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The Science of the Total Environment 314–316 (2003) 335–377

the Science of the Total Environment
An International Journal for Scientific Research into the Environment and its Relationship with Man

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A review of currently available in-stream water-quality models and their applicability for simulating dissolved oxygen in lowland rivers

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Accepted 1 January 2003

Abstract

In this paper, a review is undertaken of the major models currently in use for describing water quality in freshwater river systems. The number of existing models is large because the various studies of water quality in rivers around the world have often resulted in the construction of new 'bespoke' models designed for the particular situation of that study. However, it is worth considering models that are already available, since an existing model, suitable for the purposes of the study, will save a great deal of work and may already have been established within regulatory and legal frameworks. The models chosen here are SIMCAT, TOMCAT, QUAL2E, QUASAR, MIKE-11 and ISIS, and the potential for each model is examined in relation to the issue of simulating dissolved oxygen (DO) in lowland rivers. These models have been developed for particular purposes and this review shows that no one model can provide all of the functionality required. Furthermore, all of the models contain assumptions and limitations that need to be understood if meaningful interpretations of the model simulations are to be made. The work is concluded with the view that it is unfair to set one model against another in terms of broad applicability, but that a model of intermediate complexity, such as QUASAR, is generally well suited to simulate DO in river systems.

Keywords: Dissolved oxygen; Lowland rivers; Mass balance; Hydraulics; Solute transport; Aggregated dead zone; Water quality processes; Water-quality models, SIMCAT, TOMCAT, QUAL2E, QUASAR, MIKE-11, ISIS

1. Introduction

A sufficient supply of dissolved oxygen (DO) is vital for all higher aquatic life. The problems associated with low concentrations of DO in rivers have been recognised for over a century and the impacts of low DO concentrations or, at the extreme, anaerobic conditions in a normally well-oxygenated river system, are an unbalanced ecosystem with fish mortality, odours and other aesthetic nuisances. When DO concentrations are reduced, aquatic animals are forced to alter their breathing patterns or lower their level of activity. Both of these actions will retard their development, and can cause reproductive problems (such as increased egg mortality and defects) and/or deformities. There is a long history of using quantitative techniques to assess the impacts of pollutants on

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doi:10.1016/S0048-9697(03)00063-9

DO in river systems. These range from the basic mass balance concepts used by the Royal Commission on Pollution in 1912 through to the present sophisticated use of computer software to simulate hydrodynamics, dispersion and pollutant kinetics in the natural environment. The Royal Commission of 1912 first used the concept of water quality mass balance to determine a safe level of waste discharge into freshwaters suing a fixed dilution ratio for effluent discharges entering a river. Their approach was designed to provide sufficient dilution of effluent to minimise the impact on the DO concentrations in the receiving water, but it took no account of the dynamics and reaction kinetics and so was unable to work satisfactorily beyond a narrow range of conditions. In 1925, Streeter and Phelps derived the classic equations for simulating DO and biological oxygen demand (BOD) in rivers. These equations have formed the basis of many water-quality models that have been developed around the world since that time. In the last twenty years, with the increased use of computers in the field of hydrology, there have been a number of significant developments in the field of water-quality modelling and these have resulted in a variety of models including SIMCAT, TOMCAT, QUAL2E, QUASAR, MIKE-11 and ISIS.

A large number of textbooks cover the principals of water-quality modelling such as James (1993) and Chapra (1997), which include references to particular modelling tools. There is also a very large body of literature that describes individual models and processes, but there is little guidance on the suitability of particular models or software for specific situations or applications. To complicate matters further, a 'water-quality model' can mean anything from a simple empirical relationship, through a set of mass balance equations, to a complex software suite. In this review, an 'available model' is taken to be a distinct computer programme or other obtainable piece of software in which the user can simulate water quality in streams and rivers by supplying physical and chemical data. Furthermore, the only models considered in this review are those that are capable of simulating DO in freshwater river systems.

2. Model usage world-wide

Water-quality models are widely used by environmental regulatory bodies and water utility companies around the world, and in England and Wales the Environment Agency (EA) is perhaps the largest user. Indeed, water-quality models have been used in almost all of the water quality improvement programmes carried out by the EA over the last ten years. Thus, the use of water-quality models is largely driven by legislation and regulations, and practises therefore vary between countries as the regulatory framework varies (Rauch et al., 1998).

Regulators carry out water-quality modelling exercises both as a routine operation in consent setting and increasingly as an investigative tool in planning improvements in catchment water quality. The models currently used by the EA for simulating non-tidal waters include RQP, SIMCAT, TOMCAT, ISIS, MIKE-11 and QUASAR. Many of the more simple consents set by the EA are made by using the RQP software suite, produced by Tony Warn. This software models a single discharge using statistical techniques and provides the user with a prediction of the impact on the general quality assessment (GQA) and other standards for any given substance. Since it is designed only for simulating single discharges, the RQP software is not suitable for modelling whole rivers and so is outside the scope of this review, but its methodology is similar to that used in SIMCAT and TOMCAT.

Some of the models used by the EA, such as MIKE-11 and QUAL2E, are also widely used by institutions in many other countries, but often water-quality models will be specific to one country, one institution, or even one river catchment. Most of the widely-used models are designed to simulate the traditional set of 'sanitary determinants' such as BOD, ammonium (NH_4^+) and DO in order to set consents for effluents from sewage treatment works and other dischargers of organic waste. In setting consents, regulatory bodies such as the EA have tended to use simple models with few processes such as SIMCAT where the determinant of interest is modelled as being either conservative (i.e. it undergoes no transformations), or diminishing by a first-order decay. This simple approach allows rapid applications to be carried out, but makes no attempt to relate these determinants to the wider range of influences that can affect them, such as photosynthesis or sediment interactions. For example, an application to design for improvements in the EA's GQA should represent nitrate, ammonium and DO processes. While this could be attempted by expressing the processes affecting each determinant as conservative or diminishing simply with time, it is unlikely that such a description would be a good one since no account could be taken of the influences of one determinant on the others. In particular it would be hard to justify the use of such a model in a predictive framework where conditions may be different from those in which the model was developed. Thus, for such an application one should consider using a model with a more detailed description of the processes to simulate the stream hydrochemistry.

A literature search on in-stream water-quality modelling produced a list of well over 100 papers written in the last 5 years, and so it is clear that this is an active area of research around the world. Within this list, few papers refer to specific models and the majority of these refer to the United States Environmental Protection Agency (USEPA) model QUAL2E, with reported applications in the Americas, Europe, Asia and Australasia. The wide use of this model receives no doubt related to it being freely available on the internet together with the availability of extensive literature. However, QUAL2E has not been used greatly in the UK and this is probably because it is a steady-state model designed to calculate the 7Q10 values used to set discharge consents in the USA (Shanahan et al., 1998). The American 7Q10 values are the concentrations that might be associated with the lowest seven-consecutive-day flow, expected to have a return period of ten years, but in the UK consents are generally set on the basis of an annual mean or percentile in line with European Union Directives. Thus, US modelling practises tend towards steady-state models while models used in the UK for setting consents generally use stochastic techniques–although these two are not mutually exclusive.

The literature review revealed few European papers that referred to specific models, and instead most were related to improvements in modelling techniques rather than specific software. Furthermore, many European studies have produced models that developed by individual research centres for individual river systems and so they are not generally available or obtainable. The main exceptions to this are the MIKE series of models that is developed by the Danish Hydraulics Institute, and the Systeme Hydrologique Europeen (SHE) (Abbott et al., 1986) which have been used more widely, although the SHE model is not strictly an in-stream water-quality model. In the UK, the MIKE-11 model is used mainly for the Urban Pollution Management (or UPM) Research Programme that has been adopted in the UK by water companies and the EA for examining the risk of transient pollution of receiving waters resulting from intermittent discharges, such as combined sewer overflows (Crabtree et al., 1996).

The most used models by the EA, SIMCAT and TOMCAT, rarely appear in the literature (Jamieson and Fedra, 1996), because they are not generally used for regulation outside of the UK and this is probably due to their stochastic component as well as a lack of commercial exposure. The ISIS model developed in the UK by HR-Wallingford and a consultancy Sir William Halcrow, does appear in the literature, but there are almost no references to ISIS as a model of water quality in freshwaters, it being used instead for modelling estuaries or for the design of flood defences and weirs. The models developed as a part of the LOIS programme appear in the related literature, and of particular interest to the modelling of DO in freshwaters are the models QUASAR (Whitehead et al., 1997) and the development of that model, QUESTOR (Eatherall et al., 1998).

The use of a particular model depends on the systems to be modelled and on the legislation in place in that country. Regulatory bodies tend to use 'tried and tested' models that are generally simple, while other organisations (such as academic institutions) often use models to investigate more fundamental aspects of processes or transport mechanisms. However, these more detailed models are often only applicable to small areas or specific catchments and so are not suitable for a wider group of users. This applicability may be related to data limitations and it is necessary to match model complexity with data availability. In larger systems (i.e. $>10\,000$ km^2), water quality data are generally collected to provide qualitative analyses while intensive monitoring and data collection will only occur at the small scale (i.e. $\lesssim 10$ km^2) where the objective is to quantify model parameters for specific processes. Thus, it will generally be the case that data will need to be collated from a number of sources when modelling large systems. The limiting factor of data availability explains the popularity of hybrid/stochastic models. These models provide the necessary statistical output for relating to the water quality standards, but they also require relatively little data because they generally do not attempt to represent hydrochemical processes other than by a simple first-order decay rates. Because of this, they can be applied to almost any river catchment with no detailed knowledge of that catchment, but the assumptions made and the limitations of using a model with such simple processes must be acknowledged.

3. Model terminology

Models are usually grouped into categories based on (1) the environment modelled; (2) the purpose of the model; (3) the number of 'dimensions' considered; (4) how the processes are described; (5) whether the data used are discrete observed measurements or statistical distributions; and (6) whether temporal variability is considered as shown in Fig. 1.

The subdivisions based on purpose can be rather subjective, but they do provide useful information with regard to the limitations of a particular model. For example, hydrochemical models are designed to model the chemical and biological processes that affect the determinants of interest and the main aim of the model is to represent water chemistry. A mixing-zone model will only represent that proportion of the system that is immediately downstream of, or adjacent to, a discharge into the main water body, and a time-of-travel model provides the user with the time of arrival of pollutants downstream of an 'incident' and so is only used to simulate simple pollution incidents. Time-of-travel models do not generally include anything other than a conservative description of solute movements, but are essentially simple in-stream water-quality models. The division is used here because in-stream models are not used routinely in pollution incident assessments unless they have been calibrated specifically for that purpose.

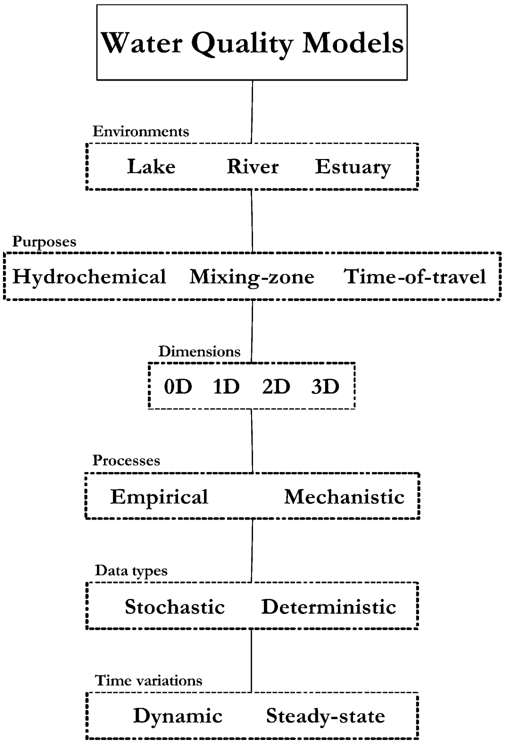

Fig. 1. Subdivisions of water-quality models in common use.

The dimensions simulated by a particular model will provide information on both the complexity of a model and also on its suitability to specific applications. A zero-dimensional (0D) model does not represent the processes of dispersion of contaminants in any direction, but simply represents the volumes and concentrations assuming that the water body is completely and instantaneously mixed. A one-dimensional (1D) model represents the water flow and the advection and dispersion of solutes in just one direction (i.e. downstream in a river model) and so the stream is assumed to be completely (and instantaneously) mixed across its width and depth. Following from this, a two-dimensional (2D) model will either simulate dispersion across the width or the depth of the stream, but not both. A width-averaged model is often used in simulating thermal stratification of deep-water bodies or when there may be layers of salt and freshwater at different depths in estuaries. Depth-averaged models are useful when the river is broad and shallow such that stratification is limited, but dispersion across the width of the river is slow. Three-dimensional (3D) models account for the water flows and solute transport in all directions. These models are highly sophisticated, and 3D water-quality models are usually reserved for large (i.e. deep and wide) estuaries where the mixing patterns are complex.

The way in which the influences on determinants are described by a model are often divided into two broad categories of empirical and mechanistic, but the distinction is not clear-cut and mechanistic descriptions will often contain empirically derived components. Empirical models make no attempt to explicitly model hydrochemical processes; instead the model inputs are related directly to its outputs by one or more relationships obtained experimentally. Because of this, some empirical models are referred to as 'black-box' models as they do not attempt to represent any mechanism. Typically, empirical models take the form of regression relationships, and are useful for investigating cause-and-effect relationships if they are used in a formal statistical environment. They are particularly useful because such models can cope with a number of inputs with minimal computation (Kirchner et al., 1993), but it is important to understand that they can only be used with any confidence within the ranges of the data used to parameterise them. Thus, an empirical model can never be used with confidence to predict long-term changes, while it is assumed that one can obtain some predictive capabilities if the models are based on physical and chemical principles (Warfvinge, 1995).

Mechanistic models simulate the changes in flow rate and water quality along a river (represented by individual reaches or stores) by attempting to represent the processes that occur in the real system. The transfer of water and solutes between stores is governed by mass-balance budgeting, and within each reach there may be additions from discharges, removal by abstractions and transformations of determinants. The rates at which these processes occur are based on the influences of a number of determinants physical, chemical and biological and the intention is that all of the rates can be derived from measured data. Thus, although such models are highly complex and data intensive, by eliminating the need for extensive calibration it is intended that such models can be applied to other systems and be used to assess the impacts of change (Bathurst and O'Connell, 1992). Unfortunately, in practise, the aim of eliminating calibration has not been realised, and mechanistic models will invariably require a certain degree of calibration. If new calibrations are required whenever a change is made to the system then, like with empirical models, the mechanistic model will only be applicable within the data range for which they were calibrated. However, if it can be shown that when the model has been calibrated once, it will reproduce reliable output over a range of situations and conditions, then it can be argued that the model can be used in a predictive framework.

A further division of models is generally made between stochastic and deterministic models. A deterministic model uses fixed input variables and there is a predetermined relationship between the inputs supplied by the user and the output variables. The calculations made by the model assume that the input and output variables are fixed (i.e. not subject to error) and so a deterministic model will always produce the same output given the same inputs. The term stochastic is used to describe several different types of model, and is often used interchangeably with 'Monte Carlo' techniques. In this review, a model is described as stochastic if the model runs many times using different input variables (such as boundary conditions or parameters) for each run that have been selected from a defined statistical distribution, and produces output also in the form of a statistical distribution. Monte Carlo methods have been devised because it has been shown that models based on the simple mass balance approach are only correct if the data used in the mass balance equation relates to the same instantaneous period of time (Warn and Brew, 1980). As soon as mean data values are used incorrect results are obtained, but if the mean values are replaced instead with distributions the solution method can be altered so that the mass balance method is repeated many times with different values taken from the specified distributions. This is Monte Carlo simulation, and can be adapted so that it is possible to apply correlations between the determinants and specify representative distribution shapes for the 'random' selection of flow and quality values.

The Monte Carlo simulation method can be applied to a single discharge or on a catchment wide basis to produce probabilistic results of mixing processes (Warn and Brew, 1980). The downstream impact can also be routed down the system as with any other water-quality model and appropriate pollutant decay processes applied to predict the statistics of the water quality at some point downstream. In this manner, the Monte Carlo approach will produce means and other statistics for concentrations along the river. The final division in Fig. 1 describes the way in which a model handles temporal variability. A steady-state model is one in which the input variables may be spatially distributed but are time invariant, and the output obtained is that which would occur if each determinant had reached an equilibrium, i.e. when $dC/dt=0$. A dynamic model, however, simulates both spatial and temporal variability. Thus, input variables and model parameters will vary with time, and the model output will also be time varying.

With such a range of different nomenclature, it is of no surprise that the terminology used to describe water-quality models can be confused and that different authors may use the same terms to describe different techniques. Further complications arise because the definitions are in no way exclusive and so a model may be both stochastic and deterministic if it is able to run in more than one 'mode'. Even within these broad terms there may be substantial variability. For example, a deterministic and mechanistic model might describe the chemistry of oxygen in a river by a series of transformations and exchanges including photosynthesis, respiration, sediment processes, the nitrification of ammonium, atmospheric reaeration, and the oxidation and biological degradation of organic matter, or it might be described as just two first-order rate constants representing an unlimited oxygen demand and continuous reaeration. At present, most stochastic models incorporate only simple processes, but this is really only due to the very long run-times that would result from multiple runs of a complex model and this is not a fundamental restriction on the application of stochastic models.

