A Method for simulation of reactive solute transport in Natural Rivers

Byunguk Kim[1], Siyoon Kwon[1], Il Won Seo[1]

[1]Seoul National University, Seoul, Republic of Korea

*Correspondence YP: seoilwon@snu.ac.kr

IAHR YPN

Hosted by Spain Water and IWHR, China

Abstract

For several decades, solute transport models have been used in order to predict behavior of solute in rivers. However, most previous studies assumed that the subject solute is conservative, and few of studies taking account of decay terms into the models which mostly employed optimization methods to determine decay parameters. Herein, we added two decay terms to the Transient Storage Model (TSM) representing volatilization and biodegradation, and proposed the method to estimate the decay parameters based on chemodynamics theories. Using this advanced model, the reactive solute transport simulation was carried out at natural river of Gam Creek, South Korea in 2020. The results revealed that there was considerable difference in resulting breakthrough curve depending on the type of chemicals. In addition, the significant regimes of decay parameters were classified using Damkohler number.

Keywords: reactive solute transport model, parameters, volatilization, biodegradation, tracer test.

Method

- We proposed the method to reflect the phenomenon of **volatilization** and **bio-degradation** of a chemical into the transient storage model (TSM)
- The numerical model was constructed for this analysis using the **finite difference method** and **Crank-Nicolson algorithm**.
- The volatilization can be interpreted as a first-order mass transfer between two-phase boundary layer that is refer to as the **Two film theory**. The concentration gradient within the quiescent boundary layers was assumed to be linear due to molecular diffusion, and mass-transfer is dominated by this diffusivity based on the Fick's law.
- To estimate the biodegradation rate, the BIOWIN model was employed which is a biodegradation half-life estimator for various chemical.

Results

- The comparison results of the estimated volatilization rate to another volatilization model and the vapor pressure showed **0.85 and 0.76 of correlation**.
- The results of simulation for the toluene, phenol, and sulfuric acid showed **57%, 12%, 24% of mass loss**, respectively, as shown in the Figure 1.
- By the Damkohler number, the decay rate can be normalized from flow velocity and travel distance as shown in the Figure 2.
- In the Figure 2, the ignorable regime means that the decay mechanism is not needed to be considered for the sake of brevity and saving of computation time. Whereas, the over-reacting regime indicates that the reaction rate could be over-estimated so that the other mixing mechanisms could be muted to function.

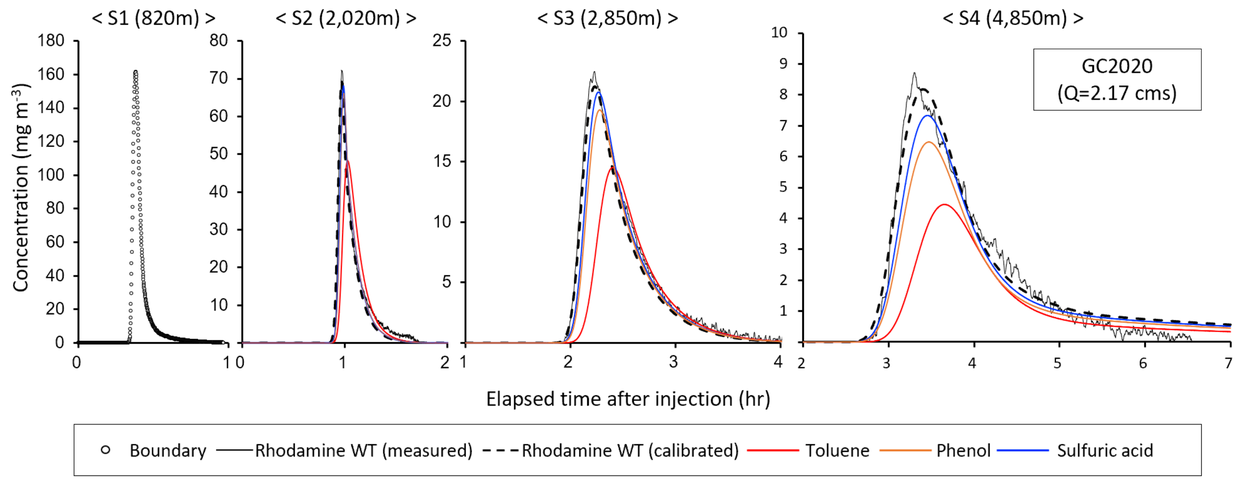

Figure 1: Resulting breakthrough curves for Rhodamine WT, toluene, phenol, and sulfuric acid

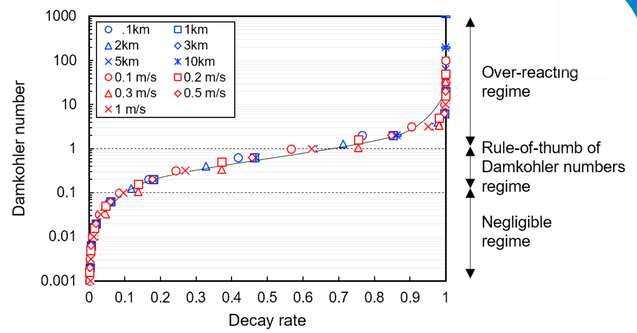

Figure 2: Classification of regimes of decay rate by the Damkohler number

Conclusions

To overcome the **limitations of precious studies that used optimization techniques** to determine the extent of decay, this study employed the pre-suggested theoretical and empirical methods to estimate the first-order reactivity parameters.

The resulting breakthrough curves from the simulations for different chemicals were considerably different indicating the inappropriateness of the conservation assumption.

Bibliography

Runkel, R. L., & Broshears, R. E. (1991). One-dimensional transport with inflow and storage (OTIS): a solute transport model for small streams (p. 85). CADSWES, Center for Advanced Decision Support for Water and Environmental Systems, Department of Civil Engineering, University of Colorado.

Whitman, W. G. (1923). The two-film theory of gas absorption. Chem. Metall. Eng., 29, 146-148.