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Modeling the fate, transport and risk of Bisphenol A and N, N-diethyltoluamide in a tropical reservoir

Xuneng Tong[1], Jingjie Zhang[2,3,4], Luhua You[2], and Karina Yew-Hoong Gin[1,2]
[1]Department of Civil & Environmental Engineering, National University of Singapore, 1 Engineering Drive 2, Singapore 117576, Singapore
[2]NUS Environmental Research Institute, National University of Singapore, 1 Create way, Create Tower, #15-02, Singapore 138602, Singapore
[3]School of Environmental Science and Engineering, Southern University of Science and Technology, Shenzhen, 518055, China
[4]Northeast Institute of Geography and Agroecology, Chinese Academy of Sciences, Changchun 130102, China

The fate and transport of emerging contaminants in aquatic environments is a complex process, which is not only determined by their own properties but can also be influenced by the surrounding environment. In this study, a comprehensive modelling framework coupling a 3D hydrodynamic--emerging contaminants module was developed to describe the fate and transport of two representative emerging contaminants, namely Bisphenol A (BPA) and N, N-diethyltoluamide (DEET) in a tropical reservoir. First, the model was calibrated and validated with BPA and DEET obtained from a historical dataset (2013-2014) in bulk water, suspended solids, pore water and sediments phase. Results revealed that the simulation performance gave “excellent simulation” results with skill scores all larger than 0.90. Subsequently, the ecological risk assessment for the reservoir was conducted using the trophic state index (TSI) and coupled species sensitivity distribution (SSD)-Risk Quotient (RQ) method. The RQ values of the study area ranged from 0.003-0.068 (BPA) and 0.001-0.014 (DEET), respectively, which suggests that the levels of studied compounds BPA and DEET may pose low risk to the aquatic ecosystem. Finally, the indirect influence of general water quality parameters such as nutrients (phosphorous) on the multi-compartment distributions of emerging contaminants was explored. Our approach lays down a comprehensive framework to better understand the dynamics of fate and transport and their potential ecological risks of emerging contaminants as well as the indirect impact of other water quality parameters on their distributions in different phases in aquatic ecosystems.