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Physics-Informed Ensemble Surrogate Modeling of Advective-Dispersive Transport Coupled with Film Intraparticle Pore Diffusion Model for Column Leaching Test

Amirhossein Ershadi, Michael Finkel, Binlong Liu, Olaf Cirpka, and Peter Grathwohl
Department of Geosciences, University of Tübingen, Tübingen, Germany (amirhossein.ershadi@student.uni-tuebingen.de)

Column leaching tests are a common approach for evaluating the leaching behavior of contaminated soil and waste materials, which are often reused for various construction purposes. The observed breakthrough curves of the contaminants are affected by the intricate dynamics of solute transport, inter-phase mass transfer, and dispersion. Disentangling these interactions requires numerical models. However, inverse modeling and parameter sensitivity analysis are often time-consuming, especially when sorption/desorption kinetics are explicitly described by intra-particle diffusion, requiring the discretization along the column axis and inside the grains. To replace such computationally expensive models, we developed a machine-learning based surrogate model employing two disparate ensemble methods (stacking and weighted distance average) within the defined parameter range based on the German standard for column leaching tests. To optimize the surrogate model, adaptive sampling methods based on three distinct infill criteria are employed. These criteria include maximizing expected improvement, the Mahalanobis distance (exploitation), and maximizing standard deviation (exploration).
The stacking surrogate model makes use of extremely randomized trees and random forest as base- and meta-model. The model shows a very good performance in emulating the behavior of the original numerical model (Relative Root Mean Squared Error = 0.09).
Our proposed surrogate model has been applied to estimate the complete posterior parameter distribution using Markov Chain Monte Carlo simulation. The impact of individual input parameters on the predictions generated by the surrogate model was analyzed using SHapley Additive exPlanations methods.