



Review

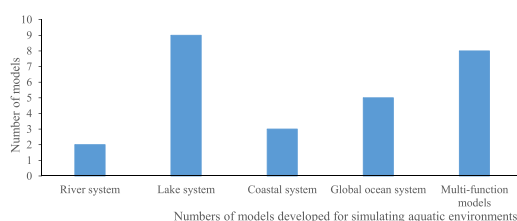
Mercury transport and fate models in aquatic systems: A review and synthesis

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HIGHLIGHTS

- A comprehensive review of mathematical models of mercury fate and transport was conducted.
- Key mercury cycling processes and environmental factors, such as fluxes and transformations, were summarized.
- Data needs and further research on the transformation mechanisms were identified.
- The mass balance model shall remain a valuable tool.

GRAPHICAL ABSTRACT



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ABSTRACT

Mercury contamination in aquatic systems has been an issue to the natural ecosystem and human health. Environmental models have become a valuable decision-making tool and play a significant role in mercury pollution control and management. This paper gives an overview of currently available models for simulating mercury transport and fate in aquatic systems. The mercury transformation mechanisms included in these models were identified, as well as data limitations in the models' application. Future advances in understanding mercury transport, cycling, and biogeochemistry in both water column and sediment will improve the robustness of current modeling applications. Moreover, additional field data are critically needed to better predict the concentrations of multi-phase mercury species in various aquatic systems, including measurements in the water column, benthic sediments, and organisms. Field data are also crucial for model calibration and validation. Without this information it will not be possible to adequately understand the environmental factors controlling mercury fate in aquatic systems. The insufficient quantity of adequate measurements and the unsatisfactory accuracy of mercury models are, in numerous cases, supplemented by mass balances since they diminish the unreliability of models. Mercury science evolves gradually with the advancement of science and technology, which requires that mathematical modeling of mercury transport and transformation should be consistently updated.

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Contents

1.	Introduction	539
2.	Model representation of the key transformation processes governing aquatic mercury cycling	539
2.1.	Hg ⁰ oxidation	539
2.2.	HgII reduction	540

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2.3.	HgII methylation	540
2.4.	MeHg degradation	541
2.5.	MeHg demethylation	541
3.	Model review	541
3.1.	River system models	542
3.2.	Lake system models	544
3.3.	Coastal and global ocean system models	544
3.4.	Model evaluation	544
4.	Data availability	544
5.	Fluxes between environmental compartments and mass balances	545
6.	Conclusion	547
	Conflict of interest	547
	Acknowledgement	547
	References	547

1. Introduction

Mercury (Hg) is a global, persistent, and bio-accumulative contaminant. In aquatic systems Hg is present in elemental, inorganic and organic forms. Elemental Hg (Hg⁰) is the most common form found in the atmosphere (Keating et al., 1997). Hg⁰ is slightly water soluble and has a large Henry's Law constant (Schroeder and Munthe, 1998; Andersson et al., 2008). Although Hg⁰ makes up only a small part of the total Hg (THg) in surface freshwater, it provides a significant pathway for the volatilization and further transport within the atmosphere. In marine environments, particularly in the Mediterranean basin, the ratio of Hg⁰/THg is significantly higher and volatilization of Hg⁰ was found to be the most important source/sink term in larger areas of the coastal and open sea (Rajar et al., 2007; Žagar et al., 2014; Kotnik et al., 2015). Besides Hg⁰, most of the Hg encountered in water, soil, sediments, and biota is in the form of inorganic Hg (HgII) and organic Hg, particularly monomethyl mercury (MeHg) (Mason et al., 1993, 1994), while dimethyl mercury (DMHg) is only present in extremely low concentrations in marine environments (Kotnik et al., 2007, 2015, 2017). HgII and MeHg can exist in the dissolved phase as well as in the colloidal and suspended phases in aquatic systems. These Hg species often undergo complex cycling and transformation processes (Krabbenhoft and Rickert, 2003; EPRI, 2006, 2013). Bio-accumulation and bio-magnification factors make MeHg the most biologically active, as well as the most toxic and perilous element for the entire food chain, including for humans, and posing great risk to wildlife and human beings (Kudo and Miyahara, 1991; Keating et al., 1997; USEPA, 2000; EFSA, 2004). Therefore, effective remediation measures must be applied so as to decrease Hg levels in heavily Hg-polluted aquatic systems (Wang et al., 2004). To effectively evaluate the potential for bioaccumulation and adequate remediation measures, both spatial and temporal distribution of Hg within aquatic systems should be characterized as completely as possible. Since the field data are often sparse and insufficient for spatial and temporal extrapolation in order to investigate the environmental impacts of different policy options, mathematical models have become a valuable tool in providing information about the possible responses of ecosystems (Knights et al., 2009).

