

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

Paul A. Burke, PhD
Johns Hopkins Applied Physics Lab
LSIC Member

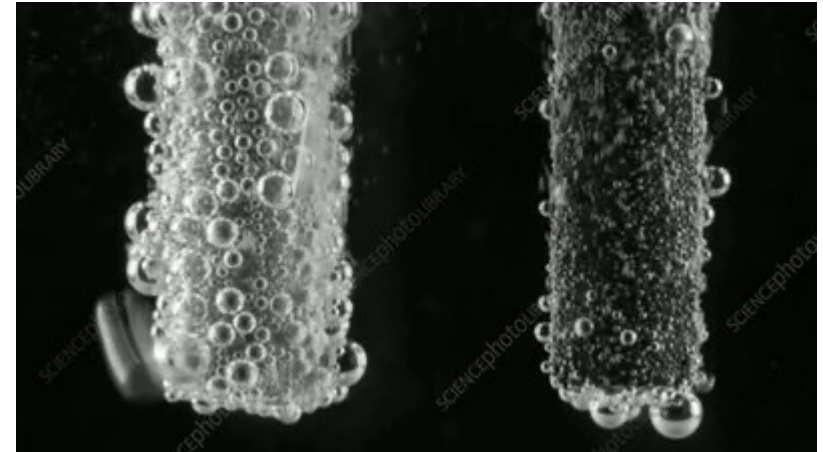
Outline

- 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



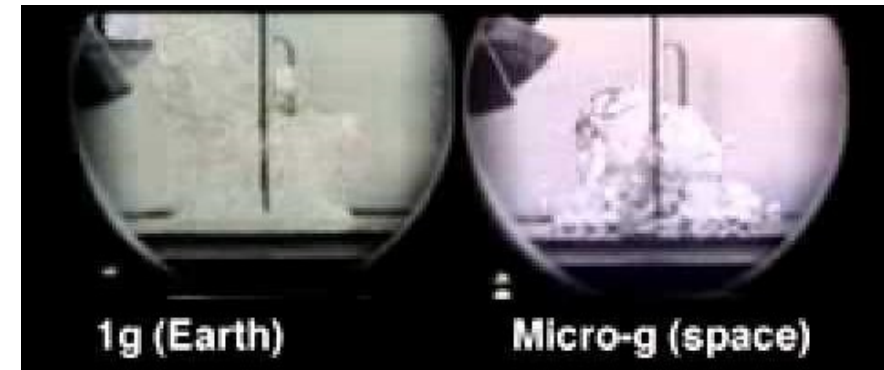
Molten Regolith Electrolysis (MRE)

- 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 *noncondensable* 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



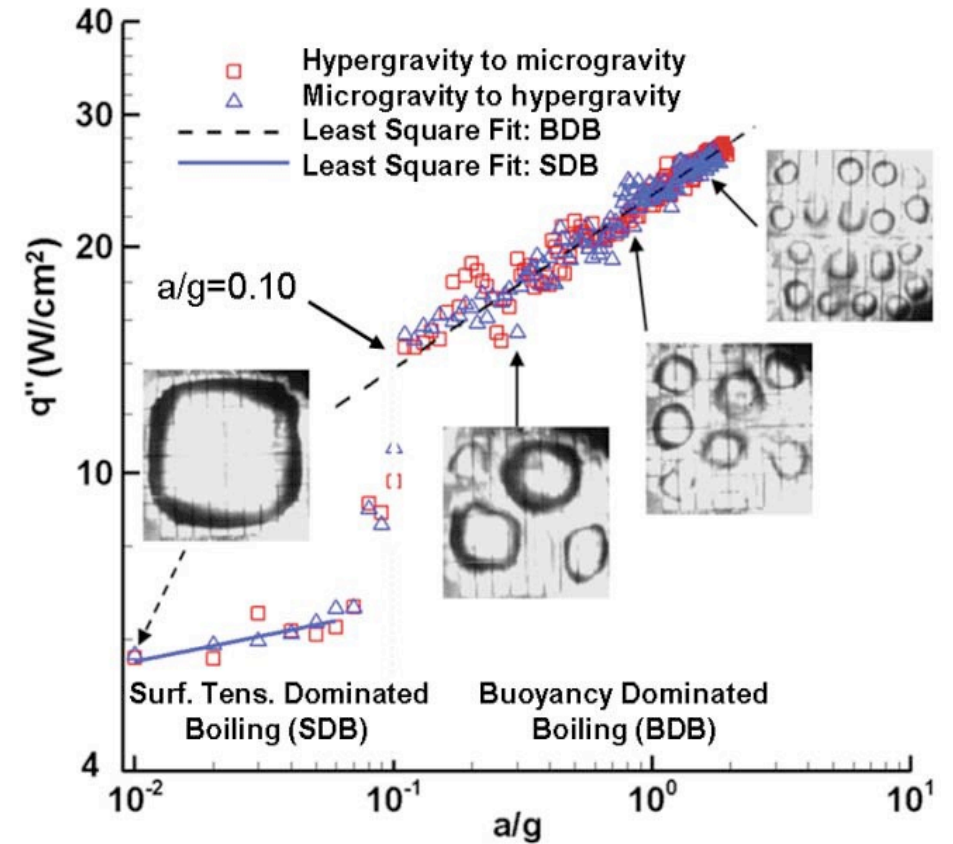
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Problems with Bubbles: Challenging the Straight Line Theory

