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Hydro-environmental modelling of riverine basins using dynamic rate and partitioning coefficients

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ABSTRACT
Details are given of the increasing global public concern relating to hydro-environmental issues and examples are cited of some of the water quality and contaminant problems now being considered by river managers on a regular basis. The limitations and restrictions of both physical and numerical hydro-environmental models are discussed and concerns raised about the increasing use being made by non-specialist river engineers and scientists of complex hydroinformatics tools – often with a minimal appreciation of the complex hydrodynamic, bio- and geo-chemical, sediment transport or computational processes involved. General details are given of numerical models used for flow, water quality, sediment transport and heavy metal concentration predictions in river basin systems and particular emphasis is focused on the influence of some master variables on two key hydro-environmental processes. These processes include the decay of coliform bacteria and the partitioning of heavy metals. Two case studies are then discussed. In the first of these studies the velocity field and faecal coliform levels were predicted for a hypothetical discharge into a freshwater lake, namely Cardiff Bay, U.K., where the effects of dynamic decay rates were found to be significant. In the second study velocity, suspended sediment and heavy metal concentration distributions were predicted along the Mersey Basin, U.K., with dynamic partitioning coefficients being found to give improved agreement between predicted and measured heavy metal fluxes.

Keywords: Hydroinformatics; river hydraulics; water quality; decay rates; sediment transport; geo-chemical modelling.

1 Introduction

1.1 Water quality concerns

In recent years there has been growing international public concern and an increased awareness of riverine pollution problems – particularly with regard to water pollution. This increasing concern relating to hydro-environmental and hydro-ecological issues has been welcomed by river engineers, scientists and managers, since the role and contribution of the engineer and scientist in combating water pollution, and the importance of accurate hydro-environmental modelling, has not always been fully appreciated by governments and society. In connection with such pollution concerns, river engineers and scientists are now involved in an increasing range of environmental impact assessment studies in most countries, with some typical examples as to the causes and problems of water pollution being given below:

(i) Sewage discharge is still one of the main forms of waste disposal to the aquatic environment and is generally released by one of two methods. Firstly, sewage can be discharged directly from outfall pipes or storm water overflows into riverine waters. Secondly, it can be discharged indirectly from diffuse sources; where, for example, farm animal waste is transported to rivers – usually under wet weather conditions – via surface stream pathways or through saturated zone groundwater flows. Such sewage discharges can include organic waste, bacteria and viruses, but in most countries direct sewage discharges into rivers have been continuously decreasing in recent years as new or more efficient wastewater treatment works are commissioned. However, the management of diffuse source inputs continues to be a major international challenge.

(ii) Industrial and chemical waste from factories etc. alongside major rivers can include the disposal of potentially dangerous substances, such as PCBs, TBT, organo-chlorines, heavy metals and acidic wastes. Such waste discharges are often released directly into many major rivers, but can also enter the aquatic system from air polluting discharges and the subsequent settling of particulate matter directly on the river surface water or on the land, only then to be transported from the land to the river system in a similar manner as to the transport of diffuse source inputs.

(iii) Intensive farming of crops on land and aquaculture within major rivers can lead to increasing nitrate and phosphate contamination from fertilizers and relatively high levels of soluble nitrogenous waste products from aquaculture. These waste solutes often lead to nutrient enrichment of the water column which, in turn, acts as a fertilizer and can thereby increase the growth of phytoplankton, potentially leading to algal blooms and eutrophication.

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(iv) Cooling water discharges, particularly from fossil fuel plants, can significantly affect aquatic life. Such discharges into large rivers can raise the local water temperature by as much as 5°C, which in turn can have a major impact on the river ecology, as well as affecting the kinetic processes for a wide range of water quality indicators.
(v) Poor flushing of relatively deep rivers or riverine embayments often leads to undesirable water quality characteristics in the form of low dissolved oxygen levels and the long-term accumulation of toxic, industrial and domestic waste, particularly during summer months.

The increased public awareness and concern relating to hydro-environmental issues, such as those cited above can be attributed to a number of factors. Some of these factors are as follows:

(i) In recent years there has been a growing awareness of the health risks associated with various forms of water pollution. For example, recent research in the U.S.A. has indicated a higher incidence of cancer of the bladder, colon and rectum in those drinking excess chlorinated water (Perera and Boffetta, 1988).
(ii) There has been a significant increase in media coverage of hydro-environmental issues in most countries, with a consequential change in public opinion. For example, the waterside development at Cardiff Bay (discussed herein), with the construction of an exclusion barrage across the mouth of two rivers, received extensive publicity at the planning and construction stage, including extensive coverage in national media.
(iii) Increased recreation and higher standards of living in many countries have also raised public awareness of most forms of water pollution. Tourism and international travel have continually been on the increase in recent years and have heightened public awareness and concern relating to the quality of water in river basins. For example, increased international travel has raised the global concerns of the health of many large rivers and particularly those rivers flowing through developing countries.
(iv) Hydro-environmental issues and concerns are now well up the political agenda in most countries. For example, in Europe concerns over climate change, EU water quality related directives and the influence of environmental pressure groups have influenced politicians of all political affiliations of the importance of hydro-environmental issues.

This increased public awareness of hydro-environmental issues and the type of water pollution examples cited above have led to a marked broadening of the role and responsibilities of river engineers and managers involved in planning assessment studies relating to water quality considerations. For example, the river engineer or manager involved in a feasibility study to determine the impact of diffuse source inputs on the hydro-ecology of a river system is increasingly expected to apply sophisticated hydroinformatics tools and then to interpret the results of complex hydrodynamic, sedimentary, biological and geo-chemical processes simulated using these tools.

