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

3
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16
17 Abstract:

18
19 To address the continental and large scale aspects of water quality assessments new modelling
20 approaches are required. This paper describes the development of a continental-scale model of
21 river water quality - WorldQual. Simple equations, consistent with the availability of data on
22 the continental-scale, are used to simulate the response of biochemical oxygen demand
23 (BOD₅) and total dissolved solids (TDS) to anthropogenic loadings and flow dilution. A
24 methodology is developed that is appropriate for scenario analysis on the continental and
25 global scale. Average monthly river water quality is modeled on a 5 arc-minute grid covering
26 all Europe. Loadings are derived from assumptions about water use, return flows and other
27 variables. The model WorldQual is tested against measured longitudinal gradients and time
28 series data at specific river locations. The model performance on European scale shows that a
29 good fit can be reached when using concentration classifications as a measure: For BOD₅, 51
30 % of the simulated data is in the same quality class as the measurements and 30 % differ only
31 by one water quality class; for TDS the respective values are 35 % and 41%. WorldQual was
32 applied to investigate the impact of climate change on resulting changes of in-stream
33 concentrations. The results for Europe show that future climate changes only have a small
34 impact on European in-stream concentration levels of BOD₅, except for the Eastern part and
35 the Black Sea region. This effect is stronger for the IPCM4-A2 scenario than for the MIMR-
36 A2 scenario.

37
38 Nomenclature

39
40 BOD₅ = Five-day biochemical oxygen demand (mg l⁻¹)

41 TDS = Total dissolved solids (mg l⁻¹)
42

43 INTRODUCTION

44
45 Over the past two decades the idea that water research and policy have not only local and
46 regional aspects but also important continental and global scale dimensions has gained
47 credence (e.g. Alcamo et al. 2008). But this new global view of water has focused mostly on
48 the quantity of water rather than its quality. The state of global water quality was assessed
49 twenty years ago (Meybeck et al. 1989) but such an effort has not been repeated since. The
50 reasons for this are not clear, but perhaps it has to do with the difficulty in evaluating water
51 quality on the large scale. In comparison to the relative ease in estimating water availability

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

61
62 Although catchment scale modelling of water and solute transport and transformations is a
63 widely used technique to study pollution pathways and effects of policies and mitigation
64 measures (e.g. Schob et al. 2006, Bärlund et al. 2007, Hesse et al. 2008, Krause et al. 2008,
65 Volk et al. 2008) there are only a few examples of continental water quality modelling
66 approaches (Seitzinger et al. 2002, Green et al. 2004, Grizzetti and Bouraoui 2006). On global
67 scale, models developed so far focus on pollution pathways and loadings within a river
68 catchment or into a river stream (e.g. Siebert 2005, Van Drecht et al. 2005, Vörösmarty et al.
69 2010).

70
71 Yet these challenges need to be met, first of all, because the lack of understanding of large
72 scale water quality patterns is a major gap in our understanding of the state of the
73 environment. Second, the assessments of the state of worldwide aquatic biodiversity and
74 threats to biodiversity require knowledge of ambient water quality and their trends. Third,
75 poor quality surface waters and groundwater pose a health hazard over large areas that need to
76 be evaluated. Finally, global drivers such as climate change are likely to have a far-reaching
77 continental and global impact on water quality. The Intergovernmental Panel on Climate
78 Change has pointed out that many of the changes expected in water quality may be negative,
79 including reduced dilution capacity of some rivers because of more frequent droughts, or
80 increased bacterial loadings to other rivers due to changes in rainfall patterns (Bates et al.,
81 2008).

82
83 To address the continental and large scale aspects of water quality assessments, we present
84 here a continental-scale model of river water quality - WorldQual. The model is generally
85 intended to address the following questions:

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

93
94 The first application of the WorldQual model is to river systems of Europe. The model itself
95 has been developed as part of the EU-funded SCENES Project (“Water Scenarios for Europe
96 and for Neighbouring States” 2006-2011) which has had the principal goal of developing new
97 scenarios of the future of water resources in Europe (Kämäri et al. 2008). Estimates of future
98 water quality are needed for two major reasons: to assess the future state of aquatic
99 ecosystems and to determine the suitability of surface water supply for different water users
100 such as industries, agriculture and the domestic sector. The aim of this paper is to describe a
101 modeling methodology to tackle some of these questions and to present results of applying
102 this methodology. For this, the paper addresses the future of Europe’s water resources as

103 impacted by climate change under natural flow conditions. Biochemical oxygen demand
104 (BOD₅) is used as a representative measure for scenario calculation but the framework is
105 generic and thus applicable to any other substance e.g. salts or total nutrients.

107 MATERIAL AND METHODS

109 *Modeling Strategy*

111
112 Before explaining the modeling strategy, it should be noted that modeling water quality on the
113 continental scale is only now becoming feasible because of new developments in large scale
114 modeling of water resources. These developments include the availability of “fine” scale
115 continental hydrologic models (5 arc-minute resolution) which allows the tracking of the
116 pathways of rivers on a continental scale grid and enables the matching of river quality
117 monitoring stations with modeled river coordinates. Another new development is the
118 computation of stream velocity which permits time of travel computations in streams on the
119 continental scale. Time of travel is a key variable in computing the longitudinal gradients of
120 non-conservative substances such as BOD₅. Finally, the development of spatially-explicit
121 water use models makes it possible to locate return flows and wastewater discharges more
122 accurately on the continental-scale.

123
124 The design of the WorldQual model is determined by its goals which are:

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

131
132 These goals influence the design criteria for the model which can be divided into:

- 133 ▪ Spatial and temporal resolution of calculations,
- 134 ▪ Water quality constituents,
- 135 ▪ Model equations.

136 137 *Spatial and Temporal Resolution*

138
139 The first decision regarding the design of WorldQual has to do with selecting the spatial and
140 temporal resolutions of the model. Since water quality can be altered very significantly and
141 quickly in the vicinity of large wastewater sources, we select a model that can compute the
142 continuous spatial change in water quality along each river reach within a 5 arc-minute grid
143 cell. Each river is divided into “reaches”, the size of a grid cell, and within each reach, the
144 model computes continuous spatial changes in water quality from the beginning to the end of
145 the reach. Only “smooth” changes are computed within the river reach since the model cannot
146 take into account every wastewater point source.

147
148 With regards to temporal resolution, we select a monthly averaging period for computing
149 water quality. This is a compromise between two cases. On one hand, it would be preferable
150 to compute water quality at daily or hourly intervals, because the model would then simulate
151 temporarily high levels of contamination. However, modeling at this time scale is not realistic
152 because it requires modeling inputs that are not available on the continental basis. On the
153 other hand, it would be preferable to compute annual average water quality because the

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

160 *Water Quality Constituents*

161
162 The next decision is to select the water quality constituents to be computed by the WorldQual
163 model. At first we select the following substances to calculate with the model, but other
164 substances will be included into the model calculations later:

- 166 ■ Biochemical oxygen demand (BOD₅) which is an indicator of the level of organic
167 pollution and its oxygen-depleting potential, and serves as a metric for the overall health
168 of aquatic ecosystems.
- 169 ■ Total dissolved solids (TDS) which is a measure of the suitability of water for household,
170 industrial and agricultural use. Since TDS does not decompose or otherwise decay in a
171 waterway, it is a useful tracer of flow inputs and outputs in a river reach and can be used
172 for validating the flow balance of a river.

173
174 These substances are also relevant indicators for studying compliance with the general
175 ecological requirements for European waters specified in the Water Framework Directive of
176 the European Union (Anon 2000). They can contribute to (but are not sufficient for)
177 determining "good ecological status" and "good chemical status" of river systems, as called
178 for by the Directive. We note again that these constituents are only the first parameters to be
179 modeled, and they will be followed by total phosphorus and total nitrogen as indicators of the
180 ecological health and level of eutrophication in rivers.

182 *Model Equations*

183
184 In selecting model equations the challenge is the same as with all river modeling, namely that
185 a compromise must be found between the desire to simulate conditions precisely, and the
186 reality that data limitations will hinder the running and testing of the model. These data
187 limitations are especially crucial for modeling water quality on the continental basis. Aim of
188 this paper is to show, that the model is generally able to work on global scale with simple
189 types of equations and with a limited amount of data input. Therefore the model presented
190 here was fed with standard values from literature or with results from other model
191 calculations as described in the next section. Therefore also, the model is not calibrated.

192
193 Solute transport in open water channels is an important topic in water quality studies. In
194 addition to any biological and biochemical reactions that may occur in river streams, polluting
195 solutes that enter water courses are transported and dispersed downstream. The ability to
196 describe and predict the effects of the transport processes on the distribution of solute
197 concentration is of great importance. In applications on such a large scale only very simple
198 approaches can be considered, such as was introduced by Chapra (1977). Based on this work
199 different formulations for conservative and non-conservative substances were derived.