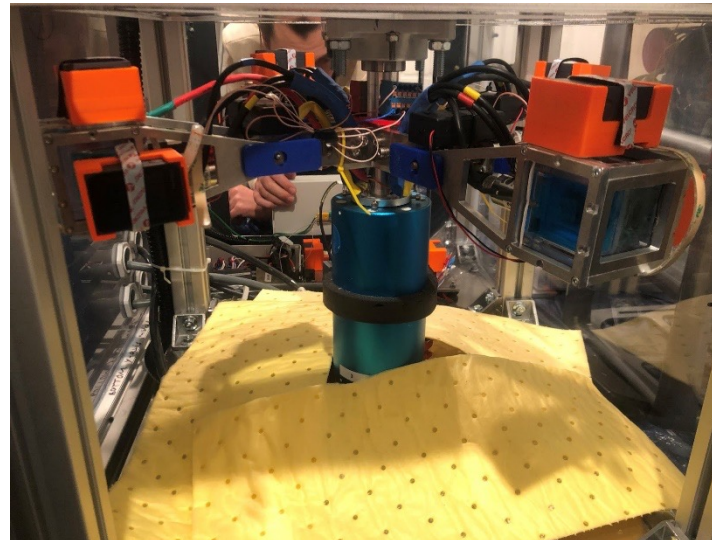
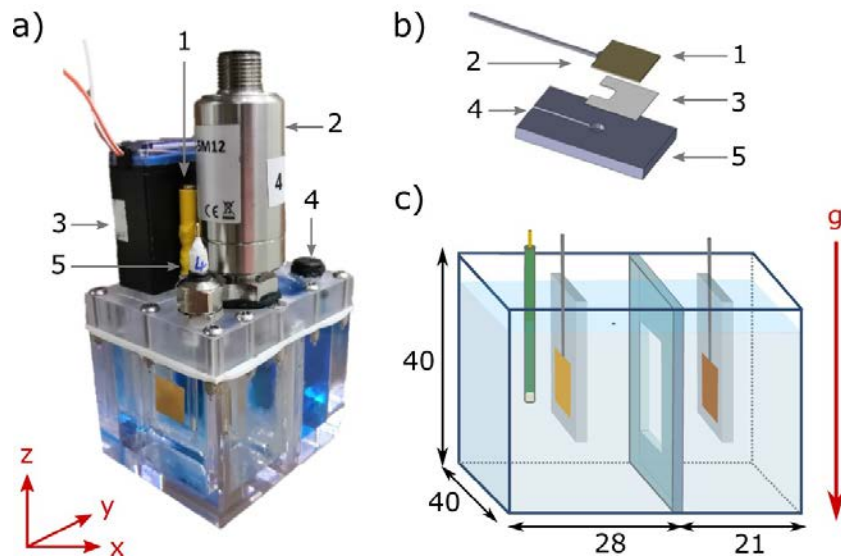
- Only recently has parabolic flights enabled partial gravity fluids research
- Not all forces which act on a bubble during growth scale linearly with gravity
 - Ex: Surface energy between the bubble and the electrode



