Article (refereed) - postprint

Williams, Richard J.; Boorman, David B. 2012 Modelling in-stream temperature and dissolved oxygen at sub-daily time steps: an application to the River Kennet, UK. *Science of the Total Environment*, 423. 104-110. 10.1016/j.scitotenv.2012.01.054

Modelling in-stream temperature and dissolved oxygen at sub-daily time steps: an application to the River Kennet, UK.

Richard J. Williams* and David B. Boorman

Centre for Ecology and Hydrology, Benson Lane, Crowmarsh Gifford, Wallingford, Oxfordshire, OX10 8BB, UK

Telephone: + 44 (0)1491 838800
Fax: + 44 (0)1491 692424
Emails: rjw@ceh.ac.uk (Williams) and dbb@ceh.ac.uk (Boorman)

*Corresponding author

ABSTRACT

The River Kennet in Southern England shows a clear diurnal signal in both temperature and dissolved oxygen concentrations through the summer months. The water quality model QUESTOR was applied in a stepwise manner (adding modelled processes or additional data) in order to simulate the flow, temperature and dissolved oxygen concentrations along a 14 km reach. The aim of the stepwise model building was to find the simplest process-based model which simulated the observed behaviour accurately. The upstream boundary used was a diurnal signal of hourly measurements of temperature and dissolved oxygen. In the initial simulations, the amplitude of the signal quickly reduced to zero as it was routed through the model; a behaviour not seen in the observed data. In order to keep the correct timing and amplitude of temperature a heating term had to be introduced into the model. For dissolved oxygen, primary production from macrophytes was introduced to better simulate the oxygen pattern. Following the modifications an excellent simulation of both temperature and dissolved oxygen was possible at an hourly resolution. It is interesting to note that it was not necessary to include nutrient limitation to the primary production model. The resulting model is not sufficiently proven to support river management but suggests that the approach has some validity and merits further development.

Keywords: Modelling, QUESTOR, Dissolved Oxygen, Temperature, Kennet.

1. INTRODUCTION

Temperature and dissolved oxygen (DO) are both fundamentally important to the biological health of rivers, and therefore to the delivery of the Water Framework Directive objectives to enhance and maintain the quality of European waters. Many species are tolerant only of specific temperature ranges (Coutant, 1977) and the River Continuum Concept (Vannote et al., 1980) states that variations in daily and seasonal water temperatures are important factors in determining the distribution of aquatic organisms. Detailed reviews of the current state of research into river temperatures has been published elsewhere (Webb et al., 2008). The specific topic of thermal regimes of rivers has also been recently reviewed (Caissie, 2006). In this latter publication, the main drivers of the thermal regime were grouped into in four classes; atmospheric conditions, topography, stream discharge and stream bed. This review also described attempts to model water temperature using regression, stochastic or deterministic approaches. Briefly, regression models usually establish a relationship with air temperature, although they sometimes also include stream flow. These models work well for monthly and weekly data, but much less well for daily data and are unsuitable for sub-daily data (Webb et al., 2008). Stochastic models usually split the modelling into two components; one for the seasonal changes and the other for short term changes, again air temperature is the usual explanatory variable. They are generally applied to predict weekly or daily temperature variations. Deterministic models are based on considerations of the energy fluxes which contribute to the heat balance of the river. They are more able than the other methods to simulating sub-daily data and can also be applied to multiple sites along river systems when incorporated into river flow models (Cox and Bolte, 2007).

Dissolved Oxygen is an important indicator of river health and used by regulators as part of the classifications for good chemical status (e.g.UK Technical Advisory Group on the Water Framework Directive, 2008). The overall level of oxygen in a river is a balance between reaeration at the water surface and loss of oxygen in satisfying chemical and microbial oxygen demands in the water column or from the river bed. Superimposed on this is a diurnal pattern due to primary production and respiration of green plants either fixed to the bed or floating in the river (Edwards and Owens, 1965; O'Connor and Di Toro, 1970; Odum, 1956). This pattern can be enhanced by the temperature dependence of some of the processes involved in the DO cycle (Loperfido et al., 2009). All these processes have been included in models (reviewed in Cox, 2003b) and many models have been developed based on these methods (reviewed in Cox, 2003a).

Despite this long-standing theoretical understanding of the diurnal DO curve, there have been relatively few published papers describing modelling of short term DO variations. Studies have looked at using models to derive rates of photosynthesis, respiration and reaeration by fitting models to diurnal DO curves (Chapra and Ditoro, 1991; Hornberger and Kelly, 1975; Williams et al., 2000). A later modelling study using QUAL2E found that a dynamic simulation of DO diurnal variation in the River Oona in Northern Ireland gave good agreement on pattern and timing but over predicted the amplitude of the signal (Shi et al., 2003). A study of the South Umpqua River, Oregon, USA used the QUAL2Kw model to set nutrient limits necessary to manage diurnal variations in pH and DO (Turner et al., 2009). Another recent study used a modification of the model of Butcher and Covington (1995) to investigate the controls on reaeration and net primary production by examination of diurnal DO signals combined with diurnal temperature patterns (Loperfido et al., 2009).

In this paper the model QUESTOR (Boorman, 2003b) is applied in a stepwise manner (process complexity and additional data were added sequentially to the model) to simulate the flow, temperature and DO concentrations along a stretch of a chalk stream in Southern England. As will be seen, a clear diurnal pattern was observed at both ends of the model reach; the aim of this study was to test whether this signal was propagated through the study reach, or whether in-stream processes were required to maintain this variability.

2. METHODS

2.1 Study Site

The Kennet is a tributary of the River Thames that flows for 40 km from Avebury in the west to its confluence with the Thames at Reading in the east. The catchment area above the confluence with the Thames is 1200 km^2 (Neal et al., 2000), comprising permeable Chalk (80%) with rural headwaters, but with some urban development along the valley. The mean daily flow at the lowest downstream site (catchment area 1033 km^2) is 9.65 m^3/s and on an annual basis river flow accounts about 38% of the catchment rainfall (Marsh and Hannaford, 2008).