4. Mechanistic water-quality modelling approaches

All the models described here are process-based or mechanistic, in that some process descriptions are included. The individual models may attempt to include many processes, or may lump several processes together, but the mechanistic models can all be assumed to have predictive capabilities to a greater or lesser extent, because they are based on physical and chemical principles. Eq. (1) provides the basic governing solute transport equation for all mechanistic water-quality models:

$$\frac{\partial \vec{c}}{\partial t} = -\vec{u}\frac{\partial \vec{c}}{\partial x} - \vec{v}\frac{\partial \vec{c}}{\partial y} - \vec{w}\frac{\partial \vec{c}}{\partial z} + \frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial \vec{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_y \frac{\partial \vec{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_z \frac{\partial \vec{c}}{\partial z}\right) + \Delta\vec{c} \qquad (1)$$

where $\vec{c}$ is an multi-dimensional mass concentration vector for each of the determinants; t is the time; x, y, and z are spatial coordinates; u, v, and w are the corresponding velocity components, ε_x, ε_y, and ε_z are turbulent diffusion coefficients for the directions x, y, and z, respectively; and $\Delta\vec{c}$ is a term representing the rates of change of determinants due to internal transformations in the reach (e.g. nitrification or reaeration). Eq. (1) also allows one to identify a useful framework and the main model elements, and these are (Rauch et al., 1998):

- the hydraulic model for deriving the velocity and turbulent diffusion components;
- the transport equation for describing movement of conservative solutes;
- the water-quality process equations that describe the transformations of determinants.

Different approaches may be taken to each of these elements and it is the combination of approaches used that generally differentiates one model from another. Thus, the approach that a particular model takes in terms of its conceptual basis; flow, transport, and process descriptions; calibration and evaluation; and also the software that allows the model to be used all define what a model is, while the terminology explained in Section 3 are used to describe what a model is capable of.

4.1. Hydrodynamics and hydraulics

The flow of water in a river can be described by using equations that conserve mass and momentum within a reach. This is known as the Navier–Stokes or Reynolds method and the actual form of the hydrodynamic model depends on the assumptions characterising turbulence. A number of complex methods are available for the solution of these equations in three dimensions, but for water-quality purposes in freshwater systems such complex 3D solutions are not usually necessary and so the Navier–Stokes model may be simplified. This is reasonable because the terms describing the diffusion of momentum due to turbulence are, in general, insignificant relative to the remaining terms in the equations (MacDonald et al., 1995). Thus, flow is often considered to be 1D (i.e. parallel to the bed) assuming that longitudinal accelerations are far more significant than those transverse or vertical. Writing equations for the conservation of mass and momentum separately results in the pair of equations called the Saint Venant equations, i.e.:

$$\frac{\partial A_x}{\partial t}+\frac{\partial Q}{\partial x}=q \quad \text{(conservation of mass)} \tag{2}$$

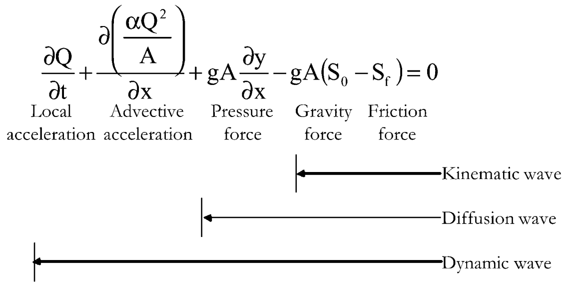

Fig. 2. The St. Venant equation for momentum and how the simpler forms may be derived by dropping terms as shown (redrawn from Chow, et al., 1988).

and

$$\frac{\partial Q}{\partial t}=gA(S_0-S_f)-gA\frac{\partial y}{\partial x}-\frac{\partial(\alpha Q^2/A)}{\partial x} \quad \text{(conservation of momentum)} \tag{3}$$

where A is the wetted area (or reach volume per unit length), t is the time, Q is the discharge, x is the distance downstream, q is the lateral inflow per unit length, g is the acceleration due to gravity, y is the depth, α is a momentum coefficient, S_0 is the bed slope and S_f is the friction slope.

As depicted in Fig. 2, the hydrodynamic model can be further simplified by dropping some of the terms from the conservation of momentum equation. Dynamic wave models solve the full equation, diffusive models ignore the acceleration terms, and kinematic models also disregard the pressure gradient term (that is essential for the description of backwater effects).

Those models taking a steady-state approach can also drop the term $\partial Q/\partial t$ since this will be equal to zero in a time-invariant system and even this can be simplified by using the semi-empirical equations of Manning and Chezy to obtain the depth and velocity in the channel:

$$Q=A\bar{U}=\frac{AR^{2/3}S_0^{1/2}}{n} \quad \text{(Manning)} \tag{4}$$

$$Q=A\bar{U}=AC\sqrt{(RS_0)} \quad \text{(Chezy)} \tag{5}$$

where $\bar{U}$ is the mean velocity; R is the hydraulic mean depth (defined as $R=A/P$, where P is the wetted perimeter); and n and C are the Manning and Chezy coefficients, respectively, which represent a roughness (or frictional) factor.

4.2. Solute transport

The transport of dissolved substances or solutes in rivers is governed by advection and turbulent diffusion as in Eq. (1). As with the hydrodynamic model, some simplifications of the transport equation can be made, for the purposes of water-quality modelling, by reducing the number of spatial dimensions considered. This is reasonable because, for relatively shallow rivers the distance of 'complete' mixing along the depth is short and thus a depth integrated (i.e. 2D) form can be applied. This integration lumps the effects of non-uniformity into a 'Fickian' advective velocity term, and the lumped diffusion parameters are called dispersion coefficients. The dispersion coefficients will be affected by the slope, morphology, and roughness, etc., but can be estimated from empirical formulae or from the results of tracer experiments.

If the river-reach being simulated is long with respect to the mixing length over the cross-section and the transport is dominated by longitudinal changes the 2D model can be integrated again to produce a 1D advection–dispersion equation (ADE) that is averaged over the cross-section of the river, i.e.:

$$\frac{\partial M}{\partial t}=\frac{\partial(VC)}{\partial t}=\frac{\partial\left(AD_{\mathrm{L}}\frac{\partial c}{\partial x}\right)}{\partial x}\mathrm{d}x-\frac{\partial(A\bar{U}C)}{\partial x}\mathrm{d}x+V\frac{\mathrm{d}C}{\mathrm{d}t}+\Delta M \tag{6}$$

where M is the mass of solute, V is the volume of water in the element ($=A\,\mathrm{d}x$), C is the concentration of the determinant, A is the cross-sectional area, D_{L} is the dispersion coefficient, x is the distance along the element, $\bar{U}$ is the mean velocity and ΔM is the net mass influence of external sources and sinks (such as discharges and abstractions). In Eq. (6), the first term represents the dispersion, the second the advection, the third internal transformations and the last external sources and sinks.

Because the model averages over the cross-section, the mass of solute is equal to the volume multiplied by its concentration, and so one can write that:

$$\frac{\partial M}{\partial t}=\frac{\partial(VC)}{\partial t}=V\frac{\partial C}{\partial t}+C\frac{\partial V}{\partial t} \tag{7}$$

In a steady-state model $\partial Q/\partial t=0$ and so $\partial V/\partial t=0$, i.e.:

$$\frac{\partial M}{\partial t}=V\frac{\partial C}{\partial t}$$

Thus, given that $V=A\,\mathrm{d}x$, the following equation can be used for steady-state simulations:

$$\frac{\partial C}{\partial t}=\frac{\partial\left(AD_{\mathrm{L}}\frac{\partial c}{\partial x}\right)}{A\partial x}-\frac{\partial(A\bar{U}C)}{A\partial x}+\frac{\mathrm{d}C}{\mathrm{d}t}+\Delta S \tag{8}$$

where ΔS is the net concentration influence of external sources and sinks.

An alternative simplification is to neglect the dispersion term and so produce an ordinary differential equation (ODE) that is easier to solve and analyse by introducing a 'travel time' as an independent variable. This integration is made by assuming that complete mixing occurs within each of a number of interconnected elements within the original reach for which the mass balance is expressed by:

$$\frac{\mathrm{d}C}{\mathrm{d}t}=Q_{\mathrm{i}}(C_{\mathrm{i}}-C)/V+\Delta C \tag{9}$$

where the subscript 'i' refers to the inflow concentration and terms without subscripts refer to the concentration in the element, which is the same as the outflow from that element; ΔC represents the internal transformations of the determinant and is equivalent to the term dC/dt in the ADE. A river simulation based on such equations is often referred to as Continually Stirred Tank Reactors in Series (CSTRS), because the model assumes perfect mixing within each element and so is similar to the design models of chemical engineers. This technique is popular because the ODE form allows for the easier formulation of methods for calibration and model evaluation when compared with partial differential equation (PDE) models, but care must be taken to ensure that the implicit or numerical dispersion introduced when solving the equations approximates that seen in the real system (Rauch et al., 1998).

4.3. Internal conversion or transformation processes

The solute transport equations described in Section 4.2 are sufficient for simulating substances that do not undergo any transformations or reactions within the reach or element (i.e. conservative substances). However without modification or extension, those equations are unable to predict the changes of determinants such as DO which are affected by a number of factors. The transformations occurring to individual determinants independent of advection, dispersion and external inputs are defined by the term dC/dt in the advection–dispersion transport equation and by the term ΔC in the CSTRS method.

The historical development of water-quality models has generally been one of maintaining a core of determinants and processes while extending the models to include additional determinants and/or process descriptions. The result of this is a general pattern of increasing complexity with time. The simplest forms of equation commonly used in water-quality models are those representing conservative determinants or first-order decay, i.e.:

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -KC \tag{10}$$

where the rate of decay is proportional to the concentration of the substance remaining, and evaluated using a coefficient K called the reaction rate parameter or rate coefficient. Simple models use equations of this form to describe the transformations affecting any determinant in a river reach, but in the case of DO this is clearly too simplistic. The classic equations of Streeter and Phelps (1925) are a combination of two first-order decays, and models of DO since then have gradually included more process descriptions and variables in an attempt to improve the simulations. Thus, a water-quality model may be constructed by the simultaneous solution of a set of equations describing each of the determinants involved. Since the greatest distinction between models tends to be the way in which the processes are described, much of the following review is concerned with recounting the way in which different models simulate the transformation processes. Most of these processes require the user to provide values for rate parameters and to calibrate these parameters in order to achieve a fit with the observed data. Generally there will not be enough time or funding for field investigations of these parameters, but clearly this route should be explored where possible. In the UK there is no one reference that provides default values for all these parameters, but one can find suggested values or estimation methods for most parameters in the USEPA report by Bowie et al. (1985), or in the models themselves.

5. A review of available in-stream models

The models selected for a more detailed review here are all mechanistic models of in-stream processes affecting river water-quality and are listed below:

1. SIMCAT
2. TOMCAT
3. QUAL2E
4. QUASAR, HERMES and QUESTOR
5. MIKE-11
6. ISIS

All the models described here are mechanistic, in that at least some of the process descriptions are included. However, as already mentioned, some of these process descriptions may be empirical or semi-empirical in nature and processes may be lumped together. The stochastic models in the list (SIMCAT and TOMCAT) make use of Monte Carlo analysis techniques.

5.1. SIMCAT

In the UK, several river water-quality modelling tools have been developed since the introduction of percentile based standards which utilise the Monte Carlo simulation approach. SIMCAT (SIMulation of CATchments) is an EA model that describes the water quality of rivers in a catchment. It is used by the EA to help plan the measures needed to improve river water quality by predicting the behaviour of water quality, as summary statistics such as the mean and 90th percentile. SIMCAT is a stochastic, 1D, steady state, deterministic model which represents inputs from point-source effluent discharges and the behaviour of solutes in the river on the basis of three types of behaviour:

- conservative substances which are assumed not to be transformed in any way such as chloride;
- non-conservative substances which decay, where a first-order (i.e. exponential) relationship is used to represent the transformation, for example BOD and nitrate;
- DO is represented by a relationship involving BOD decay, temperature and reaeration.

The river system being modelled is divided into user-defined reaches, which may be any length, but are generally taken to be the distance between tributaries or other points of interest. The model can represent more than one influence or structure in any one reach and a diffuse runoff can be specified by the user as a flow rate and quality, or be added by the model as an auto-calibration parameter.

5.1.1. Conceptual model

SIMCAT represents the river reaches as a CSTRS model as described in Section 4.2 and assumes that the condition of the stream does not vary with time. The steady-state assumption limits the model, but also allows it to be applied quickly and with relatively little data. Fig. 3 illustrates the conceptual reach model where *Q* is the flow, *C* is the concentration of the determinant of interest and the subscripts ‘o’, ‘i’, ‘t’, ‘e’ and ‘a’ refer to the outflow from the reach, the upstream input to the reach, tributary inputs to the reach, effluent discharges and abstractions, respectively. Internal transformations such as physical, chemical or biological processes in the water column are represented by the term ΔC.

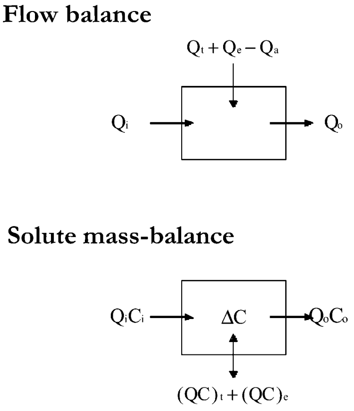

Fig. 3. Conceptualisation of the reach model used by the model SIMCAT.

From Fig. 3 it is clear that SIMCAT does not use an advection–dispersion transport model, but assumes perfect and instantaneous mixing throughout the reach, with solutes moving at the same velocity as the water. A mass balance is performed at the top of each reach using simple flow and load additions and an empirical velocity–flow relationship for that reach is used to derive the velocity of the water (and therefore the solutes). The calculated velocity is also used to compute the residence time for the reach, and then the solute concentrations are subjected to first-order decays to calculate the concentrations of the determinants that will enter the next reach.

5.1.2. Processes

SIMCAT simulates in-stream processes at steady-state (i.e. time invariant) and because the model simulates the steady state the simple load addition formula at the top of each reach is sufficient as a hydraulic model. The flow and solute mass-balances for a reach are therefore:

$$Q_o = Q_i + Q_t + Q_e - Q_a \text{ and } C_o = \frac{Q_i C_i + Q_t C_t + Q_e C_e}{Q_r + Q_t + Q_e} \tag{11}$$

The velocity of the water is calculated from the flow by the following empirically derived relationship:

$$v = aQ^b \tag{12}$$

where v is the velocity, Q is the flow rate and a and b are constants. The residence time can then be calculated by using the reach length (L) such that:

$$\tau = \frac{L}{v} \tag{13}$$

The determinants being modelled may be treated either conservatively or as having a first-order decay, and the model includes chloride (conservative), BOD (first order), ammonium (first order) and DO as a standard suite. In the case of DO the model is made slightly more complex by including atmospheric reaeration as in the Streeter and Phelps (1925) model, i.e.:

$$\frac{dC}{dt} = -K_r L + K_a (C_s - C) \tag{14}$$

where C is the DO concentration, C_s is the saturation concentration, L is the BOD, K_r is the rate of removal of BOD, and K_a is the reaeration rate coefficient which is entered as a single value by the user. The method of Elmore and Hayes (1960) is used to estimate the DO saturation concentration, i.e.:

$$C_s = 14.652 - 0.41022T + 0.0079910T^2 - 0.000077774T^3 \tag{15}$$

where T is the temperature in degrees Celsius.

5.1.3. Data requirements

The river system must be divided into a network of rivers and each river into a series of reaches which are defined between confluences or user-defined points. The connections between reaches must be defined together with physical parameters that define the extent of the system and reaction rates. Flow and quality data are entered for the top of the main river, all tributaries and any effluent discharges or abstraction in the system, and these ‘features’ are assigned to the appropriate reaches. Because SIMCAT is a stochastic model using the Monte Carlo method, the inputs are not single values, but descriptions of the statistical distribution for that determinant. The model accepts distribution descriptions as annual means and standard deviations, from the following distributions:

- Constant
- Normal
- Log-normal
- 3-Parameter log-normal

Non-parametric distributions calculated by the Weibull method may also be used, but there is a limit of 40 sets of non-parametric data because the details of each distribution must be stored in a separate file. Seasonal distributions (monthly only) can be entered in a similar manner, but in this case the data entered are monthly means and standard deviations.

5.1.4. Model operation

SIMCAT can model up to 600 reaches and can include up to 1400 ‘features’ such as rivers, discharges, abstractions, diffuse pollution, and weirs. Once the model skeleton has been assembled, the model can be run with up to 2400 shots possible. For each run, the model randomly selects values for flow and quality from the given distributions for all of the inputs and can take account of default or user-defined correlations between flow and quality at different sites. For example, the user can specify a percentage correlation between the flow rate at an effluent discharge and the flow in the receiving river. Starting at the top reach in the system, the process equations are solved for each determinant the output from this reach is then used as the inputs for the next reach in the network and so on down the system. This procedure is then repeated for the required number of shots and summary statistics for each reach are calculated from the results.