200
201 For non-conservative substances (e.g. BOD₅) the equation from Thomann and Mueller (1987)
202 was used, which describes the change in concentration of a substance c within a river reach as
203 a function of an initial concentration and of a distributed load that enters at an equal rate along
204 the river reach within a grid cell (Fig.1). The advantage of this approach is that it calls for a

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

$$211 \quad C(x) = C_0 * e^{-dec(T) \cdot x / u} + C_d * (1 - e^{-dec(T) \cdot x / u}) \quad (1)$$

212
 213 with

$$214 \quad C_0 = \frac{\sum_{i=1}^8 (Q_{in,i} * C_{in,i})}{Q_1} \quad (2)$$

$$215 \quad C_d = \frac{S_{input}}{L * A_c * dec(T)} \quad (3)$$

216 and

$$217 \quad A_c = \frac{Q}{u} = \frac{Q_0 + Q_1}{2 \cdot u} \quad (4)$$

218 and

$$219 \quad dec(T) = dec(20) * \Theta^{T-20} \quad (5)$$

220 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	$[1 / month]$
Θ	=	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	$[km^3 / month]$

222

223

224

225 Temperature dependent decay rates for BOD₅ follow equation (5) (Benham et al. 2006, Bowie
 226 et al. 1985). The decay rate at 20 °C is 0.23 1/month and the temperature correction
 227 coefficient is 1.047 (Paliwal et al. (2007), Bowie et al. (1985), Thomann and Mueller (1987),
 228 Chapra (1997)).

229

230 For conservative substances the equation from Thomann and Mueller (1987) was selected. It
231 simulates the change in an initial concentration and distributed source as it is diluted by
232 increasing flow input along the river reach. The concentration is expressed in equation (6):
233

$$234 \quad C(x) = C_0 * e^{-q_d x} + C_d * (1 - e^{-q_d x}) \quad (6)$$

235 with

$$236 \quad q_d = \ln\left(\frac{Q_1}{Q_0}\right) * \frac{1}{x} \quad (7)$$

237 and

$$238 \quad C_d = \frac{S_{input}}{Q_1} \quad (8)$$

239 where

$$241 \quad q_d = \text{coefficient for distributed inflow} \quad [1/km]$$

242

243

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

246

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

254

255 *Data input*

256

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

260

261 Hydrological variables like river discharge, cell runoff, and flow velocity will be fed by
262 output from the global model WaterGAP (Water – Global Assessment and Prognosis, Fig. 2).
263 WaterGAP is developed at the Center for Environmental Systems Research of the University
264 of Kassel, Germany. It comprises two main components, a global hydrology model and a
265 Global Water Use Model (Alcamo et al. 2003, Döll et al. 2003, Flörke and Alcamo 2004,
266 Verzano 2009). The Global Hydrology Model simulates the macro scale behaviour of the
267 terrestrial water cycle to estimate water resources. All calculations are performed on 5' grid
268 cell level to ensure that the most detailed input information available on that level can be
269 used. The Global Water Use Model of WaterGAP (Aus der Beek et al. 2010, Flörke et al.
270 2011) consists of five sub-models to determine the water withdrawals and water consumption
271 in the household, electricity, manufacturing, irrigation, and livestock sectors. In this context,
272 water withdrawals depict the total amount of water used in each sector while the consumptive
273 water use indicates the part of withdrawn water. The water use sectors only consume a part of
274 the water withdrawals and the remaining water returns into the river system. These return
275 flows are used to calculate input loadings in WorldQual.

276

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

287 *Baseline climate and scenario selection*

289 Climate forcing data used for the baseline in this study has been compiled and regionalised by
290 the Climate Research Unit (CRU) of the University of East Anglia, Norwich, UK (version TS
291 2.1, Mitchell and Jones, 2005). CRU data covers Europe in 10' resolution and monthly time
292 steps. In order to use it for the water quality modelling the dataset have simply been
293 disaggregated to a spatial resolution of 5'.

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

- 297 • IPCM-A2: IPSL-CM4, Institute Pierre Simon Laplace, France + A2 scenario (Denvil,
298 2005): high temperature increase with low precipitation increase or precipitation
299 decrease
- 300 • MIMR-A2: MIRCO3.2, Center for Climate System Research, University of Tokyo,
301 Japan + A2 scenario (Nozawa, 2005): high temperature increase, high precipitation
302 increase or low decrease.

303 The original spatial resolution (IPCM4-A2: lat 2.5° x lon 3.75°, MIMR-A2: lat 2.8° x lon
304 2.8°) was re-sampled by bilinear interpolation to 5' minutes grid cells.

305 The time frame of the climate scenarios used in the model calculations are the 2050s (2040 –
306 2069). As base year 2005 is used as it is the reference year for water use calculations in the
307 SCENES project. Scenario development in SCENES was a stakeholder driven process
308 (Kämäri et al. 2008). A characteristic feature in all storylines developed in this process was
309 the focus on climate change impacts as a major trigger to changes in human and thus societal
310 awareness and behaviour (Kok et al. 2009, Kok et al. 2011). Thus the SCENES stakeholders
311 who participated in the storyline development also played a key role in choosing an
312 appropriate IPCC SRES scenario to relate the modelling work within SCENES to the
313 storylines. Their recommendation was to concentrate on the A2 scenario only in order to
314 emphasise the trigger role of climate change in all storylines.

315 RESULTS AND DISCUSSION

316 To test the model, 15 basins across Europe were selected. These represent a range of large
317 river basins (> 9000 km² to 820 000 km²), climates (arid and humid), geogenic background
318 conditions (e.g. different salt concentrations) and degrees of anthropogenic influence (e.g.

328 different population densities and pollution loadings). Another important criterion is that at
329 least monthly measurements were available for different substances in these basins for testing
330 the model. In this paper, results from all catchments are summarised and the BOD₅ results
331 presented more detailed examination of the Ebro, Thames river basins and similarly the TDS
332 results for Ebro and Vistula basins.

333
334 Test results are presented in two formats. Firstly, longitudinal profiles show the ability of the
335 model to simulate spatial gradients of river water quality. In Figures 3 to 10 (a, b) model
336 calculations are compared to monthly average observations because this corresponds to the
337 target temporal resolution of the model. The model is tested against data from high river flow
338 periods (Figs. 3 to 10 a) and low flow periods (Figs. 3 to 10 b). The year 2000 is selected for
339 testing because of the good availability of data. The second format for testing the results is to
340 compare model calculations on yearly time series of measurements at specific locations in the
341 rivers (e.g. up- or middle stream) (Figs. 3, 4, 7, 8 c).

342
343 Because of the lack of data density the quality of model calculation can not be presented with
344 usual methods like, Nash-Sutcliff coefficients or coefficients of determination. Concentrations
345 were divided into classes and the difference of these classes between calculated and measured
346 values evaluated. The concentrations were equally distributed into 7 (BOD₅) or 9 classes
347 (TDS) in order to have comparable data sets. The resolution for BOD₅ is 5 mg/l and for TDS
348 250 mg/l. Another possibility to test the model quality is the use of the 90-percentile
349 concentration. Here a set of all available data pairs of monthly average concentrations
350 (measured and simulated) for the year 2000 is used (BOD₅: Ebro (205), Thames (50), Europe
351 (1421), TDS: Ebro (207), Vistula (306), Europe (1468)).

352
353 *BOD₅*

354
355 The results for Europe show that for the complete data set the model gives a satisfactory result
356 since 51% of reaches were predicted in the same water quality class as observed data and
357 30 % show a difference of only one class between measured and simulated values. 9 % of
358 rivers were modelled with a difference of two classes and only 8 % differ by more than two
359 classes. The 90-percentile (Tab. 2) for the measured data is 7.7 mg/l and for the calculated
360 11.0 mg/l. The modelled results generally overestimate the observed values. This is an
361 encouraging result given that the model has not been calibrated for water quality (only for
362 river flows) and is driven by national level data that has largely been reported through
363 European level databases. There will be regions where the model poorly reproduces observed
364 data due to local conditions that are not captured in European scale data. Two examples for
365 the Ebro and the Thames river basins will serve to illustrate this point.

366
367 For the Ebro, the model shows a clear underestimation of BOD₅ concentrations in comparison
368 to longitudinal measurements for high and low flow conditions as well as in the monthly time
369 series. (Figs. 3a to 3c); 20 % of the measured and calculated values belong to the same water
370 quality class, 40 % differ by one class and 13 % by two classes. 27 % show a difference of
371 more than three classes. Underestimation in the Ebro is mainly due to the estimation of
372 pollution loading of livestock. In WorldQual the loading input from livestock production is
373 generally treated as a diffuse source, but according to European Pollutant Emission Register
374 database (2010), many animal production facilities within the Ebro basin (poultry and pork)
375 discharge their wastewater directly into the river water and are thus point source inputs. This
376 phenomenon can be found mainly in the down stream region. If the inputs are modified to
377 treat the animal waste like inputs from a manufacturing point source, the modified input
378 loadings show an increase of the manufacturing loads from 1.2 t to 117.9 t, from 1.2 % of

379 total loadings to 54.7 % respective (Tab. 3). With this modified input the BOD₅ in-stream
380 concentration fit improves considerably when compared to the longitudinal measurements for
381 both high and low flow conditions (Figs. 4a and 4b). However, the BOD₅ concentration is
382 now overestimated in summer between June and September (Fig. 4c). These results are also
383 reflected by the model goodness-of-fit (Tab. 2). The difference of classes between measured
384 and calculated values are not better than with the regular input and the 90-percentile shows an
385 overestimation with 14 and 22.6 mg/l respectively (Tab. 2). More information is probably
386 needed on the timing of the animal production discharges if this aspect of the model is to be
387 improved.

