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Serpentinization and hydrocarbon formation from experiments: a machine learning approach

Fang Huang (1), Samuel Barbier (2), Muriel Andreani (2), Renbiao Tao (2), Jihua Hao (2), Osama Minhas (1), Kathleen Fontaine (1), Peter Fox (1), and Isabelle Daniel (2)

(1) Tetherless World Constellation, Rensselaer Polytechnic Institute, Troy, United States, (2) Univ Lyon, Université Lyon 1, Ens de Lyon, CNRS, UMR 5276 LGL-TPE, F-69622, Villeurbanne, France

Serpentinization is a hydrous alteration of ultramafic rocks in hydrothermal systems, which generates H2 and organic species, and can potentially contribute to origin of life. In the past decades, serpentinization has been extensively studied in labs, producing methane in highly variable amounts. Such a large experimental variability could not be easily explained. Therefore, we collected 21 papers with more than 100 experiments reporting over 400 measurements and experimental parameters. This included the pressure and temperature conditions, the type of reactor and the production concentration of >10 different kinds of organic species. However, production of these species from different groups vary largely, and it was extraordinarily difficult to identify several out of $\sim$100 parameters that really matter.

We applied a machine learning algorithm - random forest - to solve the problem. This algorithm took in all available experiment parameters, and ranked them based on their "importance", which works perfectly in our case. Based on the importance score, we found that temperature, catalytic effects from reactor, and the addition of $NaCl/NaHCO_3$ in fluids are among the most important parameters. The temperature range of possible production of CH4/C2H6 agrees with Shock et al. theoretical modeling. After detailed examination, we could show that most of the $NaCl/NaHCO_3$ products used have various levels of organic contamination. These are important preliminary results; as we continue adding more data and tune the model, the results will refine. Then it could be used to predict outcomes and guide future experiments.