1.2 Modelling restrictions

Throughout the past two decades there has been an increasing emphasis on using numerical models, rather than physical models, for predicting flow, sediment transport and water quality indicator levels in riverine systems. This increased emphasis in using numerical (or computational) models has occurred for a number of reasons, some of which are summarised below:

(i) Physical models have the over-riding disadvantage of scaling. This constraint can be particularly critical for modelling the transport of sediments and heavy metals, since these particulates cannot be scaled properly in the physical model. Furthermore, in modelling solute fluxes (including water quality indicator organisms, suspended sediments and heavy metals) the processes of dispersion, diffusion and kinetics are also not scaled properly in physical models and the measured laboratory data can lead to erroneous predictions of the corresponding concentration levels.
(ii) Physical models are increasingly perceived to be more expensive than numerical models, particularly since they generally require large laboratory resources, sophisticated electronic equipment and specialist technical support staff.
(iii) Physical models are not readily transportable, as compared to computer models which can be distributed via the Internet, using high-quality colour graphic presentations.
(iv) Physical models are not adaptable, in that a model of a particular river basin is unique to that river and cannot be used for any other river basin. In contrast, a well-tested and robust hydro-environmental numerical model can be used for a wide range of riverine studies, provided that the model limitations are appreciated and realistic.

Hence, for these and other reasons, hydroinformatics tools (embracing user-friendly numerical models) have become increasingly more attractive than physical models for most hydro-environmental studies. However, many computational model researchers, specialising in the development of hydroinformatics tools, are becoming increasingly concerned about the misuse and the unrealistic expectations of such sophisticated tools by some clients and practising river engineers and managers involved in water quality studies. For example, studies have been commissioned in the U.K. where contracts have been proposed and accepted to predict the tidal currents in large complex estuaries to within ±10% of the field measured data, for typically 70% of the measuring period. Such requirements are unrealistic in most practical cases, since – like physical models – numerical models also have a number of uncertainties. In any river basin study, the true solution of the flow and solute transport processes depends upon how accurately the solution of the model equations, the boundary conditions, the equations themselves, the empirical coefficients used to represent such processes as: the roughness, turbulence, dispersion and kinetics etc., reflect the actual hydrodynamic and bio-chemical conditions occurring in the basin. In modelling numerically the flow and water quality indicator conditions in riverine waters, there are still a large number of uncertainties included in these models.

This study focuses in particular on two of these uncertainties; these relate to the decay rate for faecal (and similar) coliform indicators and the partitioning coefficients for heavy metal fluxes. For faecal indicator decay rates, historically these rates have generally been treated as solely temperature dependent and with typical values used being as cited in the U.S. EPA models (see Brown and Barnwell, 1987). However, field and laboratory data have shown that these decay rates are also highly dependent upon solar radiation etc. Hence, in the hydro-environmental model outlined herein the decay rate has been split into two parts, including a night time decay rate and a solar radiation component giving (Kashefipour *et al.*, 2002):

$$k_B = k_n + aI^b \tag{1}$$

where k_B = total decay rate, (day^{-1}), k_n = night time decay rate (day^{-1}), I = receiving solar radiation (Wm^{-2}) and a and b = empirical constants. This refined representation of the total decay rate was applied to predict faecal coliform levels in Cardiff Bay for a hypothetical discharge, with the modified decay rate having a significant impact on the receiving water coliform distributions.

Likewise, in predicting heavy metal fluxes, such metals can enter the water column through various means. They can be input directly in either their particulate or dissolved form or in the form of re-suspension from the bed sediments. The metals can be advected with the flow in their dissolved form, or adsorbed onto the sediments and advected with the sediments (see Figure 1). In particular, Millward and Turner (1995) have established that the partitioning of heavy metals between the particulate and dissolved phase is dependent upon salinity. They established from field data an empirical relationship linking the partitioning coefficient with salinity of the following form:

$$\log_e(K_D) = b\log_e(S+1) + \log_e(K_D^0) \tag{2}$$

where K_D = partitioning coefficient (=P/C, where P = contaminant concentration adsorbed on the sediments and C = contaminant concentration in solution), S = salinity and K_D^0 = partition coefficient in freshwater. This relationship was adopted in predicting heavy metal fluxes in the Mersey and Humber estuarine basins in the U.K. and details of the former study are given herein.

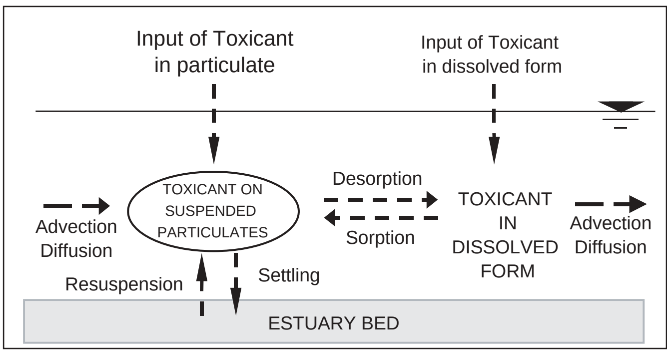

Figure 1 Schematic illustration of heavy metal processes in estuarine waters.