388

389 In contrast to Ebro, the Thames shows an overestimation of simulated values against
390 measured along river length especially for low flow conditions (Figs. 5a / b). This result is
391 confirmed by the 90-percentile (Tab. 2). For regular input only 14 % of calculated
392 concentration values belong to the same class as the measured ones, but as can be seen 70 %
393 show only a small difference of one and 16 % of two classes. One source of uncertainty may
394 be the inaccurate estimation of river flows in the Thames, especially in the upper catchment.
395 Another more important uncertainty factor concerns the share of domestic loading that,
396 especially for the middle and down stream Thames, is very high (~80%, Tab. 3). Local
397 information on domestic sewage treatment shows that within the Thames basin removal of
398 BOD is likely to be 97 % rather than 90 % used in the standard load estimation methods for
399 WorldQual (Williams et al., this issue, Butwell et al., 2009). Making this correction, the
400 simulated BOD₅ concentration fit much better to in-stream measurements (Figs. 6a / b). Only
401 the upper part of the catchment shows still an overestimation in concentrations probably due
402 to the underestimation of river flows in this region mentioned above. The 90-percentiles of
403 measured and calculated values are 2 mg/l and 4 mg/l, respectively and there are no
404 differences within the water quality classes (Tab. 2).

405

406 *TDS*

407

408 Of all calculated concentrations of European rivers 35 % belong to the same class as
409 measured values – 41 % and 14 % differ by one and two classes, respectively. Only 7 % show
410 a difference by three or more water quality classes. The calculated TDS concentration for
411 Europe is generally underestimated (Tab. 4). The 90-percentiles differ by about 400 mg/l.
412 Possible reasons can be river flow conditions and uncertainties in loading input, as for the
413 BOD₅ concentration. A third factor can be the geogenic background concentration. As can be
414 seen in Tab. 1, the background calculation is based on the geologic variation considering a
415 median salt concentration of all available non-agricultural water quality measurement points
416 within the rivers of a country (Salminen 2005). In the case that data for a country are not
417 available the drinking water mean value of 250 mg/l was used. As for BOD₅, taking account
418 of the lack of model calibration and the use of high level European data, these results are
419 encouraging.

420

421 As for BOD₅ allowance for local conditions can improve the model performance in specific
422 basins. In the Vistula river basin modelled TDS concentrations underestimate the measured
423 concentrations (Figs. 7a - c) especially in the upper part of the river. For the first 300 km the
424 measured TDS values are very high, up to 4200 mg/l. These upstream levels are due to the
425 contribution of salt effluents from the mining industry (Ericsson & Hallmans 1996,
426 Buszewski et al. 2005, Turek 2004). This input load is not accounted for in the model
427 estimated loads and therefore the 90-percentiles of measured and calculated values differ by
428 ~1600 mg/l (Tab. 4). Only 8 % of the calculated values have the same water quality class as
429 the measured values. 70 % differ by one or two classes and 22 % by three or more classes. In

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

438
439 With regular loading input the model calculates a concentration for the Ebro River that is too
440 low for low flow conditions, especially in the lower half of the river (Figs. 9a / b). The 90-
441 percentile confirms this result with a measured value of 862 mg/l against a calculated value of
442 543 mg/l (Tab 4). Main factor of TDS input within the Ebro basin is the irrigation sector
443 (~66 % with regular input, Tab. 5). There is evidence of significantly higher irrigation
444 following a monthly cycle that is clearly different from that used in the WorldQual loading
445 calculations (Causapé et al., 2006, Tedeschi et al. 2001). They report very intensive irrigation
446 practices especially in the downstream part of the Ebro for the effluents of Cinca and Segre
447 Rivers. Using these local data TDS loadings increase from 0.7 Mio t to 12.5 Mio t per year.
448 Furthermore the monthly distribution is changed. With these changes the contribution of
449 loading from the irrigation sector rises up to 97 % (Tab. 5). The results with the modified
450 input show a better result for low flow conditions and a similar one for high flow conditions
451 (Figs. 10a / b). All in all there is more dynamics along the river, but the 90-percentiles in
452 Tab. 4 show a clear overestimation of TDS concentration because of too high concentration
453 values for the months June and July.

454 455 *Scenario application: Impact of climate change on water quality*

456
457 The in-stream concentration of BOD₅ in Europe for the baseline 2005 shows that little
458 influence of loading on water quality is detected for Northern Europe (Fig. 11). In contrast,
459 the highest concentrations can be found for the Iberian Peninsula, Western Asia and Eastern
460 Mediterranean. All other rivers of Europe have low to medium BOD₅ concentrations. The
461 BOD₅ concentration in rivers for the scenario calculation is coupled with water quality
462 classes, which are used in literature and present the natural and chemical status of a river
463 system (Pettine 2004). Thereby <1 mg/l means very good and >50 mg/l means highly polluted
464 river streams. For the baseline as well as for the two scenarios all cells within a river basin
465 belong to one of these seven classes. In order to investigate the in-stream BOD₅
466 concentrations in more detail, the differences between the classes (scenario minus baseline)
467 were calculated for the IPCM4-A2 and MIMR-A2 scenarios (Figs. 12 a,b). Thereby positive
468 values (degradation of water quality), negative values (improvement of water quality) and
469 zero values (no changes) occur. The climate change scenarios have three potential effects on
470 water quality: first, the changes in precipitation lead to changes in runoff and thus in-stream
471 water availability; second, changes in air temperature affect in-stream degradation of organic
472 substances and thus the BOD₅ concentration; and third, two loading components in
473 WorldQual namely diffuse loading and wash-off from sealed areas is affected by changes in
474 precipitation.

475
476 As can be seen for both scenarios there is no change in water quality classes in most rivers of
477 Northern, middle and Western Europe. Following the IPCM4-A2 scenario in Eastern Europe
478 and in the Black Sea region the in-stream concentration will get worse by up to 2 classes
479 compared to the baseline 2005. Different patterns can be found in the MIMR-A2 scenario in
480 which only the Black Sea region will show an increase of BOD₅ concentrations.

481
482 Analyses concerning the impact of climate change on the BOD₅ decay rate and on the
483 affected loadings have shown, that they are very small and do not considerably influence the
484 in-stream concentration. The main effect for the results is the change in water availability due
485 the different climate conditions. IPCM4-A2 is drier than MIMR-A2 and therefore there will
486 be smaller river flow for IPCM4-A2. If you have no changes in loadings the effect of less
487 river availability will be an increase of concentration and a decrease of water quality.

488 489 CONCLUSIONS

490
491 This paper has presented a new global scale water quality model – WorldQual and illustrated
492 its performance through its application to modelling BOD₅ and TDS across Europe. The use
493 of such a model at the European scale has also been illustrated by considering the effects of
494 climate change on future BOD₅ concentrations.

495
496 With reference to the European rivers it has been shown that the model is robust and works in
497 the expected way. Overall of Europe, comparisons between observed and modelled
498 concentrations were encouraging given that the models were only calibrated for water flow
499 and not water quality. The aim of the model is to provide a mechanism for investigation
500 trends in water quality which might occur in response to continental scale drivers such as
501 climate change, European policy or changing populations. Global models are no substitute for
502 detailed models of individual catchments if the focus of management is at that local scale.
503 However, it has been shown that local information can improve the simulations of individual
504 river basins within the WorldQual model framework.

505
506 Because of the acceptable model performance in targeting water quality classes the modeling
507 methodology described here can be applied to scenario analysis pointing out potential water
508 quality hotspots.

509
510 The results for Europe show that future climate changes are likely to have only a small impact
511 on European in-stream concentration levels of BOD₅, except for the Eastern part and the
512 Black Sea region. In these regions, the impact on flow conditions seems to be more
513 pronounced than in other parts in Europe, leading to a potential degradation of water quality.
514 This effect is expected to be larger for the IPCM4-A2 scenario than for the MIMR-A2
515 scenario.

516
517 As a next step the model will be tested with further substances like total nitrogen and total
518 phosphorus and other scenario calculations including changing socioeconomic drivers, such
519 as treatment levels and population, which are expected to have a bigger effect on in-stream
520 water quality.

521 522 **Acknowledgements**

523
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528 of Life Sciences) and the Confederación Hidrográfica del Ebro, Zaragoza (prov. by M. Fry,
529 NERC-CEH Wallingford) for providing the in-stream water quality data for Thames, Vistula
530 and Ebro respectively used to test the model as presented in this paper. Data for calibration of
531 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
 701

COUNTRY	CONCENTRATION [mg l ⁻¹]	COUNTRY	CONCENTRATION [mg l ⁻¹]
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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 704

705 Table 2. Difference of 90-percentiles of calculated values against measured values for BOD₅
 706 in-stream concentration with regular and modified input loading [mg/l].
 707

	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

708
 709
 710
 711 Table 3. BOD₅ loadings and loading fractions 2000 for Ebro and Thames for different sectors
 712 with regular and with modified input loading.
 713

