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# Stochastic modeling of phosphorus transport in the Three Gorges Reservoir by incorporating variability associated with the phosphorus partition coefficient

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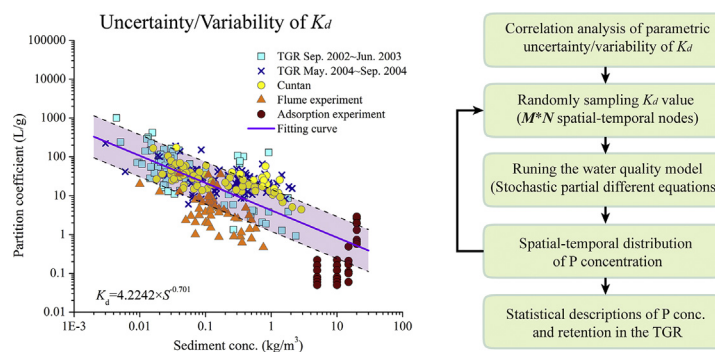
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## HIGHLIGHTS

- Characterizes variability of phosphorus (P) partition coefficient using field data.
- Parametric uncertainty generates uncertainty in the predicted P transport.
- Statistical descriptions of the P concentration and retention in the TGR.
- Stochastic model can more effectively serve as a P management tool than deterministic models.

## GRAPHICAL ABSTRACT



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## ABSTRACT

Phosphorus (P) fate and transport plays a crucial role in the ecology of rivers and reservoirs in which eutrophication is limited by P. A key uncertainty in models used to help manage P in such systems is the partitioning of P to suspended and bed sediments. By analyzing data from field and laboratory experiments, we stochastically characterize the variability of the partition coefficient ( $K_d$ ) and derive spatio-temporal solutions for P transport in the Three Gorges Reservoir (TGR). We formulate a set of stochastic partial differential equations (SPDEs) to simulate P transport by randomly sampling  $K_d$  from the measured distributions, to obtain statistical descriptions of the P concentration and retention in the TGR. The correspondence between predicted and observed P concentrations and P retention in the TGR combined with the ability to effectively characterize uncertainty suggests that a model that incorporates the observed variability can better describe P dynamics and more effectively serve as a tool for P management in the system. This study highlights the importance of considering parametric uncertainty in estimating uncertainty/variability associated with simulated P transport.

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## 1. Introduction

Phosphorus (P), one of the key nutrients affecting water quality, typically is the limiting reactant for eutrophication in rivers and reservoirs (Dai et al., 2010; Elser et al., 2007; Schindler, 2006). The ability to

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manage eutrophication is largely a function of our understanding and ability to manage P fate and behavior in these systems. In recent decades, human activities have greatly changed the inherent characteristics of many inland waters (Dai et al., 2008; Syvitski et al., 2005; Zhang et al., 1999) resulting in substantial effects on nutrients, including P. The Three Gorges Reservoir (TGR), located in the upstream Yangtze River (see Fig. 1), is the largest hydraulic project in the world. The TGR is operated to support a variety of societal benefits including flood control, hydropower generation, navigation, and water storage. Meanwhile, there are also many complex problems associated with reservoir operation including sedimentation and the accumulation of nutrients including P which controls eutrophication in the TGR (Dai et al., 2010; Wang et al., 2011). P tends to be strongly associated with suspended and bed sediment, and thus the fate and transport of sediments within these systems is integral to the understanding of the fate and behavior of P. The impoundment of the TGR substantially changed the hydrological regime and sediment fate and transport in the Yangtze River, significantly impacting the transport of P in the system. The resulting potential for eutrophication has led to serious environmental concerns (Camargo et al., 2005; Li et al., 2012; Yao et al., 2009).

Mathematical modeling is an effective tool for predicting P transport in the aqueous environment, and a great number of water quality models have been developed over recent decades (Park et al., 2008; Wang et al., 2014). Huang et al. (2015a) developed a coupled model of hydrodynamics, sediment and P transport, which was applied to predict P transport in the TGR and evaluate the effectiveness of various operating rules on sediment and P retention in the reservoir. However, these are deterministic models utilizing fixed parameters, which may not adequately characterize the parameter variability and the resulting model uncertainty. In particular, Huang et al. (2015a) observed that the model results are very sensitive to coupling between sediment and P transport which is largely controlled by the P partitioning to suspended and bed sediment. Moreover, the dissolved P likely controls eutrophication due to its high bioavailability while the transport of P or its retention in the bed sediment is largely controlled by the adsorbed P (Jarvie et al., 2006). In the current paper, the uncertainty and variability in P fate and transport associated with partitioning of P to suspended and bed sediment is explored to better understand effective P management in the TGR.

Model uncertainty has long been recognized as an important issue in water quality modeling (Dilks et al., 1992; Dotto et al., 2012), and we would like to ask how sensitive these results are to model uncertainties.

