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PRELIMINARY WATER QUALITY MODULE: STATE OF DEVELOPMENT AND PLAN FOR LINKAGE TO THE OVERALL MODELLING FRAMEWORK

Author names: Frank Voß, Anja Voß, Ilona Bärlund, Joseph Alcamo

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Authors: Frank Voß, Anja Voß, Ilona Bärlund, Joseph Alcamo
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1. Introduction

Changes in the hydrological cycle induced by global warming may affect society more than any other changes, e.g. with regard to flood and drought risks, changing water availability and water quality. The deterioration of water quality poses a risk not only to society, but also to ecosystems. Due to their complex character, the assessment of possible changes in these systems is best performed by using modelling tools.

Potential impacts on water supply have received much attention, but relatively little is known about the concomitant changes in water quality. Projected changes in air temperature and rainfall could affect river flows and, hence, the mobility and dilution of contaminants. Increased water temperatures will affect chemical reaction kinetics and, combined with deterioration in quality, freshwater ecological status. The need for a scientifically-based assessment of the potential impacts of global change on the state of surface water resources is strong for most parts of the world (Whitehead et al. 2009).

The presence of trends in water chemistry provides an indication of environmental changes and gives insight into contributing factors such as climatic variation or changes in land use and management. 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 global water quality models (Grizzetti and Bouraoui 2006, Seitzinger et al. 2002, Green et al. 2004).

WATCH will provide new insights into the inter-relationships between water, climate change, and the anthropogenic pressures upon global water systems. A global overview of the exposure of society to deteriorating water quality brought on by global-scale changes in climate, population, land use, and human activities will be obtained, leading into the development of a first model of global water quality indicators. This report aims to describe the approach to model point and diffuse source pollutant loading for a continental water quality model being developed within the EU project WATCH. In close cooperation with the SCENES project, necessary point source and diffuse loading information was prepared as input data for the in-stream water quality modelling within WATCH.
2. Concept of the modelling approach

In order to link global water resources change with water quality, WaterGAP (Water Global Assessment and Prognosis, Alcamo et al. 2003, Döll et al. 2003, Flörke and Alcamo 2004) a model that calculates water use and availability on global scale is being further developed to include a water quality module (WorldQual). The linkage between these different components is shown in Figure 1.

WaterGAP (Water Global Assessment and Prognosis) is a global model developed at the Center for Environmental Systems Research of the University of Kassel, Germany. WaterGAP 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). WaterGAP3 is currently being calibrated for Europe on a 5 grid. The Global Hydrology Model simulates the macro scale behaviour of the terrestrial water cycle to estimate water resources.

Normally, information on loading should be derived from measurements or statistics. But it is not always possible to get all values required for all sectors and all countries. In particular this is true for the water return flows from the industry and the irrigation sector, which are needed to calculate the point loadings from industry and diffuse salt loadings from irrigated agricultural areas. Therefore this information is taken from the WaterGAP model output.

The water use component of WaterGAP gives estimates about total water consumption which reduces total water availability in the hydrological component. It consists of five sub-models to determine both water withdrawals and water consumption in the household, electricity, manufacturing, irrigation, and

Figure 1: Linkage between WaterGAP (Hydrology Model and Water Use Models) and WorldQual.
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 that is lost to evapotranspiration, consumed by industrial production or humans. The water use sectors only consume a part of the water withdrawn, the remaining water returns into the river system. Return flows derived from water withdrawals within the water use models are used to calculate input loadings in WorldQual. The country-scale estimates of water use are downscaled by the model within the respective countries using demographic and socio-economic data.

The hydrological component of WaterGAP provides river discharge, flow velocity, cell runoff and urban runoff respectively, so that, together with the input loadings, in-stream concentrations can be computed. All calculations are performed on 5’ grid cell level to ensure that the most detailed input information available on that level can be used. Temporal resolution of computing time steps differs between components from daily to yearly whereas results for the WorldQual Model are provided on a monthly basis.

The WorldQual Model
The aim of this new water quality sub-model is to determine chemical fluxes in different pathways which will allow a combination of water quantity with water quality analyses. The simulated key water quality variables have been chosen to indicate the suitability of water for various purposes: household, industrial and agricultural use, as well as for the overall health of the aquatic ecosystem. Thus, the variables in the first phase will include:

- total dissolved solids (TDS),
- biochemical oxygen demand (BOD),
- total coliform bacteria (TC),
- water temperature (TW), and
- dissolved oxygen.

