Environmental Modelling & Software 80 (2016) 159–174

Contents lists available at ScienceDirect

Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft

Modeling metal-sediment interaction processes: Parameter sensitivity assessment and uncertainty analysis

Eunju Cho [a], George B. Arhonditsis [b], Jeehyeong Khim [a, *], Sewoong Chung [c, **], Tae-Young Heo [d]

[a] School of Civil, Environmental and Architectural Engineering, Korea University, Seoul, 136-701, South Korea
[b] Ecological Modeling Laboratory, Department of Physical & Environmental Sciences, University of Toronto, Toronto, Ontario, M1C 1A4, Canada
[c] Department of Environmental Engineering, Chungbuk National University, Cheongju, 362-763, South Korea
[d] Department of Information & Statistics, Chungbuk National University, Cheongju, 362-763, South Korea

A R T I C L E I N F O

Article history:
Received 7 July 2015
Received in revised form
20 November 2015
Accepted 22 February 2016
Available online xxx

Keywords:
Sediment-metal modeling
Parameter uncertainty analysis
Sensitivity analysis
Bayesian Monte Carlo
EFDC
Geum river

A B S T R A C T

Sensitivity and uncertainty analysis of contaminant fate and transport modeling have received considerable attention in the literature. In this study, our objective is to elucidate the uncertainty pertaining to micropollutant modeling in the sediment-water column interface. Our sensitivity analysis suggests that not only partitioning coefficients of metals but also critical stress values for cohesive sediment affect greatly the predictions of suspended sediment and metal concentrations. Bayesian Monte Carlo is used to quantify the propagation of parameter uncertainty through the model and obtain the posterior parameter probabilities. The delineation of periods related to different river flow regimes allowed optimizing the characterization of cohesive sediment parameters and effectively reducing the overall model uncertainty. We conclude by offering prescriptive guidelines about how Bayesian inference techniques can be integrated with contaminant modeling and improve the methodological foundation of uncertainty analysis.

1. Introduction

Micropollutants often represent a major threat to the integrity of surface waters, such as rivers, lakes, and estuaries (Hong et al., 2003; Moldovan, 2006). The complex interplay between physical and biogeochemical processes that modulates micropollutant concentrations has received considerable attention in the recent literature. Mathematical modeling offers a comprehensive means to simulate fate and transport of heavy metals/organic contaminants and to support water quality management decisions that effectively protect aquatic ecosystem functioning (Ongley et al., 1992; Ji et al., 2002; Chu and Rediske, 2012). For example, mathematical models are an integral component of all the total maximum daily load (TMDL) programs in order to determine optimal management actions that can control point and non-point pollution sources and ultimately achieve water quality standards (National Research Council, 2001).

The typical practices in micropollutant modeling view model calibration as an inverse solution problem, whereby model parameters are iteratively adjusted until the discrepancy between model outputs and observed data is minimized (Freni and Mannina, 2010). This procedure may potentially offer insights into the magnitude of ecosystem processes/causal mechanisms that shape micropollutant concentrations, but it is frequently undermined by the well-known equifinality (poor model identifiability) problem, where several distinct choices of model inputs lead to the same model outputs (many sets of parameters fit the data about equally well) (Arhonditsis et al., 2007). A main reason for the equifinality problem is that the processes used for understanding how the system works internally is of substantially higher order than what can be externally observed. Moreover, while these modeling constructs can be complex and contain significant mechanistic foundation, their application involves uncertainty contributed by model structure and parameters as well as measurement imprecision and

* Corresponding author. School of Civil, Environmental and Architectural Engineering, Korea University, Anam-dong, Seongbuk-gu, Seoul, 136-701, South Korea.
** Corresponding author. Department of Environmental Engineering, Chungbuk National University, Chungdae-ro 1, Seowon-gu, Cheongju, Chungbuk, 362-763, South Korea.
E-mail addresses: hyeong@korea.ac.kr (J. Khim), schung@chungbuk.ac.kr (S. Chung).

http://dx.doi.org/10.1016/j.envsoft.2016.02.026
1364-8152/

other data uncertainties. The structural uncertainty is not surprising because all models are drastic simplifications of reality that approximate the actual processes, i.e., essentially, all parameters are effective (spatially and temporally averaged) values unlikely to be represented by a fixed constant (Arhonditsis et al., 2007, 2008a,b). Furthermore, heavy metal/organic contaminant data are expensive, scarce, and highly variable (Freni and Mannina, 2010; Vezzaro and Mikkelsen, 2012), so individual equations which are approximately correct in controlled laboratory environments may not collectively yield an accurate picture of the processes that shape micropollutant concentrations in surface waters (Reichert, 1997; Refsgaard et al., 2005; Krysanova et al., 2007). Therefore, uncertainty analysis has been a topic of increasing importance in hydrological and water quality modeling (Freni et al., 2009; Torres and Bertrand-Krajewski, 2008; Marsili-Libelli and Giusti, 2008; Arhonditsis, 2008a,b; Shen et al., 2012; Ruark et al., 2011). Although several techniques have been implemented to evaluate parametric uncertainty (Sohn et al., 2000; Freni and Mannina, 2010), the effects of model parameters on predicted results are not well understood and can vary depending on the characteristics of modeled contaminants (Sommerfreund et al., 2010; Matthies et al., 2004).