The model can be run in four different ways. The first technique uses the data as provided by the user and is used for manual calibration; the second uses auto-calibration algorithms to check the flow and quality; the third sets effluent quality in order to achieve required river water quality objectives; and the fourth sets effluent standards that would permit no deterioration in water quality. When using the auto-calibration function of SIMCAT, the model feeds in extra flows as a function of the river length until the simulated flows match those observed in the river at flow gauges. It then calculates a series of adjustments to the quality parameters in order to match simulated quality distributions with those observed at monitoring stations. To do this, the model results are first compared with data at a monitoring station and then it calculates the adjustments that need to be made to the parameters and velocity to allow exact agreement with measured data. The model then repeats the calculations downstream of the last monitoring station using the new parameters. The new results are compared with the monitoring station data and the process of parameter adjustment is repeated, if necessary until a stable match is obtained.

5.1.5. Outputs

SIMCAT produces summary statistics (means and 90th or 95th percentiles) for each determinant for each reach and confidence limits are also provided. The latest versions of the software also include a data plotting facility which can be used to display and print results. SIMCAT estimates the confidence limits (i.e. the degree of error) of the results assuming that the distributions are normal or log-normal. It first estimates what is termed the 'effective sampling rate' (ESR):

$$\mathrm{ESR}=\frac{nl+NL}{l+L} \tag{16}$$

where l and L are the loads of a determinant in the river and n and N are the numbers of samples. The errors are then calculated by substituting the factor t_0 for the standard normal deviate for the appropriate percentile, where:

$$t_0=\frac{\sigma+\lambda\sqrt{\left(1+\frac{\sigma^2}{2\mathrm{ESR}-1}-\frac{\lambda^2}{2\mathrm{ESR}-1}\right)}}{\sqrt{\mathrm{ESR}\left(1-\frac{\lambda^2}{2\mathrm{ESR}-1}\right)}} \tag{17}$$

and

$$\sigma=z\sqrt{\mathrm{ESR}} \tag{18}$$

where z and λ are estimates of the standard normal deviate for the appropriate percentile.

5.1.6. Discussion

This approach to water-quality modelling is perhaps over-simplistic, but it is quick (aided by auto-calibration routines), easy to use and it is able to consider the errors associated with sampling rather than the errors associated with calibration found in more detailed deterministic water-quality models. However, SIMCAT is limited by the fact that there is no allowance for temporal variability and it is unlikely that the DO model will produce satisfactory results for productive rivers when there is no accounting for photosynthesis, respiration or any sediment oxygen demand, or where the reaeration rate does not vary with flow.

As with all water-quality models, the results will be limited by the quality of observed data provided, for example the distributions should be generated from large data sets if they are to be meaningful. However, the model has been used successfully in the UK for many years and is recognised in the EA as being a practical water-quality management tool to support catchment management and discharge control on a routine basis. In its current form, SIMCAT is suitable for modelling determinants in freshwater that do not rely on sediment interactions and where the simple processes simulated are a reasonable approximation of the real system. SIMCAT provides the user with annual statistics and the model can quickly run the effects of changes in effluent discharge conditions and so is useful for consent setting exercises.

5.1.7. Applicability to simulating do in lowland rivers

It is clear that the model SIMCAT is capable of producing simulations of DO in freshwater systems, and indeed it has been used by the EA for this purpose as a part of consent setting exercises. Because it is a relatively simple model in terms of processes and steady-state, the data requirements are low (although the distributions should be generated from large data sets) and this means that the model can be set up quickly. Auto-calibration routines can also improve the speed and efficiency of using this model, and the stochastic nature of SIMCAT means that it is well suited to use within the framework of UK environmental legislation. However, it is unlikely that the model will produce tight DO simulations in many situations since the processes only include a first-order decay of BOD and atmospheric reaeration. As a steady-state model, SIMCAT cannot represent temporal variability, which can be significant in lowland rivers, and although monthly distributions can be entered as an alternative to annual ones this can only provide limited improvements whilst increasing the data requirements significantly. A major concern regards the auto-calibration routines. Whilst they will certainly expedite model application, it will be too easy for an inexperienced user to accept parameter values or 'runoff' rates for the systems that are unrealistic. If the preceding limitations are accepted and understood, SIMCAT will continue to be of use to regulatory bodies such as the EA, but the lack of a dynamic mode and the overly simplistic processes suggest that this model is not particularly suitable for complex scenarios or in a predictive context.

5.2. TOMCAT

The model TOMCAT (Temporal/Overall Model for CATchments) was developed by the UK water utility company Thames Water in the early 1980s (Bowden and Brown, 1984). The model was developed to assist in the process of reviewing effluent quality standards at all Thames Water sites in order to meet river-water quality objectives. With this in mind, the model was designed so that rapid applications to any catchment were possible, it could allow the estimation of diurnal and time-of travel effects, and be able to correlate any effluent discharge to the river with the flow in the receiving water. The correlations enable TOMCAT to take account of seasonal and (some) diurnal effects in the observed quality and flow data and then reproduce these effects in the simulated data. There are number of different versions of the model adapted for specific purposes and the software is available from Thames Water.

5.2.1. Conceptual model

The conceptualisation for TOMCAT is essentially identical to that in SIMCAT, i.e. a steady-state CSTRS model, and as with SIMCAT the model takes a Monte Carlo stochastic approach. However, TOMCAT allows for more complex temporal correlations. The river system in TOMCAT is defined by a number of 'events' that are specified at the tops of rivers and reaches, confluences, effluent discharges, abstractions and monitoring sites. These events are linked by three basic processes (Bowden and Brown, 1984):

- inputs;
- internal transformations and additions to flow from runoff and groundwater;
- flow mixing and mass balance.

Where the inputs can be the distributions supplied by the user (for example at the top of a river) or the simulated flow and quality from an upstream reach. Reaches are assigned between confluences and gauging stations or wherever set by the user.

5.2.2. Processes

The flow model in TOMCAT uses the same simple flow and load additions used by SIMCAT (Eq. (11)). The process equations describing the concentrations of solutes are also identical to SIMCAT, except for those used to simulate the temperature and DO. The river temperature (T) is assumed to tend towards the air temperature (T_{air}), i.e.:

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -K_{\mathrm{T}}(T - T_{\mathrm{air}}) \qquad (19)$$

at a rate governed by a first-order rate coefficient K_T, and the DO model incorporates nitrification as well as atmospheric reaeration and the oxidation of BOD, thus:

$$\frac{dC}{dt} = K_a(C_s - C) - \frac{dL}{dt} - 4.57\frac{d[NH_4]}{dt} \tag{20}$$

where C is the concentration of DO, K_a is the reaeration rate coefficient, C_s is the saturation concentration of DO, L is the BOD concentration and $[NH_4]$ is the ammonium concentration. In TOMCAT, the reaeration rate coefficient is not determined using one of the standard empirical or semi-empirical methods, but from a 'user-supplied' reaeration parameter (K_u), the river width (W) and the cross-sectional flow area of the channel (A) i.e.:

$$K_a = \frac{K_u W}{A} \tag{21}$$

Temperature dependence is included as a linear increase in K_a with increasing temperature.

5.2.3. Data requirements

Two types of input data are required to run TOMCAT. The first is fixed values, generally physical parameters that define the extent of the system or reaction rates; the second is the flow and quality data that are used by the model as inputs to the process equations. These latter data are given as means and standard deviations of a normal distribution or of logged data (i.e. a log-normal distribution), percentage points on a non-parametric distribution, or as single values. As with SIMCAT, these distribution statistics must be generated from large data sets if they are to provide meaningful inputs to the model.

The main model structure is defined by the number of sub-catchments to be simulated, the mean monthly air temperatures, the number of 'shots' (model runs) that will be carried out and the number of 'seasons' that will be included in the model inputs together with the number of months in each season. Boundary conditions of flow and quality are supplied as single or seasonal distributions at events, and a number of reach parameters are supplied for each user-defined reach. These include:

- Reach length (km)
- Mean cross sectional area (m^2)
- Depth (m)
- Catchment number for estimating the (diffuse) catchment runoff
- Scale factor for runoff (i.e. the proportion of the total runoff for the catchment which the reach receives per km).
- Ultimate BOD concentration (mg $O_2\,l^{-1}$)
- BOD decay rate parameter (day^{-1})
- Ultimate ammonium concentration (mg NH_4-$N\,l^{-1}$)
- Ammonium decay rate parameter (day^{-1})
- Oxygen exchange rate parameter (m day^{-1})
- Thermal equilibrium rate constant (day^{-1})

Observed data are also normally included for the purpose of calibration and, at the bottom of the system, it is a requirement of the model that observed data are supplied in the form of seasonal distributions from a gauging station. Unfortunately, this means that the model cannot therefore be used in a predictive framework in terms of flow, although this is not what the model was designed for.

5.2.4. Model operation

During a model run, values are selected at random from the flow and quality distributions and, to maintain correlations with stream conditions, the random number generator can be set to be in or out of phase with flows in the river as required. TOMCAT is also able to simulate the action of storm water overflows by 'diverting' effluent discharges to an alternative outlet if the flows rise above a certain threshold. Once the input values have been chosen, the model calculates the flow and quality in each reach (from the top to the bottom of the system) by solving the process equations and this is repeated for the number of runs requested. For each simulation, TOMCAT sets up a temporal index consisting of a month-of-the-year index and an hour-of-the-day index that defines which seasonal and diurnal effects should be included. Temporal compatibility between adjacent sites is maintained by adding calculated times of travel to the hour-of-day index. The indices are allocated to successive simulations in rotation so that all 12×24 month–hour combinations are represented. This means that two 'bodies of water', for example a river reach and an effluent discharge, will only mix if they have the same temporal indices, i.e. if they arrive at the same place at the same time.

Simulated flows in the river are compared with observed data from gauging stations and are automatically calibrated to the observed data by incorporating 'catchment runoff' in addition to the user-supplied headwater (i.e. the tops of each river) and artificial (i.e. discharge and abstraction) flows. The simulated water-quality determinants are calibrated manually by adjusting the parameters until a statistical test of the distribution shows no significant difference between the modelled and observed data at each monitoring point. In this way, TOMCAT can be used for simulating the current conditions of flow and water-quality in the catchment, but the model can also be used to assess the requirements for making improvements to the quality of water in the catchment. To do this, the user is able to adjust the effluent flow rate and quality at a simulated discharge site in order to test the likely impacts on the downstream water quality. This tool can be used to see what changes to the effluent discharge would be required in order to meet legislative standards or more generally desirable conditions in the river. The user is also able to make similar changes to tributaries that have no associated flow or quality data so that the model accurately predicts the observed flow and quality below its confluence with the main river.

5.2.5. Outputs

The standard output file provides percentiles at each monitoring station in the system so that the simulations can be compared to measured values for the purposes of calibration and model evaluation. The use of temporal indices also allows the user to choose particular 'time windows' to examine. TOMCAT can also provide the user with the output from any reach and the values of inputs that were chosen for each shot. The latter feature is useful for evaluating how well the model has worked in more detail and TOMCAT includes statistical analyses such as the Kolmogorov–Smirnov, Mann–Whitney U or chi-squared tests for identifying the 'goodness of fit' between simulated and observed data.

5.2.6. Discussion

The TOMCAT model has limited functionality in terms of the processes included, but the use of seasonal statistics does allow for potentially greater accuracy than could be achieved in the similar SIMCAT model. Furthermore, the model also allows the user to obtain the results of each model run so that statistical analyses may be carried out using techniques that are not built in to the model. However, the model is less accurate than SIMCAT in the way it simulates the flow velocity as TOMCAT relies solely on the cross-sectional area of the river. This method removes the need for an empirical velocity–flow relationship, but can require arbitrary decay coefficients to account for the missing effects.

As with any water-quality model, the accuracy of the simulation is dependent on the quality of the input data, but in a stochastic method the model will also be sensitive to the form (or type) of the input distributions that are chosen. The experience of Thames Water has suggested that the assumption of a standard form of distribution (e.g. log-normal) is not always justified especially where there are significant periodic variations in the mean value of determinant. Furthermore, when the Monte Carlo simulation technique is extended to include several consecutive mixing processes (as in a catchment simulation), the errors in choosing an inadequate distribution can accumulate down the system. This can be only be mitigated by defining the input distributions as realistically as data will permit and this means that extensive monitoring and data analyses are required so that the distribution might be better described.

In its current form, TOMCAT is suitable for modelling determinants in freshwater that do not rely on sediment interactions and where the simple processes simulated are a reasonable approximation of the real system. TOMCAT provides the user with monthly and annual statistics and the model can quickly run the effects of changes in effluent discharge conditions so it is useful for consent setting exercises. However, the model would benefit from improvements in the flow and water-quality process descriptions. In particular, the DO model does not account for even simple sediment interactions, and it is hard to see how the claims of incorporating diurnal effects can be justified (with regard to the DO model) when photosynthesis and respiration are not represented.

5.2.7. Applicability to simulating do in lowland rivers

Since this model was developed by Thames Water, it is clear that TOMCAT has been used in modelling activities on the River Thames and its tributaries. The model was designed to be quick and easy to set up and to produce output suitable for comparison with UK legislation, and so in these respects it is well suited to modelling by both water utility companies and regulators. However, if the distributions of the determinants required have not already been calculated, this must be carried out using as large a data set as possible if the results are to be meaningful. Furthermore, even with excellent data, the model will be limited by the over simplistic descriptions of flow and water-quality processes, and despite the inclusion of some seasonality it is not a dynamic model and so cannot examine shorter-term variability such as diurnal effects. Therefore, like SIMCAT, TOMCAT will prove to be of use for modelling lowland rivers to organisations like water utility companies and the EA, but the lack of a dynamic mode and the overly simplistic processes (including DO) suggest that this model is not suitable for simulating anything other than the general condition of a river, nor can it be deemed suitable for predictive modelling.

5.3. QUAL2E

The QUAL2E model (Brown and Barnwell, 1987) is the latest version of the model QUAL-II (Roesner et al., 1981), which was itself developed by Tufts University and the USEPA from the model QUAL-I by F.D. Masch & Associates and the Texas Development Board in the 1960s. QUAL2E was first released in 1985 and the USEPA has used and improved this model extensively since then. The model and its manuals are available for download free of charge from their website and more recently, the model has been incorporated with other USEPA models such as HSPF and WASP5 in a GIS (Geographical Information System) environment in software called BASINS.

The QUAL2E model is a 1D, steady-state model of in-stream flow and water-quality. It simulates DO and (up to 15) associated water quality determinants along a river and its tributaries. As a steady-state model, it is limited to periods when the stream flows and any discharges are essentially constant. However, the model is able to account for the effects of meteorological diurnal variations (e.g. radiation) on certain water-quality determinants such as DO and temperature. The model is extensively documented in the user manual (Brown and Barnwell, 1987) which explains the theory behind the model and the way in which it may be implemented.

5.3.1. Conceptual model

Although QUAL2E is a steady-state model, like SIMCAT and TOMCAT, the conceptualisation is rather more advanced than those two. Fig. 4 shows a river reach that might form one part of a river system being modelled using QUAL2E. Each reach is divided into a number of sub-reaches or computational elements of equal length (Δx). Within each element flow and load additions are calculated as for SIMCAT and TOMCAT. A solute balance for any determinant (C) is then performed that considers both advective and dispersive transport along the reach. The equation used is 1D and so the model assumes that:

- the solutes are completely mixed over the cross-section;
- the advective transport is with the mean flow;
- the dispersive transport is proportional to the concentration gradient (i.e. Fick's law).

5.3.2. Processes

Like SIMCAT and TOMCAT, the flow model in QUAL2E assumes that the stream hydraulic regime is at steady-state, i.e. $\mathrm{d}Q/\mathrm{d}t = 0$. Therefore

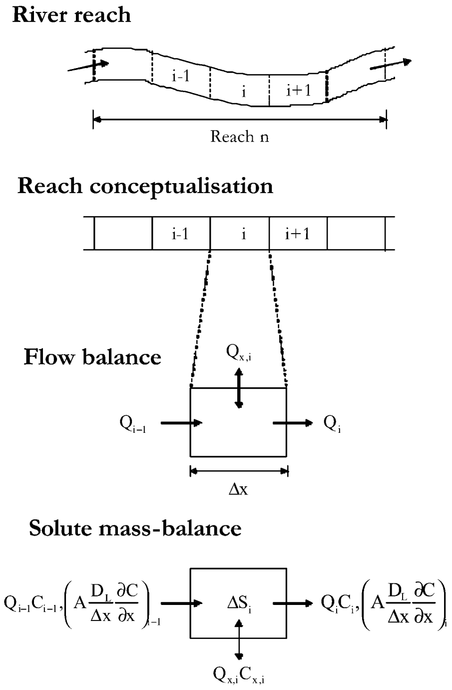

Fig. 4. A conceptualisation of the QUAL2E river reach model. (adapted from Brown and Barnwell, 1987).

the balance for a computational element can be written as:

$$Q_i = Q_{i-1} + Q_{x,i} \tag{22}$$

or

$$\left(\frac{\partial Q}{\partial t}\right)_i = Q_{x,i} \tag{23}$$

where $Q_{x,i}$ is the net sum of all external inflows (i.e. discharges minus withdrawals) to that element, and all other terms are as in Fig. 4. Once the flow in an element has been solved, the velocity area and depth are calculated using empirically derived functions, and used in the solute transport model. The solute mass balance model used by QUAL2E and described in Fig. 4 is a 1D ADE as described in Section 4.2 i.e.:

$$\frac{\partial C}{\partial t} = \frac{\partial\left(A_x D_\mathrm{L} \frac{\partial c}{\partial x}\right)}{A_x \partial x} - \frac{\partial\left(A_x \bar{U} C\right)}{A_x \partial x} + \frac{\mathrm{d}C}{\mathrm{d}t} + \Delta S \tag{24}$$

The transformations occurring to individual determinants independent of advection, dispersion and external inputs are defined by the term $\mathrm{d}C/\mathrm{d}t$ and these changes include the physical, chemical and biological processes that occur in the stream.

