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Numerical modelling of the transport and transformation of trace metals in a highly dynamic estuarine environment

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ABSTRACT

A highly accurate numerical model was developed for modeling the transport of heavy metals in estuaries. The methodology uses measurements of dissolved and particulate fractions of metals, and associated salinities to develop partitioning coefficients as a function of salinity. These relationships were incorporated into high resolution numerical models to simulate the transport of metals about the Mersey Estuary. For most of the metals the approach worked very well; however, the transport of Hg was not well simulated. The paper discusses the form of the partitioning coefficient-salinity relationships with other research in this field and makes suggestions for future research.

1. Introduction

The Mersey Estuary has become a repository for industrial deposits of heavy metals due to historically poor management of discharges into the estuary, Jones [1]. Unfortunately for water quality managers today, heavy metals manifest themselves in estuaries in different forms: dissolved in the water column, bound to suspended sediments and bound to bed sediments. This, combined with the complex hydrodynamic nature of estuaries, makes accurate modelling of the transport of heavy metals difficult. Considering metals in the water column, dissolved fractions are transported through the processes of advection and diffusion, whilst the transport of particulate adsorbed fractions are governed by sediment dynamics. A further complicating factor in understanding metal transport processes in estuaries is that the relative fraction of a metal mass between dissolved and particulate bound fractions is a function of water chemistry. Often salinity concentrations are used as surrogates for variations in water chemistry.

The UK Environment Agency have compiled a detailed database for the Mersey Estuary of simultaneous measurements of salinity and dissolved and particulate bound concentrations of heavy metals for a suite of metals. These results confirm that variations in salinity indeed induce variations in heavy metal fractions. Estuarine salinity varies both with location along an estuary and also with time at a point in the estuary depending on tidal dynamics and freshwater inflows. In the case of the Mersey Estuary variations are often large and abrupt, again contributing to the difficulty of accurately modelling heavy metal transport.

Although, a prominent case study in poor water management, the Mersey is not alone in suffering from heavy metal contamination and thus research into understanding metal transport within estuaries is highly relevant when implementing legal instruments such as the EU Water Framework Directive.

Because of the serious nature of metal contamination of the Mersey Estuary, other studies have been undertaken to define and better understand the nature of the problem of trace metal reactivity in the Mersey Estuary; Campbell et al. [2] present and discuss the distribution and behaviour of both dissolved and particulate bound nickel (Ni) in the Mersey Estuary. One of the main conclusions from their work is that the distribution of Ni throughout the Mersey Estuary is complex and clearly deviates from simple end-member mixing behaviour.

Ng et al. [3] carried out a detailed contaminant modelling study of the Humber Estuary. They outline the difficulties of making accurate predictions of heavy metals in the Humber due to many controlling variables including: salinity, pH and availability of complexing species. Within their model, the partition coefficient was allowed vary as a function of salinity in either of two ways. The paper by Ng et al. illustrates how a geochemical module based on empirically-derived partition coefficients, coupled to a two-dimensional hydrodynamic model, was developed to form the basis of a geochemical contaminant transport model. This basic approach of Ng et al. is the one followed in the research undertaken by the author; however, the authors have extended the above approach with regards to the formulation of the partition coefficients.

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Comber et al. [4] undertook research into the partitioning of trace metals between the dissolved phase and suspended solids on both the Humber Estuary and the Mersey Estuary. One of the aims of this research was to develop partition coefficients for a number of metals. A single-valued partition coefficient for Ni in the Mersey Estuary was estimated at c. 1×10^4 and the corresponding value in the Humber Estuary was estimated c. 5×10^3. The reason for the higher value of K_D in the Mersey was attributed to higher loadings of sewage into the Mersey along with differences in suspended particulate composition. The partition coefficient for Pb in the Mersey was shown to vary between 1 and 3×10^5, generally increasing with increasing salinity.

