# Physicochemical Characterization of Geologic Materials

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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. Inverse gas chromatography (iGC) enables quantification of the physicochemical properties of geologic materials using probe gases, such as volatile organic compounds. A challenge is that 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 [Denis et al. (2021), *Langmuir* 37, 6887-6897. https://doi.org/10.1021/acs.langmuir.0c03676]. Ongoing efforts include integrating iGC-determined physicochemical parameters with Subsurface Transport Over Multiple Phases-GeoThermal (STOMP-GT, https://www.pnnl.gov/projects/stomp) models to better predict vapor transport through the subsurface. In addition, in collaboration with Surface Measurement Systems (SMS), zeolite samples were tested with the new SMS high-temperature iGC. The measurements at 300 – 500 °C compared well with the PNNL-predicted partition coefficient values based on measurements of the zeolites at 110 – 130 °C. These initial efforts demonstrate how we can make predictions for temperatures that are not yet measured and highlight a need to account for potential material changes.

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