

REACTIVE TRANSPORT MODELING TO INTERPRET ENVIRONMENTAL CONDITIONS THAT MAY PRESERVE ORGANIC MOLECULES ON MARS. E.M. Hausrath¹, E.B. Rampe², D.W. Ming², P.D. Archer³, M. Millan⁴ ¹UNLV, Las Vegas, NV 89154 Elisabeth.Hausrath@unlv.edu, ²NASA Johnson Space Center, Houston, TX 77058 ³Jacobs, NASA Johnson Space Center, Houston TX 77058 ⁴Georgetown University, Washington, DC 20057

Introduction: In the search for life on Mars, organic molecules represent a critical target. Organic matter has been previously detected in Gale crater in variable concentrations and compositions [1-5]. One potential explanation for this variability is that differences in diagenetic environments may have resulted in either organic matter degradation or preservation.

In order to test this hypothesis, we are selecting samples for which both SAM and CheMin data are available, and we can therefore compare the mineralogy and geochemistry of the sample to measurements of organic matter from SAM. We are then examining the geochemical and mineralogical data to identify and quantify the degree of diagenesis exhibited by different samples, and using quantitative numerical modeling to place constraints upon past environmental conditions that may impact the preservation of organic molecules.

Based on the examination of SAM and CheMin measurements, we selected samples from Glen Torridon (GT) and Vera Rubin ridge (VRR). GT and VRR are stratigraphically equivalent, but VRR is proposed to have experienced significant late diagenetic alteration including multiple fluids with varying pH, salinity, and temperature [6]. The comparison of the geochemistry, mineralogy, and organic measurements of GT and VRR therefore allows an exciting examination of potential impacts of past diagenetic conditions on organic matter preservation. In this abstract, we present results of our ongoing numerical modeling of past environments at GT and VRR, which can be compared to results from SAM to help constrain past environmental conditions that may result in either preservation or degradation of organic matter.

Methods: We examined the mineralogy of GT and VRR to determine indicators of past aqueous conditions that we can constrain using modeling. Samples from VRR have abundant hematite and decreased clay minerals and sulfate relative to samples from GT, whereas samples from GT have more abundant clay minerals and sulfate minerals, as well as siderite in some cases (Figures 1 and 2; [6]). These minerals provide clues as to the past environments present in GT and VRR that may be important in the preservation or degradation of organic molecules, and the environments that produced them can be quantitatively constrained using reactive transport modeling.

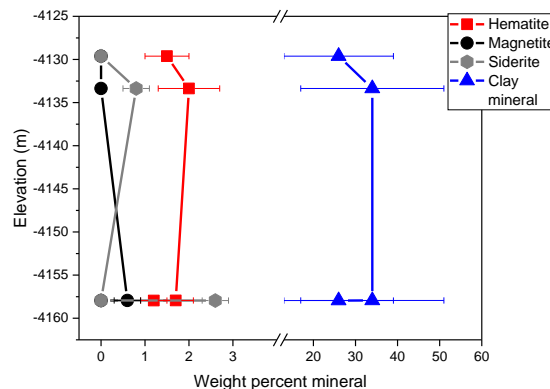


Figure 1. Mineral weight percent measured by CheMin of hematite, magnetite, siderite, and clay minerals in the samples from Glen Torridon (Aberlady, Kilmorie, Glen Etive 1 and Glen Etive 2), as reported in the PDS.

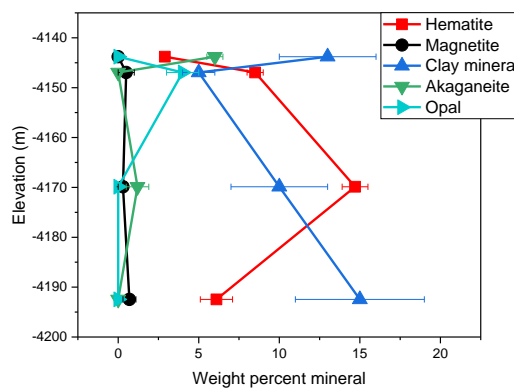


Figure 2. Mineral weight percent of hematite, magnetite, clay mineral, akaganeite, and opal measured by CheMin in samples from Vera Rubin ridge (Highfield, Rock Hall, Stoer, and Duluth), as reported in [6].

Modeling setup. Based on previous observations of significantly less diagenetic alteration of GT than VRR [6], modeling of GT was conceptualized as aqueous reaction occurring within lake sediments, including sedimentation and compaction and diffusive transport in a 1 d profile through the sediments after [7]. Input mineralogy into the reactive transport modeling was based on CheMin measurements, and included plagioclase, pyroxene, hematite, magnetite, and saponite as a pre-diagenesis mineral, with a porosity of 50%. Secondary minerals allowed to dissolve and precipitate within the model but not included as original input minerals included nontronite, a poorly crystalline

amorphous Fe silicate, ferrihydrite, jarosite, amorphous silica, gypsum, and siderite. Modeling at GT was performed at 1 °C to allow for low temperature conditions potentially present in sediments. Based on previous work [8], formation of the calcium sulfates was considered to take place during late diagenesis of the sediments, as has also previously been modeled [9].