This study focuses on the upper Kennet from Clatford just north of Marlborough to the Environment Agency gauging station at Knighton some 14 km downstream

(Figure 1). This section of the river has received extensive study related to monitoring the effects of fitting phosphorus removal technology to the sewage treatment plant (STP) at Marlborough (Jarvie et al., 2004; Neal et al., 2000; Wade et al., 2002). This is the only STP that discharges to the study river section over which mean flow increases from 0.87 m^3/s at Malborough to 2.56 m^3/s at Knighton with two significant tributaries, the River Og and the River Aldbourne with mean flows of 0.31 m^3/s and 0.21 m^3/s respectively (Marsh and Hannaford, 2008).

Figure 1

The general water quality of the River Kennet has been discussed in detail elsewhere (Jarvie et al., 2002; Neal et al., 2000; Neal et al., 2002a) and only a brief overview is given here. The river water quality is of a typical calcium bicarbonate type because of the high base flow contribution from the calcite rich Chalk. The soluble reactive phosphorus is typically 80 μg P/l rising slightly below the Marlborough STP to about 100 μg/l (this value was about 500 μg/l before the start of P removal from the effluent (Neal et al., 2010)). Nitrate values decline along the study reach from about 28 mg NO_3/l to 18 mg NO_3/l. Dissolved oxygen values are on average around saturation but there is a considerable daily fluctuation from around 50% saturated in the morning to 140% saturated in the evening (Neal et al., 2002a; Williams et al., 2000). This variation is particularly noticeable during the summer when biological activity is high. Daily temperatures show a similar variability and values are between 10 and 19 ºC during the summer and between 5 and 10 ºC in the winter.

Flynn et al. (2002) describe the macrophyte and periphyton characteristics of a 50m reach of the River Kennet within the study area. They note that macrophytes, mainly *Ranunculus*, dominate during the spring and summer months in terms of biomass, with periphitic communities becoming relatively more abundant in the autumn. This is explained by the *Ranunculus* being able to re-grow early in the season from its perennial root system, whereas periphytes take longer to re-establish.

It should be noted that the Kennet is a highly managed river with river levels maintained by a series of weirs and sluice gates and in-stream and bank-side vegetation cut, with the primary aim of providing a recreational fishery.

2.2 Water Quality Data used for modelling

For the purpose of this study the important data were DO and temperature data collected at 15 minute intervals. These data were electronically logged using a "Hydrolab" multiparameter water quality monitoring system (Omnidata Systems Ltd, UK). Dissolved oxygen was determined by a Clark-type sensor with a highly sensitive gas transfer membrane. Temperature was measured using a thermistor. Two systems were used alternately in the field. These were interchanged at weekly intervals after cleaning and recalibration. Full details of the procedures used are given by Neal et al (2002b).

2.3 Description of Model

The modelling software used for this study was QUESTOR (Eatherall et al., 1998) which provides the modelling framework for a one dimensional in-stream water quality model. The model can be tailored or developed to suit the application, for example, by changing the modelled variables or the algorithms by which processes are represented. The basic version models flow, ammonium, ammonia, nitrate, pH, DO, biochemical oxygen demand and any additional conservative determinands (Boorman, 2003b). Because of the need within this study to model within-day changes of DO and temperature, an enhanced version of the QUESTOR model was used that was developed for an European Commission funded project CHESS (Boorman, 2003a). The principle additions were the inclusion of primary production and heat transfer sub-models (Boorman, 2003a).

The algorithms used to represent the modelled determinands are similar to those used in a number of in-stream water quality models. They represent the dominant processes affecting the determinands modelled but include empirical terms and coefficients that must be set by calibration. The full set of equations used within the basic QUESTOR model is given elsewhere (Boorman, 2003b; Eatherall et al., 1998), so only those pertinent to the modelling of DO and temperature will be given here.

Within QUESTOR the river is divided into a number of reaches from the upstream boundary to the end of the modelled section. The initial selection of reaches is based on the location of confluences, diffuse (catchment) sources, discharge points, abstraction points, monitoring sites, and weirs. Once this has been done, long reaches, say those greater than 10km, can be sub-divided. The flow out of a reach is calculated based on a mass balance of river flows into the head of the reach plus contributions from point sources and diffuse sources minus abstractions (equation 1).

$$\frac{dQ}{dt} = \frac{Q_i - Q}{\tau\,(1 - c)} \qquad \text{Equation 1}$$

where, Q is the flow out of the reach (m^3/s), Q_i is total flow into the reach (m^3/s), t is the time (days) and τ is a time constant representing the average retention time in the reach given by $L/(bQ^c)$, L is length of reach (m), b and c are constants. For chemical determinands a mass balance is also performed for a reach, but there are additional terms to allow for removal or generation of the chemical species within the reach and its interactions with other determinands.

The heat model used within QUESTOR is driven by measured incoming solar radiation and an outgoing radiation flux based on water body temperature.

$$\frac{dT}{dt} = \frac{1}{\tau}(T_i - T) + k_i R_s - k_o (T + 273)^4 \qquad \text{Equation 2}$$

where T is the temperature of the out flowing water (^oC), T_i is the temperature of the water inputs (^oC), k_i is an incoming radiation factor, R_s is the incoming solar radiation (W/m^2) and k_o is an outgoing radiation factor.

For DO equation 3 was used in which DO is the DO concentration leaving the reach (mg/l), DO_i is the input DO concentrations (mg/l), W is the aerating effect of a weir (calculated from an empirical relation based on weir type and drop), P is the increase in DO from photosynthetic processes (mg/l), R is the loss of DO due to respiration (mg/l), k_{ben} is the benthic respiration rate (1/day), d is the mean depth of the reach (m), k_{rea} is the aeration coefficient at the water surface, dependent on flow velocity, depth and temperature, OCS is the DO concentration at saturation, dependent on temperature (mg/l), NH_4 is the concentration of ammonium in the water column, k_{nit} is the rate parameter for complete nitrification (1/day) which is multiplied by a factor to account for the stoichiometry of the reaction, BOD is the biochemical oxygen demand of the water column (mg/l) and k_{bod} is the rate parameter determining the loss of DO as biochemical oxygen demand decays.