QUAL2E can be used to simulate any combination of the following determinants:

- Conservative solutes (up to three);
- Temperature;
- BOD;
- Chlorophyll-*a*;
- Phosphorous (organic and dissolved);
- Nitrogen (organic, ammonium, nitrite, and nitrate);
- DO;
- Coliform bacteria;
- One arbitrary non-conservative constituent solute.

Most determinants are simulated as first-order decays but DO, nitrate, and phosphate are represented in more detail and there is also an algal model as described by Fig. 5. The model does include sediment processes, but only as a sink for substances (for example it includes a settling rate for BOD but not a re-suspension rate) or as a source of oxygen demand. Thus, QUAL2E is a much more complex model than SIMCAT and TOMCAT.

The algal model consists of growth (by photosynthesis), respiration and the settling of algae onto the sediments of the river bed, i.e.:

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \mu A - \rho A - \frac{\sigma_1}{d} A \tag{25}$$

where A is the algal biomass concentration (which

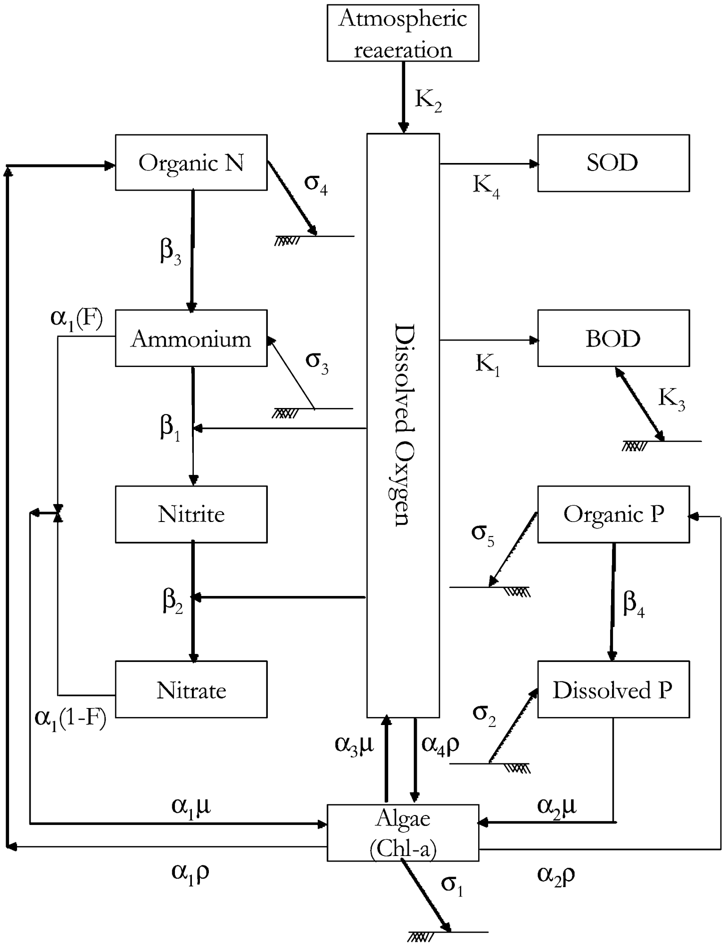

Fig. 5. A summary of the processes simulated by the model QUAL2E (adapted from Brown and Barnwell, 1987).

is directly proportional to the concentration of chlorophyll-*a*), t is the time, μ is the growth rate (which is affected by nutrient availability, light, temperature, and self-shading), ρ is the 'respiration' rate (representing the conversion of algal nitrogen and phosphorous into organic nitrogen and phosphorous), σ_1 is the settling rate and d is the depth.

The nitrogen cycle is represented by the transformations affecting organic nitrogen, ammonium (NH_4^+), nitrite (NO_2^-) and nitrate (NO_3^{2-}). The organic nitrogen is produced by the algae and removed by hydrolysis to ammonium and settling, i.e.:

$$\frac{dN_o}{dt} = \alpha_1 \rho A - \beta_3 N_o - \sigma_4 N_o \tag{26}$$

where N_o is the concentration of organic nitrogen, α_1 is the fraction of the algal biomass that is nitrogen, ρ is the algal respiration rate, β_3 is the rate coefficient parameter for the hydrolysis of organic nitrogen to ammonium, and σ_4 is the rate coefficient parameter for the settling of organic nitrogen. Thus, the ammonium concentration is increased by the hydrolysis of organic (algal) nitrogen, but is also removed from the water column by algae and by the process of nitrification. Some ammonium may also be generated in the sediments in the process of denitrification and released into the water column, i.e.:

$$\frac{d[NH_4]}{dt}=\beta_3 N_o-\beta_1[NH_4]+\frac{\sigma_3}{d}-F_1\alpha_1\mu A$$

where

$$F=\frac{P_{am}[NH_4]}{\left(P_{am}[NH_4]+(1-P_{am})[NO_3]\right)} \tag{27}$$

and where $[NH_4]$ is the concentration of ammonium, β_1 is the rate coefficient parameter for the biological oxidation of ammonium (i.e. nitrification), σ_3 is the source rate of ammonium from the sediments, F is the fraction of algal nitrogen uptake from the available ammonium, P_{am} is the preference factor for ammoniacal nitrogen over nitrate nitrogen and $[NO_3]$ is the concentration of nitrate nitrogen.

Nitrogen in the form of nitrite is produced from the ammonium in the first stage of denitrification and removed as the nitrite is further oxidised to nitrate, i.e.:

$$\frac{d[NO_2]}{dt}=\beta_1[NH_4]-\beta_2[NO_2] \tag{28}$$

where $[NO_2]$ is the concentration of nitrite nitrogen and β_2 is the rate coefficient for the oxidation of nitrite nitrogen. Finally, the nitrate in the water column is consumed by algae, i.e.:

$$\frac{d[NO_3]}{dt}=\beta_2[NO_2]-(1-F)\alpha_1\mu A \tag{29}$$

where $[NO_3]$ is the concentration of nitrate nitrogen.

The phosphorous ‘cycle’ is represented by the transformations affecting organic and dissolved phosphorous fractions. The organic phosphorous is produced by the algae and removed by a simple decay and settling, i.e.:

$$\frac{dP_o}{dt}=\alpha_2\rho A-\beta_4 P_o-\sigma_5 P_o \tag{30}$$

where P_o is the concentration of organic phosphorous, α_2 is the phosphorous content of algae, β_4 is the organic phosphorous decay rate and σ_5 is the organic phosphorous settling rate. The dissolved phosphorous arises as a result of the decay of organic phosphorous and by similar processes in the sediments, it is also consumed by algae during photosynthesis, i.e.:

$$\frac{dP_d}{dt}=\beta_4 P_o+\frac{\sigma_2}{d}-\alpha_2\mu A \tag{31}$$

where P_d is the concentration of inorganic or dissolved phosphorous, and σ_2 is the source rate of phosphorous from the sediments.

The BOD model, relates to the ultimate BOD which is diminished by biological oxidation and settling-out, i.e.:

$$\frac{dL}{dt}=-K_1L-K_3L \tag{32}$$

where L is the concentration of the ultimate BOD, K_1 is the rate of oxidation of the BOD and K_3 is the rate of BOD loss due to settling. If the only data available are for the 5-day BOD then QUAL2E uses the following conversion:

$$BOD_u=\frac{BOD_5}{(1-e^{(5K_{BOD})})} \tag{33}$$

where K_{BOD} is the BOD conversion coefficient.

The DO model incorporates the effects of the algal, nitrogen, phosphorous and BOD processes, but the DO concentration will also be influenced by atmospheric reaeration and a sediment oxygen demand i.e.:

$$\frac{dC}{dt}=K_2(C_s-C)+(\alpha_3\mu-\alpha_4\rho)A-K_1L-\frac{K_4}{d}-\alpha_5\beta_1[NH_4]-\alpha_6\beta_2[NO_2] \tag{34}$$

where C is the concentration of DO, C_s is the saturation concentration, K_2 is the reaeration rate, α_3 is the rate of photosynthetic oxygen production per unit of algal growth, α_4 is the rate of respiratory oxygen uptake per unit of algal respiration, K_4 is the rate of the sediment oxygen demand, α_5 is the rate of oxygen utilisation per unit of ammonium oxidised during nitrification, and α_6 is the rate of oxygen uptake per unit of nitrite oxidised. The reaeration rate coefficient, K_a, can be estimated by entering a value or by using one of the equations developed by Churchill et al. (1962), O'Connor and Dobbins (1958), Owens et al. (1964), Thackston and Krenkel (1969) and Langbein and Durum (1967) or Tsiovoglou and Wallace (1972); or by a simple power function of the flow, i.e. $K_a = aQ^b$. The oxygen saturation concentration is estimated using the equation developed by the American Public Health Authority (APHA, 1992):

$$\ln C_{sf} = -139.34411 + \frac{1.575701\times 10^5}{T_a} - \frac{6.642308\times 10^7}{T_a^2} + \frac{1.243800\times 10^{10}}{T_a^3} - \frac{8.621949\times 10^{11}}{T_a^4} \quad (35)$$

where C_{sf} is the freshwater DO saturation concentration (mg O_2 l^{-1}) at 1 atm, and T_a is the absolute temperature (K), which can be converted from the temperature in °C (T) by:

$$T_a = T + 273.15 \quad (36)$$

Temperature is modelled by performing a heat balance on each element. The balance accounts for heat exchanges at the air–water interface and includes the influences of radiation, convection and evaporation, i.e.:

$$H_n = H_{sn} + H_{an} - H_b - H_c - H_e \quad (37)$$

where H_n is the net heat flux through the air–water interface, H_{sn} is the net short wave solar radiation, H_{an} is the net long wave radiation, H_b is the outgoing long wave back-radiation, H_c is the convective heat flux and H_e is the heat loss by evaporation. The temperature is used to adjust most of the rate parameters included in the process equations, which are summarised in Fig. 5.

5.3.3. Data requirements

As with all of the water-quality models described here, the initial step in modelling the system is to divide the river system into reaches which are stretches of the river having (approximately) uniform hydraulic characteristics such as slope and cross-sectional area. In the standard QUAL2E model, there can be a maximum of 50 reaches and each of these is then divided into (a maximum of 20) computational elements of equal length. Since QUAL2E is a steady-state model and is not stochastic, the data requirements in terms of flow and quality data are not large since the model only requires single values of each determinant being modelled. Thus, elements at the top of tributaries or the main river will have water flow and quality data assigned to them and this is also true for elements where discharges or abstractions are simulated. At confluences the same process occurs (i.e. the external addition of water to an element), but here the model will simulate the input flow and quality. In the standard model the user can specify a maximum of seven 'headwater' elements (i.e. seven different rivers) and 25 input and withdrawal elements.

The model allows only 20 computational elements per reach and there is a limit of one 'influence' per element. For example, a computational element may contain an effluent discharge or an abstraction, but not both and this can cause problems if one needs to represent discharges which are close together. To avoid short reaches, one would have to 'pre-process' the data to estimate a combined influence or impose a layout in the model that may be rather different from the real one.

The river reach itself is the main feature for which data are required since hydraulic data, reaction rate coefficients, initial conditions and flow data are all defined for each reach rather than each element. As well as physical characteristics, a reach also requires local climatological data for the heat balance computations (wet and dry bulb temperatures, atmospheric pressure, wind velocity, and cloud cover) and rate parameters for all of the chemical and biological reactions that are simulated by QUAL2E. Table 1 lists these parameters and gives the usual range of values that might be expected—note the common use of imperial units because this is an American model.

5.3.4. Model operation

Once all of the required data have been supplied, the model simulates the changes in flow condition along the stream by computing a series of steady-state surface water profiles. QUAL2E uses a numerical solution scheme, using an implicit finite-difference method to solve the equations for flow and then the solutes for each of the elements sequentially. This is slightly different from the sequence in SIMCAT and TOMCAT, in that the model does solve from the headwaters down, but in QUAL2E the model simulates flow in all reaches first and then the solute transport and water quality, rather than solving for all determinants simultaneously.

An extension to the model called QUAL2E–UNCAS allows the user to perform uncertainty analyses by investigating model sensitivity to changes in one variable at a time (sensitivity analysis) or all of the variables at once (first-order error analysis) or by using Monte Carlo techniques. When undertaking first-order error analysis, all variables are assumed to act independently, and the relationship between the parameter and the output is assumed to be linear. This is not always correct, but does provide a useful approximation. For a Monte Carlo analysis, the user supplies an estimate of the likely variance and distribution (normal or log-normal) of each parameter, and the number of shots to be made. This technique has the advantage of there being no assumption of linearity, but at a cost of greatly increased run times.

5.3.5. Outputs

QUAL2E provides solutions to the flow and solute mass balance equations for each reach and so the output consists of single values of flow and solute concentrations for each reach for each determinant modelled. Any of the methods of uncertainty analysis may be applied to any of the determinants, but output is only available for five reaches at a time. For the first-order error analysis, the output consists of a normalised sensitivity parameter resulting from a 1% change in the parameter under test, calculated by:

$$S_{\mathrm{i,j}}=\frac{\Delta Y_{\mathrm{j}}/Y_{\mathrm{j}}}{\Delta C_{\mathrm{i}}/C_{\mathrm{i}}} \tag{38}$$

where $S_{\mathrm{i,j}}$ is the normalised sensitivity parameter for output Y_{j} to input C_{i}, C_{i} is the value of input parameter, ΔC_{i}, is the magnitude of input perturbation, Y_{j}, is the value of the output parameter and ΔY_{j} is the magnitude of the change in output parameter.

5.3.6. Discussion

The QUAL2E model is probably the most widely-used water-quality model in the world and although it is unable to handle temporal variability in a river system it does have several benefits.

- It requires only partial hydraulic data
- It does not require large amounts of data to represent the sediments
- It can simulate algae (chlorophyll-*a*)
- It includes automatic uncertainty analysis
- It is available free of charge
- The code and theoretical background behind the model are extensively documented
- It is used world-wide in a wide range of water-quality modelling exercises

However, the model is not suitable for consent setting in the UK because it is unable to provide the flows or concentrations in a reach as percentiles since it has no stochastic component. The process of setting up a deterministic model with average values can also result in unsatisfactory simulations because the use of single mean values in a mass balance model will only be correct if the data used in the mass balance equation relates to the same instantaneous period of time (Warn and Brew, 1980). Furthermore, the use of mean values might provide results that suggest that the general con-

Table 1
The rate coefficients used in QUAL2E (adapted from Brown and Barnwell, 1987)

Parameter	Units	Range	Variable within a reach?	Temperature dependent?
Ratio of chl-*a* to algal biomass	μgChla (mg A)$^{-1}$	10–100	No	No
Nitrogen fraction of algal biomass	mg N (mg A)$^{-1}$	0.07–0.09	No	No
Phosphorous fraction of algal biomass	mg P (mg A)$^{-1}$	0.01–0.02	No	No
DO production per unit of algal growth	mg O_2 (mg A)$^{-1}$	1.4–1.8	No	No
DO uptake per unit of algae 'respired'	mg O_2 (mg A)$^{-1}$	1.6–2.3	No	No
DO loss per unit of ammonium oxidation	mg O_2 (mg N)$^{-1}$	3.0–4.0	No	No
DO loss per unit of nitrite oxidised	mg O_2 (mg N)$^{-1}$	1.0–1.14	No	No
Maximum algal growth rate	day^{-1}	1.0–3.0	No	No
Algal respiration rate	day^{-1}	0.05–0.5	No	No
Michaelis-Menten half-saturation constant for light	Bru ft^{-1} min^{-3}	0.02–0.10	No	No
Michaclis-Menten half-saturation constant for nitrogen	mg N 1^{-1}	0.01–0.30	No	No
Michaelis-Menten half-saturation constant for phosphorous	mg P 1^{-1}	0.001–0.05	No	No
Non-algal light extinction coefficient	ft^{-1}		No	No
Linear algal self-shading coefficient	ft^{-1} (μg Chla r^{-1})$^{-1}$	0.002–0.02	No	No
Non-linear algal self-shading coefficient	ft^{-1} (μg Chla l$^{-2/3}$)$^{-1}$	0.0165	No	No
Algal preference for ammonium	–	0.0–1.0	No	No
Algal setting rate	ft day^{-1}	0.5–6.0	Yes	Yes
Sediment source rate for dissolved phosphorous	mg P (ft^2 day^{-1})$^{-1}$		Yes	Yes
Sediment source rate for ammonium	mg O_2 (ft^2 day^{-1})$^{-1}$		Yes	Yes
Settling rate of organic nitrogen	day^{-1}	0.001–0.1	Yes	Yes
Settling rate of organic phosphorous	day^{-1}	0.001–0.1	Yes	Yes
'Non-conservative' settling rate	day^{-1}		Yes	Yes
Sediment source rate of a 'non-conservative' solute	mg (ft^2 day^{-1})$^{-1}$		Yes	Yes
Carbonaceous BOD deoxygenation	day^{-1}	0.02–3.4	Yes	Yes
Reaeration rate coefficient	day^{-1}	0.0–100	Yes	Yes
BOD loss due to settling	day^{-1}	-0.36–0.36	Yes	Yes
Sediment oxygen demand	mg O_2 (ft^2 day^{-1})$^{-1}$		Yes	Yes
Coliform death rate coefficient	day^{-1}	0.05–4.0	Yes	Yes
'Non-conservative' decay coefficient	day^{-1}		Yes	Yes
Nitrification of ammonium to nitrite	day^{-1}	0.10–1.00	Yes	Yes
Nitrification of nitrite to nitrate	day^{-1}	0.20–2.0	Yes	Yes
Hydrolysis of organic nitrogen to ammonium	day^{-1}	0.02–0.4	Yes	Yes
Decay of organic phosphorous to dissolved phosphorous	day^{-1}	0.01–0.7	Yes	Yes

N.B. Chla represents Chlorophyll-*a* and A represents algal biomass.

dition of a system is acceptable when in fact there may be serious concerns over shorter time-scales.

