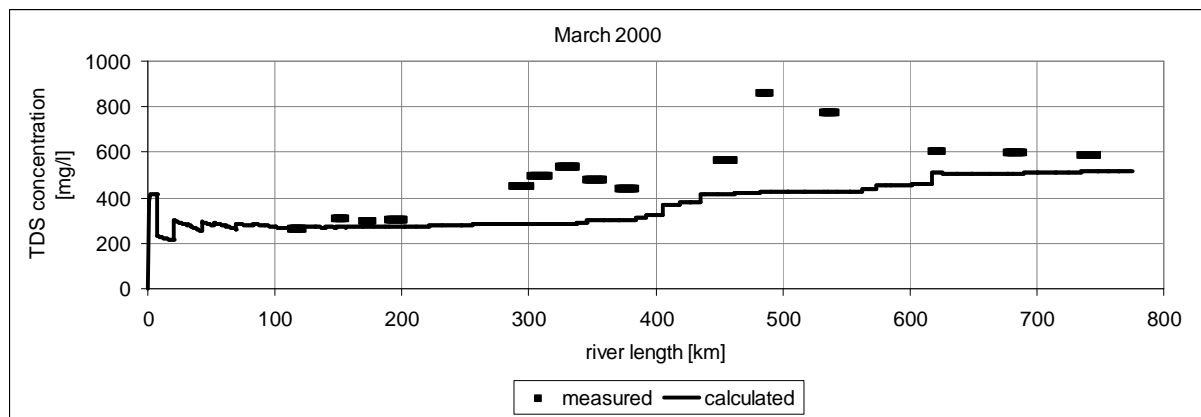


Figure 10. TDS results for Ebro River with modified input.

(a) Longitudinal profile, high flow, May 2000

(b) Longitudinal profile, low flow, March 2000

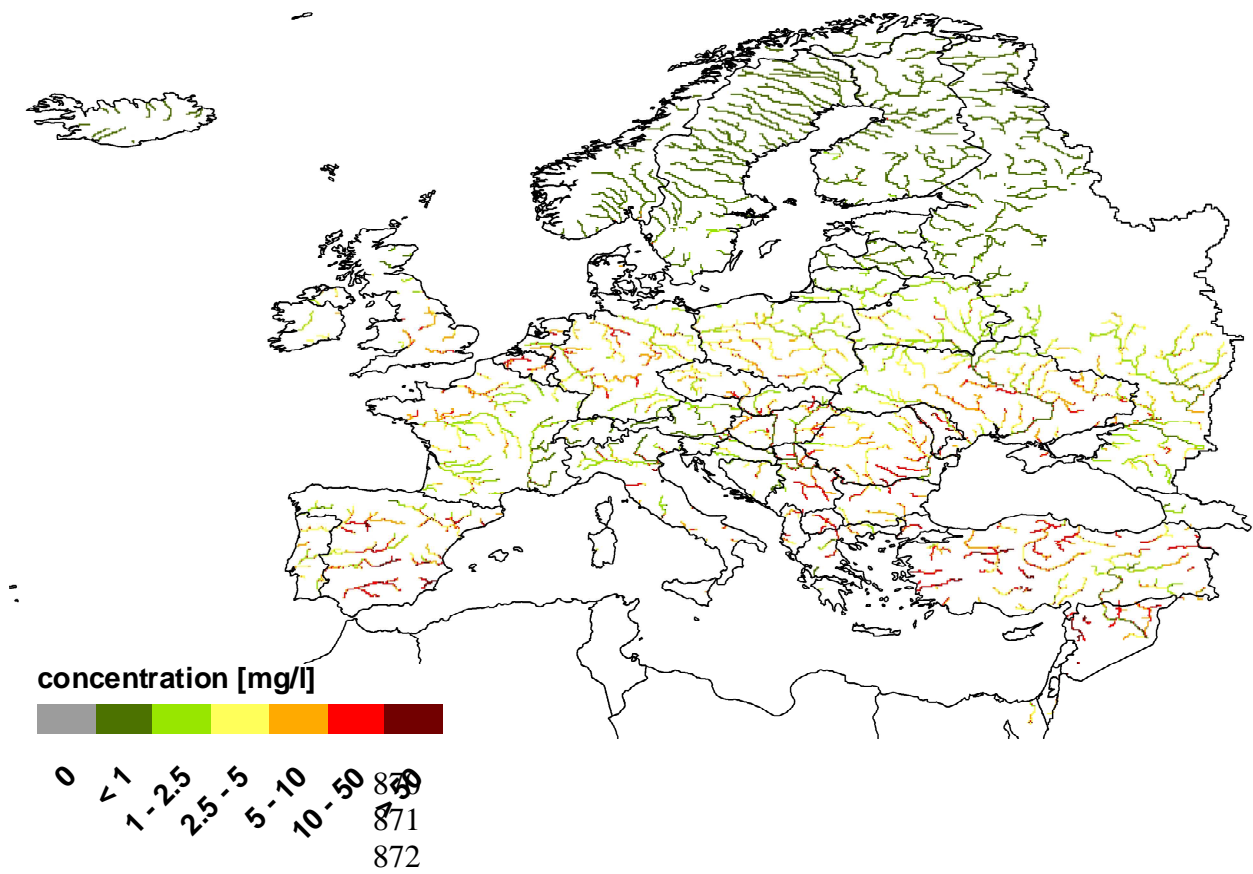


Figure 11. BOD<sub>5</sub> in-stream concentration in Europe – Baseline July 2000s.