$$
\begin{aligned}
\frac{d\,DO}{dt} = \; & \frac{1}{\tau}(DO_i - DO + W) && \text{transport} \\
& + P - R && \text{net contribution from primary production} \\
& - k_{ben}\, DO/d && \text{benthic oxygen demand} \\
& + k_{rea}\,(OCS - DO) && \text{reaeration at surface} \\
& - 4.57\, k_{nit}\, NH_4 && \text{nitrification (DO > zero)} \\
& - k_{bod}\, BOD && \text{loss due to BOD}
\end{aligned}
\qquad \text{Equation 3}
$$

Rates of respiration and photosynthesis are based on equations in the form

$$P_i = Biomass_i MaximumGrowthRate_i \; LimitingFactor_i \qquad \text{Equation 4}$$

and

$$R_i = Biomass_i MaximumGrowthRate_i RespirationFactor_i \qquad \text{Equation 5}$$

in which the subscript *i* refers to the different primary production communities. The model can represent three such communities, i.e. macrophytes, benthic algae and phytoplankton, and each of these differs in the way in interacts with its environment (Table 1). Examples of these differences are: macrophytes and benthic algae are not transported through the channel, whereas phytoplankton are; benthic algae and phytoplankton obtain nutrients from the water, whereas macrophytes can also use nutrients in the river bed; and the light conditions relate to different parts of the water column, and the air above it.

Limiting factors in the photosynthesis equation are based on the assumption that the maximum growth rate can only be achieved under optimal conditions of nutrient availability and lighting. For nutrients, i.e. nitrogen and phosphorus, it is assumed that as the nutrient concentration decreases so does the growth rate, whereas for light it is assumed that both more and less than an optimal value will limit growth. Of course primary production can itself change the light regime: for example, emergent macrophytes can shade the whole water body, while phytoplankton can limit light penetration through the water column. Temperature also influences both photosynthesis and respiration.

The other quantities required in equations 4 and 5 are the biomasses of each community. Accounting for biomass requires not only estimates of photosynthesis, respiration, and where appropriate transportation, but also an estimate of the death rate for each community. The model assumes that the death rate is also represented by the limiting factors, i.e. as the limiting factors approach zero the death rate increases.

Of course modelling primary production processes and communities is not just a question of representing the effects on DO. The growth requires nutrients which must be taken up and returned to the water column or bed, as appropriate, and death of organic plant matter contributes to the BOD.

It should be clear that to include primary production in a realistic way introduces a great deal of complexity to the basic water quality used within QUESTOR. Because of this complexity some in-stream water quality models, such as QUASAR (Whitehead et al., 1997), which was the starting point for the development of QUESTOR, estimate photosynthesis and respiration based on pre-defined values of biomass, as represented by Chlorophyll-a concentration.

Problems of complexity also meant that in developing a biomass growth model for the CHESS project as referenced above, it was not possible to make a realistic implementation of the complete primary production model outlined above because insufficient data were available to attempt calibration and validation. Instead the model was used in an indicative way to show how algal blooms may change under possible future climatic conditions (Boorman, 2003c). However, the CHESS implementation of the QUESTOR model has recently been tested and applied to investigate methods to suppress phytoplankton blooms in the River Ouse and this has increased confidence in the model equations (Hutchins et al., 2010).

The sub-daily data available for the River Kennet allows some testing of the model formulated within the CHESS project, although as will been seen this is limited to supporting the general approach rather than an attempt at validation. The approach adopted was to simulate in turn flow, temperature and DO. At each stage the questions to address by comparing model simulations with observed data are:

Are model inputs adequately described?

Are errors in the simulation random effects or systematic?

Are model simulations improved by adding additional processes?

2.4 Boundary Conditions, Inputs and Model Parameter Values

The model was run for the period 1 July 1998 to 31 December 1999 for the stretch of river from Clatford to Knighton. Hourly flow data were available for the gauging station at Marlborough just downstream of Clatford (Figure 1) and this was used as the input to the upstream end of the model. Hourly data were also available for the River Og, River Aldbourne and the Marlborough STP. Flow data for the same time period were also available close to the end of the modelled section (Knighton, Figure 1), which allowed the flow balance to be checked, and a check to be made on the dynamic response of the simulations.

Hourly average data for DO and temperature were obtained from the 15-minute Hydrolab data at Clatford and these was used as the model input data. Water quality data for all the other inputs along the modelled reach were also interpolated to give data at hourly intervals. The DO and temperature output from the model could be compared with observed Hydrolab data at Mildenhall just downstream of

Marlborough STP and at Ramsbury upstream of Knighton. Solar radiation data were available from a solarimeter placed adjacent to the Hydrolab at Mildenhall.

3. MODEL APPLICATION AND RESULTS

3.1 Flow

The first stage in the model application was to represent flow. An initial model used measured flows from the tributaries and discharges as inputs; there were no significant abstractions to include. The three tributaries represent the Rivers Kennet, Og, and Aldbourne. The last of these enters the Kennet just above the flow gauging station at Knighton, which was used to assess model performance. The success of a model of this type depends both on the calibration of the flow routing parameters, and on the proportion of the total inflow to the river that is represented by the measured inflows. The resulting simulation indicated that there was a significant underestimation of the flow at Knighton.

Examination of the catchment areas contributing to the measured tributary inflows suggested five additional surface water tributaries should be added. The flows from these were scaled from the closest gauged tributary using the ratio of the topographic catchment areas. Including these tributaries improved the flow simulations but there remained an underestimation throughout the modelled period of approximately $1m^3/s$. The difference was ascribed to a direct groundwater contribution along the length of the modelled river stretch. Ten identical groundwater elements were added along the modelled river, each making a flow contribution that has an annually variation from

0.08 m^3/s in October and November to 0.15 m^3/s in February. The inclusion of these additional flow elements and calibration of the flow routing parameters resulted, in an excellent flow simulation at Knighton (Nash-Sutcliffe efficiency of 0.99).

3.2 Temperature

For those tributaries with observed flow data, temperature data were also available. These data were also used to represent the temperature of the ungauged tributaries. The groundwater flow elements were assumed to be at a constant temperature of 10^{o}C, the approximate average of shallow groundwater in temperate regions such as the South of England (Hellawell, 1988; Schurch and Buckley, 2002). With the inputs described in this way the model was run assuming that heat was conservative.

