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Successful modelling of river dissolved oxygen dynamics requires knowledge of stream channel environments

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Abstract

Water quality in lowland rivers is sensitive to changes in flow during summer dry periods, when high temperatures and low pollutant dilution are problematic and may reduce oxygen concentrations to levels of ecological concern. A 10-year period of monitoring data was collated for a typical small lowland UK river. Two hourly-resolution applications of a process-based water quality model (QUESTOR) were made, with and without local knowledge, to establish whether specific information on stream channel hydraulics is an essential precursor to successful simulation. Results showed this information to be necessary, with considerably better goodness-of-fit statistics obtained when the local knowledge was used. In this regard, mean improvements in Nash-Sutcliffe Efficiency across all monitoring sites were from -0.33 to 0.18 and from 0.24 to 0.78 for dissolved oxygen and water temperature respectively. Percent bias was within 10% for the local model. The 10-year record also allowed a detailed characterisation of how changes in flow, as described by a comprehensive range of Indicators of Hydrological Alteration, relate to the water quality determinants. Analysis revealed these dynamics were also captured more realistically when the model was driven by local knowledge. The research concludes that river dissolved oxygen simulations driven by national-level information are of some value as screening tools, but model refinement supported by sufficient provision of local information is necessary when detailed simulations are required to support specific decision-making.

Keywords: dissolved oxygen, water temperature, river, hydraulics, water quality model, local knowledge

1. Introduction

Although the adverse overall effects of organic pollution and thermal stress on river dissolved oxygen (DO) are long known, uncertainties remain in the complex understanding of detailed process response to enable future prediction (Utz et al., 2020) which hampers the effectiveness of riverine management. Low oxygen conditions may be prevalent even in lowland rivers not experiencing high nutrient loads (Carter et al., 2021). In this context accurate modelling of DO dynamics in rivers is challenging, in as well as requiring information supporting simulation of nutrient concentrations it also requires reliable simulation of metabolism, physical reaeration and stream temperature in stream channels (Jankowski et al. 2021).

There is much welcome effort being invested in increasing the spatio-temporal extent of water quality model applications, but at the same time there is a danger of losing sight of the need for accurate and detailed models incorporating correct sensitivity to driving factors (Hrachowitz et al. 2014; Tang et al. 2019). When underpinned by a rigorous catchment hydrological model, nutrient dynamics and primary productivity can be simulated using information about climate, catchment land use and network riparian condition obtainable via GIS-based datasets. Therefore, geographically-extensive applications are achievable based upon nationally-available data resources (Abbaspour et al. 2015; Bell et al., 2021). In comparison however, the prospects for acceptable DO simulation using national-level approaches are more doubtful. In their review of commonly-used process-based DO models, Kannel et al. (2011) conclude that a single model cannot readily cover the range of functionalities required for different scales of application. More recently, in reflection of this difficulty there has been increasing focus on developing statistical DO models, in particular for large rivers, often using artificial intelligence (e.g. Csabragi et al., 2017). These can perform well using nationally-extensive low frequency water quality and runoff data, but as underlying mechanisms are not represented, correct sensitivity in predicting detailed response to change cannot be established.

The variables necessary for directly calculating DO cannot be derived from GIS-based datasets alone. Firstly, these variables include components to stream metabolism additional to those controlled by primary producers. Being related to organic carbon characteristics and sediment properties, estimation of these additional heterotrophic respiration fluxes has, despite recent technical advances, largely eluded research effort. Even if now known, this information is limited and spatio-temporally sporadic. Secondly, accurate simulation of the variability of reaeration within river networks needs detailed characterisation of river hydraulics. Although rough approximations can be made using information derived from climate and topography, 1-D models based on such data sources cannot capture local hydraulic variation. Drawbacks related to insufficient segmentation of river stretches when treated as sequences of well-mixed compartments are recognised (Warren et al., 2005). Detailed information about channel heterogeneities and the dimensions and operation of flow control structures and site-specific data and analysis represents “local knowledge”. This local contextual information is unlikely to be held in national databases and only accessible through local stakeholder interaction and site visits.

To put the likely level of need for local knowledge in context, the implications of some key structural aspects of water quality models used for large-scale application are highlighted:

- The method of model spatial discretisation determines how precisely sources of pollutants are advected, dispersed and transformed. Models use hydrological sub-catchment response units and the location of individual influences related to specific reaches of differing length (e.g. SWAT (Abbaspour et al., 2015), INCA (Jackson-Blake et al. 2016), QUAL2K (Pelletier et al. 2006)) or are based on regular grids (e.g. LTLS (Bell et al., 2021)).
- Flow routing is derived ultimately from climate data and Digital Elevation Models. From these data sources, 1-D process-based models (e.g. QUESTOR, QUAL2K, INCA and SWAT) typically use combinations of the Manning equation and Leopold-Maddox non-linear functions to relate discharge to velocity, depth and width assuming either rectangular or trapezoidal channel cross-sections. In particular, for DO the crucial consequence is whether or how the information is modified for model application using local knowledge. This is especially relevant as models applied in heavily modified urban channels employ such approaches (e.g. DUFLOW (Moreno-Rodenas et al. 2019)).
- Simulating water temperature is a fundamental precursor to accurate representation of in-river processes and is typically estimated empirically from air temperature (e.g. Mohseni and Stefan 1999; Benyahya et al., 2007). With access to (1) sub-daily solar radiation and (2) high resolution remote sensing imagery to capture riparian shade (e.g. Bachiller-Jareno et al. 2019), successful water temperature simulations using process-based approaches including those incorporating energy balance calculations are achievable (Dugdale et al., 2017) and can greatly benefit water quality simulation, in particular for modelling DO at daily or sub-daily timesteps.

To demonstrate the unique challenges of achieving spatially extensive, yet detailed and accurate, simulations of water temperature and DO in river networks, we present a case study of the River Deben, a small lowland river in East Anglia, UK. The river suffers from periodically chronic DO depletion due to oxygen demand in bed sediments related to biotic activity (Parr and Mason, 2003). Our objectives are to simulate hourly water quality dynamics over a 10-year period at successive sites along a river profile using the pseudo-1-D QUESTOR river eutrophication model (Pathak et al., 2021).

We hypothesise that DO dynamics can be simulated satisfactorily using data and information stored in national-level datasets. To test the hypothesis we run the model twice, with and without local knowledge beyond what is readily available online. If supported this would suggest that spatially extensive simulation of DO and prediction of its response to future change is achievable. The river hydrological regime is a primary control on water quality and is very sensitive to drivers of natural and anthropogenic variability and change. By considering relations between simulated water quality and indices of hydrological alteration (IHA) (Richter et al., 1996), we then compare with observed water quality to explore the extent to which the two models are correctly sensitive to hydrologically-induced change over the 10-year period. By comparison with observed data in light of model performance we consider wider implications through discussing the extent to which local knowledge is necessary for successful model application.

Structurally, first we describe the QUESTOR model and the case study river; and we define QUESTOR applications and derivation and use of IHAs (Section 2). Then in Section 3 we present results and summarise key findings. Interpretation of the findings follows in Section 4, reflecting on the value of local knowledge, discussing the importance of correctly representing water quality in low flow conditions, and identifying priority areas for model improvement.