2 Hydro-environmental model details

The type of hydro-environmental models commonly used by environmental engineers and water managers to assist in environmental impact assessment studies generally involve solving the following equations:

(i) *For flow modelling*

The numerical models used to predict the flow, water quality, and sediment and contaminant transport processes in river and estuarine waters are based on first solving the governing hydrodynamic equations. For a Cartesian co-ordinate system, with the main body of the flow in the x-direction, then the corresponding 3-D Reynolds equations for mass and momentum in the flow direction can be respectively written in a general conservative form as:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \tag{3}$$

$$\underbrace{\frac{\partial u}{\partial t}}_{(1)} + \underbrace{\frac{\partial u^2}{\partial x} + \frac{\partial uv}{\partial y} + \frac{\partial uw}{\partial z}}_{(2)} = \underbrace{X}_{(3)} \underbrace{-\frac{1}{\rho}\frac{\partial P}{\partial x}}_{(4)} \underbrace{- \frac{\partial \overline{u'u'}}{\partial x} - \frac{\partial \overline{u'v'}}{\partial y} - \frac{\partial \overline{u'w'}}{\partial z}}_{(5)} \tag{4}$$

where u, v, w = velocity components in the x, y, z co-ordinate directions respectively, t = time, X = body force in the x direction, ρ = fluid density, P = fluid pressure, $\overline{u'u'}, \overline{u'v'}, \overline{u'w'}$ = Reynolds stresses in the x direction and on the x, y, z planes respectively. Similar equations to (4) can be written to evaluate the velocity components v and w in the y and z directions respectively.

In the momentum equation above (i.e. Eq. (4)), the individual terms refer to: (1) the local acceleration, (2) the advective acceleration, (3) the body force, (4) the pressure gradient, and (5) the Reynolds stresses. For the body force term this is related to the gravitational acceleration in the vertical direction and to the relative motion effects of the earth's rotation, i.e. the Coriolis acceleration, in the x and y directions, or in the horizontal plane. The pressure gradient is related to the free surface slope and the Reynolds stresses incorporate the shear force effects arising from the bed resistance, wind action and turbulence. These latter force components, incorporated in the Reynolds stresses, each include empirical coefficients and details of these coefficients and the related formulations are given in detail in Falconer *et al*. (2001).

(ii) *For water quality, sediment and heavy metal modelling*

In modelling numerically the flux of water quality constituents, sediments or heavy metal contaminants within a river basin, the conservation equation of solute mass can first be written in general terms for a three-dimensional flow field as:

$$\frac{\partial \varphi}{\partial t} + \frac{\partial \varphi u}{\partial x} + \frac{\partial \varphi v}{\partial y} + \frac{\partial \varphi w}{\partial z} + \frac{\partial}{\partial x}\overline{u'\varphi'} + \frac{\partial}{\partial y}\overline{v'\varphi'} + \frac{\partial}{\partial z}\overline{w'\varphi'} = \varphi_S + \varphi_d + \varphi_k \tag{5}$$

where φ = time averaged solute (including suspended sediment and heavy metal) concentration, φ_S = source or sink solute input (e.g. an outfall), φ_d = solute decay or growth term, and φ_k = kinetic transformation rate for the solute.

The cross-produced terms $\overline{u'\varphi'}$ etc. represent the mass flux of solute due to the turbulent fluctuations and, by analogy with Fick's law of diffusion, these terms are generally assumed to be proportional to the mean concentration gradient and with a positive flux being in the direction of decreasing concentration. Hence, these terms can be rewritten as:

$$\left.\begin{aligned} \overline{u'\varphi'} &= -D_{tx}\frac{\partial\varphi}{\partial x} \\ \overline{v'\varphi'} &= -D_{ty}\frac{\partial\varphi}{\partial y} \\ \overline{w'\varphi'} &= -D_{tz}\frac{\partial\varphi}{\partial z} \end{aligned}\right\} \tag{6}$$

where D_{tx}, D_{ty}, D_{tz} = turbulent diffusion coefficients in the x, y, z directions. These coefficients are often associated with the eddy viscosity (ν_t) by a Schmidt number, with its value found to vary between 0.5 and 1.0. For further details on the derivation of this equation and the empirical coefficients used see Falconer and Chen (1996).

In modelling faecal coliform (or similar) the decay terms in Eq. (5) are generally expressed as a first order decay function via the following equation:

$$\phi_d = -k_B\phi \tag{7}$$

where k_B = coliform decay rate (day^{-1}), with the value of k_B being dynamically varied in the studies reported herein and as given by Eq. (1).

Based on the general advective-diffusion Eq. (5), the governing equation for suspended sediment transport processes is generally written as:

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial x}(uS) + \frac{\partial}{\partial y}(vS) + \frac{\partial}{\partial t}[(w - w_s)S] - \frac{\partial}{\partial x}\left[D_{tx}\frac{\partial S}{\partial x}\right] - \frac{\partial}{\partial y}\left[D_{ty}\frac{\partial S}{\partial y}\right] - \frac{\partial}{\partial z}\left[D_{tz}\frac{\partial S}{\partial z}\right] = S_T \tag{8}$$

where S = suspended sediment concentration and S_T = source or sink term. It should be noted that the source or sink term is introduced through the bed boundary conditions. For cohesive sediments the following bed conditions have been used (Wu *et al.*, 1999):

$$-w_s S - D_{tz}\frac{\partial S}{\partial z} = q_{dep} \quad \text{when } \tau_b \le \tau_d \quad \text{(deposition)} \tag{9a}$$

$$-w_s S - D_{tz}\frac{\partial S}{\partial z} = q_{ero} \quad \text{when } \tau_b \ge \tau_e \quad \text{(erosion)} \tag{9b}$$

$$-w_s S - D_{tz}\frac{\partial S}{\partial z} = 0 \quad \text{when } \tau_d < \tau_b < \tau_e \quad \text{(equilibrium)} \tag{9c}$$

where τ_b = bed shear stress; τ_d = critical shear stress beyond which no further deposition occurs; τ_e = critical shear stress for erosion; and q_{dep}, q_{ero} = deposition and erosion rates respectively at the bed.