The resulting model simulations showed that the diurnal variations present in the input at the top of the river had been reduced as the simulation progressed downstream, and by the end of the modelled stretch had gone. This is in contrast to the clear diurnal signal seen in the observed data at Ramsbury, the lowest site on the river for which hourly temperature data were available (Figure 2). The observed data revealed that the amplitude of diurnal variation was not constant, and also that there was some variation of the baseline temperature.

Figure 2

These problems were resolved by including the heat model described above. This required radiation data, which were available from a site adjacent to the river at Mildenhall for the periods July 1998 to March 1999 and May 1999 to September

1999. The model required the calibration of the incoming radiation factor, k_{in} and the outgoing radiation factor k_o (Equation 2) that control the gain and loss of heat. The simulation achieved by this model was remarkably good, with the variability of diurnal variation and change in baseline being very well represented (Nash-Sutcliffe efficiency = 0.85). This is illustrated for July 1999, shown in Figure 2, which shows the clear signal of the radiation, and its variation on an hourly and daily basis, in both the simulated temperature and the observed data.

3.3 Dissolved Oxygen

In the initial model of the River Kennet in which no primary production and consequent respiration is included, DO is only affected by the exchange of oxygen across the water surface. This process drives DO towards 100% saturation. As with temperature, the boundary conditions at the top of the modelled reach led to a simulation in which the initial diurnal variation in dissolved oxygen was reduced as the simulation progressed downstream, and aeration introduced only minor changes in DO. The observed data revealed that diurnal variations occurred throughout the network, and again implied an inadequacy in the model.

Primary production is an obvious process that could cause the type of observed variation in DO. It is known to occur within the real river, yet is not included in the model. The above description of the primary production model in QUESTOR noted that to include a realistic model introduces a great deal of complexity. The simplest form was to introduce a submerged macrophyte model with no transport, no nutrient limitation (i.e. the supply of nutrients from the bed is taken to be plentiful), and dependent on mean temperature and light conditions. Phytoplankton and algae continued to be excluded from the model. Macrophyte growth is known to occur throughout the modelled river stretch (Flynn et al., 2002) and this group drives the diurnal DO pattern for the River Kennet (Williams et al., 2000). Introducing even this simple model required many parameters to be set, but after some trial and error, a parameter set was found that gave excellent DO simulations. This is illustrated in Figure 3 for July 1999 which also shows that the observed DO appeared to drift from July 8th until it was reset on July 15th. During July, the model suggested that there was an increase in macrophytes of about 10%. The growth rate is seen to be driven by the radiation, with days of high and low productivity corresponding to high and low radiation inputs.

Figure 3

Because of the form of the equations 4 and 5 which control the primary production, the maximum growth rates, respiration factors and light factors values calibrated will depend on the biomass in the system, which in this case it not known. The biomass was set to an arbitrary figure and therefore, the model parameters, which were calibrated only against the DO concentrations, are themselves arbitrary. But the modelling demonstrates that primary production is an important process in maintaining the diurnal oxygen cycle along the river reaches, and that a set of model parameters can be found to match the inputs required to maintain the observed pattern. Given a set of observed macrophyte data along the river reach, this model could be parameterised to reproduce firstly macrophyte growth and then secondly the DO diurnal concentrations and these parameters would be better constrained and perhaps open to physical interpretation.

4. DISCUSSION

A model has been implemented on the River Kennet that reproduced the flow, temperature and DO during a short period for which hourly data were available to drive the model and to assess its simulations. Certain components of this model have been widely used in previous applications and have been found to be reliable and robust in application (e.g. flow routing and aeration). This prior use may give some confidence in the further use of the model. However, as noted previously (Anderson and Bates, 2001; Boorman et al., 2007; Oreskes et al., 1994) such model applications should not be considered as validation of the model, but as a failure to invalidate it.

Other aspects of the model have been used, tentatively, in previously model applications but without data to support their formulation or outputs. The data for the River Kennet provided some opportunity to explore the usefulness of the model to reproduce observed variations in temperature and DO. The step-wise approach to model building was based on a progression through the three variables, flow, temperature and DO, with complexity only being introduced to address shortcomings in the model simulations. However, the particular ways in which these problems were addressed were not the only available options and reviewing the alternatives is necessary.

The initial flow simulations were found to underestimate the observed flow throughout the year. This points to a problem with the data, rather than model, since there is no possibility to create water within the model. The underestimate was corrected by adding additional surface and groundwater contributions. The assumption in doing so is that all of the measured data are generally correct, and that the difference is the result of unmeasured contributions. While it is always wise to consider if the data used as model inputs are correct or not, it is more sensible to assume that, in the absence of other indications, all data are generally correct, rather than that any one data set contains all of the errors.

However, it is easy to explore the alternative explanation, i.e. that one or more of the flow data sets are incorrect by progressing to the temperature and DO modelling without the extra surface and groundwater elements. This assumes that the input data are good but that the data from the downstream site at Knighton are wrong, and reduces the flow throughout the entire river. In such a model there remains the same problem with the temperature simulation (i.e. no diurnal variation after the first few reaches). A reasonable conclusion is that introducing the additional flow elements has not in itself led to the requirement to improve the simulation of temperature. So regardless of the action taken in response to the flow underestimation, there is the same need to improve the model's simulation of temperature.

To improve the temperature simulation a solar heating module was included that estimated heat gain from a local measurement of incoming solar radiation. This model proved very effective in estimating the diurnal temperature variation, and the longer term variability. An alternative method of introducing this sub-daily variability would have been to change the temperature of the flow inputs on an hourly basis. As noted above, to effect a correction throughout the whole network this would have to be made to the groundwater inputs, yet evidence suggests they should be reasonably uniform throughout the year (Hellawell, 1988)

Once the temperature simulation was improved attention turned to DO. A realistic simulation of diurnal variation of DO was achieved through the introduction of primary production. Without the primary production model the only sub-daily variability comes from the aeration at the river's surface, which drives the DO content towards 100% saturation. The DO concentration corresponding to saturation is temperature dependent, with, over the normal range of temperatures found in UK rivers, higher saturation concentrations occurring at lower temperatures. Thus as the water temperature varies so does the DO concentration, with lower DO corresponding with higher temperature. Parameters in the model limit the rate at which this progresses and in fact the simulated variation in percentage saturation is from 89% to 103%.

