EGU24-21545, updated on 20 May 2024
https://doi.org/10.5194/egusphere-egu24-21545
EGU General Assembly 2024

Machine learning based metamodels for geochemical calculations in reactive transport models: Benchmark within the EURAD Joint Project

Eric Laloy[1], **Vanessa Montoya**[1], and the EURAD-DONUT Team[*]
[1]Engineered and Geosystems Analysis, Belgian Nuclear Research Centre, Belgium
[*]A full list of authors appears at the end of the abstract

Thanks to the recent progress in numerical methods, the application fields of artificial intelligence (AI) and machine learning methods (ML) are growing at a very fast pace. The EURAD (European Joint Programme on Radioactive Waste Management) community has recently started using ML for a) acceleration of numerical simulations, b) improvement of multiscale and multiphysics couplings efficiency, c) uncertainty quantification and sensitivity analysis. A number of case studies indicate that use of ML based approaches leads to overall acceleration of geochemical and reactive transport simulations from one to four orders of magnitude. The achieved speed-up depends on the chemical system, simulation code, problem formulation and the research question to be answered. Within EURAD-DONUT (Development and Improvement Of Numerical methods and Tools for modelling coupled processes), a benchmark is on-going to coordinate the relevant activities and to test a variety of ML techniques for geochemistry and reactive transport simulations in the framework of radioactive waste disposal. It aims at benchmarking several widely used geochemical codes, at generating high-quality geochemical data for training/validation of existing/new methodologies, and at providing basic guidelines about the benefits, drawbacks, and current limitations of using ML techniques.

A joint effort has resulted in the definition of benchmarks of which one is presented here. The benchmark system is relevant to the sorption of U in claystone formations (e.g. Callovo-Oxfordian, Opalinus or Boom clay). Regarding the chemical complexity, a system containing Na-Cl-U-H-O is considered as the base case, and a more complex system with the addition of calcium and carbonate (CO2) to change aqueous speciation of U. Parameters of interest, among others, are the resulting concentrations of U sorbed on edges (surface complexes), of U on ion exchange sites, and the amount of metaSchoepite, with the resulting Kd's. Following aspects are discussed: (i) Streamline the production of high-quality consistent training datasets, using the most popular geochemical solvers (PHREEQC, ORCHESTRA and GEMS). (ii) The use of different methods (e.g. Deep Neural Networks, Polynomial Chaos Expansion, Gaussian Processes, Active Learning, and other techniques to learn from the generated data. (iii) Setup appropriate metrics for the critical evaluation of the accuracy of ML models. (iv) Testing the accuracy of predictions for geochemical and reactive transport calculations.

EURAD-DONUT Team: E. Laloy 1, N.I. Prasianakis 2, D. Jacques 1, J.C.L. Meeussen 3, C. Tournassat 4, G.D. Miron 2, D. A. Kulik 2, A. Idiart 5, E. Demirer 5, E. Coene 5, B. Cochepin 6, M. Leconte 6, V. Montoya 1, M. Savino 6, 7, J. Samper II 8, M. De Lucia 9, S. V. Churakov 2,10, O. Kolditz 11, C. Yang 12, J. Samper 8, F. Claret 13 1 Engineered and Geosystems Analysis, Belgian Nuclear Research Centre, Belgium 2 Laboratory for Waste Management, Paul Scherrer Institute, CH-5232, Villigen PSI, Switzerland 3 Nuclear Research and Consultancy Group (NRG), Petten, The Netherlands 4 Institut des Sciences de la Terre d'Orléans, Université d'Orléans—CNRS/INSU—BRGM, Orléans, France 5 AMPHOS 21 Consulting, S.L., Calle Venezuela, 103, 08019, Barcelona, Spain 6 ANDRA Andra, 1/7 Rue Jean Monnet, 92290, Chatenay-Malabry, France 7 Universite Paris-Saclay, AgroParisTech, INRAE, UMR MIA-Paris, 75005, Paris, France 8 Centro de Investigaciones Científicas, ETS Ingenieros de Caminos, Universidade da Coruña, A Coruña, Spain 9 Helmholtz Centre Potsdam - GFZ German Research Centre for Geosciences, Telegrafenberg, 14473 Potsdam, Germany 10 Institute for Geological Sciences, Bern University, CH-3012, Bern, Switzerland 11 Department of Environmental Informatics, Helmholtz Centre for Environmental Research, UFZ, Leipzig, Germany 12 Environmental Data Technology Inc. San Antonio, TX USA 13 BRGM, 3 Avenue Claude Guillemin, 45060 Orléans, France