One of the most challenging processes in micropollutant modeling is the reproduction of their adsorption on the surface of cohesive sediments and their subsequent transport in the water column (Ji, 2008; Trento and Alvarez, 2011; Liu et al., 2012). In this regard, Liu et al. (2012) simulated the two-dimensional transport and distribution of heavy metals along the tidal Keelung River estuary, indicating that the partition coefficient plays an important role in the distribution of dissolved and particulate lead concentrations. In the same context, Trento and Alvarez (2011) evaluated the relative parameter sensitivity of a simple model that aimed to simulate chromium and fine sediment transport, showing that the characterization of the associated processes was predominantly driven by several parameters, such as the partition coefficients in the water column and bed sediments, the depth of the active bed sediment layer, and the mass transfer coefficient between the water column and sediment pore water. Along the same line of reasoning, Franceschini and Tsai (2010) underscored the importance of the characterization of suspended sediment processes, when modeling total polychlorinated biphenyls (PCBs) with Environmental Fluid Dynamics Code (EFDC) and Water Quality Analysis Simulation Program (WASP). Many other studies similarly emphasized that the modules that simulate toxic micropollutant concentrations are particularly sensitive to parameters related to cohesive sediments, such as settling velocity, critical stress values on sediment bed as well as to the metal partitioning coefficients (Shen et al., 2010, 2012; Ruark et al., 2011). To make matters worse, the spatial and temporal heterogeneity of the associated physical and chemical processes are important confounding factors that can profoundly inflate model uncertainty (Sohn et al., 2000; Kanso et al., 2005; Franceschini and Tsai, 2010).

In this study, our first objective is to shed light on how the uncertainty of the outputs of micropollutant modeling can be apportioned to five critical parameters; namely, the settling velocity (w_s), critical deposition stress (τ_{cd}), critical erosion stress (τ_{ce}), metal partitioning coefficient between suspended sediment and water column ($K_{d,SS}$), and metal partitioning coefficient between sediment bed and water column ($K_{d,bed}$). Specifically, we evaluate the efficiency of the local or one-step-at-a-time (OAT) sensitivity analysis method relative to the Morris Screening method. In a subsequent exercise, we implement the Bayesian Monte Carlo method to quantify uncertainty propagation of model parameters and derive posterior parameter probabilities based on the corresponding priors and observed data. Our study concludes by offering prescriptive guidelines about how Bayesian inference techniques can be integrated with contaminant modeling in order to improve the methodological foundation of uncertainty analysis.

2. Methods

2.1. Model setup-data sources

The study site for this investigation is located in the middle reach of Geum River, one of the four major rivers in Korea, where two multipurpose dams have been built. The spatial model domain begins from the Daecheong Regulation Dam to Maeogu, with a total length of 36,740 m. The cell map was constructed using a SMS (surface-water modeling system) program based on the data modification obtained from the Korean Ministry of Land, Infrastructure, and Transport (Fig. 1). There were a total of 273 active cells, which were formed by 83 longitudinal and 8 lateral cells. The average cell length and width were 429.8 m and 151.7 m, respectively. Because the construction period of the Sejongbo Dam, which included movable and fixed weirs, was from May 2009 to June 2012, different elevation data were used in 2011 and 2012 to incorporate the changes of bottom topography over time.

In this paper, we implemented the Environmental Fluid Dynamics Code (EFDC) Explorer 7, a widely used model with the capability to simulate the cohesive sediment transport and metal behavior (Elçi et al., 2007; Ji et al., 2002), developed by Dynamic Solutions International (DSI). Model calibration and verification was based on water surface elevation data measured at Hyundo

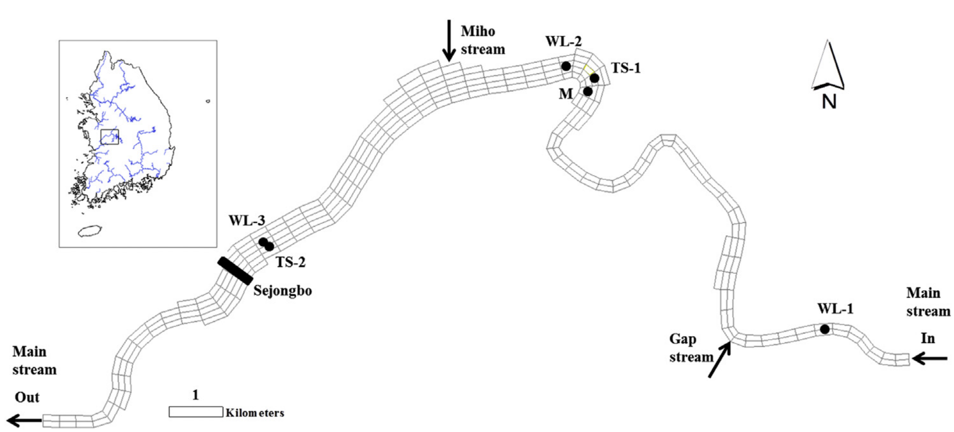

Fig. 1. Location of the Geum River in Korea, and the cell map with the boundaries and monitoring points of the water surface elevation (WL-1, WL-2, WL-3), temperature and total suspended sediment concentrations (TS-1, TS-2), and total and dissolved metal concentrations (M).