5.3.7. Applicability to simulating do in lowland rivers

The literature review did not reveal any applications of QUAL2E to UK river systems, but it has been successfully applied in many situations around the world. The extensive use of this model around the world is in part due to the fact that it is free and well documented, but the model is clearly useful for simulating water quality in freshwater systems. However, because QUAL2E has no stochastic component, it is not suitable for use with UK legislation, and the use of single values rather than statistics as inputs may also lead to errors in representing the real system.

Perhaps the greatest concern with regard to simulating DO is the fact that this is a steady-state model. The model documentation claims that some seasonality and diurnal effects are accounted for, but QUAL2E is not a dynamic model and so cannot account for shorter-term variability such as diurnal effects. Lowland rivers can show significant temporal variability over a range of scales, and it is known that that certain acceptable quality limits are exceeded from time to time (Environment Agency, 2001). This indicates that stream quality should not be judged only in terms of say yearly average indices, but that transient, intermittent deterioration of quality is also important, and may be of growing concern for the future (Whitehead et al., 1981). The problems created by variability of water quality are clearly recognised in Europe and the UK, as is evidenced by the setting of percentile limits in EC environmental directives.

5.4. QUASAR, HERMES and QUESTOR

The three models QUASAR, HERMES and QUESTOR are actually all versions of the same model called QUASAR (Whitehead et al., 1997) which was developed from a model of the Bedford Ouse (Whitehead et al., 1979, 1981). However, the differences arise because of the way in which the model and the software are used. At the present time the QUASAR model is available commercially from CEH, Wallingford as PC-QUASAR, free from The University of Reading for teaching purposes as the simplified version HERMES (Oxford Scientific Software, 1992), and on a consultancy basis from CEH, Wallingford as QUESTOR (Eatherall et al., 1998).

QUASAR (QUAlity Simulation Along River systems) describes the time-varying (i.e. dynamic) transport and transformation of solutes in branched river systems using 1D ordinary, lumped parameter differential equations of mass conservation. PC-QUASAR and QUESTOR (QUality Evaluation and Simulation TOol for River systems) also have the option of running the model stochastically using a Monte Carlo method like SIMCAT and TOMCAT. HERMES has been simplified as it is only used for teaching purposes, but PC-QUASAR and QUESTOR are capable of simulating large branched river systems with multiple influences such as effluent discharges, abstractions and weirs, etc. PC-QUASAR and QUESTOR have both been used for the freshwater component of the LOIS project, modelling fluxes along rivers in Yorkshire (Lewis et al., 1997; Eatherall et al., 1998) and by the Scottish Environment Protection Agency (SEPA) for the River Almond.

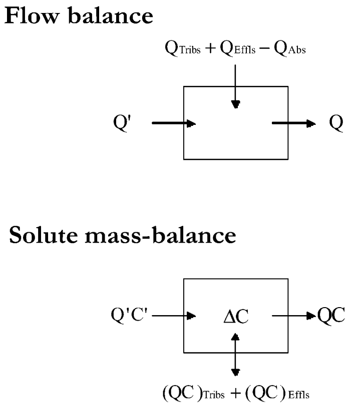

Fig. 6. A conceptualisation of the QUASAR river reach model. The subscripts Tribs, Effls and Abs refer to tributaries, effluent discharges and abstractions, respectively and ΔC represents internal transformations.

5.4.1. Conceptual model

All three models are dynamic and PC-QUASAR and QUESTOR also have stochastic ‘planning modes’. Whichever scheme is used, the conceptual model is the same, and this is the CSTSR model described in Section 4.2. Like QUAL2E, the reach can be split into a number of equally sized and completely mixed elements, but, unlike QUAL2E, influences such as abstractions, tributaries and discharges can only be added to the top element in a reach although there can be many more reaches than are allowed in QUAL2E. Like SIMCAT and TOMCAT, the time spent by the solutes in a reach or element (i.e. the residence time) is not calculated by considering the advection and dispersion of dissolved constituent, but is based only on the stream flow velocity. This has the benefit of QUASAR being able to use a much simpler (and therefore quicker) solver since the equations to be solved are ordinary rather than PDEs.

The conceptualisation of the teaching model HERMES is slightly different from that shown in Fig. 6 in that it also includes the concept of dead zones. The aggregated dead zone (ADZ) method (Beer and Young, 1983; Wallis et al., 1989a,b;

Young and Wallis, 1993) is a different approach to modelling dispersion processes than the ADE, but is related to it and can provide more accurate predictions of travel times of solutes in natural streams than the approach used in QUASAR. 'Dead zones' are considered to be areas of dynamic storage usually located around the edges of open-channel flows where some form of mixing can take place. Solutes entering a dead zone are temporarily trapped and mixed with the contents of the dead zone before being released back into the main flow. However, it is not always clear where these dead zones might be and, as well as structures at the edge of rivers, they might also be related to turbulent eddies, wakes around rougher regions, or reverse flows around pools or bends. Furthermore these dead zones may also be transient or moving. Therefore it will not be possible to directly measure the volumes of individual dead zones.

To account for all of the dead zones in a reach, the ADZ technique designates a proportion of the reach volume that is equivalent to and is representative of all of the dead zones (and other mixing processes with a similar effect) in that reach, i.e. the active mixing volume or AMZ (Young and Lees, 1993). Tracer experiments have shown that the solutes entering a river reach and being transported through it can be considered to be subjected to a pure time delay (or lag time) and mixing as the material is dispersed (Young and Wallis, 1986; Wallis et al., 1989a). The HERMES model, therefore, represents this by partitioning the time spent in the reach into a pure time delay followed by a mixing residence time. Using the principles of the CSTRS approach, as used in QUASAR, the conceptualisation of the ADZ technique is illustrated in Fig. 7 below in which it can be seen that this method assigns a proportion, rather than the whole, of the reach to be perfectly mixed—referred to as the aggregated mixing volume or AMV. The conceptual model is then equivalent to CSTRS, but with modified reach volumes and the addition of an advective time delay to account for the time taken for the leading-edge of a 'solute cloud' to be advected through the reach. Applying the ADZ technique can remove the need for using many computational elements within a reach as the dispersion characteristics are more accurately simulated (Camacho, 1997; Lees et al., 1998) and this method may, therefore, be better suited to the prediction of short time-scale events such as pollution events.

5.4.2. Processes

Although QUASAR is a dynamic model, the hydraulic model is not a full hydrodynamic model, but is relatively simple. It assumes that the density of water does not change significantly during a time-step and so the rate of change of the volume in the reach is equal to the difference between the inflow and the outflow, i.e.:

$$\frac{\mathrm{d}V}{\mathrm{d}t}=Q'-Q \tag{39}$$

where Q is the flow in the reach and Q' is the flow entering the reach. This is similar to the conventional Muskingum–Cunge method of flow routing (Nash, 1959; Cunge, 1969) which relates the storage in a reach to the inflow minus the outflow. This can be expressed in terms of the rate of change of flow instead as:

$$\frac{\mathrm{d}Q}{\mathrm{d}t}=\frac{Q'-Q}{\tau(1-c)} \tag{40}$$

where τ is called the travel time or residence time and

$$\tau=\frac{L}{v} \tag{41}$$

and

$$v=a+bQ^{c} \tag{42}$$

where L is the reach length, v is the water velocity and a, b and c are empirically derived constants for the reach.

In a perfectly mixed reach the mass is equal to the concentration of the determinant multiplied by the volume of water in the reach. Thus, it can be shown that for a conservative determinant a mass

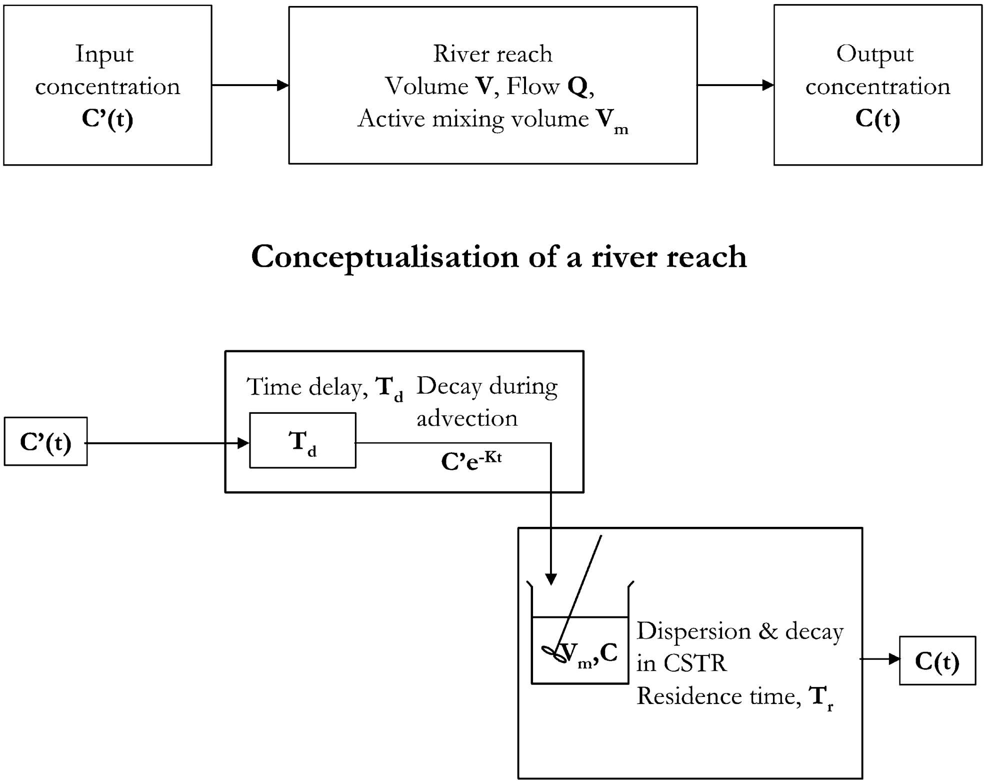

Fig. 7. Conceptualisation of river transport mechanisms using the ADZ methodology (from Lees, et al., 1998).

balance can be written as:

$$\frac{\mathrm{d}M}{\mathrm{d}t}=\frac{\mathrm{d}(VC)}{\mathrm{d}t}=Q'C'-QC \tag{43}$$

where C is the concentration of the solute in the reach and C' is the concentration of the solute entering the reach. Incorporating Eq. (40) this leads to an equation for the rate of change of the concentration with respect to time, i.e.:

$$\frac{\mathrm{d}C}{\mathrm{d}t}=\frac{Q'(C'-C)}{Q\tau} \tag{44}$$

This is equivalent to the ADE with the dispersion term removed and integrated to assume complete mixing within the element.

The version used in PC-QUASAR, HERMES and QUESTOR assumes that the flow varies only slowly relative to the time-step and that therefore Q'/Q is approximately equal to one. If this holds true then a simpler form may be derived, i.e.:

$$\frac{\mathrm{d}C}{\mathrm{d}t}=\frac{1}{\tau}(C_{\mathrm{i}}-C) \tag{45}$$

A conservative model is assumed for the simulation of water temperatures (where the temperature is assumed to be a 'heat concentration') and pH (where the mass of hydrogen ions is assumed conservative) in QUASAR, but this equation can also be used to simulate one or more other determinants that are assumed to behave conservatively. For other determinants, it follows from that the general form for a non-conservative determinant would be:

$$\frac{dC}{dt}=\frac{1}{\tau}(C_i-C)+\Delta C \tag{46}$$

where ΔC is a term representing the net accumulation in the reach of that determinant due to internal transformations, i.e. the 'sources' minus the 'sinks'.

In HERMES, the ADZ method is used and so the equations are adapted to account for the different transport model. The HERMES model partitions the time spent in the reach into a pure time delay T_d followed by a mixing residence time T_r (replacing the time constant τ) associated with the solute passage through the ADZ volume or AMZ. This is illustrated in Fig. 7, and leads to a general equation for simulating the behaviour of any water quality determinant (Lees et al., 1998), i.e.:

$$\frac{dC_{(t)}}{dt}=\frac{C'_{(t-T_d)}\,e^{-KT_d}-C_{(t)}}{T_r}+\Delta C_{(t)} \tag{47}$$

The version used in HERMES is simplified by omitting the component of decay during advection, i.e.:

$$\frac{dC_{(t)}}{dt}=\frac{C'_{(t-T_d)}-C_{(t)}}{T_r}+\Delta C_{(t)} \tag{48}$$

This is adequate for a simple teaching tool such as HERMES, but it is not clear how the term e^{-KT_d} in Eq. (47) can be defined when multiple processes affect a determinant, for example in the case of DO. Whichever form is used, the time delay and mixing residence time can be related to the standard (QUASAR) residence time by:

$$T_r=\tau-T_d=\tau\cdot\mathrm{DF} \tag{49}$$

where DF is the dispersive fraction equal to V_m/V and is therefore a measure of the fractional volume of the reach responsible for dispersion. One should note that, by using the ADZ method, the model must consider the concentrations in the reach at times other than the current time step when solving the equations.

For the rest of this section, the process equations reproduced are for the simple transport model in the original QUASAR model, but from the previous discussion it is easy to see how the equations would appear in HERMES. One should also note that, unlike QUAL2E, QUASAR uses ODEs, because of the simpler transport model. Therefore, the mass balance equations in QUASAR include the transport terms whereas those for QUAL2E do not, because transport there is calculated by the advection–dispersion PDE. The determinants and processes simulated in QUASAR are summarised in Fig. 8.