For heavy metal predictions, as outlined previously metals can exist in both the dissolved and adsorbed particulate phases in rivers and estuaries, with the distribution between these two phases being described by a partitioning coefficient K_D, as outlined in Eq. (2). For transport of metals in the dissolved phase the three-dimensional advective-diffusion is given as:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(uC) + \frac{\partial}{\partial y}(vC) + \frac{\partial}{\partial t}(wC) - \frac{\partial}{\partial x}\left[D_{tx}\frac{\partial C}{\partial x}\right] - \frac{\partial}{\partial y}\left[D_{ty}\frac{\partial C}{\partial y}\right] - \frac{\partial}{\partial z}\left[D_{tz}\frac{\partial C}{\partial z}\right] = (C_d + C_t) \tag{10}$$

where C = concentration of heavy metals dissolved in water column; C_d = source or sink of dissolved heavy metal; and C_t = transformation term from, or to, adsorbed particulate phase onto the sediments. The adsorbed particulate phase is transported with the sediments, and this process may be described by the following equation:

$$\frac{\partial SP}{\partial t} + \frac{\partial}{\partial x}(uSP) + \frac{\partial}{\partial y}(vSP) + \frac{\partial}{\partial t}[(w - w_s)SP] - \frac{\partial}{\partial x}\left[D_{tx}\frac{\partial SP}{\partial x}\right] - \frac{\partial}{\partial y}\left[D_{ty}\frac{\partial SP}{\partial y}\right] - \frac{\partial}{\partial z}\left[D_{tz}\frac{\partial SP}{\partial z}\right] = (SP_d + SP_t) \tag{11}$$

where SP = concentration of heavy metal adsorbed on the suspended sediments; w_s = the apparent sediment settling velocity; SP_d = source or sink of adsorbed particulate heavy metal; SP_t = transformation term from, or to, dissolved phase in water column. The transformation processes between the dissolved and adsorbed particulate phases are very complex. However, noting that $C_t = -SP_t$, we can avoid studying the transformation between the dissolved and adsorbed particulate phases in detail by first calculating the total heavy metal fluxes, and then dividing the dissolved and adsorbed particulate phases using a partitioning relationship of the form given in Eq. (2). The total heavy metal transport equation can be derived by summing Eqs. (10) and (11), and re-arranging the diffusion terms to give:

$$\frac{\partial C_T}{\partial t} + \frac{\partial}{\partial x}(uC_T) + \frac{\partial}{\partial y}(vC_T) + \frac{\partial}{\partial z}(wC_T) - \frac{\partial}{\partial z}(w_S P) - \frac{\partial}{\partial x}\left[D_{tx}\frac{\partial C_T}{\partial x}\right] - \frac{\partial}{\partial y}\left[D_{ty}\frac{\partial C_T}{\partial y}\right] - \frac{\partial}{\partial z}\left[D_{tz}\frac{\partial C_T}{\partial z}\right] = (C_d + SP_d + C_t + SP_t) \tag{12}$$

where C_T = concentration of total heavy metal, as given by:

$$C_T = C + SP \tag{13}$$

Substituting for the partitioning coefficient $K_D = SP/C$ in Eq. (13) gives:

$$C = \frac{C_T}{1 + K_D} \tag{14}$$

Further details of the application of this model and the numerical solution algorithm are given in Wu and Falconer (2000) and Wu *et al.* (2001).

3 Cardiff bay study

The port of Cardiff was once one of Britain's largest international trading ports and has been through a period of decline since its heyday in the 1920s. Whole scale urban regeneration of the docks area was seen as the most appropriate means of regenerating the southerly part of Cardiff and a plan to construct a 1.4 km long tidal exclusion barrage across the mouth of Cardiff Bay was given Royal Assent in 1993. The barrage was designed to create a freshwater lake of 200 hectares, incorporating the rivers Taff and Ely, with 13 km of waterfront, enhancing opportunities for recreational water use and commercial and domestic development (see Figure 2). Although the main sewage and other outfalls have been diverted from discharging into the impounded receiving waters, there are still some inputs of sewage, industrial effluents and diffuse source inputs from the river catchments, and discharges from combined sewer overflows (CSOs) during high rainfall conditions.

In studying the potential hydro-environmental challenges associated with the barrage, a 3-D hydrodynamic and water quality model study was undertaken to predict the faecal coliform levels into the receiving waters of the Bay from potential spillages and diffuse source inputs upstream and along the rivers.

The hydro-environmental model as set up for Cardiff Bay and the riverine inputs using a regular grid of 36×52 grid cells, of size 50 m, and with the downstream boundary being governed by the barrage sited across the mouth of the Bay. The 3-D model had 10 vertical layers, each of height 1.25 m. The model was run for 100 h and the time step was 1 s. A simulation was first undertaken to predict the movement of an arbitrary spillage of a conservative tracer with zero decay into the rivers Taff and Ely. The corresponding predictions were compared to the results obtained from a scaled physical model, with good agreement being obtained between both sets of results (Harris *et al.*, 2002). The model was then set up to study the impact of episodic inputs into the rivers and for a range of wind and riverine flow conditions. Some of these predictions were compared with field data, with the corresponding comparisons for different boundary conditions enabling a comprehensive set of conclusions to be drawn to indicate river basin management strategies.