There are mainly two sources for model uncertainties. One is the model structural error due to a simplified description of the natural phenomena (i.e., model assumptions using simple equations to represent complex and non-linear processes), and the degree of uncertainty in structural error is related to the degree to which these assumptions hold (Lindenschmidt et al., 2007; Radwan et al., 2004). The other is parameter uncertainty deriving from inaccurate estimation or variability of model parameters (Beck, 1987; Gong et al., 2011). Parametric uncertainty generates through the governing equations uncertainty in the predicted system behavior (Gates and Al-Zahrani, 1996a), associated with which are notions of risk, reliability, and variability that influence decision making (Hantush and Chaudhary, 2014). In this study, we focus on quantifying model parameters of the previously proposed P transport model by Huang et al. (2015a) in the TGR.

Sediment particles have a strong affinity to P due to the high specific surface areas and surface active sites (Davis and Kent, 1990; Fang et al., 2013; Wang et al., 2009). Most P in waters are adsorbed by sediment particles and transported in the particulate phase (Withers and Jarvie, 2008). The partition coefficient ( $K_d$ ) is defined as the ratio between the concentrations of particulate P (PP) and dissolved P (DP), as an indicator of the capability of sediment to retain P (Evgeny et al., 2014). The value of  $K_d$  exerts significant impacts on the simulated results, and accurate estimation of  $K_d$  is especially important for reliable model prediction. However, the value of  $K_d$  is affected by a variety of internal and external factors, such as specific surface area (Chen and Fang, 2013), mineral composition, and surface charge distribution of sediment particles (Chen et al., 2013; Huang et al., 2012). There is an inherent variability in  $K_d$  associated with both uncertainty in the parameter and the variation in sediment properties that affect the partitioning (Domènech et al., 2015). In general, these factors are inherently characterized by stochastic processes and it is most accurate to define them only by statistical distributions. In addition, sediment concentration, pH, and ionic strength also influence  $K_d$  through complex interactions with the sediment surface. These factors collectively make it difficult to accurately quantify  $K_d$ , particularly if it is seen as a deterministic, single valued function of bulk environmental properties.

Compared with deterministic models, stochastic models are more powerful due to the capability of predicting the spatio-temporal distribution of P concentration as well as associated probability of occurrence. Stochastic models can not only predict expected values, but also estimate variability in predicted system behavior and derive associated degrees of confidence (Gates and Al-Zahrani, 1996b). Stochastic models

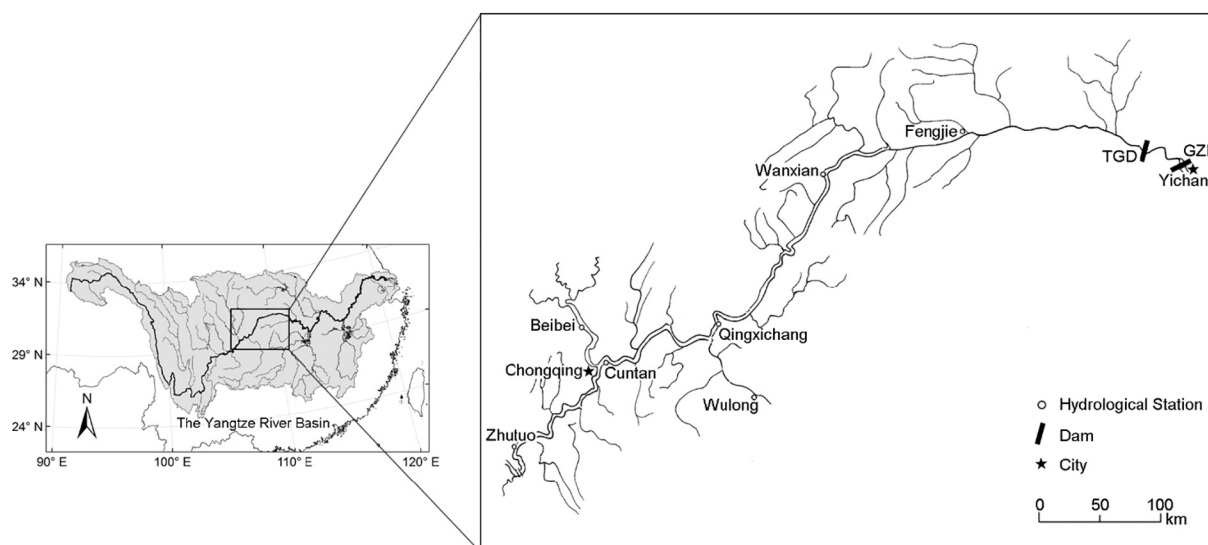


Fig. 1. Location of the Three Gorges Reservoir (left: an overview of the Yangtze River Basin; right: map of the TGR).

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