Many other researchers have also investigated behaviour in estuaries, such as Jiann et al. [5], Paucot and Wollast [6] and Zhou et al. [7]. Each of these researchers discusses the difficulties associated with describing metal behaviour in estuarine waters and the effects that salinity has on metal fractioning. The work by Paucot and Wollast is of particular interest to this research and aspects of it are discussed in detail later in this paper. Other researcher, such as Wu et al. [8], Liu et al. [9], Ouboter et al. [10] and De Smedt et al. [11], have developed various forms of estuarine metal transport models. The Cu transport model by Liu et al. is a 2D laterally averaged model; partitioning coefficients were developed from relatively few data points and the results cover less than a third of the estuary length. An interesting approach here was to relate partitioning coefficient to both salinity and SPM. Ouboter et al. developed a 1D model for the transport of Cd about the Scheldt estuary and use a chemical sub-model, CHARON, to quantify partitioning coefficients; however, details of the processes included in CHARON are not provided. Relatively few results are provided for Cd transport; a plot shows results of model output against data for one point on the estuary at a temporal resolution of months. An interesting aspect of this research is the postulated impact of algal blooms on metal concentrations. De Smedt et al. developed a simple 1D model of the Scheldt estuary and modelled the transport of a suite of metals. Salinity was modelled in order to verify the accuracy of dispersion coefficients, but was not used to determine partitioning coefficients. Partitioning coefficients were linearly related to SPM values alone. The Authors present quite good agreement between predicted values of dissolved meals and data. The research undertaken by Wu et al. used a 2D vertically integrated model for the transport of Cd and Zn, similar to the current research. This provides the most detailed information regarding spatial distributions of heavy metal concentrations. The relationship between partitioning coefficients and salinity used by Wu et al. was based on a logarithmic relationship in which partitioning values decrease with increasing salinity. Results show reasonable agreement with data; however, as shown below the variation in partitioning coefficients with salinity is highly metal specific and in general does not follow the logarithmic relationship postulated.

This paper describes research into the development of a modelling approach used to predict the transport of a suite of heavy metals about the Mersey Estuary. The metals considered during this research were: Pb, Hg, Cd, Ni, Zn and Cu. Using results provided by the Environment Agency from extensive monitoring of heavy metals in the Mersey Estuary, partitioning coefficients were developed as functions of salinity for each metal. This is the most detailed research undertaken into modelling the transport of a suite of heavy metals that the Authors are aware of. The results illustrate the significant differences in the partitioning coefficients and salinity between metals. The results also suggest that although the methodology is suitable for most metals, it needs to be used with care. In the sections below the numerical models are described, partitioning coefficients are presented along with results of heavy metal transport modelling. The final section presents a detailed discussion of the research and suggests directions for future research in this field.

2. Methodology and results

2.1. General approach

The partitioning coefficient, K_D, which gives information on the integrated effects of adsorption and desorption of metals onto and from suspended particulate matter (SPM), is defined as:

$$K_D = \frac{P}{C} \quad (1)$$

where P is the concentration of metal absorbed on suspended sediments (μg/g); C is the concentration of metal dissolved in the water column (μg/l).

The coefficient K_D is a function of spatially varied water chemistry and is notoriously difficult to quantify in marine waters ([12–14]). It is well known that, for some metals, there exists a strong functional relationship between K_D and salinity, Comber et al. [4]. In many studies salinity is used to describe variations in the partitioning coefficient for a given metal with variations in water chemistry; this approach is adopted in this research also. In order to model, hindcast and predict heavy metals, with a reasonable degree of accuracy, the following staged approach was adopted.

A hydrodynamic model of the Mersey Estuary was developed, calibrated and validated. A solute transport model was developed, calibrated and validated and used to predict salinity distributions throughout the estuary at various stages of the tide using the results from the hydrodynamic model. From field data, for each metal an expression was developed relating partition coefficient to salinity. Combining model predicted salinity and the K_D – salinity relationship, the model has the capability of computing spatially and temporally varied partition coefficients as model calculations progress forward in time. A cohesive sediment transport model of the Mersey Estuary was also developed, calibrated and validated and used to predict estimates of cohesive sediments. Finally, having predicted cohesive sediment concentrations and values of K_D at each grid point of the model for each computational timestep, the model computes the fraction of a heavy metal which is dissolved and that fraction which is absorbed onto the cohesive sediments.

2.2. Hydrodynamic model of Mersey Estuary

The Mersey Estuary is one of the largest estuaries in the UK, having a catchment of some 5000 km^2 that includes the major cities of Liverpool and Manchester. The estuary is a macro-tidal estuary with tidal ranges recorded at Gladstone Dock of between 10.5 m on extreme spring tide to 3.5 m on extreme neap tides. Freshwater inputs from the River Mersey vary between approximately 10 m^3/s and 500 m^3/s at the extremes; typical flows are in the range 20–60 m^3/s. A numerical model was developed of the estuary extending from New Brighton at the seaward end to the tidal limit at Howley Weir, Fig. 1 shows the extent of the model domain. The two-dimensional model DIVAST was used during this research. The model grid spacing was set at 100 m resulting 66,220 computational grid points. At each model grid point the bathymetry of the estuary was defined from a bathymetric survey of the estuary carried out for the Environment Agency in 2002. The Upper Estuary is a meandering channel of approximately 15 km in length; below Runcorn the estuary opens into a wide shallow basin to form the Inner Estuary with extensive mudflats and a large salt marsh on the southern bank. Further downstream the estuary converges to form the Narrows, a straight narrow channel of up to 30 m deep.