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A novel coupled biokinetic-equilibrium model to capture oyster metal bioaccumulation in a contaminated estuary (Sydney estuary, Australia)

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A B S T R A C T

Enriched concentrations of metal contaminants have been reported in surficial sediments and tissues of aquatic organisms in Sydney estuary, New South Wales, Australia. Dietary ingestion of contaminated, suspended sediments is potentially a major route of metal exposure to the filter-feeder *Saccostrea glomerata*. A dynamically coupled biokinetic-equilibrium bioaccumulation model was developed to explore sediment-oyster-metal uptake interactions. The biokinetic component simulated the sediment dynamics and oyster uptake and loss kinetics while the ion equilibrium model accounted for the metal speciation reactions. Results of a laboratory-based mesocosm experiment as well as data from the literature were used to parameterise the model. The model demonstrated a good fit of the experimental data and indicated that dissolved and particulate organic matter were important determinants of metal bioavailability to this species. The model served also as a unique tool to formulate testable hypotheses and help to better explain the bioaccumulation patterns observed from the experiment.

1. Introduction

Metal contamination in coastal waterways is a complex global environmental challenge due to high persistency, pervasiveness and ubiquitous introduction by humans (Furness and Rainbow, 1990). This is particularly relevant for cities located on, or near, estuaries, a scenario that includes 22 of the world's 32 largest cities (Ross, 1995). It is estimated that approximately one-quarter of the global population resides within 100 km of the coast (Small and Nicholls, 2003). The result has been for estuaries to become the final resting place or sink for metals that have been emitted into the hydrosphere and discharged into local tributaries through runoff from surrounding populated catchments (Tessier and Campbell, 1987).

Sydney estuary (Fig 1) located in the state of New South Wales, Australia, is extensively urbanised and has a history of heavy industry that has been linked to enriched metal concentrations in estuarine sediment (Irvine and Birch, 1998; Birch and Taylor, 1999). Elevated concentrations of metals in the epifaunal suspension filter-feeder Sydney rock oyster (*Saccostrea glomerata*) sampled from the Sydney estuary have been reported (Birch et al., 2014), with some oysters markedly exceeding background concentrations in NSW estuaries (Scanes and Roach, 1999) as well as Australian food safety standards for human consumption (FSANZ, 2006).

The high metal concentrations in sediments and tissues of ambient filter-feeding oysters coupled with their proximity suggest that resuspended sediment could be a major uptake pathway. By extension, these *sentinels of the environment* (Burns and Smith, 1981) should then be strong indicators of sediment metal contamination. However, poor to moderate correlations between elevated metal concentrations in bottom sediments (including the bioavailable and fine fraction; <62.5 μm) and suspended sediments (SS) to *S. glomerata* tissue metals have been observed for the Sydney estuary (Dafforn et al., 2012; Birch et al., 2014). This raises a question about whether the sediment is an important local source of metal bioaccumulation in epifaunal filter feeding oysters. Furthermore, if not, then what are the important determinants governing metal bioaccumulation in oysters?

A mesocosm study using sediment collected from the Sydney estuary was conducted to explore the relationship between

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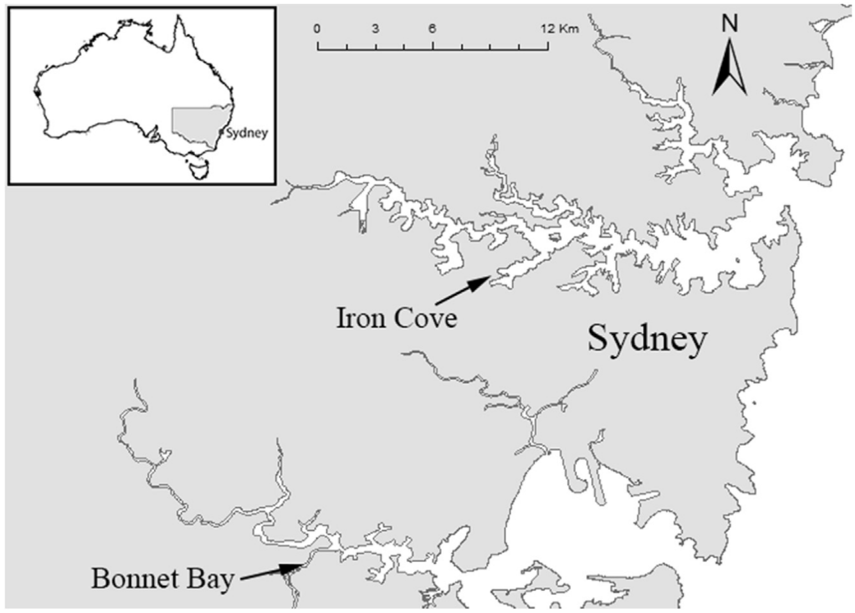