Finally, as part of a comprehensive research study, a field monitoring and model study was undertaken to investigate the impact of dynamically varying decay rates on the faecal coliform levels of the receiving waters in the rivers and the Bay. In particular, comparisons were undertaken for a range of variables and the results showed that the receiving water faecal coliform levels were highly dependent upon a number of key variables. The hydro-environmental model was first run for hypothetical spillages into the rivers and for a constant decay rate (T_{90}), both for daytime and night time, of 60 h. The model was then re-run for daytime and night time decay rates ranging from 10 to 100 h respectively and based on the representation given in Eq. (1). The difference in the predictions was significant and indicated that, for this freshwater basin, night time spillages during the autumn and winter months lead to reduced faecal coliform levels in the rivers and Bay, in comparison with corresponding spillages occurring 12 h later during the daytime (see Figure 3). Further field measurements and model predictions were undertaken, with the decay rate being related to sunlight intensity, temperature and irradiance. The corresponding test case results showed a further significant variation in the coliform levels of the receiving waters, and highlighted the need for further studies into establishing more precisely the relationship between the decay rate and a range of meteorological, hydrodynamic and bio-chemical processes. For further details of these studies see Harris *et al.* (2002).

4 Mersey basin study

The 3-D, 2-D and 1-D hydro-environmental models (namely TRIVAST, DIVAST and FASTER), developed at Cardiff University (see Lin and Falconer, 2001), were also applied to the Mersey Basin, U.K., where particular emphasis was focused on integrating a 3-D and 1-D model to cover the main basin from the coast to the tidal limits (see Figure 4) and, in particular, to

Figure 2 Photograph illustrating Cardiff Bay and barrage and the rivers Taff and Ely.

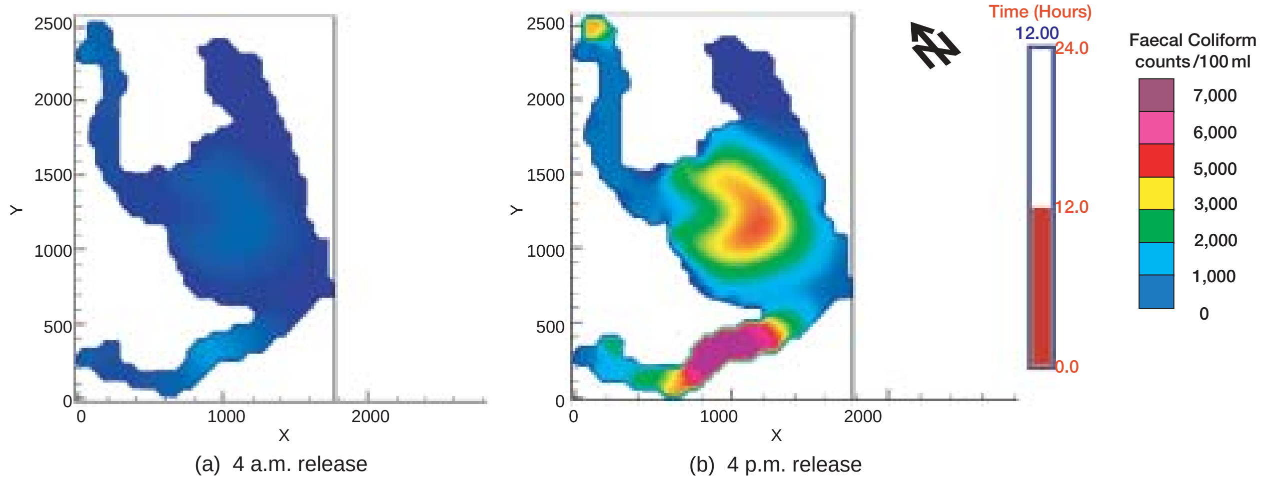

Figure 3 Predictions of Faecal Coliform Levels in rivers Taff and Ely and Cardiff Bay 12 h after arbitrary spillages at: (a) 4 a.m. and (b) 4 p.m.

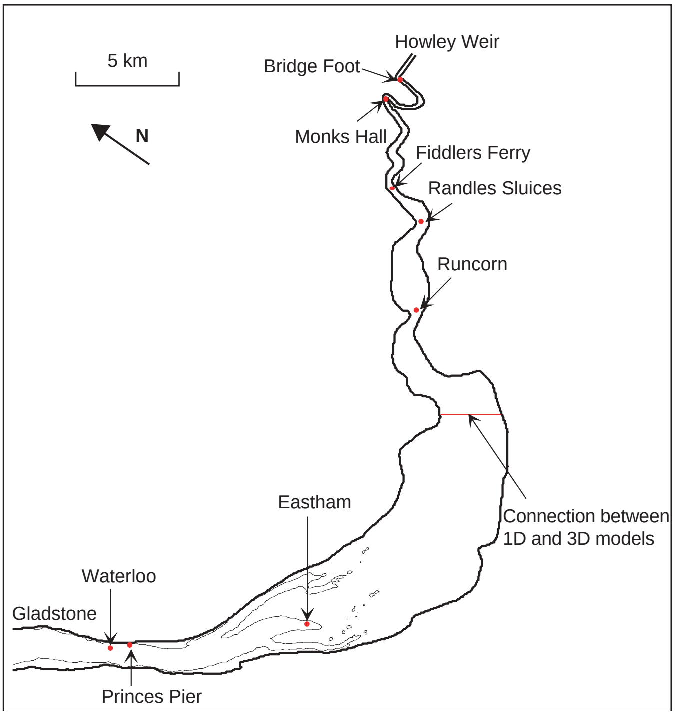

Figure 4 Plan of the Mersey estuarine basin.

predict cohesive and non-cohesive sediment fluxes and heavy metal concentration distributions in the main basin.

