

BEYOND GEOTECHNICS: THE CASE FOR THERMOCHEMICALLY-FOCUSED REGOLITH SIMULANTS K. P. Edison¹ and R. Garvey², ¹Outward Technologies, 155 Commerce St., Broomfield, CO, 80020, (kedison@outward.tech), ²Outward Technologies, 155 Commerce St., Broomfield, CO, 80020, (rgarvey@outward.tech).

Introduction: As ISRU shifts from rover mobility to high-energy processing, like molten regolith electrolysis and additive construction, the limitations of legacy simulants have become a critical bottleneck. Historically, materials were engineered for geotechnical fidelity (particle size and shear strength) to test excavation tools [3]. However, these mechanical analogs fail to replicate the complex thermochemical profiles essential for modern research, particularly with respect to elemental chemistry, volatile release, and the presence of entrapped gases in glassy rinds or water in hydrated minerals. To ensure terrestrial research scales to planetary environments, the community must move toward purpose-driven simulants that prioritize these chemical and volatile signatures over simple mechanical behavior.

The Impact of Mineralogical Impurities:

The transformation of regolith from a granular aggregate into a molten silicate fluid is governed by a complex sequence of mineralogical and thermodynamic processes. Phase transitions, partial melting, volatile release, and viscosity evolution all play critical roles in determining how regolith behaves under high-temperature conditions.

Hydrated Minerals and Fluxing Agents: One of the most significant deviations arises from the presence of hydrated minerals and alkali-rich phases. Unlike terrestrial soil, the lunar surface is essentially anhydrous. Lunar regolith formed in an extremely dry environment dominated by impact processes, solar wind implantation, and micrometeorite bombardment. Terrestrial parent rocks used to produce simulants, however, often contain hydrated minerals such as clays, zeolites, or weathering products that formed through prolonged interaction with water. During high-temperature processing, these hydrated phases release bound water and other volatiles. Even small amounts of water can act as fluxing agents in silicate systems, reducing melting temperatures and dramatically lowering viscosity [4]. Alkali elements such as sodium and potassium may further enhance this fluxing behavior. As a result, simulant melts may appear to liquefy at temperatures significantly lower than those expected for true lunar regolith compositions.

This phenomenon introduces a substantial risk in ISRU technological development. If melting behavior is artificially enhanced by terrestrial contaminants,

experimental results may suggest that less energy is required to process regolith than will be the case on the Moon or Mars. Hardware designed under these assumptions may therefore be under-engineered, potentially leading to insufficient heating capacity or inadequate containment materials when deployed in extra-terrestrial environments [1].

Outward Tech. Initiatives: To address these challenges, Outward Technologies is developing new processes for generating simulants specifically designed for thermochemical research and high-temperature processing applications. Rather than relying on a single “universal” simulant, this approach focuses on tailoring materials to specific experimental objectives. To achieve this, the development process prioritizes three key factors for creating accurate simulants for high-temperature resources: parent rock selection, agglutination, and volatile control.

Parent rock selection plays a central role in this strategy, with emphasis placed on compositions that more closely replicate the chemistry, mineralogy, and volatile content of extraterrestrial regolith. Specifically, selecting terrestrial feedstocks with reduced water content is critical to preventing artificially depressed melting points and excessive production of water vapor during high-temperature processes. The second factor involves the agglutination of the parent rock to increase the overall glass content. Agglutinates represent a major component of mature lunar soils and strongly influence melt behavior due to their glassy composition and embedded nanophase iron. Replicating the thermal and rheological effects of these features in laboratory analogs is essential during high-temperature processing. The reduction or targeted reintroduction of volatiles and fluxing agents is utilized as the concluding step. This ensures the final simulant accurately reflects the anhydrous nature of the lunar surface or the specific hydration states expected in Martian resources, thereby mitigating the risk of artificially enhanced melting and product gas generation behaviors during testing.

This framework moves away from the concept of a single standardized simulant and instead encourages the selection of materials based on relevant thermochemical parameters, including melting temperature, viscosity, dielectric properties, and heat capacity. By aligning simulant choice with the specific goals of each experiment, this approach aims to improve the

reliability of laboratory results and ensure that terrestrial testing conditions more closely approximate extra-terrestrial processing environments.

Interdisciplinary Terminology Challenges

An additional challenge in ISRU research arises from differences in terminology and conceptual frameworks between geoscientists, materials scientists, and metallurgists. While each discipline studies high-temperature silicate systems, they often describe these materials using different conventions. In materials science literature, mineral names are frequently used as shorthand for crystallographic structure types (e.g., “spinel” or “perovskite” structures referring to specific lattice symmetries). In contrast, geoscientists interpret these same terms as mineral species whose compositions and formation conditions carry geological meaning. In the context of regolith processing, this distinction can lead to ambiguity when describing phases formed during melting and crystallization [2]. Recognizing and clarifying these disciplinary differences is important for ensuring that experimental observations and material descriptions are interpreted consistently across ISRU research communities.

Conclusion: As ISRU technologies progress from laboratory demonstrations toward flight-ready systems, the fidelity of regolith simulants becomes increasingly important. If simulants used in terrestrial testing exhibit thermochemical properties that diverge significantly from those of actual lunar or Martian materials, the resulting hardware may fail under real planetary conditions. Artificially depressed melting points, altered viscosity behavior, and volatile-driven fluxing effects can all distort experimental outcomes. These discrepancies may lead to incorrect estimates of energy requirements, inaccurate predictions of material properties, or flawed assumptions during high-temperature processing for oxygen extraction and generation of byproducts.

Adopting thermochemically focused simulant standards offers a pathway toward reducing these risks. By prioritizing mineralogical accuracy, high-temperature behavior, and product gas generation, researchers can generate more reliable data on melt dynamics, structural material formation, and resource extraction processes.

Moving beyond geotechnics is therefore not merely an academic refinement; it is a practical necessity for the future of planetary infrastructure. Ensuring that terrestrial simulants accurately reproduce the anhydrous, complex mineralogy of extraterrestrial regolith will ultimately help guarantee that the systems we develop on Earth can operate successfully on the Moon and Mars.

References:

1. Edison, K. P. (2025). Melt-casting lunar regolith simulants into durable materials: feasibility, process, and simulant requirements (Doctoral dissertation, Colorado School of Mines). Colorado School of Mines Repository.
2. Lima-de-Faria, J., Hellner, E., Liebau, F., Makovicky, E., & Parthé, E. (1990). Nomenclature of inorganic structure types. Report of the international union of crystallography commission on crystallographic nomenclature subcommittee on the nomenclature of inorganic structure types. *Foundations of Crystallography*, 46(1), 1-11.
3. Slabic, A., Gruener, J. E., Kovtun, R. N., Rickman, D. L., Sibille, L., Oravec, H. A., ... & Keppta, S. (2024). Lunar regolith simulant user's guide: revision A (No. NASA/TM-20240011783). NASA.
4. Sutherland, J., Hess, K. U., Bissbort, T., Stapperfend, S., Müller, A., Hansen, T. C., ... & Dingwell, D. B. (2025). Volatile loss during heating of lunar mare simulants and related compositions. *Chemical Geology*, 123115.23115.