2. Method

2.1. Model description

QUESTOR (Quality Evaluation and Simulation Tool for River Systems) is a 1-D model of the river network representing processes controlling eutrophication and the consequences thereof (Hutchins et al. 2016). It consists of a set of reaches bounded by influences (weirs, abstractions, effluents, tributary rivers). To determine flow routing the reaches are defined of constant-width and variable-depth. Travel time, water depth and discharge are related using non-linear equations and reach-specific information on riverbed condition (Manning's N estimation) and gradient. By linking flow routing to biochemical processes (as continuously stirred tank reactors) the reach structure represents advection and dispersion. Biologically QUESTOR represents primary producers in terms of phytoplankton transported along the system (with the possibility to include plants and benthic algae). Diffuse inputs are represented by observations, process-based rainfall-runoff/diffuse pollution models or simple statistical models. Solar radiation inputs control water temperature and primary production.

2.2. Site description and model setup

The River Deben in Suffolk (UK) (Figure 1) drains a small lowland catchment of 163 km^2 (as defined at Naunton Hall gauging station (NRFA ID 35002) National Grid Reference 6322 2534). The catchment is predominant arable (79%), of low relief (maximum altitude 66 mOD) and overlays a mixture of moderately-permeable clay and permeable chalk bedrock.

The QUESTOR model of the River Deben comprises a 27.7 km slow-flowing stretch of river between the A1120 road bridge (a few kilometres downstream of the town of Debenham) and Ufford Bridge split into 13 reaches. Along this stretch there are five sites with flow and/or water quality observations. Notable amongst these are the flow gauging stations at Naunton Hall and Brandeston (3.3 and 20.8 km upstream of Ufford Bridge respectively) and the continuous water quality monitoring site at Sanctuary Bridge (Letheringham) (16.1 km upstream of Ufford Bridge).

Seven surface water tributaries are represented. Of these, the main influences from tributaries are: the main Deben and the Earl Soham tributary (which are both influenced by sewage effluent discharge and augmentation to flow from a borehole) in the upper reaches and Potsford Brook and Byng Brook.

Data to support modelling were supplied for 2010-2019 from national Environment Agency (EA) monitoring programmes. The monitoring shows the river to be vulnerable to low DO during summer. Of 71 observations at Brandeston, 6 fell below 6 mg DO L^{-1}. The earlier part of the period (2010-15) had relatively more comprehensive data coverage in tributaries and along the river from grab sampling. Solar radiation was obtained from the nearby Wattisham station and moderated by estimates of riparian canopy coverage. The estimates of riparian shade have been made using google earth imagery as shown to be realistic in other QUESTOR studies (e.g. Bachiller-Jareno et al 2019; Waylett et al. 2013). Apart from flow and water temperature which did not require calibration, the model was fitted using a process of sequential downstream site-by-site calibration for the 2010-2013 period and tested for 2014-2019. Model performance was assessed using the Nash-Sutcliffe Efficiency criterion (NSE: Nash and Sutcliffe 1970) and the percentage error in mean (PBIAS).

The model was applied at hourly resolution. A description of model determinants, processes and equations is provided in Appendix A. A biological component based on assumption of phytoplankton biomass being dominated by cool water diatoms (Equation A1) was chosen as it gives good performance in relation to hourly data from the lower River Thames (Pathak et al., 2021).

2.3. Model applications

Using the above information (Section 2.2) as a basis on which to form the bounds and data supply for the model, two applications were set up. The methods and supporting data sources described below are summarised in a table (Appendix A, Table A1).

A first application ("Basic" Model) was made without the benefit of the local knowledge. As the local knowledge related primarily to definition of channel morphological characteristics known to have a strong bearing on determinants directly related to consequences of eutrophication (DO, BOD, chlorophyll-a), only those biogeochemical parameters related to nitrogen and phosphorus species underwent site-by-site calibration. Other QUESTOR modelling studies of similar-sized rivers in lowland UK (Hutchins et al., 2020; Pathak et al., 2021) were used to help inform river hydraulic parameters and to estimate (i) the ratio of rates of water column to benthic respiration (ii) parameters related to phytoplankton dynamics. Total heterotrophic respiration was estimated in two alternative ways: "Basic (a)" by assuming rates typical of the other similar-sized rivers (0.5 d^{-1} and 0.2 d^{-1} for water column and benthic respiration respectively); and "Basic (b)" based on fitting in the calibration period the PBIAS for data aggregated across all sites. Fractional light penetration (FP) values were based on aerial photographic estimates of occupancy by riparian canopies, assumed to block 100% of direct sunlight.

A second application ("Local" Model) was set up with the benefit of local knowledge used to provide additional information to guide the process. Continuous water quality monitoring by local EA staff at Sanctuary Bridge was made available for part of the validation period (2018-2019) and therefore aided model testing. Due to the influence of the chalk aquifer on catchment hydrology and water resources, groundwater discharge contributions were included in the middle reaches. River hydraulic parameters were defined using satellite imagery, DTM, river level data, photographs of control structures and qualitative observations of channel condition in late spring. Agricultural abstraction and sewage treatment works effluent were included and characterised using local EA records. Canopy fractional penetration (FP) estimates were modified upward based on local photographic observations suggesting significant light penetration to the water surface.

2.4. Indicators of hydrological alteration

For each of the two flow gauging stations, there are three data sets of water flow. They are observed flow and simulated flow from both “Basic” Models and the “Local” Model. For better understanding the flow regime and the environmental flow, we applied the Indicators of Hydrological Alteration (IHA) to describe the variation of discharge. These biological-related hydrological indicators were proposed by Richter et al. (1996) for assessing hydrological alteration in river networks, and accepted world-wide for making linkages with water quality and ecological influences (Olden & Poff, 2003; Schneider et al., 2013; Guo et al. 2020; Valerio et al., 2021). IHA contain five hydrological dimensions of parameters, which characterize the flow regime from its magnitude, frequency, rate of change, duration and timing.

In this study, we computed two kinds of IHA. Average daily flows were used as a basis for calculating the indicators. The first matrix of 67 indicators (annual IHA) was exported from the IHA software developed by the Nature Conservancy (2009); covering monthly mean flow, magnitude and duration of annual extreme flow, timing of annual extreme events, frequency and duration of high and low pulses, and rate and frequency of flow condition changes (Appendix B, Table B1). The second matrix of indicators (short-term IHA) was modified from the annual set in order that flow events happening in defined periods (i.e., 3, 7, 14, 21 days before each specific water quality sampling date) can be emphasized. Together, 17 hydrological parameters (Appendix B, Table B2) cover the three dimensions of flow regime (magnitude of flow events, frequency of flow events, and rate of change in flow events).

3. Results

3.1. Model performance

Optimised parameters are listed for the two models (Appendix C, Table C1). When using default values for heterotrophic respiration taken from similar-sized lowland rivers, the “Basic (a)” model gave very poor performance, greatly overestimating the low DO values (for all sites: 19% < PBIAS < 22%). The alternative approach to parameter estimation (b) was therefore adopted for the remaining analysis, from now on referred to as the “Basic” model, as PBIAS and NSE were much improved (Figure 2). For two months in Spring 2011 the river was incorrectly simulated to dry up, a consequence of not using local knowledge to inform setup. Data from this period were omitted from all analysis.

Whilst both models simulated river discharge comparably, local knowledge informing hydraulic representation greatly influences river residence time and water level fluctuations. Over a 29 month period commencing in August 2017, median and 10th percentile water levels at Letheringham Mill (14.5 km upstream of Ufford Bridge) were 0.73 and 0.67 m respectively. This small variation was reflected by both the “Local” model (0.45 and 0.40 m respectively for median and 10th percentile) and the “Basic” model (0.13 and 0.10 m respectively for median and 10th percentile). It was to be expected that water level observations would be higher than simulated estimates due to substantial submerged macrophyte presence, which are not accounted for in the model. However, although the “Local” model appears to simulate acceptable water levels, the “Basic” model simulations are clearly unrealistically low.