The Mersey estuary and river basin has received high loads of toxic, persistent and bio-accumulative organic and inorganic compounds over many years and the basin has been renowned for receiving major discharges of mercury, lead and organochlorine compounds, including polychlorinated biphenyls (PCBs). Over the last decade the Environment Agency (North West Region) has achieved a significant improvement in the water quality in the Mersey Basin by virtue of a coherent recovery programme defined by the Mersey Estuary Management Plan (Jones, 2000). However, major challenges still remain, including the fact that the sediments in the estuary and its salt marshes have high contaminant concentrations from the past and may provide a significant source of toxins in the future. Thus, this study involved refining a suite of hydro-environmental models to predict the basin hydrodynamics and geochemistry, to contribute to the on-going restoration plan for the Mersey Basin.

Estuarine basins such as the Mersey often consist of three distinct regions according to the physical nature of the flow, i.e. a deep region close to the mouth of the estuary, which is frequently 3-D in nature, a large shallow region along the inner part of the estuary, which may be 2-D in nature, and a narrow meandering region towards the upper part of the basin, which is often 1-D in nature. To model efficiently and accurately this complex system, an implicitly coupled 3-D and 1-D model was developed to replace the common approach of using overlapping models. An implicitly coupled model has many advantages over an overlapping model. In particular, it eliminates the explicit exchange of boundary data between the individual models at the overlapping zone, with the previous approach often causing model instability. The implicit coupled model developed for this study was fully mass conservative, whereas overlapping models are generally not fully mass conservative across the overlapping zone.

The integrated model was set up for the Mersey Basin from New Brighton, the seaward open boundary, to Howley Weir, the landward open boundary. The model area was represented horizontally using two grid systems, i.e. a three- and a one-dimensional grid. The two-dimensional plan domain covered the region from New Brighton to Hale, which was represented horizontally using a mesh of 216 × 116 uniform grid squares, each with a length of 100 m. For this 3-D model reach seven layers were used in the vertical plane, with the thickness of the top layer being 4 m at mean water level, and with the other layers each being 3 m thick. The one-dimensional part of the model covered the region from Hale to Howley Weir, which was represented using 80 segments, and with the extensive bathymetric data needed for each reach being obtained from recent bathymetric surveys undertaken in 1997 by HR Wallingford Ltd and ABP. The refined model was firstly calibrated against extensive hydrodynamic, salt and suspended sediment concentration field data, collected along the Mersey Basin by the Environment Agency. The model was then applied to the Mersey to investigate the sorption and desorption of dissolved metals onto, and from, the suspended sediments in the basin, and to study the impact of the heavily contaminated bed sediments and load inputs on the water contamination levels within the basin.

The calibrated model was first run to simulate zinc and cadmium fluxes in the basin for the field survey conditions, undertaken on 25th June and 20th October 1998. In considering only the June data simulations herein, the data were recorded for a spring tide, of range 8.47 m, and with high tide reaching Liverpool at about 12:45. The daily fresh water input from the River Mersey was approximately 3,600 Ml, with the corresponding input being 7,100 Ml for the October dataset. The survey boat started from the Buoy C1 in the Outer Estuary at 10:56 on 25th June and traversed to Monks Hall in the Upper Estuary. Samples were collected at 20 locations along the estuary and the travel time was about 3.5 h.

A typical model prediction of the velocity field and dissolved zinc concentration distribution is shown in Figure 5, for the top layer and for the region close to the mouth of the estuary. Likewise, Figure 6 shows a comparison between the model predicted and the measured salinity levels along the basin. The field data and model predictions were tidally corrected to enable the predicted concentrations to be compared directly with the field data. From the comparison it can be seen that the calibrated model predictions were in good agreement with the observed data, particularly at the head of the basin where the salinity gradient was expected to have a significant effect on influencing the partitioning of heavy metals. A typical comparison between the predicted and measured suspended sediment concentrations along the estuary for the June survey data is shown in Figure 7. Again the predicted suspended sediment concentrations agreed reasonably well with the field data, although the model underestimated the peak level of the suspended sediment concentration. The predicted maximum suspended sediment concentration at Monks Hall was 483.5 mg/l, which was about 16.8% lower than the measured peak value of 581 mg/l.

To investigate the impact of the input loads on the distribution of heavy metal concentrations along the Mersey Basin, the model was then run both with and without input metal loads from the

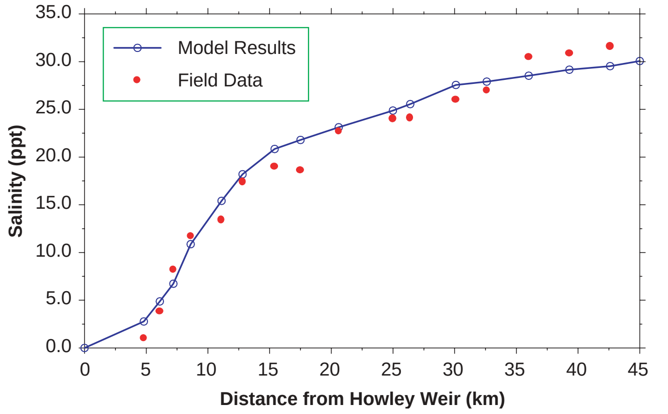

Figure 6 Comparison of predicted and measured axial salinity distribution on 25 June 1998.