It is interesting to compare the macrophyte growth model approach developed in this paper with the regression modelling of Flynn et al (2002). In the latter, regression equations were developed using a number of environmental variables (flow, radiation, sediment and phosphorus concentration) to predict the variability in different measures of the macrophyte and periphyton communities. The best regressions, in terms of highest R^2, linked biomass to flow rate (inversely) and *Ranunculus* growth to net solar radiation. Including measured soluble reactive phosphorus and suspended sediment did not add to the predictive ability of the regression models. Both of these independent variables (flow and radiation) are very much seasonal indicators, and highly correlated. In developing the macrophyte growth model in this application, radiation was also found to be essential, and the assumption of a plentiful nutrient supply, i.e. there was no need to include a nutrient limitation term in the model, is supported by the regression modelling.

It is interesting that nutrient limitation was not required in the simulation model. As described earlier the model code included nutrient limitation, but it wasn’t necessary to enable this addition complexity. This could be because the assumption that the primary production is mainly by macrophytes and that they have access to limitless, or renewed, nutrient resources is valid. but it may be the case that nutrient limitation was not important, but that this is the case only for the limited period of this simulation. Understanding this is crucial for river management since there is a widespread assumption that primary production is highly dependent on nutrient availability, and can be controlled by managing nutrient input to rivers, from both point and diffuse sources.

While the above discussion makes the case that better process representation is the most reasonable way of explaining and improving the model’s representation of the real system it does not justify the exact form of the final model, or provide model parameters, that might be used elsewhere. The final form of the model as used in this study was the form that was just complicated enough to represent the available observed data. Considerable investigative fieldwork prior to an additional monitoring campaign would be required to justify it. For example, what evidence can be found to justify the added groundwater flows and their temperature regime; what programme of biomass sampling could be instigated to inform the macrophyte growth modelling (e.g. extending the sampling approach of Flynn et al (2002) from one site to the entire reach); and what data would help explore the issue of nutrient limitation.

Some of these issues have been investigated in recent work with the QUESTOR model which suggests that the algal growth model can reproduce observations in the River Humber, UK (Hutchins et al., 2010); this supports (or at least does not invalidate) a different part of the primary production system of equations proposed. However, the work on the Humber, like that on the Kennet, uses available data opportunistically, and again highlights the need for purpose-specific data gathering.

It is useful for water quality models to be able to simulate the diurnal pattern of oxygen and temperature variations in rivers, because biological systems are sensitive to these two factors. Concentrations of DO can go from levels that would qualify them has high quality water to levels that would be low quality waters within the space of one day (Neal et al., 1998; Williams et al., 2000). In the future it is possible that climate change will increase river temperatures, decrease the general levels of DO in rivers (Cox and Whitehead, 2009; Johnson et al., 2009; Whitehead et al., 2009) and increase phytoplankton levels (Hutchins et al., 2010) thus making the diurnal DO minima and the temperature maximums potentially even more important to understand. These diurnal changes could be controlled by light (Loperfido et al., 2009) or by nutrient levels (Turner et al., 2009), appropriate use of models can provide information for river basin managers on which is appropriate in any given situation.

5. CONCLUSIONS

The QUESTOR model has been applied to the a 14 km stretch of the River Kennet in a stepwise manner in order to achieve good quality simulation of the observed diurnal patterns of temperature and dissolved oxygen. These patterns were reproduced by introducing processes known to occur in the real world, i.e. a heating term for temperature and primary production and respiration terms for DO. The need for addition model complexity has been based on a series of step-wise model experiments and a consideration, and dismissal, of alternative mechanisms to explain the observed variability.

The resulting model is still very much a prototype that needs to be tested against other data sets and in other conditions. However the results obtained show promise in giving an insight into how flow, nutrient and radiation regimes combine to influence the growth of macrophytes. Such an insight can inform the future management of rivers, e.g. whether increased shading could be a local method of controlling macrophyte growth, and whether nutrient reduction will be effective in controlling in-stream primary productivity. Understanding controls on primary production can make a significant contribution to the informed management of river systems and the objective of improving, or maintaining, healthy river ecosystems.

6. REFERENCES

Anderson MG, Bates PD. Validation of Hydraulic Models In: Anderson MG, Bates PD, editors. Model Validation: Perspectives in Hydrological Science. John Wiley and Sons, Chichester, UK, 2001, pp. 512.

Boorman D, Williams R, Hutchins M, Penning E, Groot S, Icke J. A model selection protocol to support the use of models for water management. Hydrology and Earth System Sciences 2007; 11: 634-646.

Boorman DB. Climate, Hydrochemistry and Economics of Surface-water Systems (CHESS): adding a European dimension to the catchment modelling experience developed under LOIS. The Science of The Total Environment 2003a; 314-316: 411-437.

Boorman DB. LOIS in-stream water quality modelling. Part 1. Catchments and methods. The Science of The Total Environment 2003b; 314-316: 379-395.

Butcher JB, Covington S. Dissolved-Oxygen Analysis with Temperature-Dependence. Journal of Environmental Engineering-Asce 1995; 121: 756-759.

Caissie D. The thermal regime of rivers: a review. Freshwater Biology 2006; 51: 1389-1406.

Chapra SC, Ditoro DM. Delta Method for Estimating Primary Production, Respiration, and Reaeration in Streams. Journal of Environmental Engineering-ASCE 1991; 117: 640-655.

Coutant CC. Compilation of Temperature Preference Data. Canadian Journal of Fisheries and Aquatic Sciences 1977; 34: 739-745.

Cox BA. A review of currently available in-stream water-quality models and their applicability for simulating dissolved oxygen in lowland rivers. The Science of the Total Environment 2003a; 314: 335-377.

Cox BA. A review of dissolved oxygen modelling techniques for lowland rivers. The Science of the Total Environment 2003b; 314-316: 303-334.

Cox BA, Whitehead PG. Impacts of climate change scenarios on dissolved oxygen in the River Thames, UK. Hydrology Research 2009; 40: 138-152.