	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

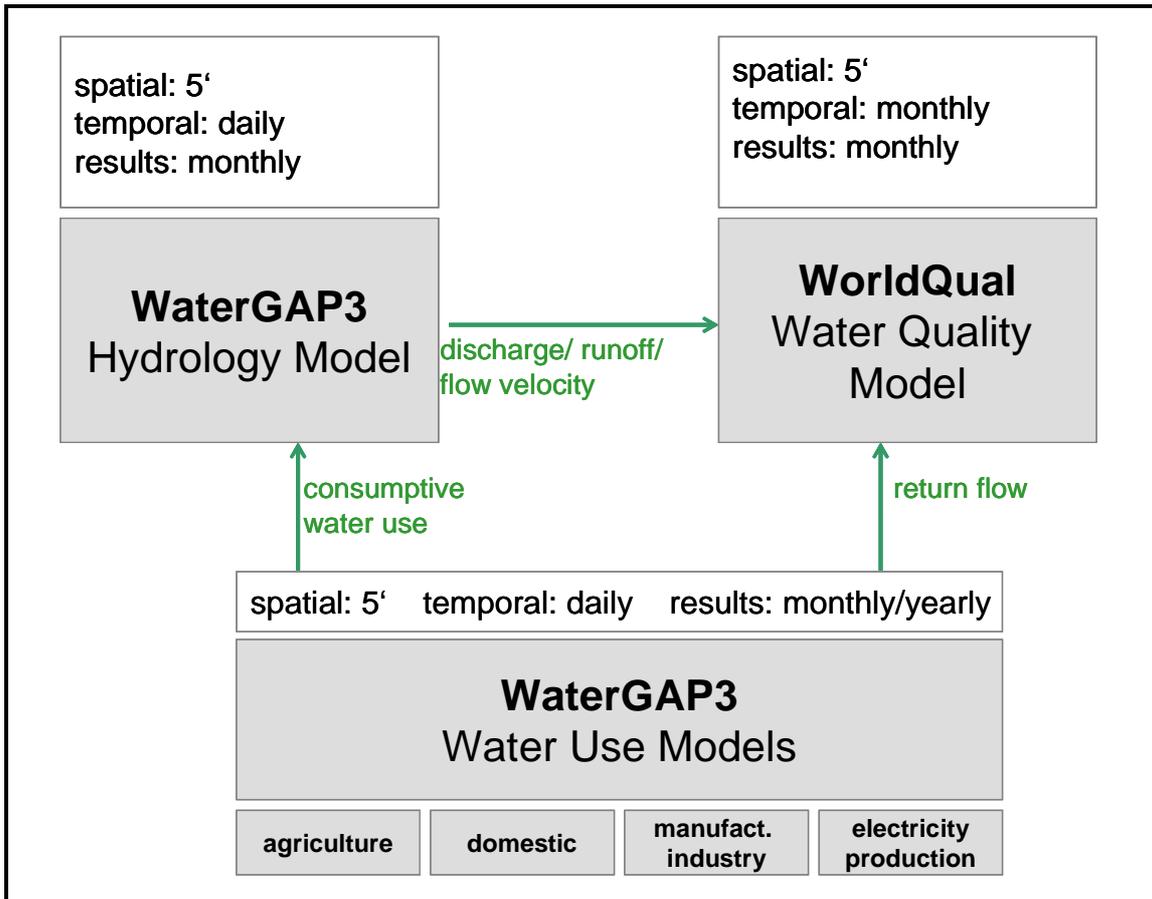
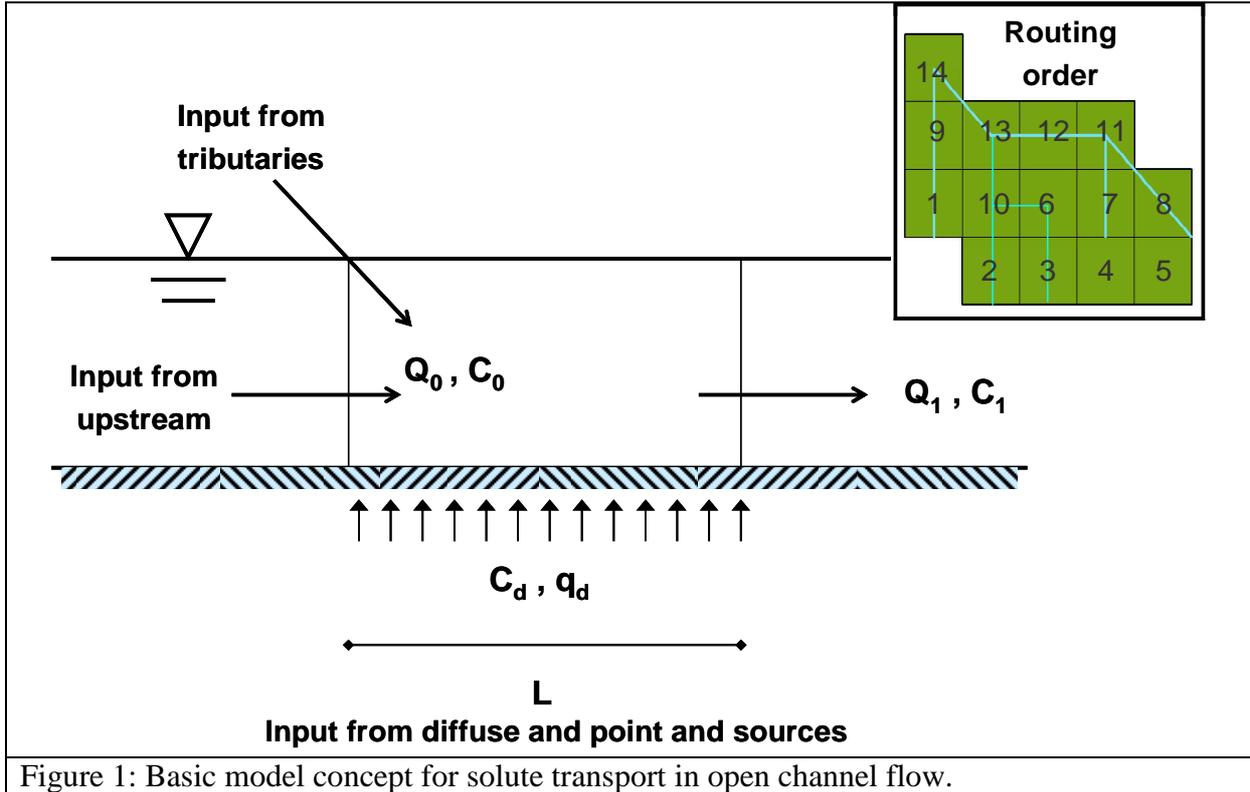
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 717 Table 4. Difference of 90-percentiles of calculated values against measured values for TDS
 718 in-stream concentration with regular and modified input loading [mg/l].
 719

	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

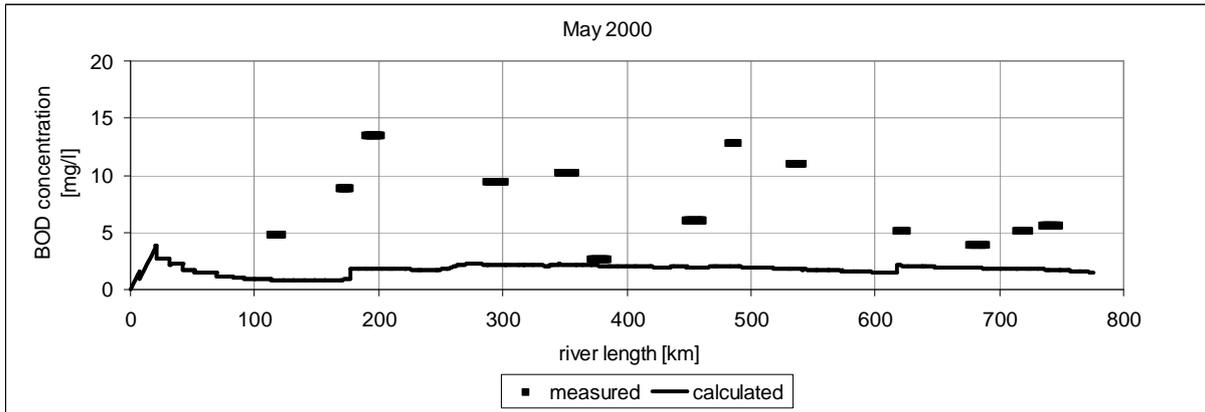
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 723 Table 5. TDS loadings and loading fractions 2000 for Ebro and Thames for different sectors
 724 with regular and with modified input loading.
 725

		industry	domestic	scattered settlements	urban runoff	diffuse	total
		Ebro - regular	[t/a]	1 201	15 075	16	2
	[%]	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