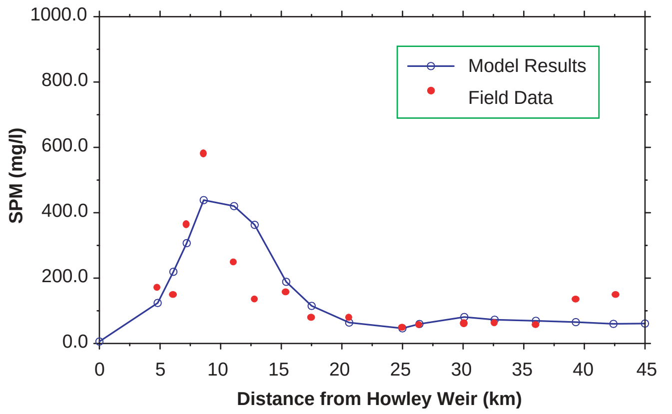

Figure 7 Comparison of predicted and measured axial suspended sediment distribution on 25 June 1998.

River Weaver and the sewage works at Liverpool and Warrington; details of these loads are given in Millward *et al.* 2001. The metal distribution on the bed sediments was estimated from spot data provided by the Environment Agency and the empirical constants used to determine the partitioning coefficient (i.e. K_D^0 and b), were provided by the University of Plymouth (see Millward

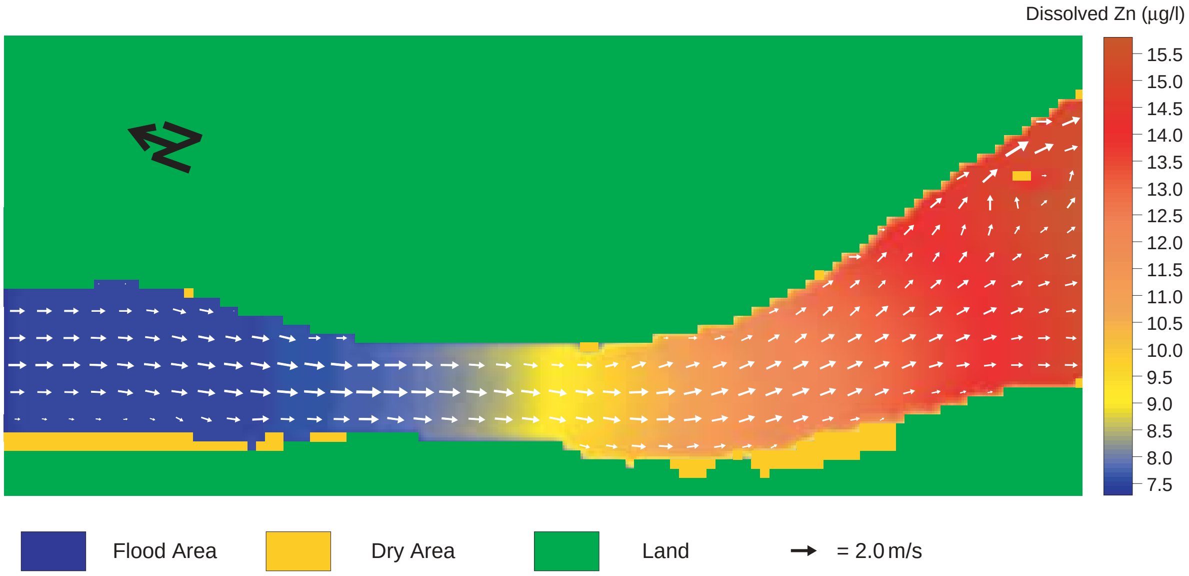

Figure 5 Predicted velocities and dissolved zinc concentrations for top layer.

et al. 2001). For the case of zinc the modified empirical constants for K_D^0 and b were found to be 6,000 and 0.299 respectively. Figure 8 shows the model predicted and measured dissolved zinc distribution along the basin. From this comparison it can be seen that the predicted values of the peak concentration of dissolved zinc agreed well with the measured data, but the location of the peak dissolved zinc concentration differed between both sets of results. Figure 9 shows the model predicted dissolved zinc distribution along the estuary for no bed load inputs in the model. These results indicated the contribution of the contaminated bed sediments on the dissolved zinc concentrations in the water column. In comparing the resulting prediction in Figures 8 and 9 it can be seen that the contaminated bed sediments are predicted to have contributed noticeably to the axial dissolved zinc concentrations along the estuary.

In addition to zinc, cadmium was modelled and Figure 10 shows a comparison between the model predicted and measured dissolved cadmium concentrations along the basin. The empirical constants K_D^0 and b, used to estimate the partitioning of cadmium between the adsorbed and dissolved metal fractions, were found to be 41,700 and −0.45 respectively for the model. Again the predicted dissolved cadmium distribution agreed reasonable well with the field data, with the desorption process generally being well reproduced in the model. In particular, the field data and the model predictions confirmed that the partitioning coefficient

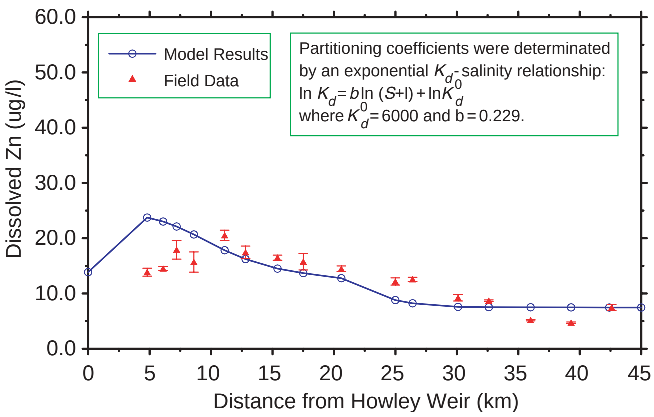

Figure 8 Comparison of predicted and measured axial dissolved zinc distribution on 25 June 1998 with contaminated bed sediments.