The “Local” model also performed considerably better than the “Basic” model for all water quality determinants (Appendix C, Table C2) and simulated most water quality determinants with little bias. Overall levels of nitrate, ammonium, DO and temperature were modelled acceptably (PBIAS < 20% at all sites). In contrast, the “Basic” model had overall tendency for underestimation. The exception is SRP which was substantially overestimated at all sites by both models (“Local” model PBIAS: 13-121%). The largest mismatches were in the autumn. Reliable chlorophyll-a data were not available and could only be inferred indirectly from nutrient, oxygen and BOD dynamics. The “Local” model correctly simulated depletion of nutrients in the early summer and simulated BOD at Brandeston over a 6 year period (>300 measurements) with minimal bias (PBIAS = 0.5%). In comparison the "Basic" model greatly underestimated BOD (PBIAS value of -82% (or -52% under the "Basic (a)" application)) at Brandeston and gave much greater overestimation of SRP (PBIAS: 146-330%). In summary, in terms of mean levels across all monitoring sites, the percentage improvement in PBIAS gained over the 10 year period by invoking the "Local" model was 18%, 55%, 66% and 47% for temperature, nitrate, SRP and DO respectively.

In terms of PBIAS and NSE criteria the benefits gained by including local knowledge and how the level of improvement varies along the river is shown for water temperature and concentrations of nitrate and dissolved oxygen (Figure 2). The "Basic" model does not provide values of NSE above zero for DO, suggesting that based on nationally-available data alone the model cannot provide an adequate simulation in systems of this type. The inclusion of local knowledge resulted in much better representation of time-series response (NSE) for temperature and DO. There was also improvement for nitrate, although this was only moderate as the "Basic" model shows good performance in this respect. Whilst overestimation of SRP was more acute in upstream reaches, performance of the "Local" model generally declined slightly downstream, possibly due to increasing uncertainty in local knowledge in particular regarding volumetric contributions to river flow. Differences between the performance of the two models and its variation between sites is shown for DO and water temperature (Figure 3). For temperature, compared to the "Basic" model, there is less scatter in "Local" model performance. At Naunton Hall there is less bias (i.e. less underestimation). The "Basic" model failed to represent variation in DO either sufficiently or correctly, a shortcoming less apparent for the "Local" model.

3.2. Detailed assessment of response in data and models

The differences in model performance as evaluated by comparison with hourly data at Sanctuary Bridge show the "Local" model to perform better than the "Basic" model (Figure 4). The "Local" model better captures the extent of diurnal cycling. Both models have a tendency to underestimate late summer and autumn water temperatures.

The oxygen holding capacity of water is reduced under increasing water temperature and theoretically this will lead to inverse relationships in natural river waters. Whilst this appears the overriding control at Brandeston Bridge as represented in the "Basic" model, it does not reflect observations (Figure 5). A more complex relationship is revealed by the data, suggesting the influence of other factors on DO concentration not related to temperature. This subtlety is only captured in the "Local" model.

At Brandeston Bridge and Naunton Hall, where flow data from gauging stations are available, water quality response (Temperature and DO) was assessed in terms of indicators of hydrological alteration (IHA). The degree to which the two models capture relationships at an annual level between IHA and typical summer water temperatures (90th percentile) is shown (Figure 6). For the "Local" model there is better agreement with observations for the majority of indicators, as demonstrated by many points plotting much closer to the 1:1 line than for the "Basic" model. There were insufficient DO data.

In addition, short-term response was investigated. A set of Short Term IHAs were each regressed in turn against instantaneous water temperatures and DO concentrations and the strength of relationships analysed statistically. These relationships were compared between those derived from observed data, and from simulations at all corresponding time points using both "Basic" and "Local" models. The types of relationship observed between IHA and water temperature are clearly better reproduced by the "Local" model (Figure 7) and the correlation coefficients are in closer agreement. The process when repeated for DO revealed similar results, although there are fewer observed data. At Naunton Hall, the majority of IHA indicators result in disagreement in the direction of relationship between observed and "Basic" model simulation (opposite sign of r value). When using the "Local" model there is much better agreement.

4. Discussion

4.1. Improvements in model performance achieved through local knowledge

Comparison of results from the "Basic" and "Local" models with observations demonstrates the improved performance gained for a range of determinants by including local knowledge in model setup, almost exclusively manifested in terms of a more realistic representation of river hydraulics. Of the sources of local knowledge previously outlined (Table A1), those that have specifically enabled better model performance are as follows:

- Groundwater modelling (Environment Agency, 2019) and British Geological Survey monitoring (Shand et al., 2007) informed estimation of groundwater discharges and water quality signatures in middle reaches flowing through areas underlain by chalk.
- Local information about water use for agriculture and groundwater pumping to augment river flow provide more informed estimates of abstractions along the river channel and tributary flow estimates respectively.
- Geo-referenced photographs of weirs and mill gates allowed artificial influences on reaeration to be estimated more accurately. Typically "Basic" modelling can only include default values for an incomplete subset of all structures that are included on OS digital data sets.
- Continuous water level data provided by local EA staff, which allowed better specification of river hydraulic parameters.
- Photographs of river condition enabled a better specification on a reach-specific basis of widths, roughness and hydraulic parameters, alongside better estimation of light penetration through riparian tree canopies.

Applying local knowledge has resulted in better simulation of water temperature, a variable fundamental in controlling water quality dynamics. The considerable mismatches in the "Basic" model as demonstrated by scatter in Figure 3, is considerably reduced when using the "Local" model. With local knowledge good fits are achieved in November to April periods whereas without it there is underestimation. Underestimation is still apparent during the summer, for which the reasons are unclear but could be attributable to model input uncertainties concerning either shading effects or estimated groundwater temperature. By achieving a more realistic representation of the response of water level to change in flow inputs and consequent representation of velocity, the "Local" model reflects diurnal temperature fluctuations well (Figure 4). The "Basic" model greatly overestimates such fluctuations.

There is uncertainty in autotroph response in the Deben system due to lack of representative chlorophyll-a data. Observations of BOD at Brandeston Bridge in the first half of the study period when coupled with DO give indirect evidence of phytoplankton growth and decay. Consequently, the "Local" model application achieved BOD simulations with minimal bias whereas the "Basic" model greatly underestimated BOD. Concentration of nitrogen species were largely simulated acceptably by both models (Table C2, Figure 2). Overestimation of SRP was apparent throughout the network, especially in upper reaches, most acutely in late summer, and by both "Local" and "Basic" models (Table C2). As sources are comprehensively accounted for in the "Local" model, the implication is that in-channel uptake fluxes not represented in model structure are important. Plausible mechanisms of in-channel uptake are abiotic (co-precipitation with calcite or adsorption to sediment) or biotic (macrophyte uptake). Significant abiotic SRP uptake has not been consistently identified from a synthesis of river modelling studies (Jackson-Blake et al. 2017). Photographic evidence shows macrophytes to be plentiful in the upstream Deben, but quantifying their impact on nutrient levels is not straightforward due to difficulties in making representative biomass estimation.

Simulation of DO is improved when using local knowledge (Table C2, Figure 2). Notably, the “Basic” model fails to represent the apparent complexity of influences on DO beyond the fundamental temperature control (Figure 5). In this respect the “Local” model provides clear improvement, yet whilst levels are generally simulated acceptably it is clear that the variation in DO (not captured by the “Basic” model) is still not represented sufficiently or accurately (Figure 3). At Sanctuary Bridge, DO is overestimated (PBIAS = 29%) especially in summer (see Section 4.3).