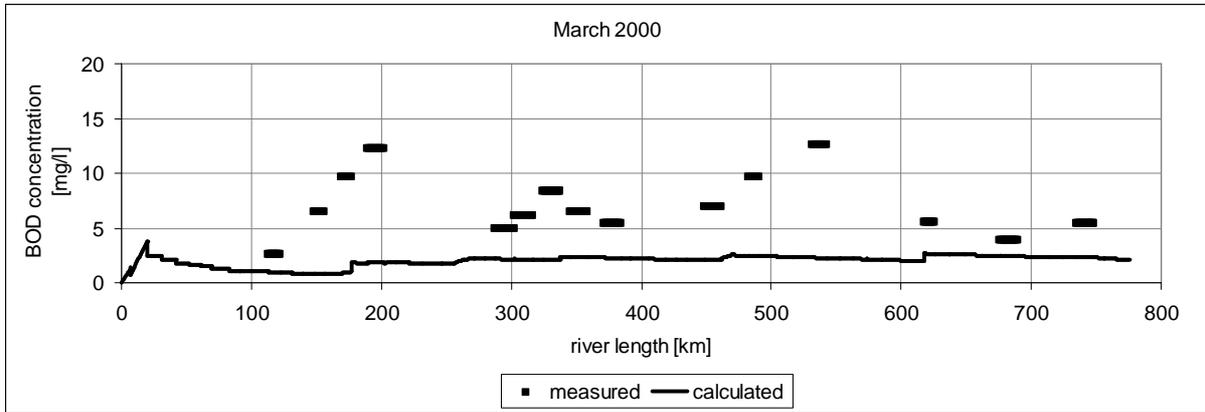
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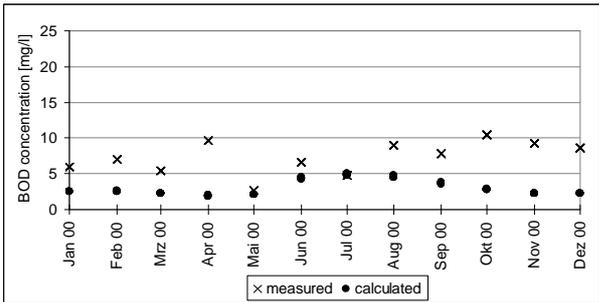
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737 (b)
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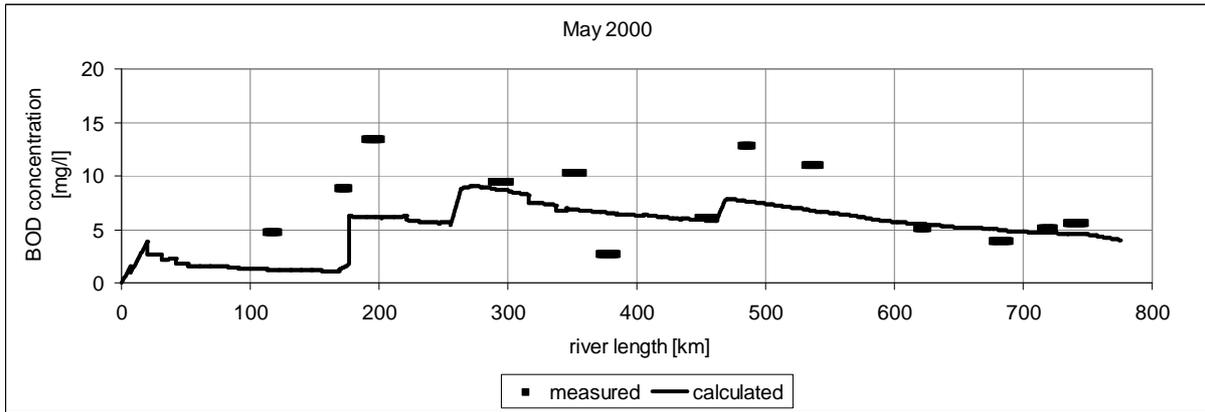
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742 (c)
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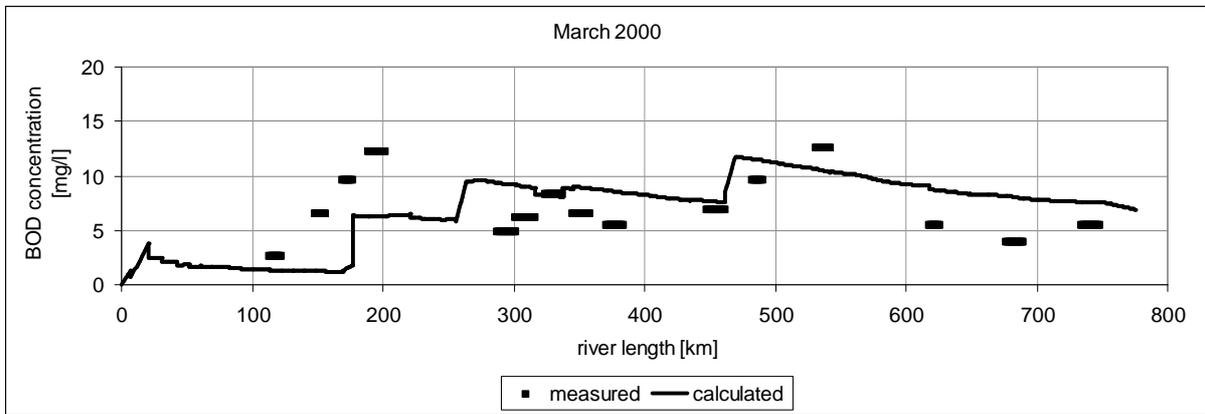
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Figure 3. BOD₅ results for Ebro River with regular input.
(a) Longitudinal profile, high flow, May 2000
(b) Longitudinal profile, low flow, March 2000
(c) Time series – middlestream

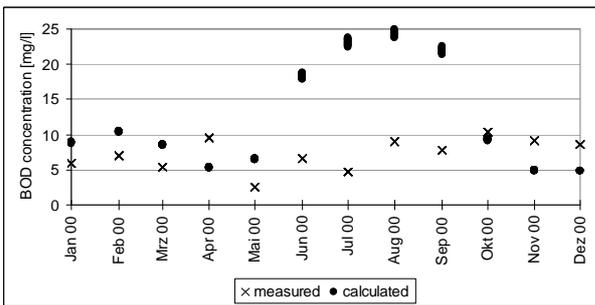
753 (a)
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760 (c)
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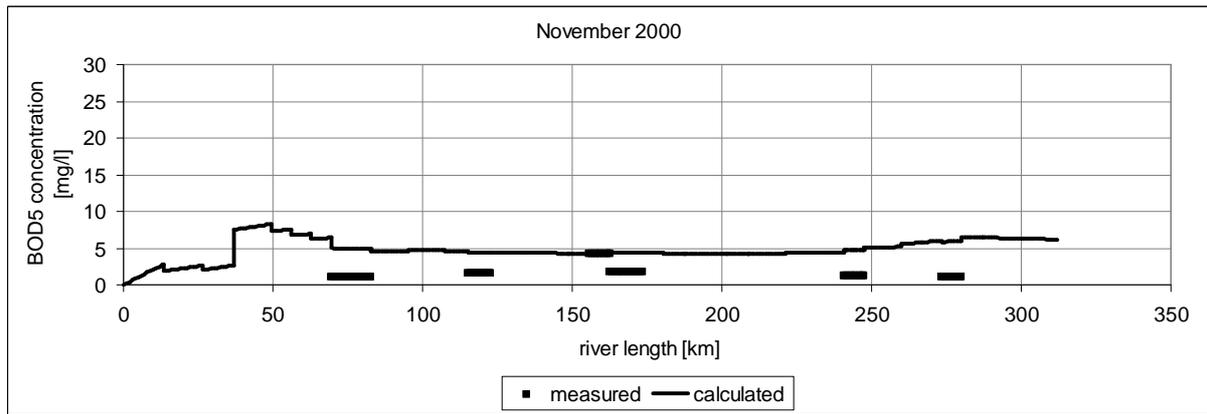


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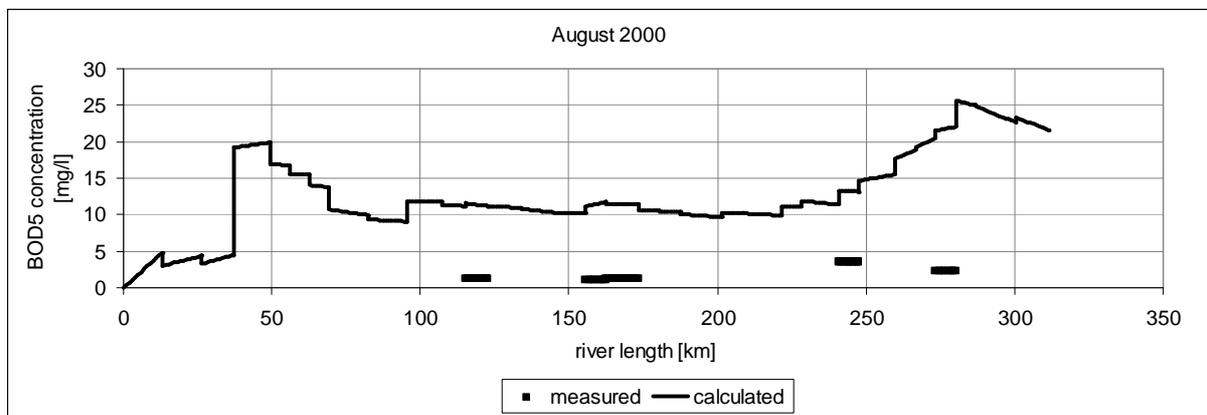
Figure 4. BOD₅ results for Ebro River with modified input.