Cox MM, Bolte JP. A spatially explicit network-based model for estimating stream temperature distribution. Environmental Modelling & Software 2007; 22: 502-514.

Eatherall A, Boorman DB, Williams RJ, Kowe R. Modelling in-stream water quality in LOIS. Science of the Total Environment 1998; 210: 499-517.

Edwards RW, Owens M. The Oxygen Balance of Streams and the Industrial Society. Oxford, UK: Blackwell, 1965.

Flynn NJ, Snook DL, Wade AJ, Jarvie HP. Macrophyte and periphyton dynamics in a UK Cretaceous chalk stream: the River Kennet, a tributary of the Thames. Science of the Total Environment 2002; 282: 143-157.

Hellawell JM. RIVER REGULATION AND NATURE CONSERVATION. Regulated Rivers Research and Management 1988; 2: 425-444.

Hornberger GM, Kelly MG. Atmospheric Reaeration in River using Prodcutivity Analysis. Journal of the Environmental Engineering Division ACSE 1975; 101: 729-739.

Hutchins MG, Johnson AC, Deflandre-Vlandas A, Comber S, Posen P, Boorman D. Which offers more scope to suppress river phytoplankton blooms: Reducing nutrient pollution or riparian shading? Science of the Total Environment 2010; 408: 5065-5077.

Jarvie HP, Neal C, Williams RJ. Assessing Changes in Phosphorus Concentrations in Relation to In-Stream Plant Ecology in Lowland Permeable Catchments: Bringing Ecosystem Functioning Into Water Quality Monitoring. Water, Air, and Soil Pollution: Focus 2004; 4: 641-655.

Jarvie HP, Neal C, Williams RJ, Neal M, Wickham HD, Hill LK, et al. Phosphorus sources, speciation and dynamics in the lowland eutrophic River Kennet, UK. Science of the Total Environment 2002; 282: 175-203.

Johnson AC, Acreman MC, Dunbar MJ, Feist SW, Giacomello AM, Gozlan RE, et al. The British river of the future: How climate change and human activity might affect two contrasting river ecosystems in England. Science of the Total Environment 2009; 407: 4787-4798.

Loperfido JV, Just CL, Schnoor JL. High-Frequency Diel Dissolved Oxygen Stream Data Modeled for Variable Temperature and Scale. Journal of Environmental Engineering-Asce 2009; 135: 1250-1256.

Marsh TJ, Hannaford J. UK Hydrometric Register. In: Marsh TJ, Hannaford J, editors. Hydrometric data UK series. Centre for Ecology and Hydrology, Wallingford, UK, 2008, pp. 210.

Neal C, Harrow M, Williams RJ. Dissolved carbon dioxide and oxygen in the River Thames: Spring-summer 1997. Science of the Total Environment 1998; 210: 205-217.

Neal C, Jarvie HP, Howarth SM, Whitehead PG, Williams RJ, Neal M, et al. The water quality of the River Kennet: initial observations on a lowland chalk stream impacted by sewage inputs and phosphorus remediation. Science of the Total Environment 2000; 251/252: 477-495.

Neal C, Jarvie HP, Williams R, Love A, Neal M, Wickham H, et al. Declines in phosphorus concentration in the upper River Thames (UK): Links to sewage effluent cleanup and extended end-member mixing analysis. Science of the Total Environment 2010; 408: 1315-1330.

Neal C, Jarvie HP, Williams RJ, Neal M, Wickham H, Hill L. Phosphorus-calcium carbonate saturation relationships in a lowland chalk river impacted by sewage inputs and phosphorus remediation: an assessment of phosphorus self-cleansing mechanisms in natural waters. Science of the Total Environment 2002a; 282: 295-310.

Neal C, Watts C, Williams RJ, Neal M, Hill L, Wickham H. Diurnal and longer term patterns in carbon dioxide and calcite saturation for the River Kennet, south-eastern England. Science of the Total Environment 2002b; 282: 205-231.

O'Connor DJ, Di Toro DM. Photosynthesis and Oxygen Balance in Streams. Journal of the Sanitary Engineering Division 1970; 92: 547-571.

Odum HT. Primary Production in Flowing Waters. Limnology and Oceanography 1956; 1: 102-117.

Oreskes N, Shraderfrechette K, Belitz K. VERIFICATION, VALIDATION, AND CONFIRMATION OF NUMERICAL-MODELS IN THE EARTH-SCIENCES. Science 1994; 263: 641-646.

Schurch M, Buckley D. Integrating geophysical and hydrochemical borehole-log measurements to characterize the Chalk aquifer, Berkshire, United Kingdom. Hydrogeology Journal 2002; 10: 610-627.

Shi J, Douglas R, Rippey B, Jordan P. Modelling the diurnal variation of dissolved oxygen concentration in the River Oona. In: Brebbia CA, Almorza D, Sales D, editors. Water Pollution Vii - Modelling, Measuring and Prediction. 9. Wit Press, Southampton, 2003, pp. 403-412.

Turner DF, Pelletier GJ, Kasper B. Dissolved Oxygen and pH Modeling of a Periphyton Dominated, Nutrient Enriched River. Journal of Environmental Engineering-Asce 2009; 135: 645-652.

UK Technical Advisory Group on the Water Framework Directive. UK Environmental Standards and Conditions (Phase 1) - Final Report, London, UK, 2008, pp. 73.

Vannote RL, Minshall W, Cummins KW, Sedall JR, Cushing CE. The River Continuum Concept. Canadian Journal of Fisheries and Aquatic Sciences 1980; 37: 130-137.

Wade AJ, Whitehead PG, Hornberger GM, Jarvie HP, Flynn N. On modelling the impacts of phosphorus stripping at sewage works on in-stream phosphorus and macrophyte/epiphyte dynamics: A case study for the River Kennet. Science of the Total Environment 2002; 282-283: 395-415.

Webb BW, Hannah DM, Moore RD, Brown LE, Nobilis F. Recent advances in stream and river temperature research. Hydrological Processes 2008; 22: 902-918.

Whitehead PG, Wilby RL, Battarbee RW, Kernan M, Wade AJ. A review of the potential impacts of climate change on surface water quality. Hydrological Sciences Journal-Journal Des Sciences Hydrologiques 2009; 54: 101-123.