Although the overestimation of SRP might imply problematic consequences in terms of overall water quality simulation, DO is not directly affected by SRP in the Deben. Here, observed SRP are above a level where it becomes limiting for phytoplankton growth which would have consequences for DO. Other studies of systems transitioning from heterotrophic to autotrophic control have found DO response to be insensitive to phosphorus. Using Boosted Regression Tree approaches in the Thames, Pathak et al. (2021) found primary productivity and eutrophication impacts to be insensitive to nutrients. Likewise Wang et al. (2018) made similar conclusions from process-based model sensitivity analysis in situations of excess nutrient supply.

4.2. The importance of understanding flow controls on water quality in dry periods

Water quality in lowland river systems such as the Deben is especially sensitive to changes in flow during dry periods (Mosley, 2015). In this context, environmental regulators recognise the fine balance needed between river quality considerations, maintaining groundwater resources and supporting agricultural activity (Defra, 2019). Consequently much focus is given to the implications of river flow augmentation and inter-basin transfers. Therefore relationships between the suite of IHAs and measures of water quality response provide important contextual information of the mechanisms operating in these systems.

Realistic capture of relationships between determinants represents a fundamental measure of the worth of the respective model applications. From the interpretation of correlation coefficients based on multi-year datasets (Figures 6 and 7) it is clearly demonstrated that the “Local” model better represents strength of correlations between water quality and hydrological indicators than the “Basic” model. This finding is consistent and robust across a range of IHAs both for individual (short-term IHA) and aggregated (annual IHA) categories. As IHAs were normalised between the categories it is noteworthy that IHAs relating to flow magnitude are more strongly correlated with water temperature at an aggregated level than at an individual level. Frequency-related IHAs show higher correlations at the individual level. Rate of change IHAs rarely show high correlation. The analysis was performed for fundamental integrated indicators, namely water temperature and DO, whose inter-relationships are clearly also better represented by the “Local” model (Figure 5). However, it is also clear there is still considerable mismatch; and possibilities for rectifying these problems are explored below.

4.3. Needs for and prospects for further improving DO simulation

At Sanctuary Bridge very low oxygen levels were observed from a continuous monitoring system (10^{th} percentile DO values of 2.83 and 1.12 mg/L in 2018 and 2019 respectively). Various possible reasons why both models overestimated these low values, which could potentially be rectified within the existing structure, were investigated: (1) much lower levels of DO in groundwater than suggested by Shand et al. (2007), (2) accelerated benthic algal and macrophyte growth throughout reaches which could reconcile the SRP overestimation and, through undesirable eutrophic consequences, deplete the DO, (3) slower-flowing deeper river channel. By making appropriate model adjustments, the first two were shown to have no discernible effect whereas the third only reduced mismatch if waters were implausibly slow-flowing and deep (> 5m).

Other potentially plausible explanations exist but their exploration extends beyond the specific issues at Sanctuary Bridge and also beyond the overall scope of the QUESTOR model. They thereby also cover wider considerations beyond the case study and highlight both shortcomings and opportunities for further improving water quality models:

- Sluice-controlled damming of rivers can result in flow stagnation and periods of low DO in specific locations.
- Localised abundant submergent vegetation can contribute to reduction in flow velocity and a supply of BOD towards the end of the growing season. Reaches with elevated macrophyte biomass may show higher gross primary productivity (GPP) and ecosystem respiration (ER) than elsewhere (Alnoee et al. 2021). In the Deben however, although Sanctuary Bridge DO data implies high ER there is no evidence of elevated GPP.
- Assumptions underpinning simple 1-D model structures may lead to difficulty representing the hydraulic conditions to which water quality is very sensitive.
- Allowance should be made that rather than reflecting the main channel, measurements may represent dead zones of markedly reduced flow conveyance. Such areas of limited main channel mixing are possibly influenced by anoxic bed sediment environments.
- In addition to supply from upstream sewage effluent solids, very high levels of benthic respiration may locally arise from abundant overhanging vegetation supplying organic matter. In the Deben application, high levels were nevertheless inferred in the "Local" model, and a further increase revealed little additional reduction in simulated DO. Quantifying benthic respiration is highly uncertain due to difficulties in measurement (Hutchins et al., 2020). Novel methods incorporating aquatic eddy covariance (Berg et al. 2003) can provide a step-change in understanding at a local level but are time-consuming and an expensive investment.

With sufficient access to local knowledge many of these challenges can likely be overcome using 2-D approaches (e.g. Knightes et al. 2019). Alternatively, aggregated dead zone models employed to improve simulation of pollutant dispersion (e.g. Lees et al., 2000) might be adapted to better capture local variability in DO.

5. Conclusions

Evidence from a modelling study of the River Deben (UK) suggests that although a process-based water quality model (QUESTOR) driven solely by national-level data sources can likely simulate nutrient concentrations acceptably in such environments it cannot achieve satisfactory results for DO. A clear improvement in performance is obtained when specific local knowledge of hydrology and flow routing is included to inform the model application. Improvements were shown to arise from efforts to identify (i) dam operations, (ii) dead zones, whose significance can be pinpointed from detailed meta-data from the monitoring programme, and (iii) macrophyte prevalence.

The implications of the study are wide-ranging. In shallow slow-flowing rivers in dry lowland areas of flat terrain, processes controlling water temperature and DO are very sensitive to changes in flow regime during low flow periods in summer. The Deben is typical of such a river found in south-eastern UK and, as is often the case, the challenges are exacerbated by macrophyte overgrowth in channels and flow regulation. Unsurprisingly, findings from the Deben study reveal patchy model performance (Section 4.1), poorer than that achieved by QUESTOR in larger lowland rivers such as the Thames (Pathak et al., 2021), and an inability to fully reconcile changes in flow with changes in water quality (Section 4.2). The findings demonstrate that insufficient contextual information behind water quality observations can still hamper model performance and the observations necessary to support improvements can remain elusive.

For investigating DO response, challenges associated with characterising river hydraulics, representing benthic environments and quantifying the influence of macrophytes mean that national-scale water quality model structures are best used as screening tools. Greater caution is needed for more detailed simulation, which would benefit from the considerations and recommendations outlined in Section 4.3. Overall, detailed local knowledge leads to better water quality simulation and can support model improvements and lead to improved process understanding. Whilst this provides greater insights and confidence for management decisions, the greater information requirements are challenging for conducting national-scale assessments. Frameworks that facilitate screening and increasingly refined modelling, proportional to local problems, allow more appropriate management solutions to be developed.

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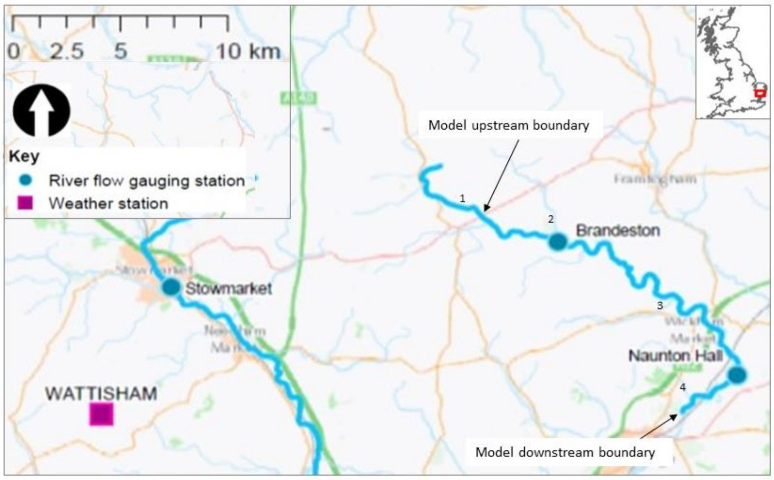

Figure 1: Location map of River Deben (Suffolk, UK), showing extent of the model system. Locations of tributaries mentioned in the text: (1) Deben, (2) Earl Soham tributary, (3) Potsford Brook, (4) Byng Brook.