- (a) Longitudinal profile, high flow, May 2000
- (b) Longitudinal profile, low flow, March 2000
- (c) Time series – middlestream

773 (a)
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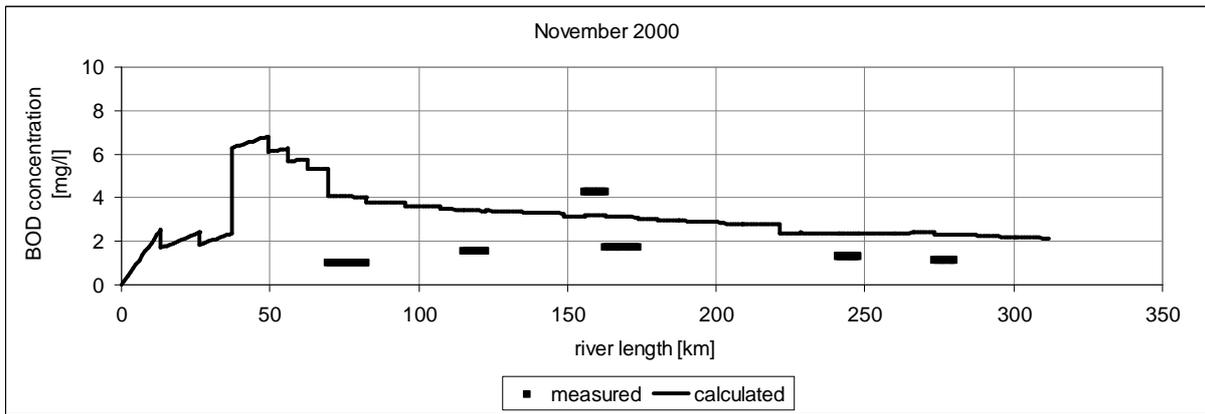
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778 (b)
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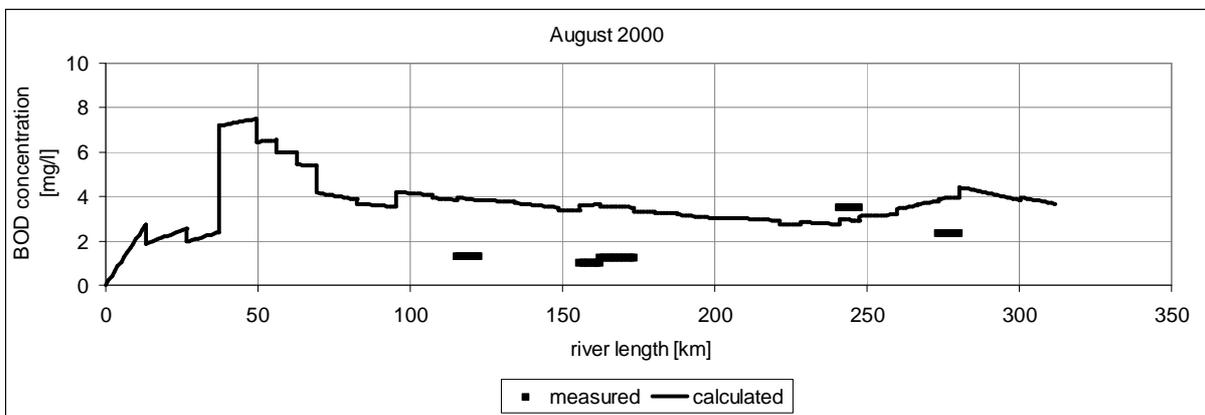
Figure 5. BOD₅ results for Thames River with regular input.
(a) Longitudinal profile, high flow, November 2000
(b) Longitudinal profile, low flow, August 2000

788 (a)
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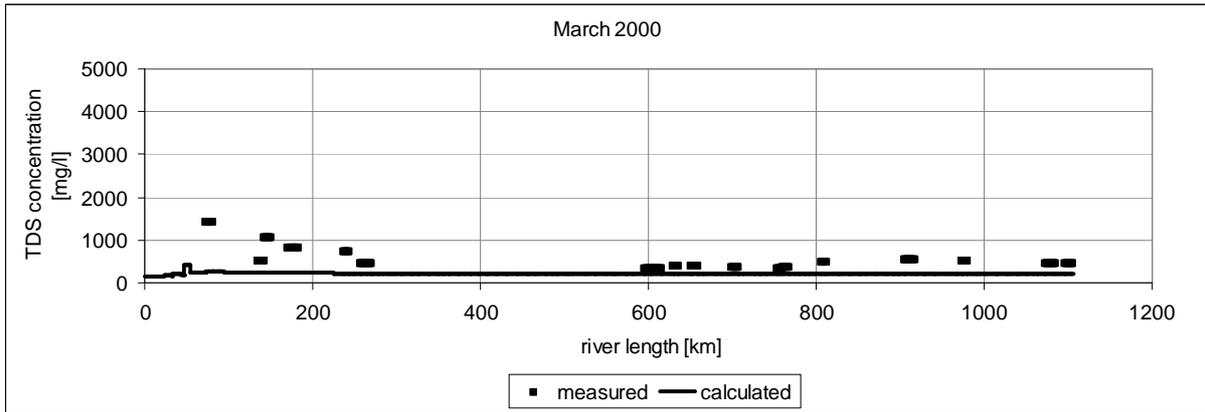
(b)



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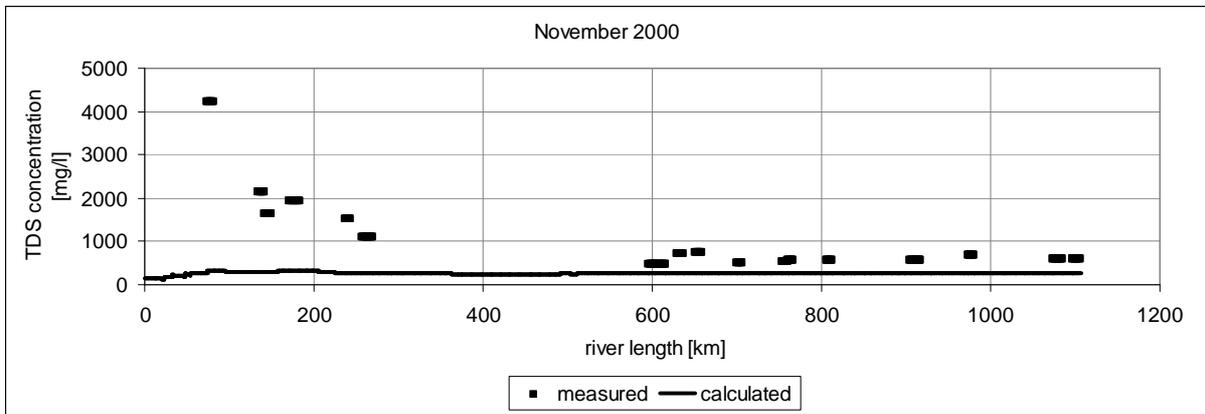
Figure 6. BOD₅ results for Thames River with modified input.
(a) Longitudinal profile, high flow, November 2000
(b) Longitudinal profile, low flow, August 2000

802 (a)
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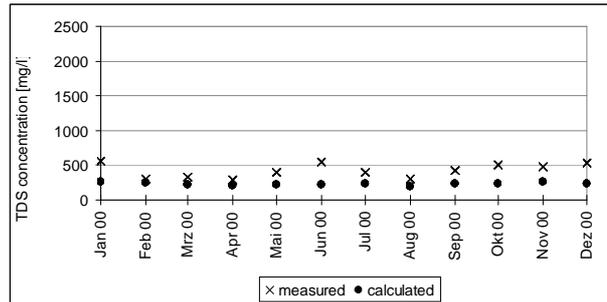
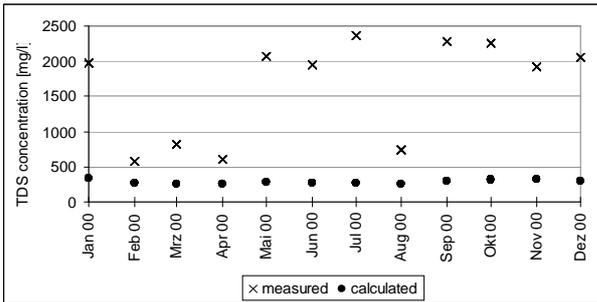
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(b)



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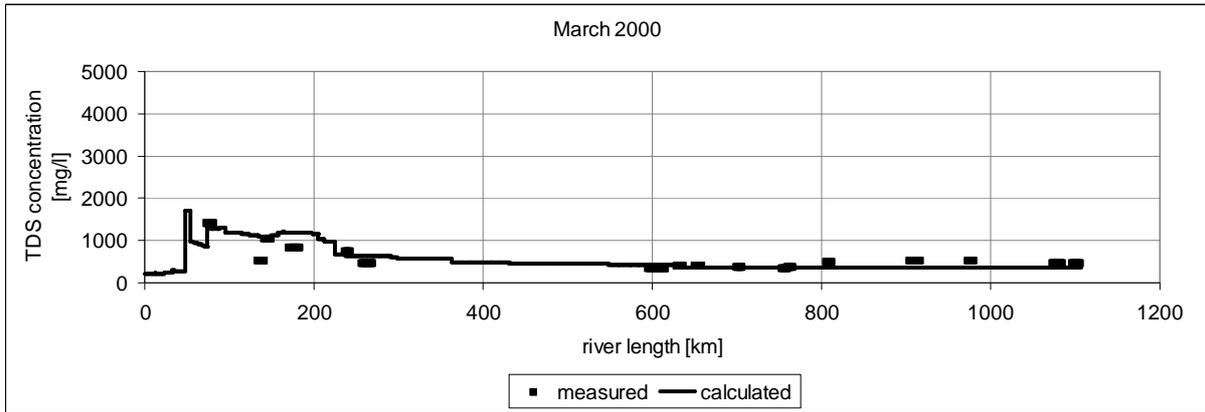
(c)



