Lawrence Livermore National Laboratory

L-SURF (LLNL Surface Complexation-Ion Exchange Database)

The L-SURF code provides a new, alternative approach to simulate metal-mineral interactions.

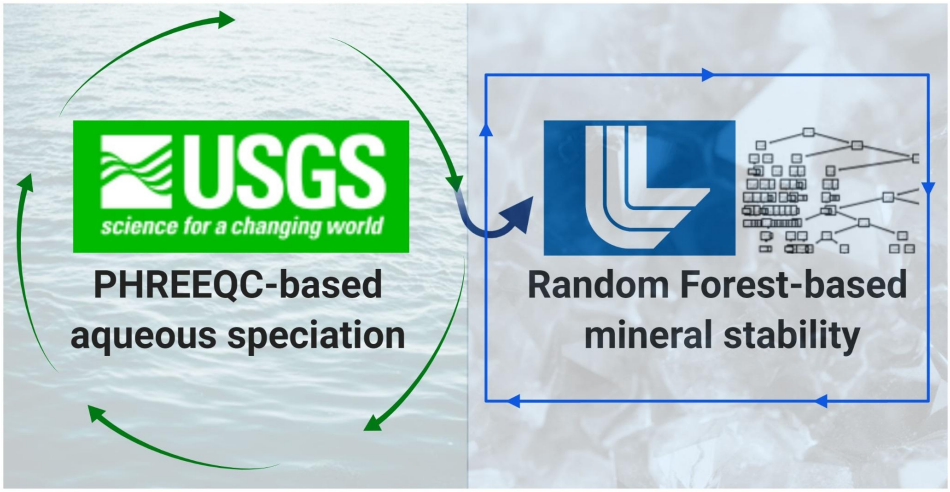
Description

Historically, reactive transport models have provided important simulation results on the mobility and fate of radionuclides in subsurface geologic systems. The effectiveness of these models depends in part on surface complexation models (SCMs) that provide geochemically informed sorption-based retardation information. This work demonstrates a first-of-its-kind hybrid random forest ML approach that serves as an alternative method to quantifying metal-mineral sorption processes. At its core, the random forest ML approach is motivated by a successful effort in digitizing raw sorption community data contained in the RES3T database (i.e., LLNL Surface Complexation-Ion Exchange Database). Our new hybrid ML model incorporates important geochemical information through aqueous speciation calculations while also implementing a data-driven random forest decision making process to determine mineral sorption phenomena. Named the LLNL Speciation Updated Random Forest (L-SURF) model, this code provides a new, alternative approach to simulate metal-mineral interactions. A test-case for Uranium-Quartz sorption is presented in the example code package.

Category

Software

Learn more



References

1. Chang, Elliott, Zavarin, Mavrik, Beverly, Linda, Wainwright, Haruko(August 2023) , https://doi.org/10.1016/j.apgeochem.2023.105731, Applied Geochemistry, 155