EXPLORING THE CHALLENGES OF MOLTEN REGOLITH ELECTROLYSIS AND OXYGEN PRODUCTION ON THE LUNAR SURFACE.

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Introduction: In the coming decade, national space agencies and private companies plan to establish a Lunar presence. In-situ resource utilization (ISRU) technologies may power, construct, and sustain this next generation of Lunar (and eventual Martian) space exploration. Molten regolith electrolysis (MRE) is a candidate ISRU technology with the ability to produce economically useful amounts of oxygen and metallic alloys [1]. The MRE process produces oxygen by passing an electric potential difference through melted regolith. Molten salt electrolysis, an MRE analog on Earth, has already proven viable in its production of oxygen [2].

While fluid behavior has been studied considerably in microgravity and 1 g, the effects of partial gravity (such as 1/6th g on the Moon) on fluids are not yet well characterized or understood. In reduced gravity, both buoyancy and surface tension effects must be considered. Unexpected problems in fluid systems continue to occur under reduced gravity levels [3-7]. Several researchers have modeled and experimentally characterized fluids in partial gravity. Through a series of parabolic flights, Lomax, et. al., for example, found that oxygen-generating water electrolysis in Lunar gravity is 11% less efficient than the same system in Earth's gravity. Due to the lack of experimental platforms in partial gravity, and limited modeling results, many open questions remain pertaining to fluid behavior in reduced gravity.

Two questions specifically motivated this research: What challenges will MRE systems face when operating on the Lunar surface? Will any of these challenges cause MRE to stall and fail? To investigate the problems an MRE system may experience on the Moon, computational fluid dynamic (CFD) models were developed to model MRE and water electrolysis in Lunar gravity and 1 g.

Scope of Work: The CFD models study the formation, growth, and detachment of oxygen bubbles formed via water electrolysis and MRE at Lunar gravity and 1 g. Exhaustive experimental and computational studies of bubble formation remains difficult to achieve due to the small time and length scales over which bubbles form, as well as bubbles' high sensitivity to various interdependent factors [6-7]. Taking this into consideration, the research models a simplified electrolysis experiment, which includes a single bubble nucleation site on the electrode. Although not operationally realistic, single bubble modeling is a common approach and allows for the detailed study of bubble behavior across all stages of a bubble's life [7-8]. Multiple nucleation sites are a potential area of future research, but due to limitations on time and computational resources, a single nucleation site was chosen.

The variables tested in this modeling effort were: choice of fluid, gravity level, electrode orientation (Fig. 1), and electrode surface roughness. Water electrolysis and MRE models were run in 1 g and Lunar gravity. In both water electrolysis and MRE, models were run with two different electrode orientations (parallel and perpendicular to the gravity vector) and three different electrode surface roughness values (smooth, medium, and rough). The electrode orientation simulates a design choice in the MRE system, and the surface roughness simulates material selection and electrode degradation.

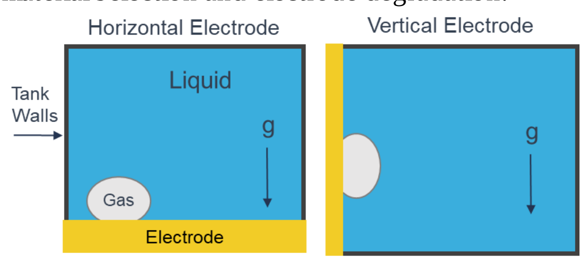

Figure 1. Two electrode orientations were tested: horizontal (left) and vertical (right).

CFD Methodology: The CFD models were developed using OpenFOAM's interFoam solver, a two-phase, isothermal, incompressible, transient, immiscible, volume of fluid (VOF) solver. The model includes a structured mesh, which was developed in Gmsh. The geometry includes a fluid chamber, with an electrode (containing the single 2 mm radius bubble nucleation site) on one of the chamber walls and an outlet on the top of the chamber. The chamber is 15 cm by 10 cm by 10 cm. All model runs were run in parallel across six cores.