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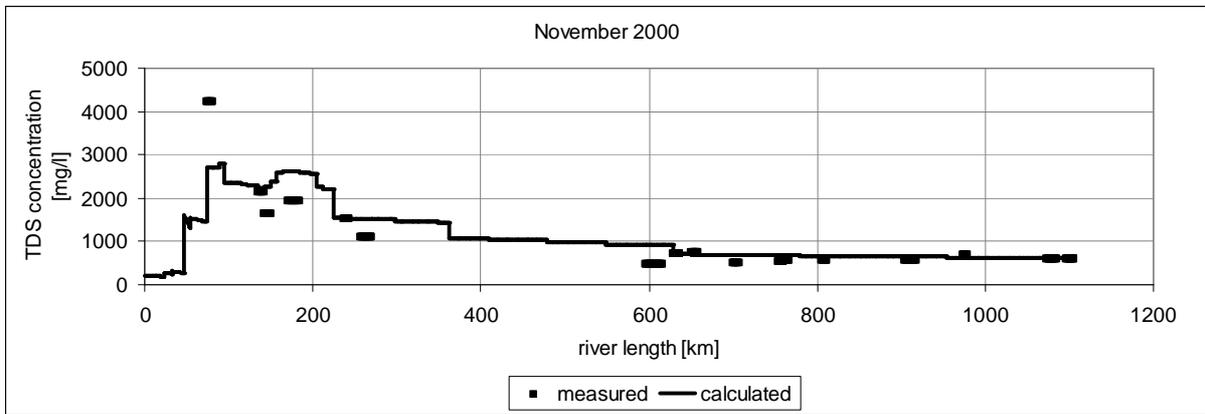
Figure 7. TDS results for Vistula River with regular input.
(a) Longitudinal profile, high flow, March 2000
(b) Longitudinal profile, low flow, November 2000
(c) Time series – upper- and middlestream

822 (a)
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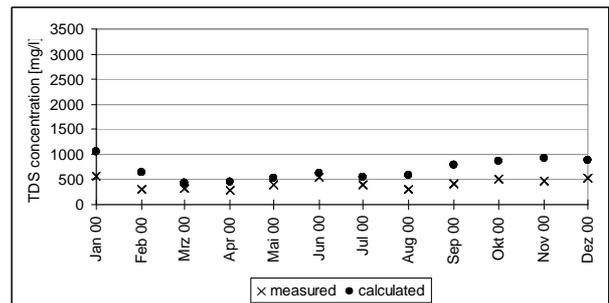
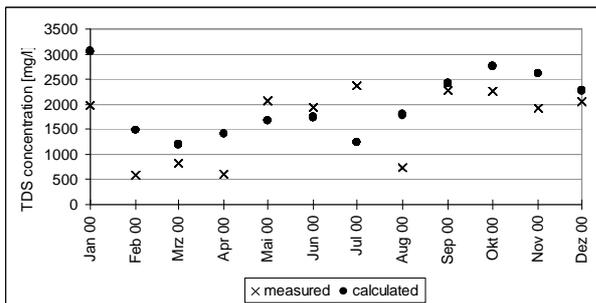
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(b)



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(c)



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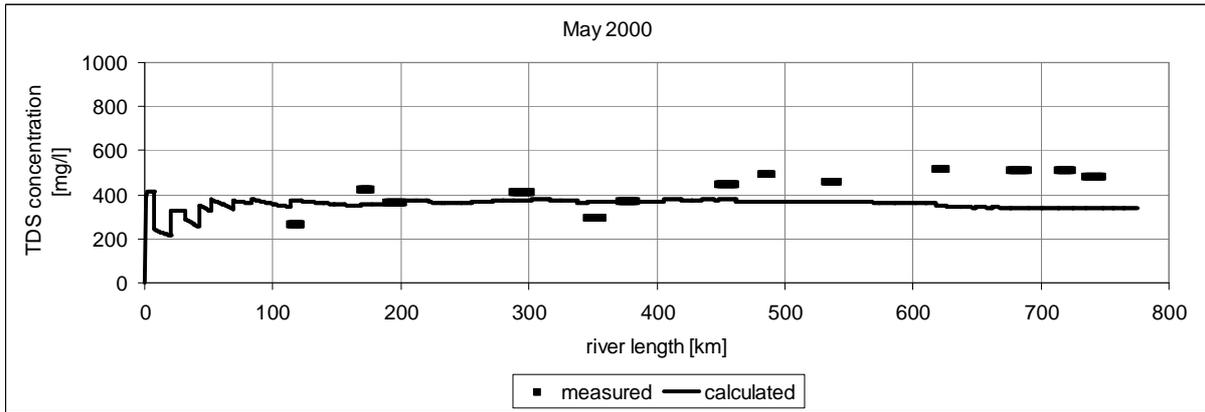
Figure 8. TDS results for Vistula River with modified input.

(a) Longitudinal profile, high flow, March 2000

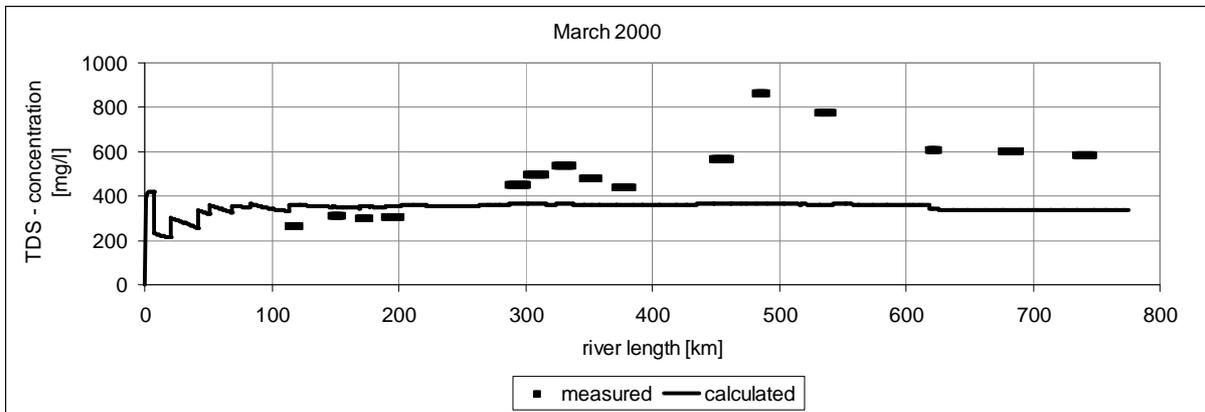
(b) Longitudinal profile, low flow, November 2000

(c) Time series – upper- and middlestream

842 (a)
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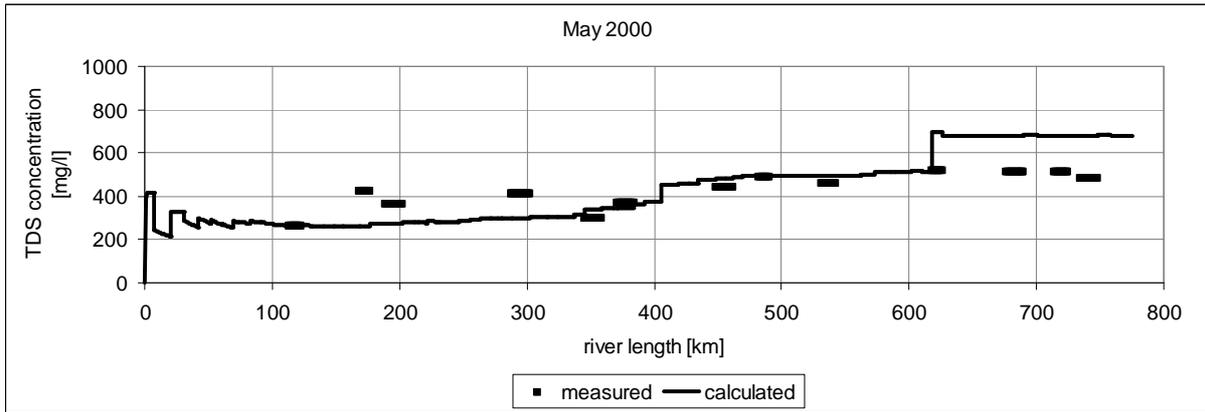


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847 (b)
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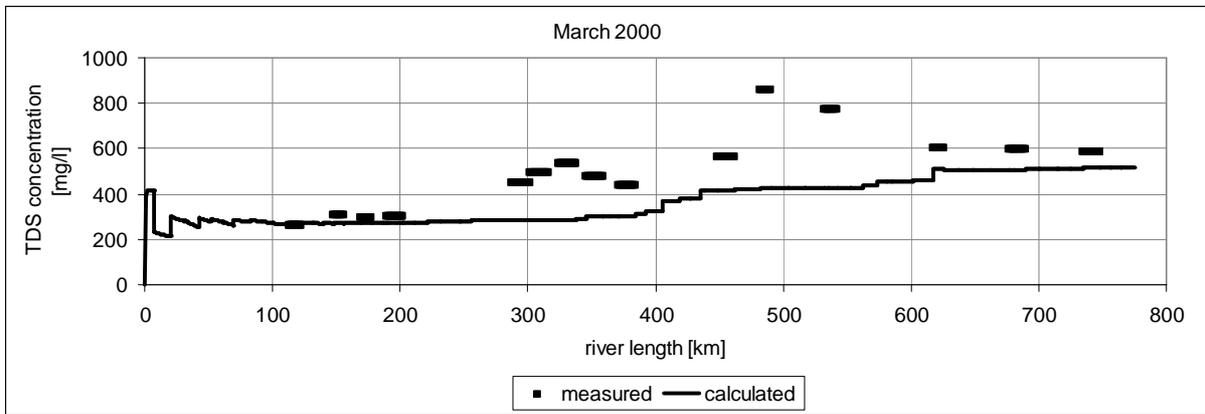