Total dissolved solids is a measure of the suitability of water for household, industrial and agricultural use; coliform bacteria is an indicator for the suitability of water for tourism (swimming and other water contact activities); biochemical oxygen demand and dissolved oxygen, which are strongly water temperature dependent, are indicators of the level of organic pollution and overall health of aquatic ecosystems.

This paper describes the first steps in developing the approaches to quantify point source and diffuse pollution loading for BOD, TDS and TC. This is achieved by calculating national point source and diffuse loading and distributing the load according to certain rules across the grid system used in WaterGAP. A schematic overview of modelling concepts is described by means of flowcharts (Figure 2). Generally we distinguish 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 irrigation return flows or livestock farming), and
- also from natural background sources.

All the different sources of input loadings will be shortly described in the next paragraphs. For a more detailed description the reader is referred to the SCENES report ‘Assessment of current water pollution loads in Europe’. For the in-stream solute transport, basic approaches and model formulation will be described in this report.

Considering the poor global coverage of existing water quality data, we will concentrate on modelling and model testing on the European scale in the first phase.
Figure 2: Main concepts of modelling point source and diffuse pollution loadings on national scale and downscaling the total amount on grid cell level. The upper panel shows the methodology for BOD and TC, in the lower scheme the concept for TDS is introduced.
**Point Sources of Pollution**

Point source pollution arises from three main sources, domestic effluent, urban runoff and manufacturing discharges. The approaches taken to predict these loads and downscaling them to a grid square are described below.

**Domestic Effluent**

The national load estimates were calculated as the total influent load to the countries sewage treatment works. These estimates were based on urban and rural populations, urban and rural connectivity (%), and an estimate of per capita emission factor of a given determinant Y.

The values of the emission factors for BOD, TC and TDS, were found in the literature. For TDS only an average value of the emission factor of 45.6 mgL⁻¹ was available (UNEP 2000). However, for BOD values in domestic wastewater for selected regions and countries were available from the Intergovernmental Panel on Climate Change (IPCC 2006).

The estimates of urban and rural populations were provided by the CESR using data from the HYDE database (History Database of the Global Environment, version 3). The connectivity data was derived from the publicly available data and were taken from two main data sources (i.e. Eurostat and the World Health Organisation & UNICEF Joint Monitoring Program Data (JMP)).

The national load for a given determinant Y must be distributed across all country cells and then the appropriate treatment removal is applied in order to estimate the effluent in each grid cell. The present methodology was developed by adapting the method employed by Grizetti and Bouraoui (2006) for nitrogen and phosphorous. In order to derive monthly values, yearly amounts were divided by the factor 12.

The concept and flow of information are explained in Figure 3.

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**Figure 3**: Procedure to derive national load estimates from domestic effluents.
**Urban Runoff**

There are a number of methods for estimating pollution loads from paved areas in urban areas. The method selected for this study was based on the concept of event mean concentration (EMCs). This method assumes that the concentration of chemical runoff in an urban rainfall event is principally determined by the volume of the runoff and that each event has a typical concentration (the EMC). The load from paved urban areas is then simply the product of the EMC and the annual runoff from that area. Mitchell (2005) lists the reasons for adopting this approach. These volume-concentration methods often perform better than regression models. Observations made in the UK, suggest that the mean EMC of a site is not correlated with the annual runoff volume. Many pollutants can be addressed with this method and to add new ones is straightforward when appropriate data become available.

The urban influent load for a grid cell is added to the domestic load for the grid square. This load then gets treated in the same way as proposed for the domestic effluent. The total amount of urban runoff is taken as direct output from the WaterGAP – hydrology model. The concept and flow of information are explained in Figure 4.

![Figure 4: Procedure to derive national load estimates from urban runoff.](image-url)
**Manufacturing Discharges**

The method adopted here was to try to establish typical concentrations of each of the determinants of interest for six main manufacturing sectors using, if possible, different values for each country. Here we make use of the total return flow from the manufacturing industry in each country as given by the WaterGAP - water use model. 

The manufacturing sectors used in this model are food, textiles, paper, metal, chemicals and other. The typical concentrations of these effluents were obtained from two sources of data, the Emission Inventory from the International Commission for the Protection of the Danube River (ICPDR 2005) and from a literature search. In this analysis it has been assumed that all manufacturing discharges would receive further treatment. For each industrial discharge, the concentrations of the chemicals discharged were estimated by dividing the chemical load by the discharge volume to produce the data required to estimate country loads.

