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Modelling trace metal concentration distributions in estuarine waters

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Abstract

Details are given of a numerical model study of the fate and transport of trace metals in estuarine waters, with particular application to the Mersey Estuary, located along the northwest coast of England. A dynamically integrated model was first developed, including a two-dimensional depth-integrated model and a one-dimensional cross-sectional averaged model. This model was then refined to predict the hydrodynamic and sediment and trace metal transport processes in the Mersey Estuary. Details are given of the development of a governing equation of the total trace metal transport, including both dissolved and particulate metals. The model was first calibrated against field data, collected during spring and neap tidal cycles, for water levels, salinity and suspended sediment. The calibrated model was then used to investigate the trace metal transport processes in the Mersey Estuary, with the partition coefficient between the dissolved and adsorbed particulate phases being modelled as a function of salinity. Comparisons were also made between the model predictions and field-measured data along the estuary. Reasonable agreement between the model results and field data has been obtained, indicating that the novel approach to model metal concentration distributions is capable of representing the fate and transport of trace metals in estuarine environments and can be used as computer-based tool for the environment management of estuarine waters.

Keywords: estuary; hydrodynamics; sediment transport; trace metals; numerical modelling

1. Introduction

Many UK estuaries have suffered environmental damage due to the discharge of effluents from manufacturing processes and wastewater from centres of population over several decades. Although estuarine water quality is generally improving, as a result of the remedial actions implemented over the past 20 years, many potentially harmful chemicals, such as trace metals, still remain embedded within erodable sediments. Trace metals generally exist in two phases in estuarine waters, i.e., in the dissolved phase in the water column and in the particulate phase adsorbed on the sediments. The behaviour of trace metals in the aquatic environment is strongly influenced by adsorption to organic and inorganic particles. The dissolved fraction of the trace metals may be transported through the water column via the processes of advection and dispersion, while the adsorbed particulate fraction may be transported with the sediments, which are governed by sediment dynamics. The partition of a trace metal between its dissolved and adsorbed particulate fractions depends on the physical and chemical characteristics of the suspended particles, together with various ambient conditions, such as: salinity, pH, type and concentration of dissolved organic matter (Turner et al., 2001; Turner and Millward, 2002).

Fine sediments act as a source (or sink) for the organic chemicals and trace metals entering (or leaving) the water

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column with sediments contaminated by trace metals being a potential threat to the aquatic environment. Resuspension of contaminated bed sediments caused by strong tidal currents or dredging operations may release a significant amount of trace metals into the water column, and this desorption of contaminants from their particulate phase can have a pronounced impact on the aquatic environment and ecosystem. Numerical models provide a valuable tool for predicting the fate and transport of trace metals in estuarine environments and are increasingly used for such hydro-environmental management studies of estuarine waters. However, computer-based tools for predicting such trace metal concentration distributions and concentrations, although they can support decision-making by the regulatory authorities, marine environment agencies and industry, are still used relatively infrequently (Ng et al., 1996). Coupled numerical models involving hydrodynamic and contaminant geochemistry processes are very few in number, and they are largely research oriented, rather than being applied tools for managing estuarine and coastal waters.

The paper gives details of the development of a novel approach in modelling trace metal concentration distributions and the application of the model to the Mersey Estuary, located along the north western coast of England, for the prediction of the fate and transport of trace metals. Details are given of the development of a governing equation for the total trace metal transport, including both dissolved and particulate metals as a combined flux, in contrast to previous model studies reported in the literature where the dissolved and particulate metal processes have been treated independently (e.g. Ng et al., 1996). Details are also given of the integration of a two-dimensional depth-integrated estuarine model and a one-dimensional cross-sectional averaged river model and the application of the model to simulate the hydrodynamic and sediment and trace metal transport processes in the Mersey Estuary. The model was calibrated against six sets of field measured time series data, collected during spring and neap tidal cycles, for water levels, salinity and suspended sediment concentrations. The calibrated model was then used to investigate trace metal transport processes in the estuary, with the partition coefficient between the dissolved and adsorbed particulate phases being modelled as a function of salinity (Turner and Millward, 1994).

2. Mathematical model

2.1. Hydrodynamic model

In modelling estuarine and riverine processes, the modelling domain often covers areas of different physical characteristics, e.g. large water basins with a two- or three-dimensional flow structure and narrow meandering channels with a predominately one-dimensional flow structure. When a two-dimensional numerical model is used for such cases the detailed bathymetric features of a narrow meandering channel may not be well represented unless a very fine grid system is used, thereby increasing the computing time significantly. Similarly, if a one-dimensional model is used then the two-dimensional flow features in the wider part of an estuary or river may not be well resolved. For many engineering problems these physical features are prevalent in many estuarine and riverine waters. Therefore, a combined 2-D and 1-D model has been developed in this study to predict accurately the hydrodynamic and water quality processes in the estuarine and riverine waters.

The hydrodynamic model used to predict the water elevations and velocity fields in coastal, estuarine and riverine waters initially involves the solution of the governing equations of fluid flow. The two-dimensional hydrodynamic equations are generally based on the depth-integrated 3-D Reynolds equations for incompressible and unsteady turbulent flows, with the effects of the earth's rotation, bottom friction and wind shear being included to give (see Falconer, 1993):

$$\frac{\partial \zeta}{\partial t}+\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}=0 \tag{1}$$

$$\frac{\partial q_x}{\partial t}+\beta\frac{\partial U q_x}{\partial x}+\beta\frac{\partial V q_x}{\partial y}=f q_y-gH\frac{\partial \zeta}{\partial x}+\frac{\tau_{xw}}{\rho}-\frac{\tau_{xb}}{\rho}+\bar{\varepsilon}H\left[\frac{\partial^2 U}{\partial x^2}+\frac{\partial^2 U}{\partial y^2}\right] \tag{2}$$

$$\frac{\partial q_y}{\partial t}+\beta\frac{\partial U q_y}{\partial x}+\beta\frac{\partial V q_y}{\partial y}=-f q_x-gH\frac{\partial \zeta}{\partial y}+\frac{\tau_{yw}}{\rho}-\frac{\tau_{yb}}{\rho}+\bar{\varepsilon}H\left[\frac{\partial^2 V}{\partial x^2}+\frac{\partial^2 V}{\partial y^2}\right] \tag{3}$$

where $H=\zeta+h$ = total water column depth; ζ = water elevation above (or below) datum; h = water depth below datum; U, V = depth-averaged velocity components in x, y directions; $q_x=UH$, $q_y=VH$ = unit width discharge components (or depth-integrated velocities) in x, y directions; β = momentum correction factor; f = Coriolis parameter; g = gravitational acceleration; τ_{xw}, τ_{yw} = surface wind shear stress components in x, y directions; τ_{xb}, τ_{yb} = bed shear stress components in x, y directions; and $\bar{\varepsilon}$ = depth average eddy viscosity.

The components of the wind stress at the free surface are given as (Falconer et al., 2001):

$$\tau_{xw}=C_d\rho_a W_s W_x,\quad \tau_{yw}=C_d\rho_a W_s W_y \tag{4}$$

where C_d = resistance coefficient; ρ_a = air density; W_x, W_y = wind velocity components in the x, y directions,