The nitrate concentration in a reach is simulated as being affected by nitrification and denitrification and so:

$$\frac{d[\mathrm{NO_3}]}{dt}=\frac{1}{\tau}\left([\mathrm{NO_3}]'-[\mathrm{NO_3}]\right)+K_1[\mathrm{NH_4}]-K_2[\mathrm{NO_3}] \tag{50}$$

where $[\mathrm{NO_3}]$ is the concentration of nitrate, $[\mathrm{NH_4}]$ is the concentration of ammonium, K_1 is the nitrification rate coefficient and K_2 is the denitrification rate coefficient. Similarly the ammonium concentration is reduced by nitrification and so:

$$\frac{d[\mathrm{NH_4}]}{dt}=\frac{1}{\tau}\left([\mathrm{NH_4}]'-[\mathrm{NH_4}]\right)-K_1[\mathrm{NH_4}] \tag{51}$$

The concentration of DO in the river is simulated as being affected by algal photosynthesis and respiration, a sediment oxygen demand, reaeration, nitrification and BOD, i.e.:

$$\frac{dC}{dt}=\frac{1}{\tau}(C'-C+\mathrm{WEIR})+P-R-K_3C+K_4(C_s-C)-4.57K_1[\mathrm{NH_4}]-K_5L \tag{52}$$

where C is the DO concentration and WEIR is the increase in DO concentration due to a weir or other structure in the reach, which is calculated using an empirical relationship with the weir type and height. P is the rate of (algal) photosynthetic oxygen production, R is the rate of oxygen uptake due to algal respiration, K_3 is the rate coefficient for the sediment oxygen demand, K_4 is the reaeration rate coefficient, C_s is the DO saturation

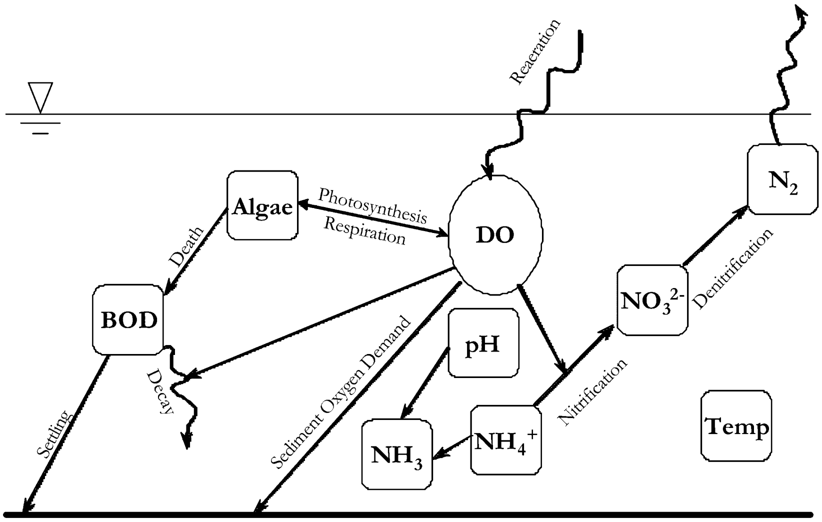

Fig. 8. A summary of the determinants and processes simulated by QUASAR (after Whitehead, et al. 1997).

concentration, L is the BOD concentration and K_5 is rate parameter for BOD oxidation. The reaeration rate coefficient is estimated using an equation attributed to Owens et al. (1964) and the photosynthesis rate is based on an empirical relationship with radiation and algal concentration. In QUASAR, the method of Elmore and Hayes (1960) is used to estimate the DO saturation concentration as in SIMCAT (Eq. (15)).

BOD in the water column is simulated as being removed by biological oxidation and sedimentation and there is a contribution to the BOD due to dead algae, i.e.:

$$\frac{dL}{dt}=\frac{1}{\tau}(L'-L)-K_5L-K_{10}L+K_{11}\text{Chla} \tag{53}$$

where L is the BOD concentration, K_{10} is rate coefficient for sedimentation, K_{11} is the rate coefficient for the increase in BOD due to algal death, and Chla is the concentration of chlorophyll-*a* representing the algal (biomass) concentration.

5.4.3. Data requirements

The data required to run QUASAR can be broadly divided into four categories: catchment structure and geographical information; boundary conditions, i.e. the water flow and quality inputs to the system; observed data for the purposes of calibration and evaluation of the model, and reach parameters consisting of the rate coefficients specific to each reach. These data are summarised below:

Catchment structure

- Locations of reach boundaries (generally selected at river confluences, weirs, discharges, abstractions, and monitoring sites);

Boundary conditions

- Flow and quality data for: the top of the main river, the tops of any tributaries, effluent discharges, and abstractions.

Reach parameters (in HERMES these parameters are set for the whole system):

- Velocity–flow relationship parameters;
- Length, width and depth;
- Number of sub-reaches or computational elements;
- Weir type and height;
- Ammonium nitrification rate coefficient;
- Denitrification rate coefficient;
- Oxygen loss to the sediment oxygen demand rate coefficient;
- BOD oxidation rate coefficient;

- Photosynthetic oxygen production rate coefficient (for chlorophyll-*a* concentrations below 50 $\mu g\,l^{-1}$);
- Photosynthetic oxygen production rate coefficient (for chlorophyll-*a* concentrations above 50 $\mu g\,l^{-1}$);
- Algal respiration rate coefficients;
- BOD sedimentation rate coefficient;
- Algal death rate coefficient.

The rate coefficients are all specified by the user for the value at 20 °C and where appropriate the model takes account of the effect of temperature on their value. In the current versions of QUASAR it is also necessary to specify algal concentrations in each reach or for the whole system, as there is no algal model.

If dispersion effects are important in a river system, it will be important to select the number of reach elements carefully such that the introduced implicit or numerical dispersion is roughly equal to that of the actual system (Lees et al., 1998). However, in HERMES, it is not necessary to define sub-reaches or computational elements within a reach, because HERMES uses the ADZ technique to simulate dispersion in the reach. For the HERMES model, parameters representing the dead zones in each reach are required in addition to the parameter list above. ADZ research (Beer and Young, 1983; Wallis et al., 1989a,b; Young and Wallis, 1993) has led to the formulation of two methodologies for estimation of the advection and dispersion parameters. The first approach is a simple subjective method that uses derived relationships from observed concentration–time data measured at two downstream locations (Wallis et al., 1989b); while the second objective is based on the Simple Refined Instrumental Variable (SRIV) (Young, 1984, 1992) method of system identification. Although the latter method is theoretically superior, the former method is simpler to use and is relatively accurate if reliable tracer data are available.

When QUASAR is run dynamically, time-series of flow and quality are used as the inputs (or boundary conditions) and, in a complex system the process of compiling such a data set can be very laborious. In PC-QUASAR the time series consist of daily or monthly means for the period of interest, but in QUESTOR the model can be run with a wider range of time-steps and the frequency of the input data should reflect the choice made. In the stochastic mode of each model, the user supplies flow and quality data as means and standard deviations of a normal or log-normal distribution, or as lower and upper boundaries of a rectangular distribution.

5.4.4. Model operation

Simple flow and load addition equations are used at the top of each reach (i.e. in the first computational element) for all flows entering (or being abstracted from) that reach and so all influences such as discharges and abstractions are considered to enter at the beginning of the reach. The solution of the mass-balance equations for flow and the determinants being simulated is then made in each element and the results of these calculations are used as input for the next element. At the end of a reach the results are stored and then used as the upstream influence on the next reach. In dynamic mode, this is performed once per time-step, in stochastic mode the model selects vales randomly from the input distributions and runs for thirty ‘time-steps’ or until a there is little change in the result if this is sooner. Unlike SIMCAT and TOMCAT, there is no ability in QUASAR to correlate flow or quality values chosen from the distributions.

The set of ODEs are solved using an efficient finite difference method namely a fourth-order Runge–Kutta technique which can adapt according to the local conditions in the solution. This method allows for the simultaneous solution of the model equations and thereby ensures that no single process represented by the equations takes precedence over another. Because the QUASAR model consists of ODEs rather than the PDEs used in QUAL2E, it has an easier formulation and calibration and model evaluation will also be easier.

5.4.5. Outputs

In dynamic simulations, a time-series of flow and quality may be obtained for each reach at the frequency specified by the user. In QUESTOR there is also the ability to output data at a lower frequency than the computational time-step. This is useful for better representing diurnal influences while not generating excessive amounts of output data. In stochastic simulations, the results of each run are stored and used to generate frequency distributions from which statistics such as the mean, standard deviation and percentiles may be extracted.

5.4.6. Discussion

This 'family' of models has been used extensively by the EA as a planning tool and during the LOIS project to simulate dynamic changes in water quality in the Yorkshire Ouse river system (Lewis et al., 1997; Eatherall et al., 1998). The basic hydraulic model reduces the data requirements and also simplifies the process of calibration and results in relatively quick runtimes. However, this simple approach is not always sufficient, and where there are rapid changes in the flow rate or water quality the model may not be satisfactory. Certainly the model can not cope with any backflows or loops in the river system, and, unlike SIMCAT, TOMCAT and QUAL2E, QUASAR has no method for incorporating the effects of runoff. If this is required, it must be estimated externally and added as a point source or tributary flow. Furthermore, although the model is simple, when run as a dynamic model the data requirements for a large river system can be prohibitive.

The model is suitable for planning purposes and consent setting by using the stochastic capabilities, but this feature is rather limited when compared with SIMCAT and TOMCAT. QUASAR would be of more use for these purposes if more distribution types could be used, if monthly statistics could be used and particularly if correlations between the main river and tributaries and discharges and concentrations could be set.

5.4.7. Applicability to simulating do in lowland rivers

The QUASAR model has been used to simulate the water-quality of the Bedford Ouse (Whitehead et al., 1979, 1981) and has been used extensively as a part of the LOIS work (Lewis et al., 1997; Eatherall et al., 1998). The model satisfies many of the inadequacies of SIMCAT and TOMCAT in that the process descriptions are much more complete, and improves on QUAL2E as well, because it can run dynamically and stochastically, but the data requirements for running this model are considerable for dynamic simulations. In some catchments, this could prevent the model from, being applied successfully, but in many of the larger UK rivers this should not to be an issue. Of more concern is the flow representation, which is rather simple for a dynamic model and will not cope with complex flow patterns such as backflows. However, in non-tidal rivers this should not be an issue other than during extreme flow conditions. As a stochastic model, QUASAR should be improved to include correlations and an increased number of distribution types as available in SIMCAT and TOMCAT, but as a dynamic model QUASAR seems to be well suited to modelling large freshwater river systems provided there are sufficient data.

5.5. MIKE-11

MIKE-11 has been developed by the Danish Hydraulic Institute (DHI) and forms part of a suite of software marketed by themselves and other consultants in the UK and Europe. The model has been developed from the DHI's system 11 originally released in 1972 and is marketed as a modular package based around a 1D full-hydrodynamic model that simulates the dynamic water movements in a river or stream. The modules that may be added include those that simulate advection–dispersion, water quality, sediment transport, eutrophication, and rainfall-runoff. MIKE-11 is widely used as a hydraulic model by flood defence workers in the EA, but it is also used as a water-quality model as part of the Urban Pollution Management (UPM) methodology where it is used to assess the impact of intermittent discharges on rivers and estuaries. Because it uses a full-hydrodynamic model it is capable of modelling tidal sections of rivers as well as in freshwater applications.

5.5.1. Conceptual model

MIKE-11 consists of a set of modules that comprise a 1D model of flow and quality in rivers and estuaries. The hydrodynamic module simulates dynamic flows in rivers and estuaries and can be applied to branched and looped networks. Because the model is 1D, the scheme assumes that the flow conditions are homogeneous within the channel although flow over structures such as weirs can be simulated. The transport of solutes is simulated by an advection–dispersion module which solves the same 1D equation of conservation of mass as QUAL2E, but in MIKE-11 a dynamic solution is provided. Thus, the conceptual model is still that of reaches in series, but here the flow is modelled explicitly using the full-hydrodynamic equations and the ADE is solved dynamically.

The advection–dispersion module can simulate first-order decays of determinants, but for more advanced simulation one must use the water quality module. In MIKE-11, the water quality can be simulated at one of six different levels of complexity. For DO modelling, the increasing levels of complexity can be summarised thus:

- Level 1—First-order decay of BOD and DO plus reaeration and temperature effects.
- Level 2—As above plus BOD sediment exchanges (i.e. settling and re-suspension) and a sediment oxygen demand (SOD).
- Level 3—As above plus ammonium and nitrate balances without denitrification. This adds an oxygen demand due to nitrification.
- Level 4—As above plus denitrification.
- Level 5—As above plus a ‘delayed’ oxygen demand due to the settled BOD, but without the nitrogen components of ammonium and nitrate. BOD is now modelled as dissolved, suspended and settled fractions.
- Level 6—As above plus ammonium and nitrate. Cohesive and non-cohesive sediment processes may also be included for BOD.

Phosphorous and coliform processes may also be added to any of the levels. Other water-quality modules include: eutrophication, heavy metals, iron oxidation, nutrient transport, and wetlands. In each case the module can be run with or without sediment processes.

5.5.2. Processes

The hydrodynamic module is the core of the system and this solves either the full hydrodynamic (or St. Venant) equations or one of the two simpler versions called diffusive wave and kinematic wave equations as described in Section 4.1. The friction slope term can be estimated using empirical formulae such as those of Manning or Chezy. Using Manning’s method:

$$S_{\mathrm{f}}=\frac{Q|Q|}{K^2} \tag{54}$$

and

$$K=\frac{A^{5/3}}{nP^{2/3}} \tag{55}$$

where K is called the conveyance, n is Manning’s friction coefficient and P is the wetted perimeter. The velocity can then be estimated using the stream cross-section and friction parameters and the method of Manning or Chezy. The simpler versions are useful in steeper rivers where there will be no backwater effects because the St. Venant equations require complex numerical solutions. MIKE-11 uses an efficient implicit finite-difference model to solve the equations, but the solution of full hydrodynamic model can result in long runtimes.

Temperature is computed as being the result of the difference between the solar energy input in the daytime and the energy loss due to emitted heat radiation, i.e.:

$$\frac{\mathrm{d}T}{\mathrm{d}t}=I_{\mathrm{s}}-I_{\mathrm{r}} \tag{56}$$

where T is the temperature, t is the time, I_{s} is the solar energy input and I_{r} is the emitted heat loss.

The DO model, like QUASAR, accounts for photosynthetic production, respiration, atmospheric reaeration, BOD decay and nitrification and the number of terms included depends on the level of model being run. Up to and including level four, this can be expressed as:

$$\frac{\mathrm{d}C}{\mathrm{d}t}=P_{(t)}-R+K_{\mathrm{a}}(C_{\mathrm{s}}-C)-K_{\mathrm{bod}}L \\ -\alpha_1K_{\mathrm{ni}t}[\mathrm{NH_4}]^{e_4}-K_{\mathrm{SOD}} \tag{57}$$

where C is the DO concentration C_s is the saturation concentration, K_a is the reaeration rate coefficient, K_{bod} is the BOD decay rate coefficient, L is the BOD concentration, α_1 is the amount of oxygen used in converting a unit mass of ammonium to nitrate in nitrification, K_{nit} is the nitrification rate coefficient, $[NH_4]$ is the ammonium concentration, e_4, is a coefficient characterising the concentration dependence of nitrification, and K_{sod} is the ('baseline') sediment oxygen demand rate. Note the BOD may be split into dissolved particulate and settled fractions in levels five and six, and in this case three BOD degradation terms will be required. In this situation a settled BOD will occur in addition to the baseline SOD. Strictly speaking, this does not change the 1D nature of the model, but simply includes partitions within each element or reach where different processes may occur. The reaeration rate coefficient can be estimated by using the methods of Thyssen et al. (1987) and O'Connor and Dobbins (1958), or Churchill et al. (1962). Alternatively, the user may enter a measured rate or another method.

The simulation of BOD (L) at level four includes biological oxidation or degradation settling and re-suspension, i.e.:

$$\frac{dL}{dt} = -K_{bod}L - K_{set}\mathrm{BOD} + K_{sus} \tag{58}$$

where K_{set} is the settling rate coefficient and K_{sus} is a term expressing the rate or re-suspension. At levels five and six the BOD is separated into dissolved, particulate and settled fractions with individual rate parameters, and sedimentation and re-suspension will affect particulate and settled BOD differently than as expressed in Eq. (58). The BOD degradation rate coefficient is calculated as:

$$K_{bod} = K_1 L \frac{C^2}{K_2 + C^2} \theta_{BOD}^{(T-20)} \tag{59}$$

where K_1 is a rate coefficient for the oxidation of BOD, C is the DO concentration, K_2 is a coefficient describing the influence of DO concentration on the BOD decay and θ_{BOD} is a coefficient for the effect of temperature on the reaction rate. This model assumes that BOD degradation will decrease under anaerobic conditions because without oxygen, the bacteria responsible for degradation will be unable to survive.

The MIKE-11 description of the nitrogen cycle includes the nitrification of ammonium, the release of ammonium during respiration, the uptake of ammonium during photosynthesis and the denitrification of nitrate. Thus, the equation used to describe the ammonium transformations is:

$$\frac{d[NH_4]}{dt} = -K_{nit}[\mathrm{NH_4}]^{e_4} - \alpha_3 P + \alpha_4 R \tag{60}$$

where α_3 is the amount of ammonium uptake per unit mass of photosynthetic oxygen production, and α_4 is the amount of ammonium produced per unit mass of oxygen consumed in respiration. The nitrate transformations are described by:

$$\frac{d[NO_3]}{dt} = K_{nit}[\mathrm{NH_4}]^{e_4} - K_{den}[\mathrm{NO_3}]^{e_6} \tag{61}$$

where $[NO_3]$ is the nitrate concentration, K_{den} is the denitrification rate coefficient and e_6 is a coefficient characterising the concentration dependence of denitrification. At levels three and four it is only the immediate oxygen demand that is considered, but at levels five and six a delayed nitrogenous oxygen demand may also be included. A further option is to alter the reaction rate order for nitrification and denitrification from first order to one half or zero order provided the rate coefficients are also adjusted.

5.5.3. Data requirements

The MIKE-11 software allows the user to draw the river network on a screen using the mouse and this can then be corrected to the actual distances in a table. A series of editors in the interface allows the user to enter cross-section and hydrodynamic, advection–dispersion and water-quality parameters which are referenced to the network by the distance along the river. Tops of rivers and tributaries (i.e. the headwaters), discharges and abstractions are referred to as boundary conditions and each of these is linked to a time-series of flow and quality entered in an editor. Ideally, these time-series will include dry weather flow periods and storm events for the purposes of calibration and evaluating the model's performance.