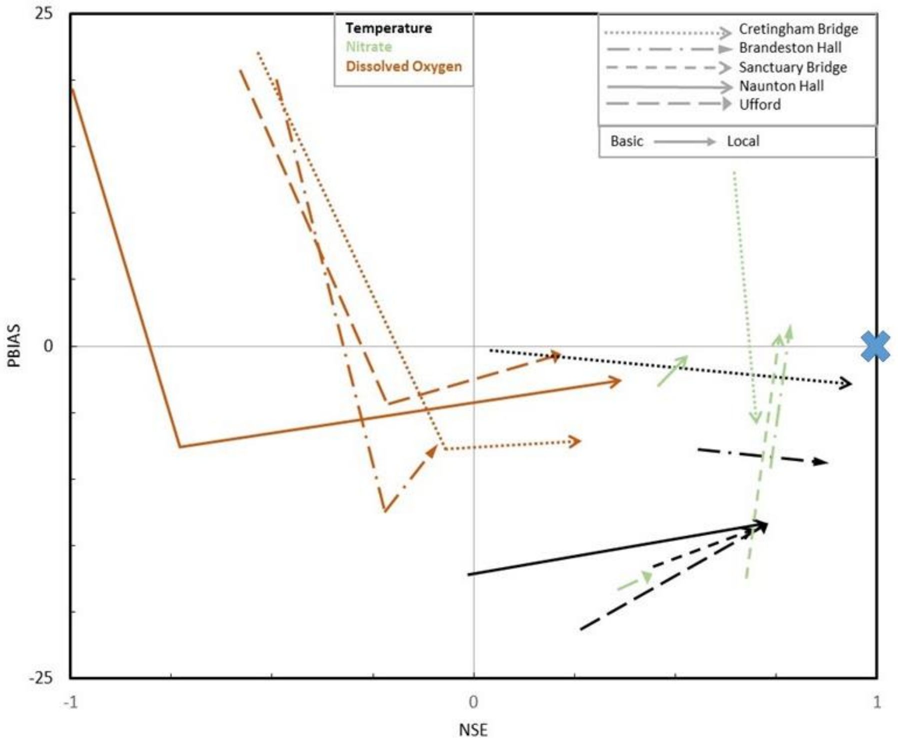

Figure 2: Level of improvement gained during the validation period (2014-2019) in terms of NSE (Nash-Sutcliffe Efficiency) and PBIAS (percent error in mean) when switching between basic model (start of arrow) and model incorporating local knowledge (end of arrow) for simulation of three determinants (temperature, nitrate and dissolved oxygen). The “X” marks optimal location with zero errors. For DO the arrows represent the change from “Basic (a)” to “Local” with the mid-point (break-point) representing “Basic (b)”. DO at Sanctuary Bridge not shown as PBIAS >25 (Table C2): see Section 4.3.

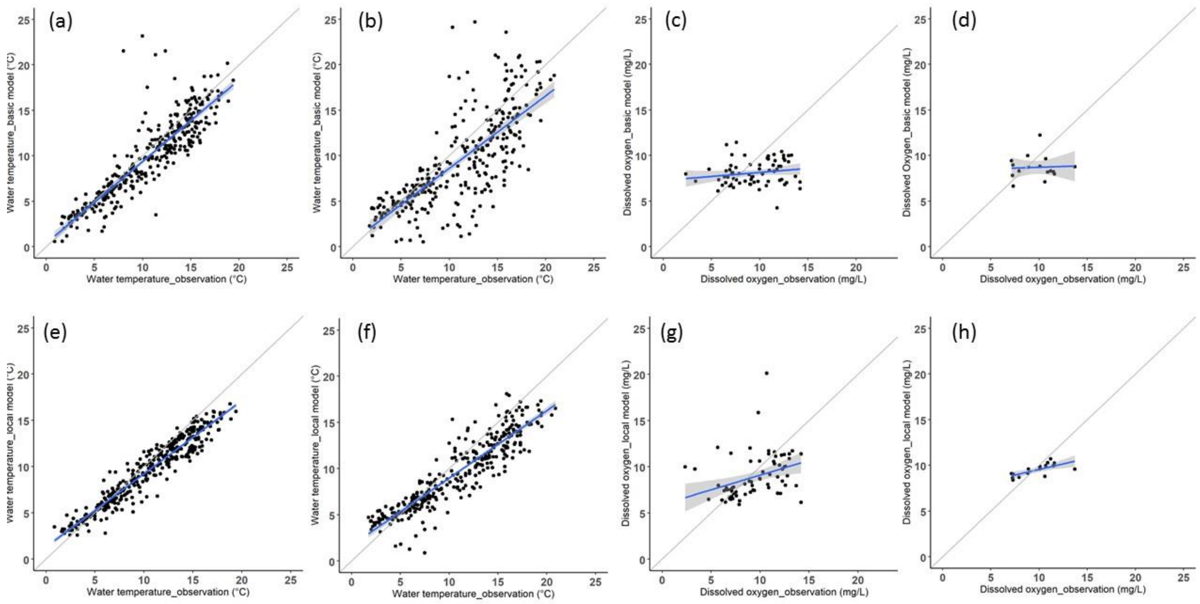

Figure 3: Scatterplots relating observed and simulated water quality with best fit regression lines and 95% confidence intervals. Graphs cover the "Basic" model (a-d) and the "Local" model (e-h): water temperature at (a) Brandeston Bridge (b) Naunton Hall, DO at (c) Brandeston Bridge (d) Naunton Hall, water temperature at (e) Brandeston Bridge (f) Naunton Hall, DO at (g) Brandeston Bridge (h) Naunton Hall.

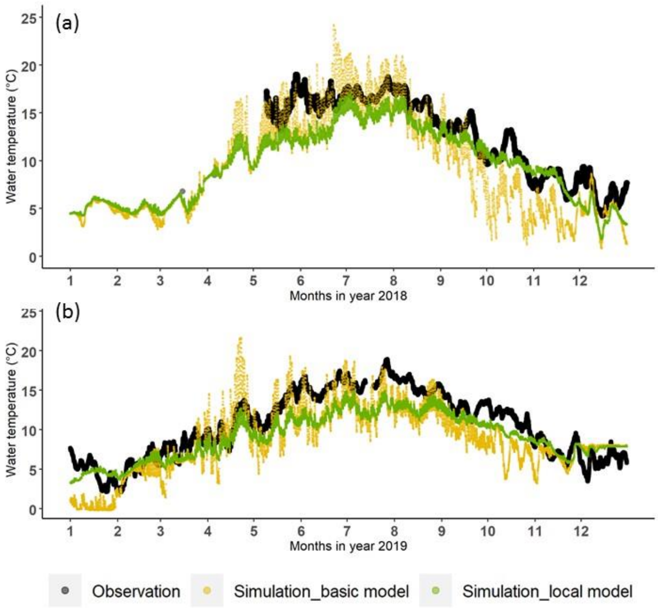

Figure 4: Time-series plots of observed and simulated hourly water temperature at Sanctuary Bridge for (a) 2018 and (b) 2019.

