World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

Performance Evaluation of Using Genetic Programming Based Surrogate Models for Approximating Simulation Complex Geochemical Transport Processes

Authors : Hamed K. Esfahani, Bithin Datta

Abstract : Transport of reactive chemical contaminant species in groundwater aquifers is a complex and highly non-linear physical and geochemical process especially for real life scenarios. Simulating this transport process involves solving complex nonlinear equations and generally requires huge computational time for a given aquifer study area. Development of optimal remediation strategies in aquifers may require repeated solution of such complex numerical simulation models. To overcome this computational limitation and improve the computational feasibility of large number of repeated simulations, Genetic Programming based trained surrogate models are developed to approximately simulate such complex transport processes. Transport process of acid mine drainage, a hazardous pollutant is first simulated using a numerical simulated model: HYDROGEOCHEM 5.0 for a contaminated aquifer in a historic mine site. Simulation model solution results for an illustrative contaminated aquifer site is then approximated by training and testing a Genetic Programming (GP) based surrogate model. Performance evaluation of the ensemble GP models as surrogate models for the reactive species transport in groundwater demonstrates the feasibility of its use and the associated computational advantages. The results show the efficiency and feasibility of using ensemble GP surrogate models as approximate simulators of complex hydrogeologic and geochemical processes in a contaminated groundwater aquifer incorporating uncertainties in historic mine site.

Keywords : geochemical transport simulation, acid mine drainage, surrogate models, ensemble genetic programming, contaminated aquifers, mine sites
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020