Goldschmidt 2022 Abstract
https://doi.org/10.46427/gold2022.9835

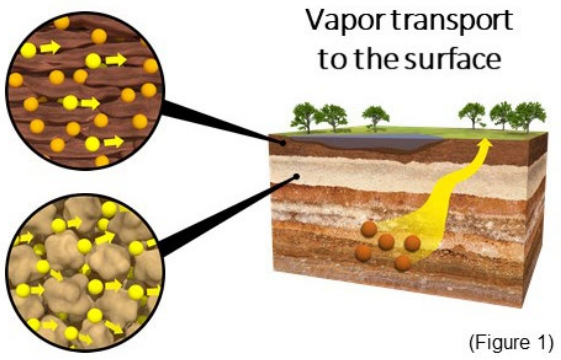
Elucidating physicochemical properties of geologic materials using inverse gas chromatography and modeling

DR. ELIZABETH H DENIS, PHD, MARK L ROCKHOLD, ANJELICA BAUTISTA, NICHOLAS L HUGGETT, GUOHUI WANG, MARK D WHITE AND APRIL J CARMAN

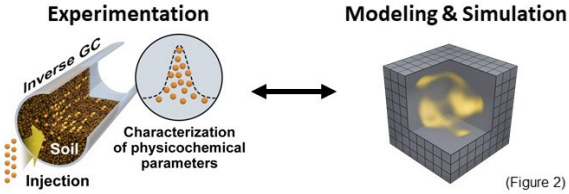
Pacific Northwest National Laboratory

Presenting Author: elizabeth.denis@pnnl.gov

A goal of this work is to better understand the chemistry of gas-solid interactions and how volatile compounds are transported through geologic materials under different temperature and humidity conditions (Figure 1). Inverse gas chromatography (IGC) allows us to characterize and quantify the physicochemical properties of geologic materials using probe gases, such as volatile organic compounds and noble gases. Geologic materials are typically heterogeneous, both physically and chemically. Characterizing the properties of individual organic and inorganic components can help elucidate the primary factors influencing volatile interactions in more complex mixtures. Recent work has demonstrated that IGC is effective in analyzing key physicochemical parameters (e.g., partition coefficient, diffusion coefficient, and heat of adsorption) used for modeling subsurface gas transport [1]. Ongoing efforts involve integrating IGC-determined physicochemical parameters with Subsurface Transport Over Multiple Phases-GeoThermal (STOMP-GT, [2]) models to better predict vapor transport through the subsurface (Figure 2). Initially, STOMP-GT is being used to create a 2D cylindrical model that simulates IGC conditions. In an iterative process, the model is being validated based on experimental results. Ultimately, experimentation helps produce the scientific understanding and physicochemical parameters that will enable more effective modeling and prediction of subsurface gas transport.



(Figure 1)



(Figure 2)

References

[1] Denis, Fraga, Huggett, Weaver, Rush, Dockendorff, Breton-Vega & Carman (2021), *Langmuir* 37, 6887-6897. https://doi.org/10.1021/acs.langmuir.0c03676

[2] STOMP. https://www.pnnl.gov/projects/stomp