Fig. 1. Sydney estuary, New South Wales, Australia.

sediment-bound metals and oyster-metal bioaccumulation patterns (Lee et al., 2016). The outcomes and observations of these mesocosm experiments were then used to help parameterise a process-based model aimed at simulating the experimental conditions. This model can be used not only to try and replicate the mesocosm experimental results but also to supplement them by further investigating the processes that might be occurring.

Uptake of a metal by an organism may be markedly affect by its speciation, thus a central challenge to modelling the temporal patterns of trace metal speciation occurring in the mesocosm experiment (and in natural waters more generally) is that biophysical processes are often quantified in terms of days, months and even years while metal speciation reactions can be almost instantaneous (Hofmann et al., 2008). Many of the slower transformations that occur in aquatic environments such as the physiological feeding responses of oysters are competently addressed using kinetic rate constants (e.g. Richards and Chaloupka, 2009), but rapid processes such as that associated with metal speciation reactions are not. Instead, an approach based on steady-state conditions using equilibria theory (van der Lee, 1998) is often more suitable if the speciation reactions are assumed to be instantaneous (Hofmann et al., 2008). However, there is an increasing need to dynamically couple these equilibrium and kinetic processes into the same modelling framework so that the linkages between metal speciation, sediment resuspension and oyster biodynamics can be simulated (Richards et al., 2010).

The aim of this paper is to develop a coupled equilibrium-biokinetic bioaccumulation model for exploring relationships between resuspended, contaminated sediments and metal bioaccumulation in *S. glomerata* tissue. The performance of the model is tested by using the results of the mesocosm experiment as a case study to parameterise the model and aims to simulate and reproduce the experimental results. The model is also used to better understand key underlying processes that were not revealed by the experimental measurements, but may have markedly influenced the observed metal bioaccumulation patterns in *S. glomerata*. The use of a biokinetic modelling approach (Richards and Chaloupka, 2009) enables the temporal evolution of metal uptake, bioaccumulation and depuration (loss) to be simulated by factoring in the physiological feeding responses of the oyster alongside the dynamics of metal-sediment resuspension. Extending the biokinetic model to include an equilibrium metal speciation model enables investigation of the role of speciation as a mediator of metal bioaccumulation in the oysters. Furthermore, it addresses the challenge of integrating fast processes (e.g. many metal speciation reactions) within the biokinetic model where processes may be several orders of magnitude slower.

2. Material and methods

2.1. Model description

The coupled model (Fig 2) is represented by a biokinetic model comprised of a system of coupled ordinary differential equations dynamically linked to a metal speciation model (the equilibrium model). For each time step, the equilibrium model first calculated the speciation patterns for the seven metals based on the current total aqueous metal concentrations (Me_T). The metal speciation calculations were then inputted into the biokinetic model, which enabled the Me_T to be updated based on the sediment and oyster physiological dynamics. For the initial time step (t_0), the initial conditions applied to the biokinetic model were used as input for the equilibrium model.

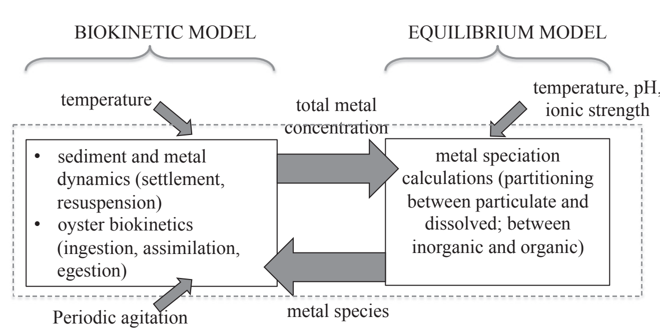

Fig. 2. Conceptualisation of the coupled biokinetic – equilibrium model.