The downscaling to the grid squares was based on the return flow from the manufacturing industry calculated in the WaterGAP - water use model. It is important to emphasize that the national load from direct emissions is discharged without treatment to water courses, whereas national load from indirect emissions is treated via sewage treatment works before being discharged to rivers. In this analysis only indirect emissions were considered.

There was no data available for the fraction of treatment for industrial discharges. Within European countries, industrial wastewaters were generally considered as treated via secondary or tertiary treatment, thus proportions were derived from the fraction of treatment values used for downscaling the domestic load. In order to derive monthly values, yearly amounts were simply divided by the factor 12.

The concept and flow of information are explained in Figure 5.

**Figure 5: Procedure to derive national load estimates from industrial discharges.**
**Diffuse Sources of Pollution**

Diffuse pollution does not only originate from one discrete source, in fact it comes from many different sources like atmospheric deposition or natural background. Important diffuse sources for BOD, TC and TDS are the use of agricultural areas and the nonpoint effluents from scattered settlements. The approaches to calculate the loads from scattered settlements and agriculture are described below.

**Scattered Settlements**

The national load estimates from scattered settlements are based on the fractions of urban and rural population that is not connected to public waste water treatment plants. The per capita emission factor of a given determinant Y is the same as for the effluents from the domestic point sources. Like the input from domestic point sources the input from scattered settlements must be distributed across all country cells and then the appropriate treatment removal applied in order to estimate the effluent in each grid cell.

Sewage treatment from scattered settlements is much more variable than from domestic point sources. One typical treatment is septic tanks, but there are also small private treatment plants with high removal rates of pollution substances. In the calculations it has been assumed that the average treatment level of scattered settlements is similar to the secondary treatment level of public waste water treatment plants. Monthly estimates are calculated from yearly loadings divided by the factor 12.

The concept and flow of information are explained in Figure 6.

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**Figure 6: Procedure to derive national load estimates from scattered settlements.**
**Agricultural Input**

Although both, TDS and BOD (and to some extent also TC), originate from agricultural areas, different approaches have been used to calculate the loadings. TDS comes more from irrigated or salt affected soils in semiarid or arid regions and BOD and TC respectively from the livestock based agriculture.

**TDS**

Besides industrial and urban areas, also agricultural areas contribute to the salt emissions into a river system (Davis & Cornwell, 1999). In this analysis it is assumed that the main part of the agricultural salt emissions come from water return flow from irrigated agriculture. The estimation of salt loadings is a function of the salt concentration of the irrigation water return flow within a certain salt emission potential class (SEPC) and the amount of irrigation water return flow. Irrigation water return flow is provided by the WaterGAP – water use model and is provided on a monthly time basis. The concept and flow of information are explained in Figure 7.

In order to calculate the SEPC, information about the natural, primary salinity of soils and the manmade, secondary salinity are used. The main problem of secondary soil salinisation is the application of unsustainable irrigation practices in salt endangered regions. The lack of financial resources often prevents the use of state-of-the-art irrigation methods, or the treatment of irrigation water. Thus, the SEPC is a combination of natural salt classes (SC) and GDP (gross domestic product) classes.

Natural salt classes (SC) are a combination of primary salt enriched soils (S), and arid-humid climate conditions (H). Primary salt enriched soils were taken from the FAO soil map of the world (FAO, 2000). The soil types Solonetz and Solonchaks and soils with calcic or calcaric layers were assumed to be salt enriched soils. These salt enriched soils are divided into two classes, geogenic background salt content (S0), salt enriched soil (S1).

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*Figure 7: Procedure to derive national load estimates from irrigation return flow.*
Table 1: Concentrations (mgL⁻¹) of salt used in salt emission classes based on natural salt class (SC) and Classes based on Gross Domestic Product (GDPC).

