CFD Modeling of Molten Regolith Electrolysis and Water Electrolysis, Scaled Across Gravity Levels

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LSIC Member
Outline

• The use and benefits of Molten Regolith Electrolysis (MRE)
• Problems with bubbles
• Water Electrolysis as a baseline
• Modeling methodology
• CFD Results
• Scaling across gravity
• Future Work
Molten Regolith Electrolysis (MRE)

• In the scope of ISRU, MRE could have multiple applications
  1. In-situ production of oxygen
  2. In-situ production of metal alloys

• MRE analogs on Earth (such as molten salt electrolysis) have proven to be viable in its production of oxygen (Lomax, 2019)
Why Bubbles Matter in Space Applications

• In reduced gravity, bubbles can show up unexpectedly
  - Practical:
    ▪ Reduced flow in heat pipes due to entrapped bubbles (STS-43) and failure due to *noncondensible* gas evolution
    ▪ Microfluidic experiments encounter entrapped bubbles
  - Life-threatening:
    ▪ Heat exchangers/cooling systems for Lunar nuclear power plants
    ▪ Interruption of life support systems and waste collection systems
    ▪ Air bubbles found in IV bags
    ▪ Anecdotal stories from astronauts confirm these to be frequent occurrences
Problems with Bubbles: Challenging the Straight Line Theory

• Only recently has parabolic flights enabled partial gravity fluids research

• Not all forces which act on a bubble during growth scale linearly with gravity
  - Ex: Surface energy between the bubble and the electrode

Plot of heat flux versus gravity levels with a discontinuous increase across boiling regimes (Kim, 2014)
Water Electrolysis

• Lomax et. al. conducted 1 g ground tests and parabolic flight tests of water electrolysis
• Water electrolysis is a familiar, well-understood baseline (which passes safety reviews for parabolic flights)
• Centrifugal electrolysis cell run from microgravity to 8 g
Experimental Findings of Water Electrolysis Runs
(Lomax, et al, 2021)

- Stalling of electrolysis due to decreased bubble detachment
- Bubble detachment scales nonlinearly with gravity
- 11% reduction in efficiency at Lunar gravity

\[ V_{\text{detach}} \propto g^{-1.5} \]

\[ d_{c \text{ max}} \propto \frac{1}{\sqrt{g}} \]
CFD Modeling of Electrolysis

• OpenFOAM’s InterFoam solver:
  - Volume of Fluid method of interface tracking
  - Immiscible Multiphase
  - Transient
  - Isothermal
  - Incompressible
• Use axisymmetric geometry
• Structured Mesh
• Run on 8-cores
• 2 mm radius nucleation site (from which the bubble would nucleate and grow
• 10 cm by 15 cm tank of liquid
• Tested both horizontal and vertical electrode (perpendicular and parallel to gravity vector)
Variables Tested

- Types of Electrolysis:
  - Water
  - Molten Lunar Regolith

- Gravitational Acceleration:
  - 1 g
  - Lunar Gravity (1/6th g)

- Orientation of Electrode:
  - Horizontal
  - Vertical
Physical Properties being Modeled

- The physical properties of water and Molten Lunar Regolith were used
- Major variations were in density, viscosity, surface tension, and temperature

<table>
<thead>
<tr>
<th>Physical Property</th>
<th>Water Value</th>
<th>Regolith Value (referenced from Humbert)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acceleration due to gravity on Earth</td>
<td>9.81 m/s²</td>
<td>9.81 m/s²</td>
</tr>
<tr>
<td>Acceleration due to gravity on the Moon</td>
<td>1.625 m/s²</td>
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</tr>
<tr>
<td>Temperature as measured in lab</td>
<td>25°C</td>
<td>1800°C</td>
</tr>
<tr>
<td>Surface Tension between liquid and gas</td>
<td>0.0720 N/m</td>
<td>475 N/m</td>
</tr>
<tr>
<td>Gas Density</td>
<td>1.184 kg/m³</td>
<td>1.184 kg/m³</td>
</tr>
<tr>
<td>Liquid density</td>
<td>997 kg/m³</td>
<td>2600 kg/m³</td>
</tr>
<tr>
<td>Kinematic viscosity of Gas</td>
<td>15.62 * 10⁻⁶ m²/s</td>
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<tr>
<td>Kinematic viscosity of Liquid</td>
<td>0.893 * 10⁻⁶ m²/s</td>
<td>1.923 * 10⁻⁴ m²/s</td>
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</table>
CFD Results – Water Electrolysis

• When scaling from 1 g to Lunar gravity, the time to bubble detachment increases by over 3.8 times (for horizontal) and by 4.2 (for vertical)

• An increase in bubble size is seen when the electrode is vertical, due to increased bubble spread

• When electrode is vertical, bubble tends to stay attached to the electrode for part of its rise – could possibly be used to induce other bubble detachment

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CFD Results – MRE

• When scaling from 1 g to Lunar gravity, the time to bubble detachment increases by nearly 3 times

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<td>1 g</td>
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<td>7.075</td>
</tr>
<tr>
<td>1/6 g</td>
<td>Horizontal</td>
<td>20.75</td>
</tr>
<tr>
<td>1 g</td>
<td>Vertical</td>
<td>Limited due to CFD computation time</td>
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Comparing MRE to Water Electrolysis

- We see nearly 45x increase in bubble time to detachment in MRE, compared to water electrolysis

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Water Electrolysis CFD Results

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MRE Electrolysis CFD Results
Problems Encountered When Modeling MRE

- When modeling a vertical electrode for MRE, bubble detachment has not yet been observed
  - In the first case run, the bubble grew so large about the nucleation site that it attached itself to an adjacent tank wall
  - In second case run, bubble continued to grow, but never detached in computation time allotted

- Computation time increases when fluid and material properties are changed: density, viscosity, etc.
  - MRE CFD Computation time ranges from 12 hours (1 g) to 72 hours (Lunar g)
Accessing Feasibility of MRE

• Due to dramatic increases in surface tension and viscosity, bubbles produced by MRE are much less likely to detach, especially in Lunar gravity

• Vertical electrode geometries encourage bubble spreading, which increases attachment force (delaying bubble detachment)

• A lack of bubble detachment could cause electrode stalling and a decrease in electrolytic efficiency

• There appears to be methods to induce bubble detachment in MRE (such as electrode orientation)
Future Work

• Investigate other ways to induce premature bubble detachment:
  - Model multiple nucleation sites
  - Test various angles of electrode
  - Induce cross flow over nucleation sites
  - Model various surface finishes
    ▪ Surface roughness
    ▪ Coatings

• Measure bubble rise velocity

• Test and model various gravity regimes to understand the full scaling effects
Acknowledgements

Modeling work was supported and paid for by the Lunar Surface Innovation Initiative (LSII)
Lunar Surface Innovation Consortium
Water Electrolysis CFD Results

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<td>36.427</td>
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