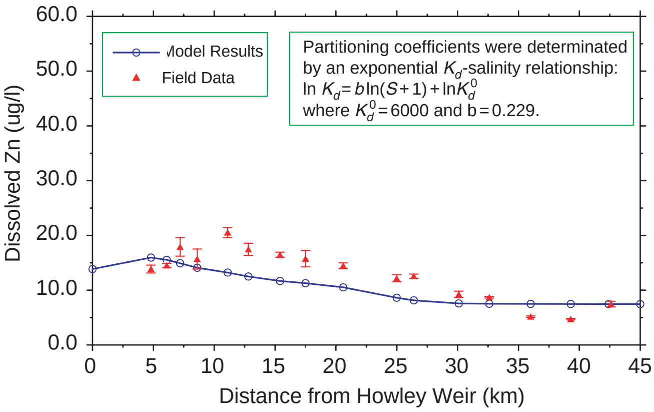

Figure 9 Comparison of predicted and measured axial dissolved zinc distribution on 25 June 1998 without contaminated bed sediments.

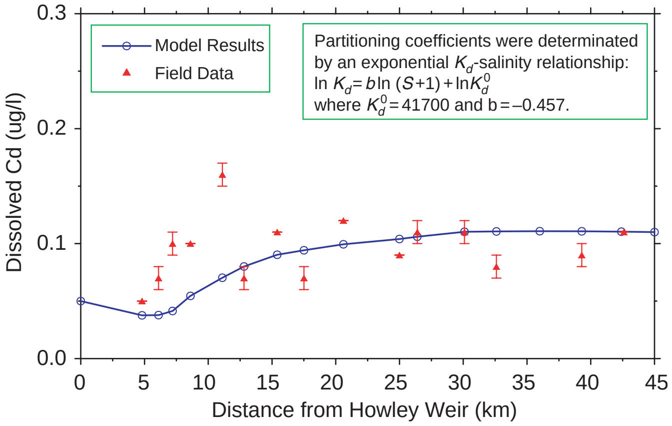

Figure 10 Comparison of predicted and measured axial dissolved cadmium distribution on 25 June 1998.

was highly dependent upon the salinity local levels (see Millward *et al*. 2001).

5 Conclusions

In recent years there has been a significant increase in public awareness of a wide range of hydro-environmental issues. Current day hydroinformatics tools (or models) provide wide scope for use in river basin management and can provide valuable and extensive information for hydro-environmental river engineers and managers. However, it is important to appreciate that these modelling tools have limitations, primarily governed by our lack of understanding of some complex hydrodynamic, bio-chemical, morphological and geo-chemical processes. Nevertheless, despite these limitations, it is also important to appreciate that such predictions are not possible using traditional scaled physical models, since a range of processes, including: bed friction, turbulence, diffusion, dispersion, decay and metal partitioning, are all generally scaled incorrectly in such models. Although much emphasis in recent years has focused on modelling accurately some of these processes, other complex processes have often been simplified considerably in such hydroinformatics tools. Two such processes include the decay of coliform bacteria and the partitioning of heavy metals. In general these processes have been modelled using constant coefficients and in this study the empirical coefficients have been refined to relate their values to known master variables, such as irradiance and salinity respectively.

Details are given of two such model studies to investigate the significance of dynamically relating these coefficients to various master variables. The first study was for Cardiff Bay, U.K., where it was found that the receiving water faecal coliform levels in the freshwater bay were highly dependent upon the value of the decay rate. The decay rate was made functionally dependent upon daytime and night time conditions, sunlight intensity, water temperature and irradiance. In comparison with a constant decay rate, the receiving water coliform levels for two hypothetical spillages were found to vary significantly with the value of the decay rate and several key water-management strategies were indicated.

Details are also given of the application of the model to the Mersey Estuary Basin, U.K., where 3-D and 1-D hydro-environmental models have been integrated to enable the complex basin domain, of significantly varying width, to be modelled more precisely. The integrated model was also refined to predict the cohesive sediment, suspended sediment and geo-chemical processes more accurately in the estuary and river basin. A new approach was also developed to predict the metal fluxes in this model. This approach involved first calculating the total metal flux in the water column and then separating this flux into the dissolved and particulate metal fractions. This subdivision of the total metal flux into its constituents was based on a salinity-dependent partitioning coefficient, and was found to be more accurate than calculating the dissolved and particulate concentrations separately (see Ng *et al.*, 1996).

These refined models were set up to simulate the hydrodynamic processes and the salinity, sediment and heavy metal concentration distributions along the Mersey Estuary Basin, from the coast to the tidal limits. The 3-D and 1-D integrated model was firstly calibrated against field data collected for the Mersey by the Environment Agency. The model was then tested to investigate the partitioning of heavy metals and then applied to study the impact of contaminated bed sediments on the water contamination levels of the estuary. The model generally showed good agreement between the predicted and measured concentration distributions for dissolved zinc and cadmium and further showed that the contaminated bed sediments had a marked impact on the metal concentration levels along the estuary. This study highlighted that removing the outfall source inflows alone may not in the short term necessarily clean up a river basin from toxic contaminants; in particular, any contaminated sediments may lead to persistent water contamination problems.

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