<table>
<thead>
<tr>
<th></th>
<th>GDPC 1</th>
<th>GDPC 2</th>
<th>GDPC 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>SC 1</td>
<td>250</td>
<td>250</td>
<td>250</td>
</tr>
<tr>
<td>SC 2</td>
<td>250</td>
<td>500</td>
<td>500</td>
</tr>
<tr>
<td>SC 3</td>
<td>250</td>
<td>750</td>
<td>750</td>
</tr>
<tr>
<td>SC 4</td>
<td>500</td>
<td>750</td>
<td>1000</td>
</tr>
</tbody>
</table>

Furthermore, there are more salt affected soils under arid than under humid conditions. Low precipitation and high evaporation can cause a low water discharge and an increase of salt affected soils in endangered regions. The small water amount which can drain off into the river system is assumed to have a high salt concentration. Also arid and humid conditions are divided into two classes; humid (H1) and arid (H2). This classification is based on land cover implemented in WaterGAP, where grassland/steppe, hot desert, scrubland, and savanna are considered as arid, the remaining land cover classes are humid (Weiß 2008). Altogether four natural salt classes result from the combination of naturally salt enriched soils and arid-humid climate conditions: SC1 combines S0 and H1, SC2 combines S1 and H1, SC3 combines S0 and H2 and SC4 combines S1 and H2.

GDP classes (GDPC) are used to give likely irrigation technique standards of a country. Three GDP classes are differentiated: countries in GDP class 1 (> 10000 US$) are able to use the best irrigation techniques. Here the salt concentration in irrigation water is low. Countries in class 3 (< 1001 US$) are not able to use highly technical irrigation systems and the salt concentration in irrigation water can be high depending on the natural salt classes.

Finally, the salt concentration in irrigation water return flow results from the salt emission potential class. The salt emission potential is divided into four classes (see Table 1) in relation to the natural salt classes (SC) and the GDP classes (GDPC). The concentrations used for the four different classes were derived from Follett & Soltanpour (1999), who describe the salinity hazard of irrigation water depending on the dissolved salt content. Additionally, it was assumed that every country tried to use the best irrigation technique that was available, and that high saline irrigation water (> 2000 mg/l) is not used. For the background salt concentration within the rivers of a country the median concentration (derived from electric conductivity) of all available non agricultural water quality measurement points are used (Salminen 2005). In the case that data for a country are not available the drinking water mean value of Germany (250 mg/l) (TrinkwV, 2001) is used.
**BOD and TC**

We tested three different ways to estimate the diffuse BOD and TC loadings. Amongst a nitrogen correlation method and a calibrated export coefficient method we made use of a livestock based method, which seems to be on the global scale the most appropriate approach concerning the data availability. In the livestock based version it is assumed that the main source of BOD and TC emissions from agriculture comes from livestock. The calculations are based on an emission factor from livestock and the number of livestock units within a country. There also exist a retention rate in soil that includes decay and transformations processes. The emission factor used is the same for all countries. It is a product of the concentration in livestock manure and the amount of manure per livestock unit. The national livestock numbers for 1995 were derived from FAO and sub national statistics, which were edited and provided by the Institute of Physical Geography, Frankfurt University (Siebert 2005). Retention rates in the soil are assumed to be in the range of 95%. In order to generate grid cell loadings the national load is downscaled depending on the number of livestock units per grid cell. Cell runoff calculated by the WaterGAP - hydrology model is used to compute total loadings and is provided on a monthly time basis.

The concept and flow of information are explained in Figure 8.

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**Figure 8: Procedure to derive national load estimates from livestock farming.**
In-stream Water Temperature

Water temperature is an important and highly sensitive variable that affects physical, chemical, and biological processes in flowing waters (Hannah et al. 2008). Mean water temperature is known to have significant variation at the basin-scale related, in particular, to the source of stream water and to stream characteristics including altitude, azimuth, and length or riparian woodland cover.

In this first phase of development we want to make use of a linear relationship between mean monthly air temperature and mean monthly water temperature. For the mean monthly air temperature we use the CRU data set. A combination of the datasets CRU TS 2.1 and CRU TS 1.2 (Mitchell and Jones 2005, Mitchell et al. 2004) is used to force WorldQual Model. The CRU TS 1.2 dataset has a spatial resolution of 10'. However this dataset covers Europe only. Hence, the dataset of higher resolution (CRU TS 1.2) is used in the covered grid cells, whereas in all other regions the CRU TS 2.1 is applied. Data for water temperature were provided from UNEP GemsWater and SCENES project partners. Single point measurements for water temperature at water quality gauges were also aggregated to mean monthly values and compared to that value of mean air temperature given in the corresponding grid cell. In this sense there are in total 9943 air-water temperature data pairs available for all over Europe, covering a time period between 01/1990 and 12/2002.