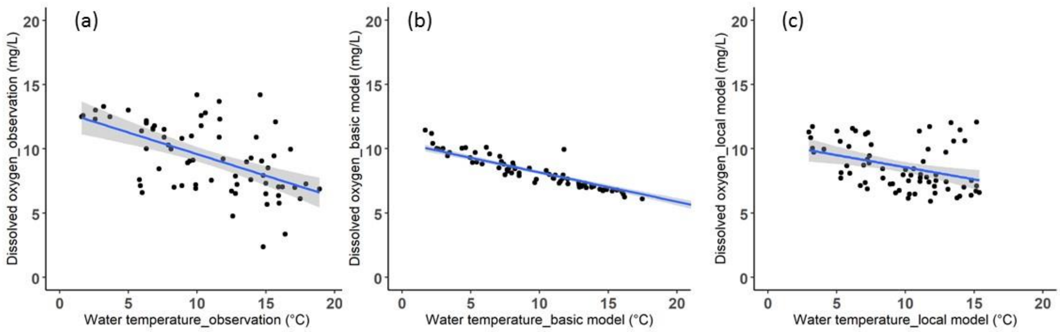

Figure 5: Relationships between water temperature and DO with best fit line and 95% confidence interval for (a) paired observations, (b) paired "Basic" model simulations (c) paired "Local" model simulations. Points plotted for simulations at all times when paired observations available.

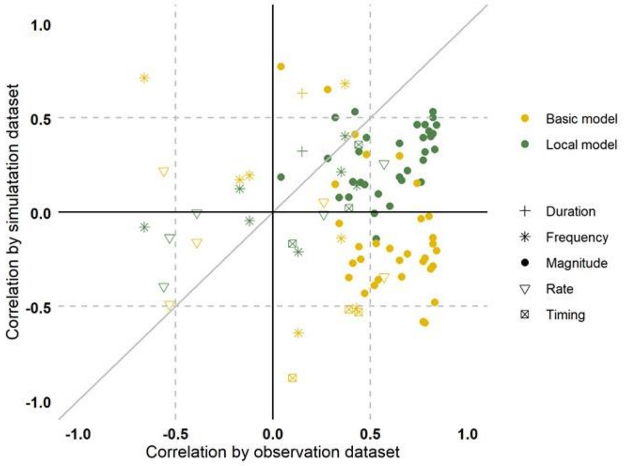

Figure 6: Plot of paired correlation coefficients derived by observations and simulations. Correlations relate annual IHAs and annual 90th percentile water temperature for each of the 10 years (2010 -2019). Points are discriminated by model application ("Basic" or "Local") and by categorical type of IHA. Data are pooled from Brandeston Bridge and Naunton Hall.

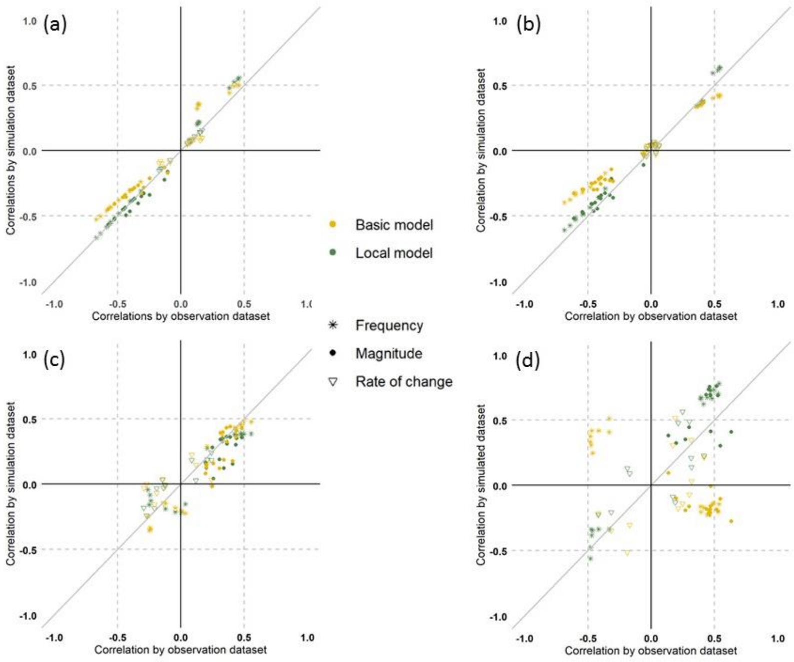

Figure 7: Plot of paired correlation coefficients derived by observations and simulations. Correlations relate short term IHAs with instantaneous 2010-2019 water quality representing (a) water temperature at Brandeston Bridge (b) water temperature at Naunton Hall, (c) DO at Brandeston Bridge (d) DO at Naunton Hall. Points are discriminated by model application ("Basic" or "Local") and by categorical type of IHA.

Supplementary Material

Appendix A. Theoretical basis to QUESTOR and information requirements

QUESTOR simulates Chlorophyll-a (Phytoplankton), Biochemical Oxygen Demand (BOD), Dissolved Oxygen (DO), Inorganic (P-in, equating to soluble reactive fraction) and Organic Phosphorus, Nitrate, Particulate Organic Nitrogen, Ammonium, pH, Temperature, Flow and Photosynthetically-Active Radiation in the water column. Processes that the QUESTOR model represents are aeration, BOD Decay, Deamination, Nitrification, Denitrification, Benthic Oxygen Demand, BOD Sedimentation, P Mineralisation, in conjunction with a biological sub-model of Phytoplankton (comprising Growth, Respiration and Death), which includes nutrient uptake and release. To simulate the hydrological and chemical variables the configuration of QUESTOR as described by Boorman (2003) was used. The full sets of equations used are given elsewhere (Boorman, 2003) so only those equations directly impinging on phytoplankton and DO concentrations are given here.

With the exception of phytoplankton growth (see Equation A.1) temperature dependencies are based on the Arrhenius equation whereby:
$k = k_{ref}\, \vartheta^{(T-Tref)}$
$T_{ref} = 20$ °C
ϑ = Arrhenius factor for temperature dependencies (θ =1.08)

A.1. Phytoplankton model

Biomass is linked to Chl-a using a fixed stoichiometry model with the ratio Chl-a:C:N:P of 1:50:10:1.

__**Equation A.1:**__ Shows the photosynthetic rate with respect to biomass and temperature. An optimal temperature model for cool water diatoms (with “opt” and “range” parameters) is used:

$$k^{pho} = Phy.\,k_{ref}^{pho}.\,e(-(T-opt)^2/range^2).\,f(N).\,f(L)$$

k^{pho} = Photosynthesitc rate (day^{-1}),
Phy = Concentration of Chl-a (mg L^{-1})
T = Temperature (°C),
opt = 14 °C
range = 8 °C
f (N) and *f(L)* = limitation factors for nutrients and light, each holding values between 0 and 1
k^{pho}_{ref} = Maximum phytoplankton growth rate (day^{-1}) at $T_{ref.}$

__**Equation A.2:**__ Calculates the maximum photosynthetic rate and the limitations by nutrients, this has been taken from Michaelis Menten kinetics

$$f(N) = \min\left(\frac{N}{N+k_N}, \frac{P}{P+k_P}\right)$$

N = Nitrate-N plus Ammonium-N (mg L^{-1})
P = Inorganic-P (equivalent to SRP) plus Organic-P (mg L^{-1})
Where k_N = 0.1 and k_P = 0.01 mg L^{-1}

__**Equation A.3:**__ Light limitation, attenuation with depth is described by the Beer-Lambert Law

$$\gamma = \gamma_{base} + L_{SS}.\,SS + L_{Phy}.\,Phy$$

γ_{base} = light extinction coefficient in clean water (0.01 m^{-1})
SS = concentration of suspended sediment (mg L^{-1})
L_{ss} = Light attenuation with depth due to suspended sediment (m^{-1} mg^{-1} L)
L_{phy} = Light attenuation with depth due to phytoplankton (m^{-1} mg^{-1} L)