Whitehead PG, Williams RJ, Lewis DR. Quality simulation along river systems (QUASAR): Model theory and development. Science of the Total Environment 1997; 194: 447-456.

Williams RJ, White C, Harrow ML, Neal C. Temporal and small-scale spatial variations of dissolved oxygen in the Rivers Thames, Pang and Kennet, UK. Science of the Total Environment 2000; 251: 497-510.

Figure Captions

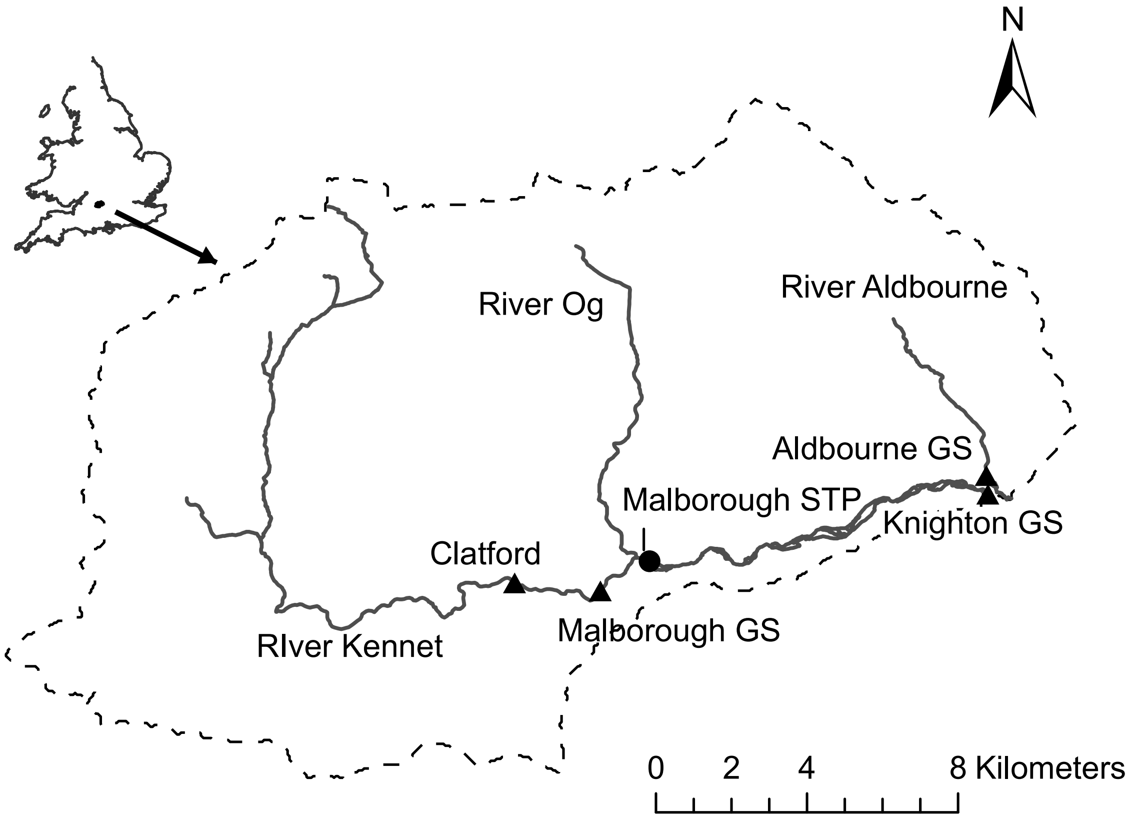
Figure 1 Location and main features of the modelled section of the River Kennet – Clatford to Knighton. GS = gauging station, STP = sewage treatment plant.

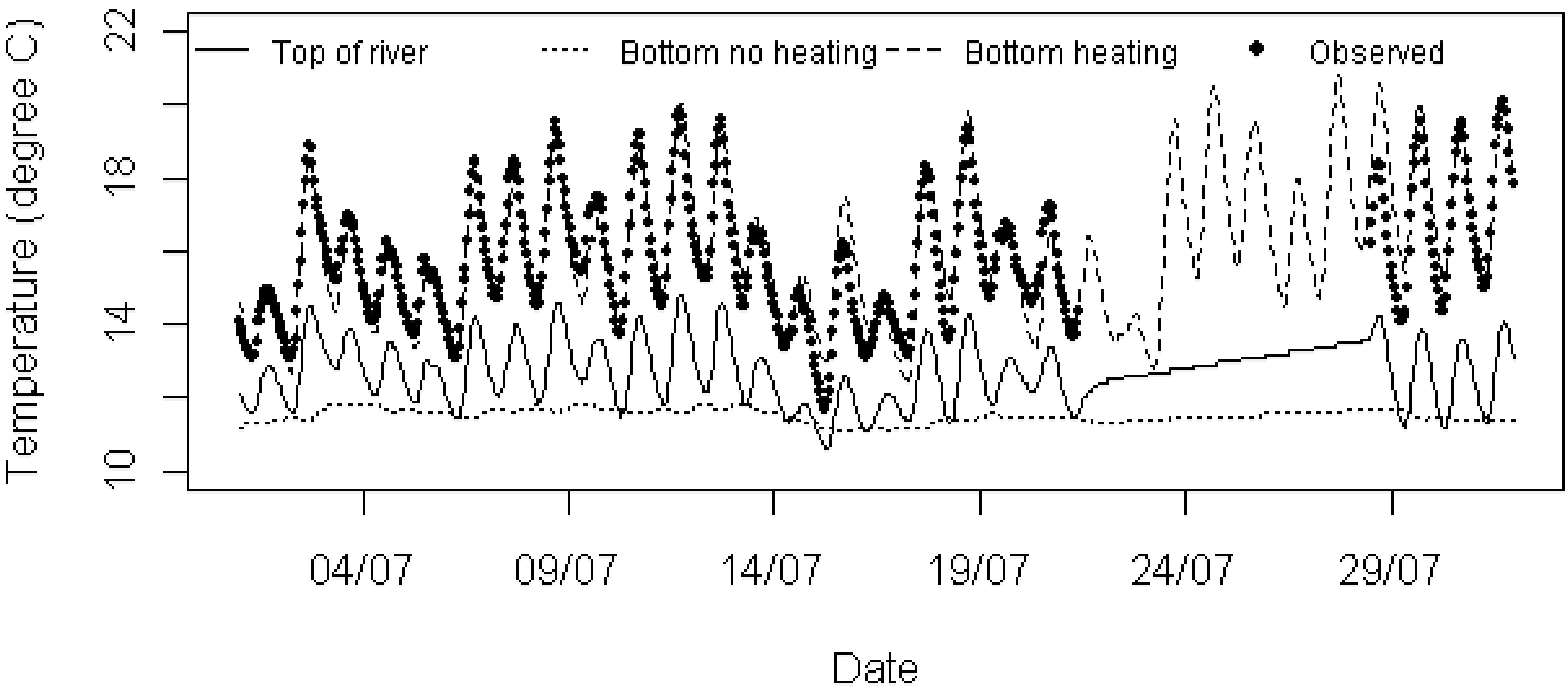
Figure 2 Simulation of river water temperatures in the river Kennet during July 1999 showing the temperature at the topmost modelled reach and the bottom modelled reach (Ramsbury) with and without the heating model. Observed data are shown for Ramsbury. The flat line from 21st to 29th is a period of missing input data.