These data pairs were analysed resulting in the assumption that a sigmoid-curve fitting would lead to best results in deriving water instream temperatures out of air temperatures (see also Figure 9).

\[
T(\text{water}) = \frac{C_0}{1 + e^{(C_1 + C_2 + T(\text{air}))}}
\]

Figure 9: Relationship between mean monthly air temperature and mean monthly water temperature. Type of formula for curve fitting is shown in the upper right corner.
**Solute Transport**

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. Due to application on such a large scale only very simple approaches can be considered.

Such a simple approach was first introduced by Chapra in 1977. Based on this work we derived different formulations for conservative (e.g. TDS) and non-conservative substances (e.g. BOD and TC). The basic concept for these formulations is shown in Figure 10.

We assume that input from direct upstream and from other tributaries enters the grid cell right at the beginning of each cell and defines the upstream concentration $C_0$. All the input from diffuse and point sources reaching the river network within a cell is distributed uniformly all over the river length. For conservative substances, loadings entering the channel are dissolved in distributed inflow $q_d$, whereas for non-conservative determinants only the substance itself is distributed longitudinally. In total, additional loadings from within a cell define the concentration $C_d$. Concentration in downstream flow is defined as $C_1$. Downstream routing is similar to the routing procedure in the WaterGAP – hydrology model with a predefined routing order (from upstream to downstream).

![Figure 10: Basic model concept for solute transport in open channel flow.](image)

The mathematical formulation for non-conservative substances is given in equation (1) assuming a temperature dependent decay rate $\text{dec}(T)$:

$$C(x) = C_0 e^{- \text{dec}(T) x / u} + C_d \left(1 - e^{- \text{dec}(T) x / u}\right)$$

(1)
with

\[ C_0 = \sum_{i=1}^{s} (Q_{in,i} \cdot C_{in,i}) / Q_i \]  \hspace{1cm} (2)

\[ C_d = \frac{S_{input}}{L \cdot A_c \cdot dec(T)} \]  \hspace{1cm} (3)

and

\[ A_c = \frac{Q}{u} = \frac{Q_0 + Q_1}{2 \cdot u} \]  \hspace{1cm} (4)

and

\[ dec(T) = dec(20) \cdot \Theta^{T-20} \]  \hspace{1cm} (5)

where

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

The concentration for conservative substances is expressed in equation (6):

\[ C(x) = C_0 e^{-q_d x} + C_d (1 - e^{-q_d x}) \]  \hspace{1cm} (6)

with

\[ q_d = \ln \left( \frac{Q_i}{Q_0} \right) \cdot \frac{1}{x} \]  \hspace{1cm} (7)

and

\[ C_d = \frac{S_{input}}{Q_i} \]  \hspace{1cm} (8)

where

\( q_d \) = coefficient for distributed inflow \hspace{1cm} \left[ \text{1/km} \right]
Temperature dependent decay rates for both BOD and TC follow equation (5) (Benham et al. 2006, Bowie et al. 1985), but differ in constant decay rate at 20°C $\text{dec}(20)$ and the temperature correction coefficient $\theta$. In this study we used values given in Table 2 (ranges for $\text{dec}(20)$ and $\theta$ found in the literature in brackets below).

Table 2: Ranges for $\text{dec}(20)$ and $\theta$ given in stated literature.

<table>
<thead>
<tr>
<th></th>
<th>$\text{dec}(20)$ in rivers [1/day]</th>
<th>References</th>
<th>$\theta$ []</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>TC</td>
<td>0.990 (0.01 – 7.99)</td>
<td>Moore et al. (1988), Crane S. R. and J. A. Moore (1986), Rosen (2000), Thomann and Mueller (1987), Bowie et al. (1985)</td>
<td>1.07 (0.08 – 1.2)</td>
<td>Pachepsky et al. (2006), Parajuli et al. (2009), Bowie et al. (1985)</td>
</tr>
<tr>
<td>BOD</td>
<td>0.23 (0.02 – 5.6) (in shallow rivers 1.6)</td>
<td>Paliwal et al. (2007), Bowie et al. (1985), Helfand J. and D. Dilks (2001)</td>
<td>1.047 (1.02 – 1.15)</td>
<td>Chapra (1997), Thomann and Mueller (1987), Bowie et al (1985), Helfand, J. and D. Dilks (2001)</td>
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</tbody>
</table>
3. Preliminary Results

This report aims to describe general trends in water quality over recent years. Due to the poor global coverage of existing water quality data, we will concentrate on modelling and model testing on the European scale. The model results have been tested against measured data in 14 European river basins along the river length for different data input conditions and dates (see also Figure 11).