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



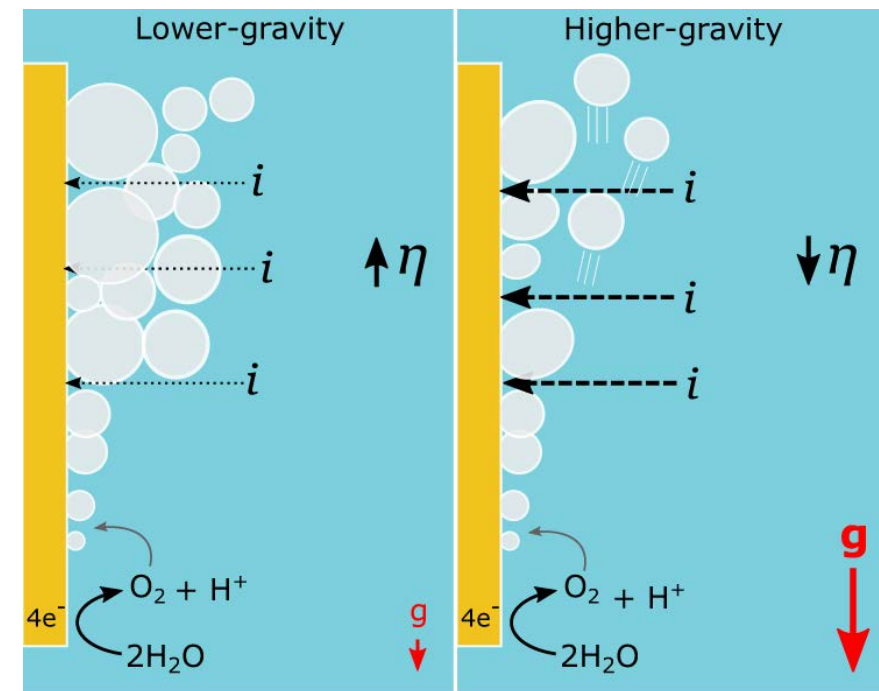
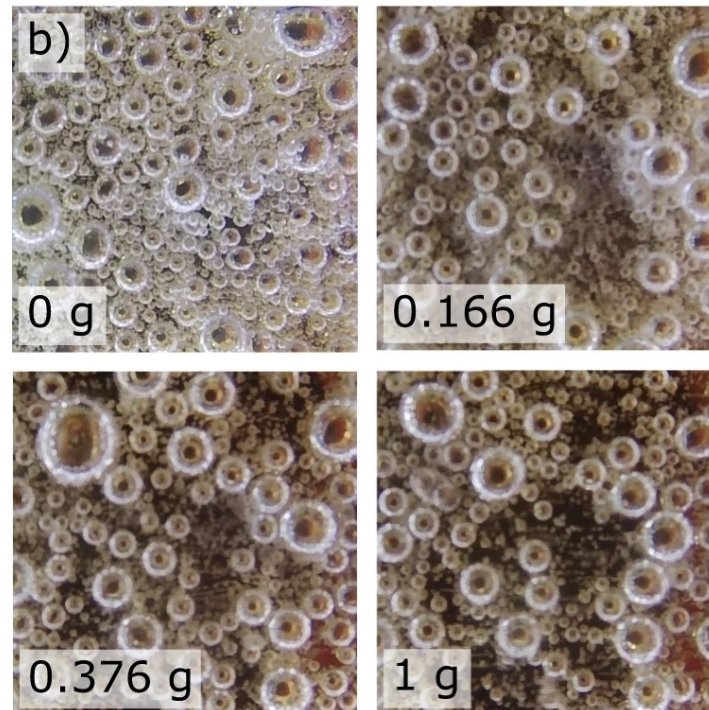
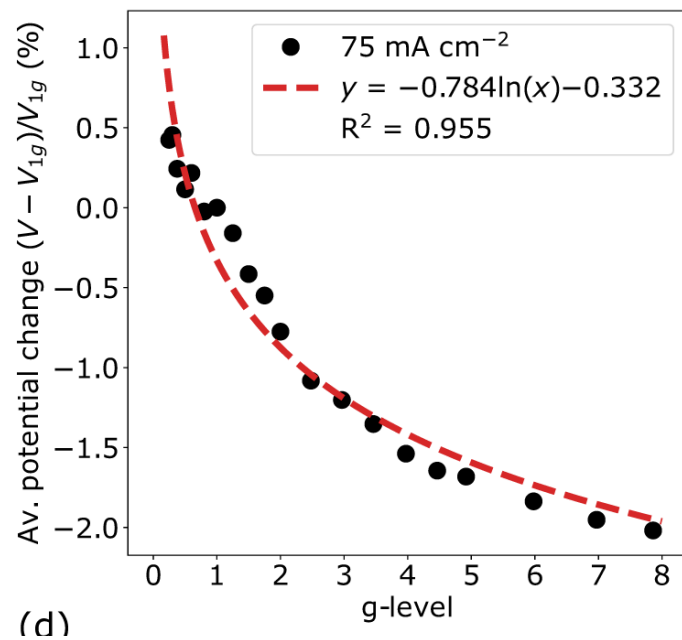
Experimental Findings of Water Electrolysis Runs