Reactive transport modeling was also used to model diagenesis at VRR [6]. Based on the presence of jarosite and akaganeite [6], solutions were interpreted to be acidic, oxic, and Fe-containing. Input minerals were based on the CheMin measurements of VRR samples Highfield, Rock Hall, Stoer, and Duluth as reported in [6]. Secondary minerals allowed to dissolve and precipitate but not included as initial inputs in the model included nontronite, a poorly crystalline amorphous Fe silicate, ferrihydrite, jarosite, amorphous silica, saponite, and hematite. Modeling in VRR was performed at 50 °C based on previous evidence of high temperature fluids in this region of Gale crater [6]. Modeling of both GT and VRR was performed using CrunchFlow [10], which has been previously used to model a variety of terrestrial and martian environments including terrestrial and martian basalts [11], martian carbonates [11] and phosphates [12], the Stimson unit [9], and the Murray formation [13].

Results: Modeling results can help place quantitative constraints on the formation and diagenetic conditions of past environments in GT and VRR (Figures 3 and 4). For example, hematite and nontronite precipitation in the modeling of VRR occurred under acidic (pH = 3) and oxidizing conditions that may degrade organics, and ongoing modeling can help yield additional insights. These types of results can then be compared to measurements from SAM, to help constrain conditions that impact the preservation or degradation of organic molecules.

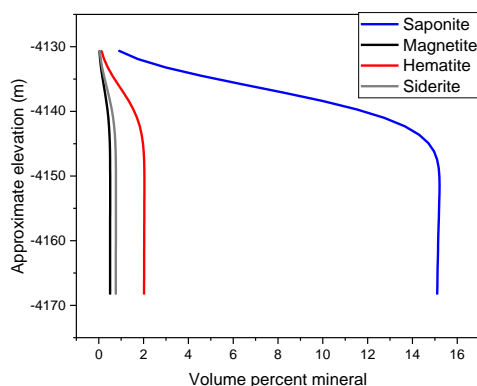


Figure 3. Volume percent saponite, magnetite, hematite, and siderite modeled in Glen Torridon.

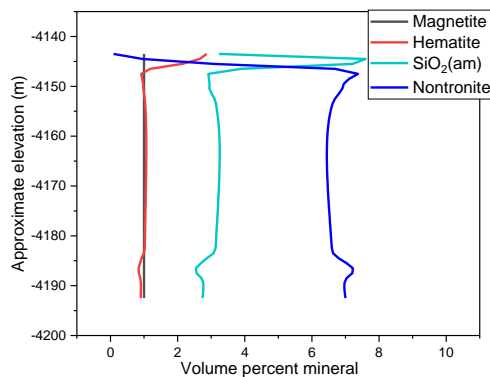


Figure 4. Volume percent magnetite, hematite, amorphous silica, and nontronite modeled in VRR.

The SAM analyses of the Kilmarie sample from Glen Torridon GC-MS detected no clear evidence of indigenous organic molecules, but EGA detections of CO₂ and CO may indicate oxalate or organic oxidation products [14]. EGA analyses of VRR samples indicate the formation of CO₂ and CO from all samples, consistent with oxidized compounds such as oxalate [15].

Conclusions and future work: This continued work will allow quantitative constraints to be placed on the characteristics of past alteration at Gale crater that are important to preservation or degradation of organic molecules. Importantly, these constraints will allow a better understanding of the types of environments in which organic molecules may be found on Mars, helping to detect environments conducive to biosignature preservation, with important implications for sample return from Mars.

References: [1]. Eigenbrode, J.L., et al. *Science*, 2018. **360**(6393): p. 1096-1101. [2]. Szopa, C., et al., *Astrobiology*, 2020. **20**(2): p. 292-306. [3]. Freissinet, C., et al. *Journal of Geophysical Research: Planets*, 2015: p. 2014JE004737. [4]. Ming, D., et al., *Science*, 2014. **343**(6169): p. 1245267. [5]. Leshin, L., et al., *Science*, 2013. **341**(6153): p. 1238937. [6]. Rampe, E.B., et al. *Journal of Geophysical Research: Planets*, 2020. **125**(9): p. e2019JE006306. [7]. Arora, B., et al. *Computational Geosciences*, 2015. **19**(3): p. 613-633. [8]. Yen, A., et al., *Multiple stages of aqueous alteration along fractures in mudstone and sandstone strata in Gale Crater, Mars*. *Earth and Planetary Science Letters*, 2017. **471**: p. 186-198. [9]. Hausrath, E.M., et al. *Earth and Planetary Science Letters*, 2018. **491**: p. 1-10. [10]. Steefel, C.I., *CrunchFlow - Multicomponent reactive flow and transport software*. 2010: Berkeley, CA. [11]. Hausrath, E.M., et al. *Geology*, 2008. **36**(1): p. 67-70. [12]. Adcock, C.T. and E.M. Hausrath, *Astrobiology*, 2015. **15**(12): p. 1060-1075. [13]. Hausrath, E.M., et al. *ACS Earth and Space Chemistry*, submitted. [14]. Millan, M., et al., *American Geophysical Union*. 2019: San Francisco. [15]. McAdam, A.C., et al. *Journal of Geophysical Research: Planets*, 2020. **125**(11): p. e2019JE006309.