Figure 11: Locations of measurement gauges for water quality data across Europe covering 14 European river basins (marked with red dots along the river channel).

In the following sections we will describe preliminary results for BOD, TC and TDS for the Danube river basin. National loadings have been used as described above, to get gridded loading information. In this study we will concentrate on the illustration of model performance in terms of comparison between measured and calculated water quality data. Please note that measured data is in most cases a point measurement not revealing the whole dynamic within one month and the whole grid cell.
Biochemical Oxygen Demand

Biochemical oxygen demand is an indicator of the level of organic pollution and the overall health of aquatic ecosystems. Main input loadings come from manufacturing discharges and domestic effluents. Based on the rough estimates of gridded input information, longitudinal profiles for BOD5 in January and July 2002 in the River Danube were calculated (upper and middle diagram in Figure 12). In January the level of BOD5 concentrations can be met in general. Even for higher peaks 1500 km downstream the spring calculated data are in line with measured data. In July 2002 upstream mean level domain in concentration can also be met and is about 1.5 mg/l. After approximately 1200 km downstream the spring measured concentration is getting higher which can not be captured within our modelling approach. Due to considerable underestimates of total input loadings in July 2002 these high levels in concentration can not be achieved.

In the lower chart of Figure 12 a time series of BOD5 concentration in the Danube at Wilkowo (near the Danube delta) is shown. Data of two measuring stations are drawn, showing also the range of concentration within one grid cell. Calculated time series indicate high dynamics which is not the case for the measured time series. This can be seen as consequence of too high decay rates. Modelling results show high seasonal variability with respect to this parameter. Refining it (current value 0.23 day⁻¹) would definitely lead to better results. But at this stage of development model calibration could not be performed.
Figure 12: Upper chart - Longitudinal profile of BOD5-concentrations for the Danube River in January 2002.
Middle chart - Longitudinal profile of BOD5-concentrations for the Danube River in July 2002.
**Total Coliform Bacteria**

Coliform bacteria are an indicator for the suitability of water for tourism (swimming and other water contact activities). Main sources come from domestic effluent and from scattered settlements. Figure 13 (upper and middle panel) show longitudinal profiles for TC in the Danube River in January and July 2002 as well as a time series (lower panel) for TC concentrations in the Danube at station Wilkowo. Again, the measured concentration in parts of the river can not exactly be captured. In January concentrations in TC are overestimated and in July most the time concentrations are a little bit too low. In both cases this is due to a mismatch in input loadings. In July for example, that high input loadings can not be achieved, which is the reason for the underestimation at river kilometre 1.000. But also too high simulated river discharges can lead to a mismatch in TC concentration, which is the case for the downstream area of the Danube (after kilometre 1.800 in July 2002; see middle diagram in Figure 13). However looking at the time series for TC concentration at Wilkowo (see lower diagram in Figure 13), calculated concentration seems to be higher than measured data, leading to the assumption that input, especially in winter time, is too high and temperature dependent decay rates are assumed to be too low.
Total Dissolved Solids

Total dissolved solids is a measure of the suitability of water for household, industrial and agricultural use. Not only the input associated with the return flow from irrigated areas is important, but also geogenic background concentration.

A shift in background concentration would lead to higher concentration not only at Wilkowo, but also across the whole river basin (see Figure 14). As water quantity for the River Danube is balanced, a better estimate of this background concentration would refine dynamic and level of TDS concentration in the Danube.

Figure 14: Longitudinal profile of TDS-concentrations for the Danube River in July 2002.
In-stream Water Temperature

Figure 15 illustrates performance of measured and calculated monthly in-stream water temperatures for the River Danube. Two types of curve fitting to the original data are shown. On the one hand the sigmoid curve fitting as described in Chapter 2 is illustrated including all data pairs available across Europe, on the other hand a simple linear correlation is used based on the Danube data solely. Two measuring stations were chosen (one upstream and the most downstream one) to demonstrate the influence of river basin characteristics on water temperature. In general, both functions give similar results for the middle domain of water temperature, whereas the sigmoid curve tends to give higher maximum temperatures. In case of the most downstream station this leads to a better representation of high water temperatures, for the upstream station water temperatures are overestimated. The linear regression function tends to estimate lower minimum water temperatures and at least for the downstream station this leads to a better representation of measured data.
Figure 15: Water temperature in the Danube river basin (upper panel: measured and calculated data for an upstream station; lower panel: measured and calculated data for a downstream station).