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852 Figure 9. TDS results for Ebro River with regular input.
853 (a) Longitudinal profile, high flow, May 2000
854 (b) Longitudinal profile, low flow, March 2000
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856 (a)
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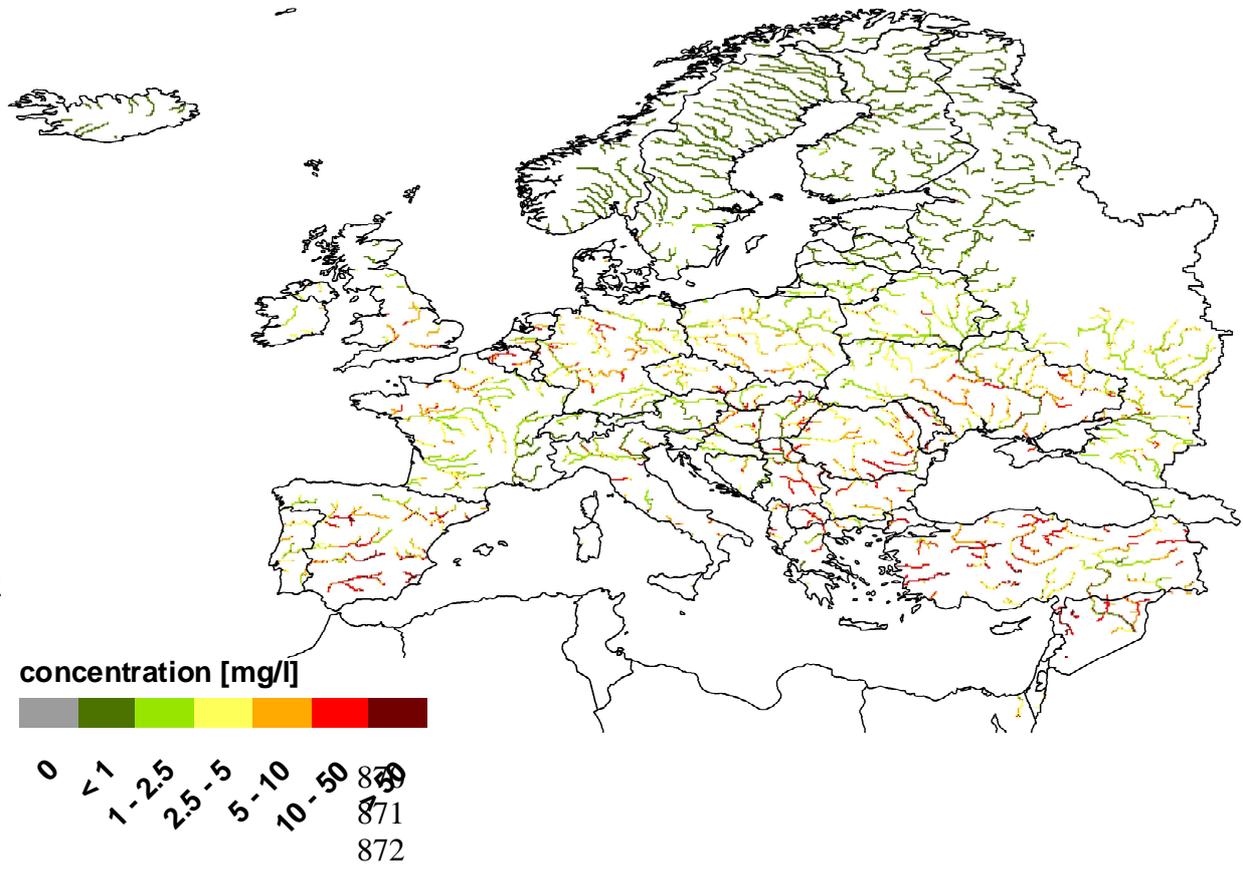


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861 (b)
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Figure 10. TDS results for Ebro River with modified input.
(a) Longitudinal profile, high flow, May 2000
(b) Longitudinal profile, low flow, March 2000

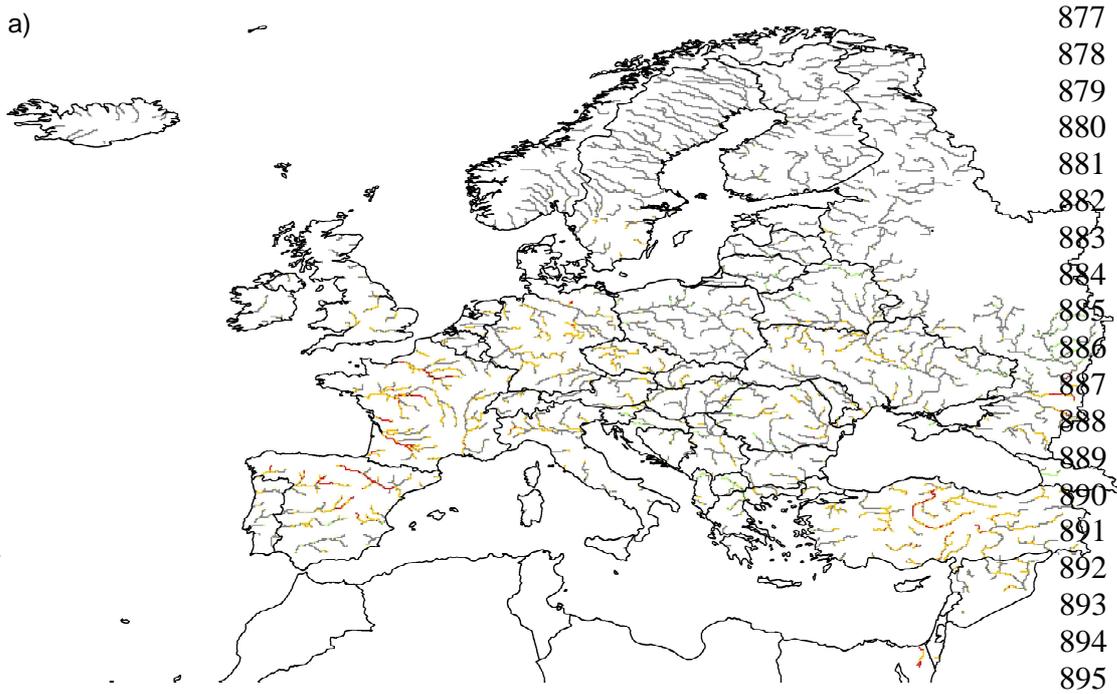


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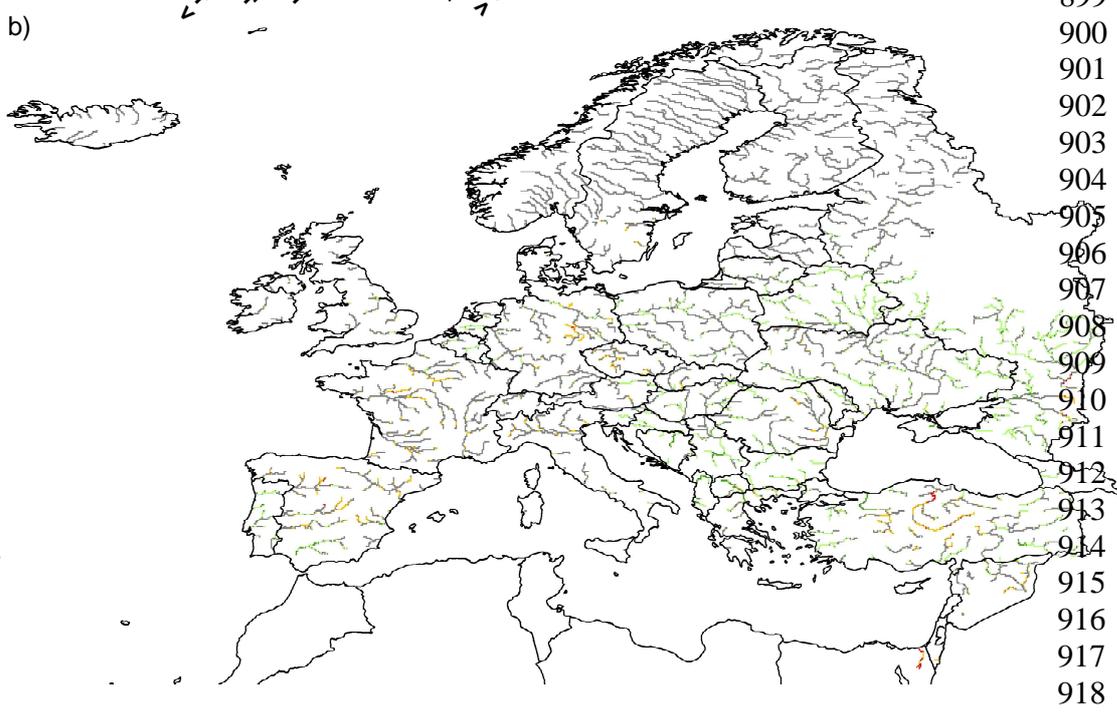
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875 Figure 11. BOD₅ in-stream concentration in Europe – Baseline July 2000s.

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Figure 12. Effect of climate change on BOD₅ 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