Standard boundary conditions were used in the model. All parts of the model include an isothermal boundary condition. All chamber walls and the electrode use boundary conditions of fixed flux pressure and no slip. The outlet was modeled as open to atmosphere. The bubble nucleation site was modeled as an inlet with a constant, uniform velocity profile into the liquid. The electrode's surface roughness was varied by changing the contact angle boundary condition on the electrode's surface. The higher the contact angle, the rougher the surface (Fig. 2).

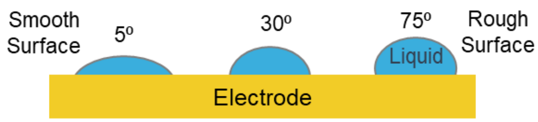

Figure 2. Three surface roughness values were tested using contact angle boundary conditions.

Simplifying assumptions were made. In contrast to a multiphysics simulation, this CFD model does not model the formation and precipitation of metals from the regolith, nor the spontaneous nucleation of gas across multiple nucleation sites. The model was designed to study the formation, growth, spreading, and detachment of a gas bubble from a single nucleation site on the electrode. The model also assumes a homogeneous regolith melt.

Results: CFD results have been obtained for both MRE and water electrolysis in Lunar gravity and 1 g, across three electrode surface roughness values. Detailed tabulated results will be presented at the conference. Due to space constraints, important insights from the results are summarized in the following sections. For a visual representation, sample CFD results are shown in Figure 3.

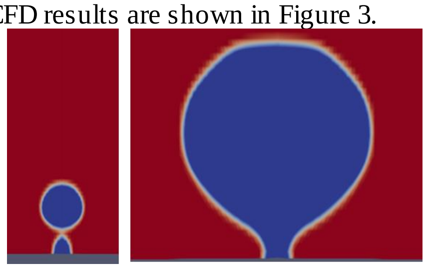

Figure 3. Bubble formed via water electrolysis (left) and MRE (right) in 1g. Nucleation site radius - 2 mm.

Discussion of Results: Reduced gravity levels affected both water electrolysis and MRE by increasing the time to bubble detachment and bubble volume. This is a significant insight into MRE at Lunar gravity. If bubbles remain attached to the electrode and continue to grow, the MRE process could stall, or reduce the rate of oxygen production.

Dependence on gravity level. The results show that MRE is less dependent upon gravity level than water electrolysis. Bubble volumes in water electrolysis increase by approximately four times when scaling from 1 g to Lunar gravity, whereas, bubble volumes in MRE increase in size by less than three times when scaling from 1 g to Lunar gravity.

Effects of electrode orientation. It was found that electrode orientation affects bubble behavior. Compared to horizontal electrodes, vertical electrodes result in larger bubbles and longer time to detachment. In the vertical orientation when a bubble spreads along the electrode (due to buoyancy), the contact surface area and surface tension force on the bubble increase, thus opposing detachment [6]. It is important to note that when multiple nucleation sites are incorporated into future models, vertical electrodes may allow bubbles to spread and encourage detachment of neighboring bubbles.

Surface properties of the electrode. MRE is significantly dependent upon electrode surface properties, specifically surface roughness. For rough electrodes, bubbles in MRE spread along the surface and take 100's of seconds to detach. This is especially concerning when considering that electrode degradation may produce rough surfaces.

Conclusions: The results provide important insight into the efficiency and feasibility of MRE on the Lunar surface. Due to the high surface tension and viscosity of molten regolith, and considering the discussion above, bubbles produced by MRE grow very large and detach at low rates, especially in Lunar gravity. A lack of bubble detachment could cause stalling of MRE, a decrease in electrolytic efficiency, and low oxygen production rates. Fortunately, there appears to be mitigation techniques. These could include: electrode orientation, electrode surface modifications/coatings, vibration, and cross flow over nucleation sites. Future designers of large-scale MRE systems expected to operate on the Lunar surface must consider gravity level, electrode orientation, electrode surface finish and degradation, and regolith composition.

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