Water-quality parameters are entered in a water quality file and default values are suggested initially. Rates can be set globally or for specific reaches identified by the distances along the river to which they apply. One must also choose the length of the run and a time-step in a simulation editor. The parameters specific to the water-quality model are listed in Table 2.

5.5.4. Model operation

Like QUAL2E, the model completes the flow simulation before solute transport and water-quality processes are simulated. Once this has been completed successfully, the model can be run for water quality using existing hydrodynamic results to save time. The hydrodynamic module contains an implicit, finite difference computation of the hydrodynamic equations and both subcritical and supercritical flow can be described by means of a numerical scheme which adapts according to the local flow conditions. Once a hydrodynamic run has been completed the advection–dispersion module can be run to simulate solute transport in the rivers. The advection–dispersion module solves the 1D ADE (as used by QUAL2E) using an implicit finite difference scheme and the results are used by the water-quality module to simulate the water-quality or this module can simulate the first-order decay of a determinant. The mass balances for the water-quality determinants are calculated for all reaches at all time-steps using a rational extrapolation method in an integrated two-step procedure with the advection–dispersion module.

5.5.5. Outputs

Following successful model simulations MIKE-11 provides the user with time-series of flow, depth and concentrations for each determinant for each reach. Since this data set can be large the user can specify a 'save-step' interval like QUESTOR such that, for example, daily values are produced from a model with an hourly frequency. The MIKE-11 software also provides numerous charting and statistical options to describe the results.

5.5.6. Discussion

The MIKE-11 model is an advanced model of flow and water-quality in streams. It can simulate the hydrodynamics of branched and looped rivers and estuaries, and can be used to simulate solute transport and transformations in complex river systems. However, a common problem for complex process models like MIKE-11 is the need for large amounts of data that may not always be available. MIKE-11 attempts to avoid this problem by allowing the user to run the model at different levels of water-quality complexity, so that it can be run even with limited data, but it is likely that there will be great difficulty in simulating some determinants well with such simple descriptions. Furthermore, with very limited data it would not be clear whether or not the chosen parameter set is unique and so the model would benefit from parameter estimation routines.

Like QUASAR, the MIKE-11 model is dynamic and so the data requirements are far greater than for a steady-state model like QUAL2E, because time-series rather than single values are required for influences. A further requirement in MIKE-11, which is not needed in QUASAR, is that channel cross-sections are needed at reach boundaries for the hydrodynamic model. The number of water-quality parameters required by MIKE-11 is actually less than the number required by QUAL2E, but it is more then in QUASAR and, because this is a dynamic model, the calibration and evaluation of results will be a far greater task for the user than in QUAL2E Finally, the use of a hydrodynamic model and the ADE requires that PDEs are solved rather than the ODEs used by QUASAR and so the MIKE-11 will not run as quickly and is unlikely to be as straightforward to calibrate.

5.5.7. Applicability to simulating do in lowland rivers

From the literature search, the model MIKE-11 has been applied as a water-quality model to the River Derwent, near Derby in central England (Crabtree et al., 1996) and the Yamuna River, near

Table 2
A list of parameters and coefficients required for the water-quality module of MIKE-11

Parameter	Description
Lat	Latitude
$I_{s,max}$	Maximum heat radiation from the river
I_r	Emitted heat radiation from the river
ϕ_r	Displacement of the time of maximum stream temperature from noon (12 p.m.)
K_a-type	Reaeration method and its temperature dependency
R, θ_R	Respiration of plants and animals at 20 °C and its temperature dependency
P_{max}	Maximum oxygen production (i.e. photosynthesis) rate
ϕ_p	Displacement of the maximum oxygen production from noon (12 p.m.)
K_{SOD}, θ_{SOD}	Baseline SOD decay rate at 20 °C and its temperature dependency
K_{BOD}, θ_{BOD}	Decay rate for dissolved BOD at 20 °C and its temperature dependency. At levels five and six need to separate this for dissolved, particulate and settled fractions
K_1	Biological oxidation (degradation) of BOD
K_2	Influence of DO concentration on the BOD decay
v_{set}	Settling velocity of (particulate) BOD
K_{sus}	Resuspension of (settled) BOD from the bed
v_{crit}	Critical flow velocity below which there is no re-suspension
β_{SOD}	Sediment oxygen adsorption constant (levels 5 and 6 only)
L_{crit}	Critical concentration of (settled) BOD in the river bed below which there is no re-suspension whatever the velocity
α_1	Oxygen demand by nitrification per unit mass of ammonium converted to nitrate
α_2	Rate of ammonium release as (dissolved/suspended/settled) BOD decays
α_3	Rate of uptake of ammonium in plants proportional to net photosynthesis
α_4	Rate of ammonium uptake in bacteria proportional to the BOD degradation (i.e. respiration)
n_{nit}	The nitrification reaction rate order (1, 0.5, or 0)
K_{nit}, θ_{nit}	Nitrification rate constant at 20 °C and its temperature dependency
e_4	Concentration dependence of nitrification
n_{den}	Denitrification reaction rate order (1, 0.5, or 0)
K_{den}, θ_{den}	Denitrification rate constant at 20 °C and its temperature dependency
e_6	Concentration dependence of denitrification

Delhi in northern India (Kazmi and Hansen, 1997). The model is clearly well suited to complex systems and can cope with complex flow patterns such as backflows and loops in the system. The processes simulated are also comprehensive, although the level of complexity is perhaps too great at level six, because the data requirements will be too high and the calibration will be difficult. If instead the model is used at too low a level the ease of setting up the model may cause a user to erroneously assume that they have a calibrated model representing the most important processes in the river, while in fact given a scarce dataset the model may calibrate equally well using several combinations of parameters, any of which may most accurately reflect the in-stream processes. In this case, a simpler model could provide equally good results given the amount of data available and would not be so easily misinterpreted. A final issue is that MIKE-11 lacks a stochastic component and this means that the model cannot be used in relation to UK legislation.

5.6. ISIS

The ISIS model has been developed by HR Wallingford from earlier models such as ONDA and SALMON-Q and the software has been developed and marketed by the consultancy Halcrow UK. ISIS is a dynamic model capable of simulating flow and water-quality and has been used by the EA, but more as a flow model for the flood defence groups than for water-quality modelling. Like MIKE-11 it is modular comprising the following:

- Short term flood hydrology and long term hydrology including subsurface interaction.

- Flow routing and full hydrodynamic simulations.
- Simple water quality analysis for urban pollution management.
- More comprehensive water-quality analysis using the quality + module
- Sediment transport modelling.

The model structure is therefore very similar to MIKE-11, although the actual water-quality process representations are different. The ISIS Quality module simulates a range of water quality determinants including: general conservative and decaying pollutants, coliforms, salt, temperature, pH, DO, BOD, organic and oxidised nitrogen, ammonium, phytoplankton (floating algae), macrophytes (fixed, rooted aquatic plants), benthic algae (algae on the river bed), adsorbed phosphorus, silicates, and cohesive sediments. It is also able to model some sediment–water column processes. It is not necessary to model all of the determinants in a particular simulation; however some of these variables and processes interact.

5.6.1. Conceptual model

The conceptual model is very similar to that in MIKE-11, and as with MIKE-11, the St. Venant equations for the hydrodynamics are solved and the transport of solutes is modelled by a finite difference approximation to the 1D ADE. Transformations of the determinants can occur as described by the process equations in the quality module. As the equation is only 1D all of the variables obviously represent averages across the cross-section. However, the requirements of the sediment–water interaction modelling demand that each element is divided. In this case, this is achieved by partitioning the reach vertically into four sub components as shown in Fig. 9.

The four components are (HR Wallingford and Halcrow UK, 1998):

- Water column—the main body of water through which dissolved and suspended substances are transported.
- Bed—the consolidated mud that has settled out of the water column and cannot be re-suspended.

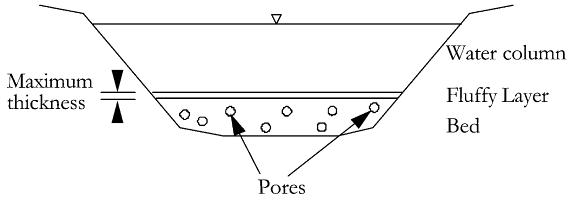

Fig. 9. Vertical structure of the ISIS Quality model (HR Wallingford and Halcrow UK, 1998).

- 'Fluffy layer'—the unconsolidated layer of mud that lies above the consolidated mud of the bed and has a lower density. Settled matter falls into this layer initially and once filled to its maximum thickness any additional settled material causes an equal amount to pass into the bed.
- Pore water—water trapped in pores within the consolidated mud. The rate of transfer of dissolved substances into the pore water is proportional to the deposition rate.

The contents of one layer are able to interact with the contents of an adjacent layer. This means that the contents of the fluffy layer can interact with the water column and the bed material and pore water can interact, but are isolated from the water column unless re-suspended. Erosion of the fluffy layer and bed material will return their contents and that of the pore water to the water column.

5.6.2. Processes

The water-quality processes in ISIS are incorporated into the ADE when the quality module is included. This is the same method used by QUAL2E and MIKE-11, but in ISIS there are two different methods for calculating the dispersion coefficient, D. The first is used for estuaries and the second for rivers:

$$D=D_0+D_1\frac{Q}{A_0U_0}+D_2\frac{\mathrm{d}S/\mathrm{d}x}{S_0/L_0} \tag{62}$$

or

$$D=\mathrm{Max}(D_0,D_1u_*b) \tag{63}$$

where D_0, D_1, and D_2 are empirical constants (and D_0 is a lower limit, D_1 represents tidal mixing and D_2 represents the effect of the salinity gradient on dispersion), Q is the flow rate, U_0 is the peak velocity at the downstream (or seaward) boundary, A_0 is a representative cross-sectional area at the downstream boundary, S_0 is a representative salinity, L_0 is a representative limit of saline intrusion, u_* is the shear velocity and b is the width at the water surface.

The form of the process equations for each determinant is the same as in QUAL2E and MIKE-11, i.e. they represent the internal transformations term in the ADE. In ISIS, the temperature is assumed to decay towards an equilibrium temperature, i.e.

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -K_\mathrm{T}(T - T_\mathrm{base}) \tag{64}$$

where K_T is the heat transfer coefficient and T_base is the equilibrium water temperature. When the water temperature exceeds the equilibrium temperature the water will cool otherwise it heats up unless the temperature is T_base in which case there is no heat transfer.

The DO model includes the oxygen demand due to BOD, the nitrification of ammonium, the oxidation of nitrite to nitrate, atmospheric reaeration and the effects of phytoplankton (i.e. photosynthesis and respiration). The BOD is divided into fast and slow decay components, where the fast BOD represents the dissolved fraction and the slow BOD represents a particulate BOD fraction. The decay of BOD is therefore represented by two temperature dependent first-order reactions.

The reaeration rate parameter can be calculated either as a simple function of temperature or by using a combination of equations formulated by Owens, et al. (1964), O'Connor and Dobbins (1958), and Churchill et al. (1962). The actual form of the equations used is modified from the original equations and the reaeration rate parameter (K_a) is expressed as a function of the width and cross-sectional area, i.e.:

$$K_\mathrm{a} = f_\mathrm{a}\frac{b}{A} \tag{65}$$

where f_a is the transfer velocity (based on the quoted equations), b is the reach width at the water surface and A is the cross-sectional area.

The DO model in ISIS thus uses the following equation,

$$\begin{aligned}\frac{\mathrm{d}C}{\mathrm{d}t} = {} & -K_\mathrm{f} - K_\mathrm{s} - 3.43K_\mathrm{am}[\mathrm{NH_4}] \\ & -1.14K_\mathrm{no2}[\mathrm{NO_2}] + K_\mathrm{a}(C_\mathrm{s} - C) \\ & + \frac{8}{3}[(P-R)\mathrm{AC} - K_\mathrm{dc}\mathrm{DC}]\end{aligned} \tag{66}$$

where C is the DO concentration, K_f is the decay rate coefficient for fast BOD ($\mathrm{BOD_f}$), K_s is the decay rate coefficient for slow BOD ($\mathrm{BOD_s}$), K_am is the rate coefficient for the nitrification of ammonium to nitrite, $[\mathrm{NH_4}]$ is the concentration of ammonium, K_no2 is the rate coefficient for the oxidation of nitrite to nitrate, K_a is the reaeration rate parameter, C_s is the saturation concentration of DO, P is the rate of photosynthetic oxygen production, R is the respiration rate, AC is the dry-weight of algal carbon as a concentration, K_dc is the rate coefficient for the oxidation of detrital carbon and DC is the concentration of detrital carbon.

The BOD model in ISIS divides the BOD into fast and slow components. Otherwise the BOD model is similar to those in the other models described, i.e.:

$$\frac{\mathrm{d}L}{\mathrm{d}t} = -K_\mathrm{f} - K_\mathrm{s} \tag{67}$$

the rate parameters are temperature dependent and the proportions of each BOD fraction can be estimated by using the following relationship:

$$\mathrm{BOD_u} = \frac{\mathrm{BOD_5}}{1 - \left[(1-\alpha)\mathrm{e}^{-5K_\mathrm{f}} + \alpha\mathrm{e}^{-5K_\mathrm{s}}\right]} \tag{68}$$

where $\mathrm{BOD_u}$ is the ultimate BOD and $\mathrm{BOD_5}$ is the five-day BOD which is equivalent to the fast BOD ($\mathrm{BOD_f}$). In the other models, BOD will cease to decay if the DO levels drop to zero, but in ISIS the decay can continue using oxygen produced from denitrification and the decay of sulphates to hydrogen sulphide.

Nitrogen is modelled in ISIS as organic nitrogen, ammonium, and the oxidised forms nitrite and nitrate. The organic nitrogen can be hydrolysed to ammonium and is produced when detrital carbon is oxidised, i.e.:

$$\frac{dN_o}{dt} = -K_{hyd}N_o + \text{rphtn } K_{dc}\text{DC} \tag{69}$$

where N_o is the concentration of organic nitrogen, K_{hyd} is the reaction rate coefficient for hydrolysis, rphtn is the nutrient to carbon ratio for nitrogen for phytoplankton, K_{dc} is the decay rate parameter for the decay of detrital carbon and DC is the concentration of detrital carbon.

Ammonium is simulated as being nitrified to nitrite (when there is sufficient oxygen) as a first-order decay, i.e.:

$$\frac{d[NH_4]}{dt} = K_{hyd}N_o - K_{am}[NH_4] \tag{70}$$

where $[NH_4]$ is the ammonium concentration, K_{am} is the rate coefficient for the nitrification of ammonium to nitrite and:

$$K_{am,T} = K_{am,20}\left(1+\frac{\alpha}{100}\right)^{T-20}\left(1+\frac{\beta}{100}\right)^{S-S_0}\left(1+\frac{\gamma}{100}\right)^{SS-SS_0} \tag{71}$$

where $K_{am,T}$ is the nitrification rate parameter at temperature T, $K_{am,20}$ is the nitrification rate parameter at 20 °C, α is a temperature dependence factor, β is a salinity dependence factor, S is the salinity, S_0 is a reference salinity, γ is a suspended solids dependence factor, SS is the suspended sediments concentration, and SS_0 is a reference concentration of suspended solids. An equilibrium exists between ionised (NH_4^+) and unionised forms of ammonia (NH_3) and the proportion of each that exists in a body of water depends on the pH and temperature (T). In ISIS, this relationship is included as:

$$[NH_3] = \frac{[NH_4^+]}{1+10^x} \tag{72}$$

and

$$x = 10.055 - 0.0324T - \text{pH} \tag{73}$$

where higher pH values (i.e. lower concentrations of hydrogen ions) allow a greater proportion of ammoniacal nitrogen to exist in the unionised form (i.e. as NH_3). The primary purpose in ISIS for simulating pH is to determine the concentration of unionised ammonia which is toxic to aquatic life.

Nitrite, is the result of oxidising ammonium during nitrification, but under anoxic conditions or conditions with very little oxygen, oxygen demand in the water may be met by denitrification, thus:

$$\frac{d[NO_2]}{dt} = K_{am}[NH_4] - 0.58\frac{[NO_2]}{[NO_3]+[NO_2]} \tag{74}$$

where $[NO_2]$ is the nitrite concentration and $[NO_3]$ is the nitrate concentration. The first term only applies when there is sufficient oxygen and the second term only applies when the DO concentration is close to zero. Like nitrite, nitrate may also act as a source of oxygen under anoxic conditions, but it is also taken up by plants during photosynthesis and is formed from the oxidation of nitrite, i.e.:

$$\frac{d[NO_3]}{dt} = K_{no2}[NO_2] - 0.35\frac{[NO_3]}{[NO_3]+[NO_2]} - \text{rphtn}\cdot P\cdot \text{AC} \tag{75}$$

where rphtn is the nutrient to carbon ratio for nitrogen for phytoplankton, P is the rate of production, AC is the dry-weight of algal carbon. Macrophytes (if simulated) also take-up nitrogen in the form of nitrate, but in ISIS this is assumed to be only taken from the pore water not the water column itself.