Numerous models have been developed to simulate Hg transport and transformations in aquatic systems: from simple mass balance models to complicated biogeochemical models computing hydrodynamics, water quality, and sediment transport together with Hg processes. Hg in aquatic systems was initially examined with a mechanistic model by Harris (1991). This is a compartment (zero-dimensional) model for simulating Hg cycling in lakes, and it assumes the total mixing of all quantities in the water body under examination (Rajar et al., 1997). Hg was additionally modeled with contaminant simulators, such as the use of the Estuarine Contaminant Simulator (ECOS) to evaluate Hg accumulation in sediments and recovery time in a coastal lagoon (Abreu et al., 1998). This model is quite simple, and can only be used to simulate THg concentrations (Harris et al., 1993). Some researchers developed project-based models to simulate main

transformation processes in Hg cycling. For example, Rajar et al. (1997) modeled Hg cycling in the Gulf of Trieste where the main biochemical processes such as sedimentation, methylation, and demethylation were simulated. Over time, this model became the PCFLOW3D model. Another example is the modeling of the biogeochemical cycle of Hg with the Mercury Cycling Model (MCM) in lakes (Hudson et al., 1994). The MCM model simulates the transport and transformation reactions in each of the main lake compartments based on principles of mass conservation, chemical equilibria, and kinetics, as well as ecosystem bioenergetics (Leonard et al., 1995). This model has been widely used to study Hg dynamics in lakes (Hudson et al., 1994; Leonard et al., 1995; Knights and Ambrose, 2007), and the latest version is named Dynamic Mercury Cycling Model (D-MCM). Researchers, such as Massoudieh et al. (2010) and EPRI (2013), have also tried over the past 10 years to couple the Hg cycling model with a sediment diagenesis model so as to better capture the methylation process. These advances in Hg science bring new insight for Hg modeling in aquatic systems. However, a systematic review and summary of these models does not exist, except for some brief overviews, such as described in Wang et al. (2004), Massoudieh et al. (2010), or Gworek et al. (2016).

A comprehensive literature review of Hg simulation models in aquatic systems is given in this paper. The key processes and environmental factors governing Hg transport and fate were reviewed in order to better understand and, if possible, evaluate, the system processes of Hg simulations.

2. Model representation of the key transformation processes governing aquatic mercury cycling

Key transformation processes governing Hg cycling in aquatic systems include: 1) Hg⁰ oxidation, 2) HgII reduction, 3) HgII methylation, 4) MeHg degradation, and 5) MeHg demethylation (Harris et al., 2003), which are depicted in Fig. 1.

2.1. Hg⁰ oxidation

Hg⁰ can be relatively quickly oxidized by various reagents, mainly oxygen but also nitrates, nitrites, iron hydroxides, iron phosphates, sulfate, sulfur, and carbon dioxide (Stein et al., 1996). Photooxidation has also been reported in literatures (Lalonde et al., 2001; Lalonde et al., 2004; Garcia et al., 2005; He et al., 2014). Oxidation from Hg⁰ to HgII has generally been simulated as first-order degradation in the models (Rajar et al., 1997; Bale, 2000; Harris et al., 2003; Gandhi et al., 2007; Ethier et al., 2012), and an oxidation rate constant (k_{ox}) is employed. Generally, k_{ox} ranges from 0.001 to 0.1 day⁻¹ (Allison and Allison, 2005). A high photooxidation rate (34.56 day⁻¹) was reported by He et al. (2014), and the Hg⁰ photooxidation rate is much higher in the presence of both carbonate and nitrate than in the presence of carbonate, nitrate, or dissolved organic matter alone. The addition of dissolved organic matter to the solution of carbonate and nitrate decreased the

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