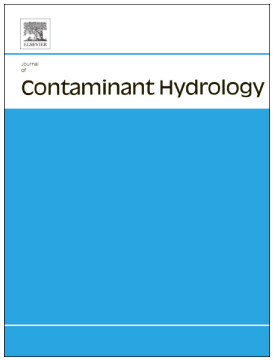

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Parameterizing Sorption Isotherms Using a Hybrid Global-Local Fitting Procedure

L. Shawn Matott[1,*], Anshuman Singh[2], Alan J. Rabideau[3]

[1] – University at Buffalo, Center for Computational Research, Buffalo NY
[2] – Department of Civil Engineering, National Institute of Technology, Patna, India
[3] – University at Buffalo, Department of Civil, Structural and Environmental Engineering, Buffalo NY
[*] – Corresponding author, lsmatott@buffalo.edu, ph. 716-881-7566, fax 716-849-6656

Abstract

Predictive modeling of the transport and remediation of groundwater contaminants requires an accurate description of the sorption process, which is usually provided by fitting an isotherm model to site-specific laboratory data. Commonly used calibration procedures, listed in order of increasing sophistication, include: trial-and-error, linearization, non-linear regression, global search, and hybrid global-local search. Given the considerable variability in fitting procedures applied in published isotherm studies, we investigate d the importance of algorithm selection through a series of numerical experiments involving 13 previously published sorption datasets. These datasets, considered representative of state-of-the-art for isotherm experiments, had been previously analyzed using trial-and-error, linearization, or non-linear regression methods. The isotherm expressions were re-fit using a 3-stage hybrid global-local search procedure (i.e. global search using particle swarm optimization followed by Powell's derivative free local search method and Gauss-Marquardt-Levenberg non-linear regression). The re-fitted expressions were then compared to previously published fits in terms of the optimized weighted sum of squared residuals (WSSR) fitness function, the final estimated parameters, and the influence on contaminant transport predictions – where easily computed concentration-dependent contaminant retardation factors served as a surrogate measure of likely transport behavior. Results suggest that many of the previously published calibrated isotherm parameter sets were local minima. In some cases, the updated hybrid global-local search yielded order-of-