The phytoplankton model includes the photosynthesis, respiration and mortality of algae, i.e.:

$$\frac{\mathrm{d\,AC}}{\mathrm{d}t}=(P-R-M_{\mathrm{p}})\mathrm{AC} \tag{76}$$

where AC is the dry-weight of algal carbon, P is the production rate, R is the respiration rate, and M_{p} is a mortality constant. Thus, unlike the models described previously, ISIS represents algae by the dry weight of algal carbon, rather than by chlorophyll-*a*. The rate of growth of algae is dependent on the species and the temperature and is assumed to be limited by the intensity of light reaching them and the availability of nutrients (nitrogen, phosphorous and silicon). Thus, the daily algal production is calculated by multiplying the maximum growth rate for the species being modelled, the light limitation factor and the limitation factors for each included nutrient. In ISIS, this is represented by:

$$P_{\mathrm{max}}=\mathrm{e}^{(2.303mT+c)} \tag{77}$$

and

$$P=P_{\mathrm{max}}\mu_{\mathrm{light}}\,\mathrm{Min}(\mu_{\mathrm{N}},\mu_{\mathrm{P}},\mu_{\mathrm{Si}}) \tag{78}$$

where P_{max} is the maximum possible rate, μ_{light} is the light limitation factor and μ_{N}, μ_{P}, and μ_{Si} are the nutrient limitation factors for nitrogen phosphorous and silicon, respectively. The light availability is represented by μ_{light} (Steele and Baird, 1965):

$$\mu_{\mathrm{light}}=\frac{I\,\mathrm{e}^{(1-I/I_{\mathrm{max}})}}{I_{\mathrm{max}}}\quad\text{and}\quad I=I_0\,\mathrm{e}^{-kz} \tag{79}$$

where I is the light intensity at the water surface, z is the depth and k is an attenuation factor related to the algal and suspended solids concentrations. To represent nutrient limitations a Michaelis–Menten equation, using a half-saturation constant, is used for each nutrient (although the inclusion of silica is optional), i.e.:

$$\mu_{\mathrm{N,P,Si}}=\frac{C_{\mathrm{N,P,Si}}}{k_{\mathrm{N,P,Si}}+C_{\mathrm{N,P,Si}}} \tag{80}$$

where μ is the nutrient limitation factor, C is the concentration of the nutrient and k is the half-saturation constant for the nutrient.

Phytoplankton respiration (R) is included as a function of the temperature using:

$$R_T=R_{20}\theta_{10}^{(T-20)/10} \tag{81}$$

where θ_{10} is the temperature dependency coefficient. Phytoplankton death (or mortality) is simulated as a first-order process with a fixed rate constant and the dead algae contribute to the detrital carbon in the water column.

The death of algae produces suspended detrital carbon which may be oxidised (like BOD) and in the process of oxidation releases of nutrients into the water column. Detrital carbon is assumed to be particulate and suspended in the water sediment and so can settle onto the bed where it becomes incorporated into the fluffy bed layer. This 'bed detrital carbon' decays at the same rate as the suspended detrital carbon and the nitrogen produced is 'recycled' as organic nitrogen, the phosphorus as orthophosphate and the silicon as silica. The proportions of detritus that are nitrogen, phosphorus or silicon are determined by nutrient to carbon ratios. Thus,

$$\frac{\mathrm{d\,DC}}{\mathrm{d}t}=M_{\mathrm{p}}\mathrm{AC}-\left(K_{\mathrm{dc}}+\frac{v_{\mathrm{sdc}}}{d}\right)\mathrm{DC}\quad\text{and}$$
$$K_{\mathrm{dc},T}=K_{\mathrm{dc},20}\left(1+\frac{\alpha_{\mathrm{dc}}}{100}\right)^{T-20} \tag{82}$$

where DC is the concentration of (suspended) detrital; carbon, v_{sdc} is the settling velocity for suspended detrital carbon, d is the depth and α_{dc} is a temperature dependence coefficient for the decay rate. As well as material settling on the fluffy layer, it can also be eroded from it. The rate of deposition is controlled by a settling velocity and the water column sediment concentration. Erosion is governed by the bed stress which is a function of overall friction, water velocity and the average density of the water. Thus, the amount of sediment on the bed is represented by the equation:

$$\frac{\mathrm{d}m}{\mathrm{d}t}=v\cdot\mathrm{SS}-M_{\mathrm{e}}(T_{\mathrm{b}}-T_e) \tag{83}$$

where m is the mass of sediment per unit bed area, v is the settling velocity, SS is the suspended sediment concentration, M_e is the erosion rate constant, T_e is the critical erosion stress of the bed and T_b is the bed stress, where:

$$T_b = \frac{f_{\text{bed}} u|u|\rho}{8} \tag{84}$$

where f_{bed} is the overall friction factor, u is the stream flow velocity and ρ is the average density of the water.

Benthic algae and macrophytes may also be simulated using ISIS. For benthic algae, the rates of production, respiration and mortality are all determined in the same way as for phytoplankton, i.e.:

$$\frac{\mathrm{d\,BA}}{\mathrm{d}t} = (P - R - M_{\text{ba}})\text{BA} \tag{85}$$

where BA is the dry-weight of carbon in the benthic algae, and M_{ba} is the mortality rate for benthic algae. However, macrophytes are assumed to make all of their oxygen exchanges (photosynthesis and respiration) in the atmosphere not the water column and macrophyte mortality (M) is simulated as a function of salinity (S):

$$M = \frac{M_{\text{mac}}(10 - S) + 0.9(S - 3)}{7} \quad \text{for}$$
$$\text{S} \leq 10‰ \quad M = 0.9 \tag{86}$$

where M_{mac} is the rate at a salinity of 3‰ (parts per thousand). Although the oxygen produced by macrophytes during photosynthesis is assumed to escape into the atmosphere, it is assumed that a proportion of the production of macrophytes (pexu1) is lost into the water column. Thus, the macrophytes (MC) are represented by:

$$\frac{\mathrm{d\,MC}}{\mathrm{d}t} = \left[(1 - \text{pexu1})P - M\right]\text{MC} \tag{87}$$

Both benthic algae and macrophytes also contribute towards the detrital carbon on death, but both supply carbon directly to the bed store (rather than being suspended as with phytoplankton sourced detrital carbon) and a proportion (plea1) of the macrophyte production is also lost by leaching, thus:

$$\frac{\mathrm{d\,DC_{bed}}}{\mathrm{d}t} = M_{\text{ba}}\text{BA} + M(1 - \text{plea1})P \cdot \text{MP} \tag{88}$$

5.6.3. Data requirements

In common with other dynamic water-quality models, ISIS requires boundary conditions of flow and water-quality time-series at the beginning of the network and at the top of each tributary being simulated. As with MIKE-11 the model also requires flow and water quality data at the downstream boundary because of the full-hydrodynamic representation. ISIS uses the channel shape to calculate depth and area from the flow rate and the shape is defined by cross-sections that the user must supply. Between sections the model assumes that the channel is uniform in cross-section, but it can simulate changes within reaches (such as general changes in shape or structures) using more cross-sectional data. This can be important if structures such as bridges and weirs are present. Furthermore, ISIS uses simulated depth, velocity and slope values to estimate the rate of reaeration and so, if insufficient cross-sections are supplied, this can lead to a reduction in accuracy.

The boundary conditions of flow and water quality provided can be time-series or the quality data can be inputted as seasonal stochastic data. Influences such as effluent discharges or abstractions can only enter where a cross-section has been supplied, and tributary confluences require cross-sections upstream and downstream of the confluence in the main river. Discharges and abstractions may be entered as time-series or as statistics, but the statistical method is not straightforward, because it asks for shape functions (rather than say means and standard deviations). These shape functions are rather complex to derive and require hourly data for many days. Thus, this is not a simple method to implement and is also limited in that ISIS is unable to account for correlations between inputs as TOMCAT does.

Problems can arise in applying ISIS because it is a complex process model and so requires a large number of rate parameters to be specified and many of the parameters required are rarely or never measured. For example, once the sediment processes are chosen to be simulated, it is necessary to supply data for most determinants and their processes for each layer. For example, data may be required for BOD in the water column (slow and fast), in the fluffy and consolidated bed layers and in the pore water for each site and these data will often not be available. For example pore water concentrations are rarely measured outside of a laboratory. If the data are not provided, the model will still run on the default assumption of an initial condition of zero, but this can have a serious impact on not only the accuracy of the model, but also on the relative ease of calibration too. Unlike the other models described in this review, ISIS represents algae by the dry weight of algal carbon, rather than by chlorophyll-*a*. Again this is a more elegant description, but it will be affected by a lack of data, since most routine measurements are of chlorophyll-*a*. A relationship between the two could be devised, but this is then little better than the semi-empirical methods employed by other models to use chlorophyll-*a* rather than carbon as an indicator of the algal population.

5.6.4. Model operation

Once the data files have been compiled, ISIS first simulates the flow in the rivers at steady-state. This generates a set of initial conditions that can be used by the model to run a dynamic flow simulation. Like MIKE-11, this hydrodynamic run must be completed for the whole system before any simulation of water-quality can be made, and like MIKE-11 once the flow model has been calibrated satisfactorily the results can then be stored and used for any number of quality runs in the future to save time. This is particularly useful, because the run times in ISIS can be rather long. Calibration must be carried out by the user (there are no automatic routines included) and obviously this is done for flow and then the water-quality determinants. In ISIS this can be a difficult operation given the number of determinants and parameters, especially if the sediments are included in a simulation.

5.6.5. Outputs

A successful run of the model produces time-series of flow and water-quality at user-defined time steps for each cross-section. ISIS has a built in interface to display the data and it can plot some measured/observed data for comparative purposes. However, the format of the graphs is fixed and this means that often one must often resort to exporting the data into another software package for charting.

5.6.6. Discussion

ISIS is clearly a comprehensive package of software and is the most complex of the mechanistic models described here. However, it is not often used for water-quality modelling due to the difficulty in collating sufficient data to run the model. The in-reach processes are wide-ranging, but the whole system is limited, because fixed parameters are used throughout the model. This means that, in a large system where there could be quite different flow regimes, the model uses the same parameters for processes such as BOD settling and ammonium decay for all river reaches in the system being modelled. This may be mitigated by detailed calibration of parameters such as the depth and the sediment shear velocity, but these terms will not always be known to the accuracy required. Furthermore, fixed rate parameters can not allow for any small-scale variability such as the rapid removal of substances like ammonium downstream of STWs. A number of improvements might be recommended and these include:

- improved data entry, given the requirements of the model;
- the ability to enter data as simple statistics such as the mean and standard deviation;
- reduced data requirements in general, for example, pore water concentrations could be estimated as some proportion of the concentration in the water column where data are not available;
- spatially variable parameters;
- improved presentation of results and improved exporting of the results;

5.6.7. Applicability to simulating do in lowland rivers

The literature review did not reveal any applications of ISIS as a water-quality model, although it is more widely used in flood simulation applications. The lack of presence in the literature is quite likely to be related to the high cost of the software. Expensive software is more often used in commercial than academic situations and so the results of applications do not often make it into the public literature. However, the hydrodynamic model allows ISIS to cope with the full range of flows seen in lowland rivers and it can even account for floods that leave the confines of the river bank.

The water quality processes that can be simulated are numerous and the preceding sections have shown that the ISIS model is the most complex of all the water-quality models described in this review. Thus, one might expect that (given that these are mechanistic models that try to describe real-world processes affecting determinants) this should be the most accurate of those models. However, many of the parameters required are rarely or never measured and a lack of data will lead to uncertainty that may not be correctly identified, especially by more inexperienced users. Even where there is a great deal of data associated with a large river system, this may not be sufficient for a simulation of ISIS using its full functionality. Furthermore, ISIS would benefit from the ability to enter data in a more simple statistical format than the shape functions, such as means and standard deviations on a define distribution.

6. Conclusions and recommendations for modelling dissolved oxygen in lowland rivers

At the current time there are many excellent and elegant models for studying environmental processes and new models appear regularly that further enhance our understanding of those processes and provide tools for water utility managers and regulators alike. There are, therefore, many water-quality models in use today that are not mentioned here, but most do not satisfy the requirement of availability, i.e., a distinct computer programme or other obtainable piece of software in which the user can simulate water quality in streams and rivers by supplying physical and chemical data. Often, this is because the research institutions and universities active in model development do not have the financial resources to develop the model as a ‘user friendly’ piece of software, since the development and testing of a suitable interface can be a very expensive part of model development. As a result, such models only tend to be available commercially with high purchase and licence costs.

Models have been developed for particular purposes and it is perhaps unfair to set one against the other in terms of broad applicability. However, from the review undertaken here, an ideal model would possess the following properties (Whitehead, 1980):

- It should be a truly dynamic model capable of accepting time-varying inputs of the upstream water quality, which are used to compute time varying output responses downstream;
- It should provide a reasonable mathematical approximation of the physical, chemical and biological changes occurring in the river system and should be compared with real data collected from the river at a sufficiently high frequency and for a sufficiently long period of time;
- The model should be as simple as possible whilst retaining the ability to adequately characterise the important aspects of the system behaviour;
- It should be able to account for the inevitable errors associated with laboratory analysis and sampling, and account for the uncertainty associated with imprecise knowledge of the pertinent physical, chemical and biological mechanisms.

The models described here have been described as being either steady-state or dynamic and, since all of the models are mechanistic, they will all (to a greater or lesser degree) provide a reasonable mathematical approximation of the physical, chemical and biological changes. Furthermore all of the models can accept observed data for the purposes of calibration and model evaluation. In terms of processes, the models reviewed in this review can be divided into three levels of complexity,

- Simple—SIMCAT and TOMCAT
- Intermediate—QUAL2E and QUASAR
- Complex—MIKE-11 and ISIS

The question, therefore, is which level of complexity is required to meet the demands of simulating DO in lowland rivers? The simple models will be unable to determine which processes dominates the control of DO concentrations in rivers, because they do not include a sufficient number of processes, and so SIMCAT and TOMCAT can be discounted. Perhaps then, the complex models MIKE-11 and ISIS should be considered since they include a large number of processes that can be investigated in terms of DO and other aspects of water chemistry? Unfortunately, the data requirements of these models are prohibitive if all processes are to be involved and the complexity of any model should be consistent with the quality and quantity of data available for its application (Eatherall et al., 1998). Furthermore, the financial cost of these models must also be considered and the common lack of data suggests that it is difficult to justify the time and costs required to set up a very complex river water-quality model.

Model complexity is not confined to the number of processes simulated and the mathematical formulation should also be considered. For example, the QUASAR model is a set of lumped parameter, ODEs that draws upon standard elements of chemical engineering reactor analysis (Himmelblau and Bischoff, 1968; Whitehead et al., 1979). This idealisation is clearly not as flexible as full hydrodynamic models incorporating ADEs, but it does approximates the properties of those distributed parameter, PDE representations and this form has been tested favourably in several water quality studies (Thomann, 1972; Beck and Young, 1975; Whitehead et al., 1979, 1981, 1984, 1995; Lewis et al., 1997; Eatherall et al., 1998). The principle advantages of this model over the more complex PDE descriptions used by MIKE-11 and ISIS are (Whitehead et al., 1981):

- the simplified computation required to solve the equations in the case of lumped parameter ODEs;
- the availability of statistically efficient algorithms for model identification and parameter estimation that can readily be applied to equations of the lumped parameter form;
- the availability of extensive control system methods which are best suited to and ODE model and which may be used for management purposes.

Therefore, it is the intermediate models that perhaps offer the best framework in which to investigate DO in lowland rivers and it is also desirable that a dynamic model be applied rather than a steady-state model. The steady-state modelling approach has been questioned on the following technical grounds: the probability distribution of downstream water quality which underlies the guidelines for the setting of consent conditions for effluent discharges depends on short-term interactions between the upstream flow and quality and these interactions are not considered by a steady state model (Warn, 1982). In relation to DO models the deficiencies of steady state models have also been highlighted by Beck and Young (1975) who state that ‘for any forecasting, parameter estimation, or control applications two factors are of considerable importance. Firstly, a river system in unlikely to be in a steady state since this implies that the BOD and DO inputs and outputs, as well as the volumetric flow-rate, are time-invariant; therefore a dynamic model should be assumed. Secondly, it is not constructive to use the model unless it has been shown to be a reasonable description of the true nature of the system.’ Thus, the usefulness of the steady state modelling approach can be somewhat limited and a dynamic approach is required to account for the flow and water quality interactions.

It is therefore recommended that, in general, the model QUASAR is well suited to investigating DO in lowland river systems. This model also benefits from a stochastic mode and this can be used in two ways: (a) to investigate the errors associated with laboratory analysis and sampling, and the uncertainty associated with imprecise knowledge of model parameters and process mechanisms; (b) to provide model results in a form suitable for comparison with the guidelines and standards in EC Directives and legislation in the UK. However, it is clear from this review that, like all models, the QUASAR model has a number of limitations, and these must be either addressed or acknowledged. Moreover model uncertainty must be quantified and understood if meaningful interpretations of model output are to be made.

Acknowledgments

This review results from a NERC/Environment Agency funded Ph.D. (GT2/97/3/EA), and the author is grateful to NERC and the Environment Agency for the financial support granted, also to Paul Whitehead (The University of Reading) and Colin Neal (CEH, Wallingford) for supervising the project.

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