EU_func_sigmoid (red line) is the fitted sigmoid curve based on all data across Europe, DANUBE_func (green line) is the linear interpolation function based on the Danube data solely.
5. Conclusions and Outlook

In this study preliminary estimates of recent trends in water quality in Europe especially in the Danube river basin are presented, including parameters like BOD, TC, TDS and water temperature. The specific aim of this paper was to provide background information on the new WorldQual model to be capable of operating on global scale. It provides insight in getting national loadings for the above mentioned indicators covering both, point and diffuse sources. These data sets have been put together to drive a grid based water quality model with a view to estimate the impacts on water quality of socio-economic and policy driven changes. The WaterGAP model has already been used to show impacts on water resources from such drivers (Flörke & Alcamo 2004, Alcamo et al. 2007, Weiß et al. 2007, Bärlund et al. 2008) and similar techniques will be used for combined water quality and water quantity backward as well as forward looks.

Not only for point sources but also for diffusive sources it is difficult to assess at this scale how good the methods presented in this report are at estimating the loading across Europe because of the paucity of easily accessible datasets at this scale. As an example, for the River Danube industrial and domestic effluent loads of BOD are available separately (ICPDR 2005). This source gave an estimate of approximately 342 tyr⁻¹ for the domestic load and 60 tyr⁻¹ for the industrial load, compared to the calculated values of 433 and 523 tyr⁻¹ respectively. The domestic estimate is in quite good agreement, but there is almost an order of magnitude overestimate in the BOD load from industry.

There is a need to gather more observed data to further test and refine these methods. Currently no data have been found with which to test the TDS loading information. Further data collation will be a priority in the next stages of the project.

Beside this, a refined model validation for the WaterGAP – hydrology model is essential to get right estimates of river discharges. Both, refined water quantity and information on input loadings, will lead to a better representation of measured water quality data as shown with preliminary results for BOD, TC and TDS. At this stage in model development model calibration could not be performed. Especially temperature dependent decay rates are very sensitive in model calculations and have to be improved.

In calculating the water temperature, we tested two different modelling approaches. First we made use of a linear regression based on data for a distinct river basin solely. Second a sigmoid curve fitting for all available pairs of air/water temperature data was implemented. In the Danube catchment both procedures resulted in an adequate reproduction of measured time series. This was done also for the other catchments where sufficient data was available leading to similar results. Finally we suggest to make use of regionalized regression functions to cover areas all over the world. Due to a slightly better overall representation of mean monthly water temperatures, which can also be seen in other river basins, fitting the sigmoid curve should be preferred.

In general modelling results show a promising step forward in building the first model of surface water quality to be capable in operating on the global scale. The data set presented in this study and the resulting outputs from the WorldQual model will form a baseline against which the impact of future scenarios can then be measured.
Next Steps and Linkage to the Modelling Framework

The data set presented in this study and the resulting outputs from the WorldQual model will form a baseline against which the impact of future scenarios can be measured. The next stage, and running alongside further refinement, is to provide plausible future scenarios. The difficulty comes in quantifying how fairly qualitative scenarios can be interpreted in terms of changed model parameters and input variables. This quantification step is part of WP6.3. In this way it will be possible for the first time to try to quantify water quality futures across continental scale which will result from socioeconomic storylines.

In the next phase of development we will concentrate a little bit more on water temperature modelling. This will include both further development of model formulation and compilation of the data for running and testing the model. Herein we will test regression of water temperature and air temperature in different regions (climatic zones) or especially for different river basins. Afterwards it is planned to set up a first modelling approach for dissolved oxygen (DO), which is known to be strongly correlated with water temperature.

All the developed approaches can easily be linked to the overall modelling framework. As already shown in Figure 1, data for e.g. river discharge, runoff, flow velocity, water use, and sectoral return flows are provided by the WaterGAP model. All the input data needed for water quality modelling is stored within a database, and the WorldQual model is also linked to that database, so that the data mentioned above can be replaced with input data provided from other models. Data has to be provided on a 5’ grid scale level, otherwise we will lose the aspired high level of spatial resolution which is important for water quality modelling.

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