Equation A.4: Photolimitation with respect to phytoplankton-specific optimum intensities (Steele, 1962)

$$f(L) = \frac{2.718}{\gamma d}.\left[e^{-\frac{R_S L_1 L_2}{L_{opt}}e^{-\gamma d}} - e^{-\frac{R_S L_1 L_2}{L_{opt}}}\right]$$

γd = Water column depth (m),
R_s = Radiation at the surface not reflected (W m^{-2}) (i.e. input solar radiation x 0.6)
L_1 = Fraction of incoming radiation that is visible light (0.5)
L_2 = Fraction of visible light used for phytoplankton (0.5)
L_{opt} = Optimum light intensity for phytoplankton (60 W m^{-2})

Equation A.5: Respiration

$$k^{res} = Phy.k_{ref}^{res}.k_{ref}^{pho}.\theta^{(T-Tref)}$$

$k^{res}{}_{ref}$ = reference respiration rate for phytoplankton (day^{-1})

Equation A.6: Death

$$k^{death} = Phy.k_{ref}^{death}.k_{ref}^{pho}.\left[1-\left(f(N).f(L)\right)\right].\theta^{(T-Tref)}$$

$k^{death}{}_{ref}$ = reference death rate for phytoplankton (day^{-1})

Death is a combination of grazing and non-predatory mortality.

A.2. Dissolved Oxygen model

Equation A.7: Change in Dissolved Oxygen.

$$\frac{dDO}{dt} = \frac{1}{T}(DO_i - DO + W) + (P - R) - (k_{ben}DO/dep) + k_{rea}(OCS - DO) - 4.57k_{nit}NH_4 - k_{bod}BOD$$

Where:
T = a time constant representing the average retention time in the reach. This is defined by L/(bQ^c) in which *L* is length of reach (m), Q is flow out of reach (m^3s^{-1}) and b and c are reach specific constants.
DO = DO concentration leaving the reach (mgL^{-1})
DO_i = input DO concentration (mgL^{-1})
W = aerating effect of a weir as calculated from an empirical relationship based on weir type and height
P = k^{pho}(133.3Phy) = DO increase due to photosynthesis
R = k^{res}(133.3Phy) = DO decrease due to respiration
k_{ben} = benthic respiration rate (day^{-1})
dep = mean water depth of reach (m)

k_{bod}= rate of loss of DO as BOD decays (day^{-1})
k_{nit} = rate coefficient for complete nitrification (day^{-1})
NH_4 = concentration of ammonium in water column (mg L^{-1})
k_{rea} = aeration coefficient at the water surface (day^{-1}) (dependent on velocity (v), depth (d) and temperature (T): $k_{rea} = 5.32\ v^{0.67}\ 1.024^{T-20} d^{-1.85}$)
OCS = DO concentration at saturation (mg L^{-1})

The amount of oxygen produced in photosynthesis (P) or consumed in respiration (R) per unit mass of algae. For each 1 mg of chlorophyll-a 133.3 mg of oxygen are produced. This same ratio applies for oxygen consumption in respiration, and in additions to BOD on phytoplankton death.

A.3. Biochemical oxygen demand model

<u>Equation A.8:</u> Change in biochemical oxygen demand:

$$\frac{dBOD}{dt} = \frac{1}{\tau}(BOD_i - BOD) - k_{bod}BOD - \frac{(v_{sed}BOD)}{dep} + k^{death}(133.3Phy)$$

Where:
BOD = BOD concentration leaving the reach (mgL^{-1})
BOD_i = input DO concentration (mgL^{-1}) (mean from all sources)
v_{sed} = settling velocity of BOD. A value of 0.25 ms^{-1} was used.

A.4. River water temperature model

<u>Equation A.9:</u> Change in water temperature is defined as follows:

$$\frac{dT}{dt} = \frac{1}{\tau}(T_i - T) - \frac{H(R_s - R_o)}{dep}$$

Where:
T_i = mean temperature (°C) from all sources
T = temperature in water leaving the reach (°C)
R_o = outgoing long-wave radiation (Wm^{-2})
H = heat flux coefficient (0.005 m^{-1})
The largest component for the outgoing radiation is the long wave back radiation which is given by R_o=0.97 σ T^4 (in which 0.97 is the emissivity constant of a water surface and σ is the Stefan-Boltzman constant (5.67051 10^{-8} Wm^{-2} k^{-4}) and T is the temperature in ^oK)

Reference

Boorman DB, 2003. LOIS in-stream water quality modelling. Part 1. Catchments and methods. *Science of the Total Environment* 314: 379-395.

Information	"Basic" model	"Local" model
Water quality data	[1]Periodic national-level monitoring only	Periodic monitoring; and local [4]continuous sensor-based monitoring at Sanctuary Bridge
River flow data	[2]Daily gauging station data from national level monitoring	Daily gauging station data from national level monitoring
Solar radiation data	[3]Hourly measurements from nearby Wattisham weather station from national network	Hourly measurements from nearby Wattisham weather station from national network
Groundwater discharge influences	No	Yes. In middle reaches. Estimated from local groundwater modelling (flow) and monitoring (quality).
Abstraction and effluent influences	No	Yes. Two agricultural abstractions (Wickham Market, Kettleburgh) and one sewage treatment works (Wickham Market).
Calibration of nutrient-related parameters	Yes	Yes
Calibration of ecosystem-metabolism related parameters	No. Estimated from other QUESTOR modelling in similar lowland UK river systems (a), or based on fitting average DO PBIAS across all Deben sites (b)	Yes
Information used to define hydraulic parameters	Stream width and gradient, estimated from catchment area and other QUESTOR applications.	Stream width from satellite imagery/aerial photography. Channel gradient from DTM. River level data from two locations (middle reaches). Roughness and macrophyte abundance estimated from qualitative stream bed observations (multi-site).
Channel control structures	Weirs identified from Ordnance Survey topographic maps. Default values used for characterisation.	Additional information provided from local photographic sources (EA staff).
Fractional light penetration	Percent riparian tree occupancy from aerial photography. 0% penetration through canopy assumed	Aerial photography, supported by local photographic qualitative observations.

Table A1: Information used to support Deben model applications. National-level data sets available to support the "Basic" model: (1) Environment Agency Water Quality Archive data accessible from a portal: http://environment.data.gov.uk/water-quality/view/landing. (2) Daily river flow data accessed via UKCEH National River Flow Archive: http://nrfa.ceh.ac.uk/data/search. (3) Solar radiation observations accessed at the British Atmospheric Data Centre (http://archive.ceda.ac.uk/). "Local" model supported by (4) YSI multi-parameter 6600 sonde including temperature and dissolved oxygen sensors. Sanctuary Bridge is an additional site not covered by national monitoring[1].