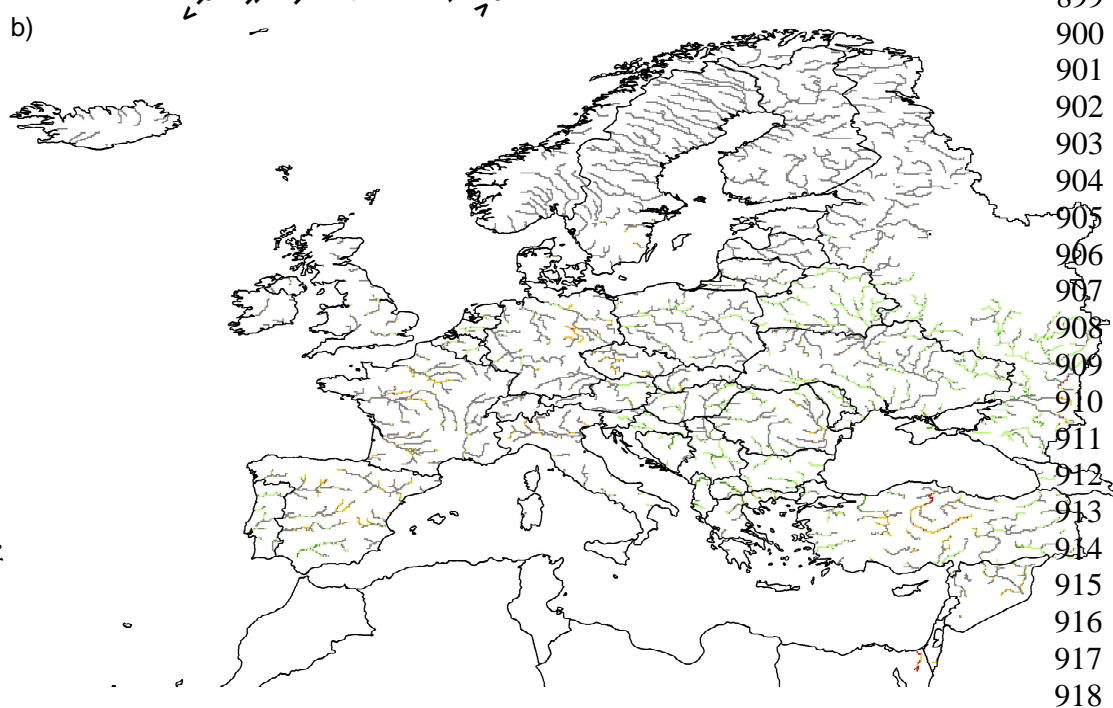
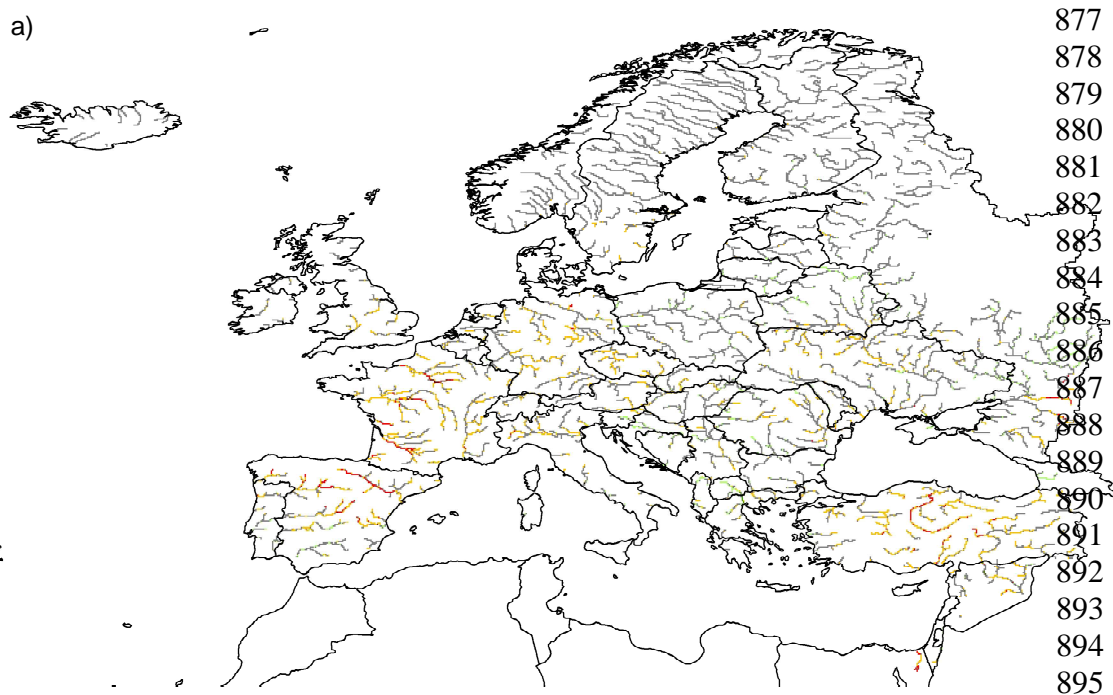


Figure 12. Effect of climate change on BOD<sub>5</sub> in-stream concentration in Europe.  
 (a) Changes in water quality classes in July (2000s vs. 2050s) under IPCM4-A2 climate  
 (b) Changes in water quality classes in July (2000s vs. 2050s) under MIMR-A2 climate