Figure 3 Simulated and observed dissolved oxygen concentrations at Ramsbury for on the River Kennet July 1999 with and without the macrophyte model implemented. The observed values from the 9th to the 15th show sensor drift. Data are missing from 21st to the 29th.

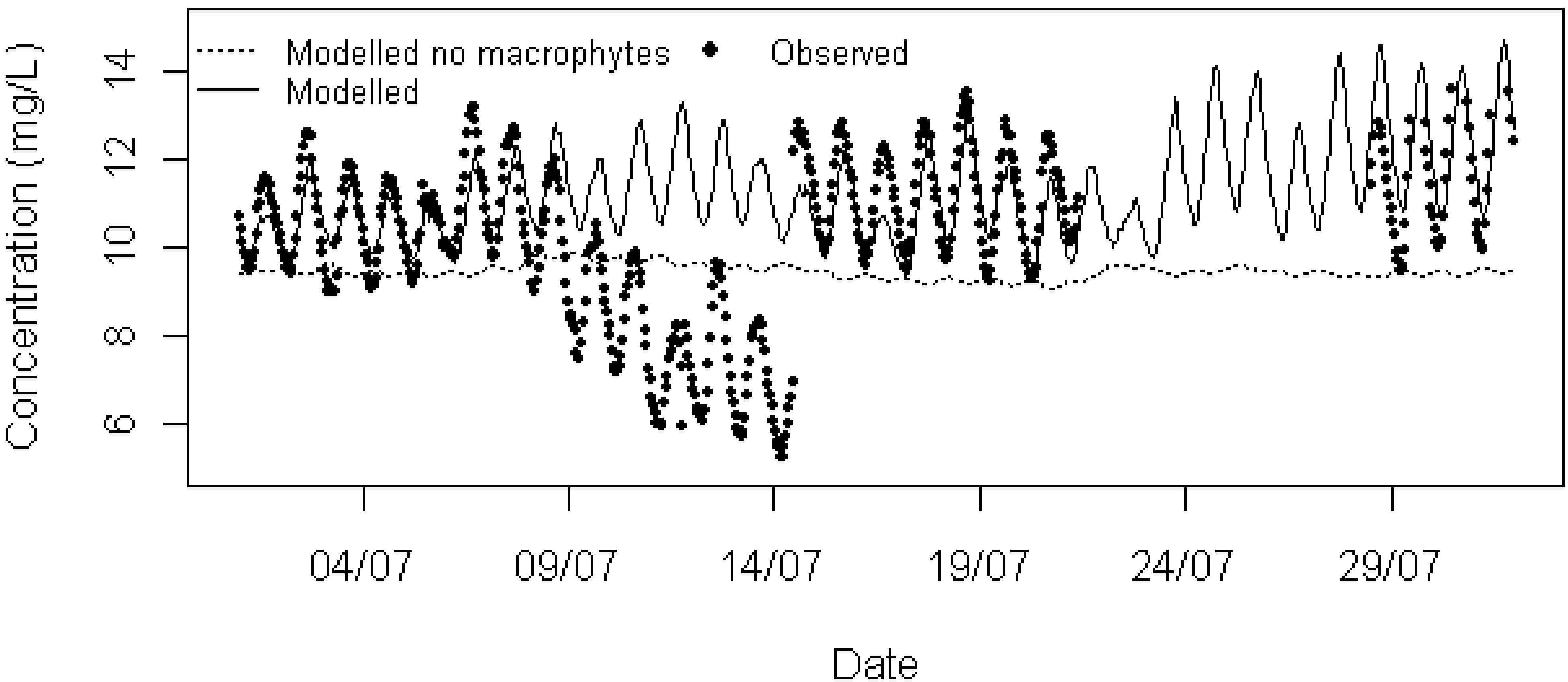
Table 1 *Summary of the differences in the ways in which the three river primary production communities represented in QUESTOR interact with their environment.*

Interaction	**Macrophytes**	**Benthic Algae**	**Phytoplankton**
Transport through river network	No – only in extreme events.	No – only in extreme events.	Yes
Temperature	Air, water and bed.	Water and possibly bed	Water
Light	Above surface to bed.	Bed	Water column
DO exchange	Air and water	Water	Water
Nutrient exchange	Bed and water	Water	Water
BOD on death	Bed and possibly water	Bed and possibly water	Water


N
River Og
River Aldbourne
Aldbourne GS
Malborough STP
Knighton GS
Clatford
RIver Kennet
Malborough GS
0
2
4
8 Kilometers



Top of river
Bottom no heating
Bottom heating
Observed
Temperature (degree C)
10
14
18
22
04/07
09/07
14/07
19/07
24/07
29/07
Date



Modelled no macrophytes
Observed
Modelled
Concentration (mg/L)
6
8
10
12
14
04/07
09/07
14/07
19/07
24/07
29/07
Date