Appendix B: Indicators of hydrological alteration

Annual IHA code	Parameter	Dimension	Annual IHA code	Parameter	Dimension
IHA_01	Mean value for January	Magnitude	IHA_34	January Low Flow	Magnitude
IHA_02	Mean value for February	Magnitude	IHA_35	February Low Flow	Magnitude
IHA_03	Mean value for March	Magnitude	IHA_36	March Low Flow	Magnitude
IHA_04	Mean value for April	Magnitude	IHA_37	April Low Flow	Magnitude
IHA_05	Mean value for May	Magnitude	IHA_38	May Low Flow	Magnitude
IHA_06	Mean value for June	Magnitude	IHA_39	June Low Flow	Magnitude
IHA_07	Mean value for July	Magnitude	IHA_40	July Low Flow	Magnitude
IHA_08	Mean value for August	Magnitude	IHA_41	August Low Flow	Magnitude
IHA_09	Mean value for September	Magnitude	IHA_42	September Low Flow	Magnitude
IHA_10	Mean value for October	Magnitude	IHA_43	October Low Flow	Magnitude
IHA_11	Mean value for November	Magnitude	IHA_44	November Low Flow	Magnitude
IHA_12	Mean value for December	Magnitude	IHA_45	December Low Flow	Magnitude
IHA_13	1-day minimum	Magnitude	IHA_46	Extreme low peak	Magnitude
IHA_14	3-day minimum	Magnitude	IHA_47	Extreme low duration	Duration
IHA_15	7-day minimum	Magnitude	IHA_48	Extreme low timing	Timing
IHA_16	30-day minimum	Magnitude	IHA_49	Extreme low freq.	Frequency
IHA_17	90-day minimum	Magnitude	IHA_50	High flow peak	Magnitude
IHA_18	1-day maximum	Magnitude	IHA_51	High flow duration	Duration
IHA_19	3-day maximum	Magnitude	IHA_52	High flow timing	Timing
IHA_20	7-day maximum	Magnitude	IHA_53	High flow frequency	Frequency
IHA_21	30-day maximum	Magnitude	IHA_54	High flow rise rate	Rate
IHA_22	90-day maximum	Magnitude	IHA_55	High flow fall rate	Rate
IHA_23	Number of zero days	Magnitude	IHA_56	Small Flood peak	Magnitude
IHA_24	Base flow index	Magnitude	IHA_57	Small Flood duration	Duration
IHA_25	Date of minimum	Timing	IHA_58	Small Flood timing	Timing
IHA_26	Date of maximum	Timing	IHA_59	Small Flood frequency	Frequency
IHA_27	Low pulse count	Frequency	IHA_60	Small Flood rise rate	Rate
IHA_28	Low pulse duration	Frequency	IHA_61	Small Flood fall rate	Rate
IHA_29	High pulse count	Frequency	IHA_62	Large flood peak	Magnitude
IHA_30	High pulse duration	Frequency	IHA_63	Large flood duration	Duration
IHA_31	Rise rate	Rate	IHA_64	Large flood timing	Timing
IHA_32	Fall rate	Rate	IHA_65	Large flood frequency	Frequency
IHA_33	Number of reversals	Rate	IHA_66	Large flood rise rate	Rate
			IHA_67	Large flood fall rate	Rate

Table B1. List of annual indicators of hydrological alteration.

Code	Meaning (N=3, 7,14, 21)	Dimension
MA1	Mean of flow in N days	Magnitude
MA2	Median of flow in N days	Magnitude
MA3	Coefficient of variation in N days	Magnitude
MA4	Skewness of N days flows	Magnitude
ML1	Low flood pulse count N days	Frequency
ML2	The percentage of low flood pulse count in N days	Frequency
MH1	Number of occurrences during N days	Frequency
MH2	The percentage of low flood pulse count in N days	Frequency
EL1	Extreme low flow count N days	Frequency
EL2	The percentage of extreme low flood pulse count in N days	Frequency
EH1	Extreme high flow count N days	Frequency
EH2	The percentage of extreme high flood pulse count in N days	Frequency
RC	Mean rate of change in N days	Rate
RH1	Numbers of day change rises in N days	Rate
RH2	Percentage of day change rises	Rate
RL1	Numbers of day change decline in N days	Rate
RL2	Percentage of day change decline	Rate

Table B2. List of short-term indicators of hydrological alteration and their meaning.

Appendix C: Model parameter values and goodness-of-fit statistics

			"Basic" Model										"Local" Model									
Reach	Monitoring Site	Distance (km) upstream of Ufford Br	Width (m)	P	R	D	^{5}k	^{4}k	^{10}k	^{6}k	^{8}k	^{9}k	Width (m)	P	R	D	^{5}k	^{4}k	^{10}k	^{6}k	^{8}k	^{9}k
1	Cretingham Br	24.0	4.0	d	d	d	12.0	4.8	0	2.4	0.12	0	2.6	3.84	0.15	0.42	1.2	1.2	0	2.4	0.12	0
2	Brandeston Br	20.8	4.0	d	d	d	12.0	4.8	0	0.48	0.072	0	3.4	3.84	0.15	0.42	1.2	1.2	0	0.48	0.072	0
4	Sanctuary Br	16.1	4.0	d	d	d	12.0	4.8	0	1.44	0.144	0	3.6-3.8	3.84	0.15	0.42	1.8	1.8	0	1.44	0.144	0
11	Naunton Hall	3.3	6.0-8.0	d	d	d	12.0	4.8	0	0.48	0	0	3.5-5.0	3.84	0.15	0.42	1.8	1.8	0	0.48	0	0
13	Ufford Br	0.0	8.0	d	d	d	12.0	4.8	0	2.4	0	0	4.7	3.84	0.15	0.42	1.8	1.8	0	2.4	0	0

Table C1: Optimised parameter values (day^{-1}) (note values are converted to $hour^{-1}$ for model application) where:

Daily phytoplankton parameters: P = k^{pho}_{ref}, R = k^{res}_{ref}, D = k^{death}_{ref}

Default values used = d

FP values: basic model = 0.64, local model = 0.77

BOD decay = ^{5}k

Benthic OD = ^{4}k

Deamination = ^{10}k

Nitrification = ^{6}k

Denitrification = ^{8}k

P mineralisation = ^{9}k

	SRP	PP	NH4	NO3	SS	Temp	DO	BOD	Flow
N									
Cretingham	76		41	76		77	76		
Brandeston	323	309	352	360	340	354	71	56	hourly
Sanctuary	41		41	41	21	*14670	*14670		
Naunton	607	603	607	607	603	318	16		
Ufford	29		29	28		37	28	9	hourly
"LOCAL" MODEL									
Cretingham	-2.1/98		0.74/-23	0.69/-5.8		0.92/-3.1	0.25/-7.1		
Brandeston	-8.6/121	0.13/-5.0	0.05/-20	0.77/1.8	0.52/-40	0.86/-8.8	-0.1/-7.4	-2.2/0.5	0.99/-2.5
Sanctuary	-8.1/84		-5.7/9.7	0.75/0.9	0.35/-37	*0.72/-13.3	*0.03/29		
Naunton	-1.1/33	-0.11/-44	-0.08/-6.5	0.52/-0.7	-0.06/-59	0.71/-13.3	0.35/-2.8		0.58/-23
Ufford	-0.57/13		-24/150	0.43/-17		0.68/-13.6	0.20/-0.7		
"BASIC" MODEL									
Cretingham	-8.5/200		0.78/-4.2	0.63/13		0.03/-0.4	-0.1/-7.6		
Brandeston	-36/267	0.10/-39	0.04/-3.9	0.73/-8.6	0.52/-44	0.55/-7.9	-0.24/-12.6	-3.2/-81.9	0.99/-8.8
Sanctuary	-64/330		-7.3/19.5	0.67/-16.9	0.18/-43	*0.41/-17.0	*-0.33/32		
Naunton	-19/146	-0.22/-57	-0.48/48	0.44/-2.4	-0.07/-63	-0.03/-16.9	-0.76/-7.6		0.58/-31.5
Ufford	-11/181		-131/319	0.38/-17.4	0.18/-52	0.25/-21.0	-0.23/-4.2		

Table C2: Number of observations (N) and paired NSE/PBIAS values for local and basic model (2010-2019). Goodness of fit values shown for validation test period 2014-2019. *2018-19 continuous monitoring data, in a heterogeneous river reach environment (DO omitted from Figure 2, discussed in Section 4.3)