(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

$$V_{detach} \propto g^{-1.5}$$

$$d_{c\ max} \propto 1/\sqrt{g}$$

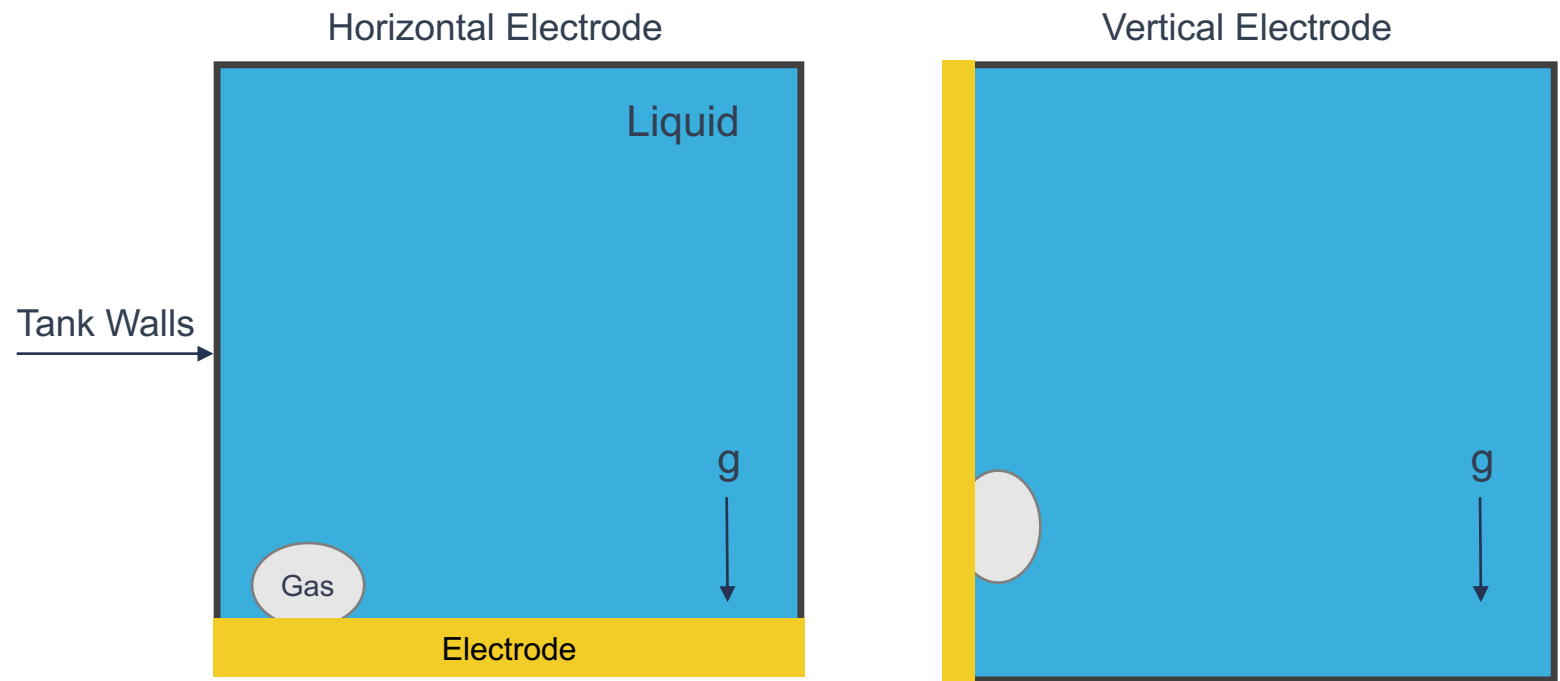


CFD Modeling of Electrolysis

- 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

Physical Property	Water Value	Regolith Value (referenced from Humbert)
Acceleration due to gravity on Earth	9.81 m/s ²	9.81 m/s ²
Acceleration due to gravity on the Moon	1.625 m/s ²	1.625 m/s ²
Temperature as measured in lab	25° C	1800° C
Surface Tension between liquid and gas	0.0720 N/m	475 N/m
Gas Density	1.184 kg/m ³	1.184 kg/m ³
Liquid density	997 kg/m ³	2600 kg/m ³
Kinematic viscosity of Gas	15.62 * 10 ⁻⁶ m ² /s	15.62 * 10 ⁻⁶ m ² /s
Kinematic viscosity of Liquid	0.893 * 10 ⁻⁶ m ² /s	1.923 * 10 ⁻⁴ m ² /s

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

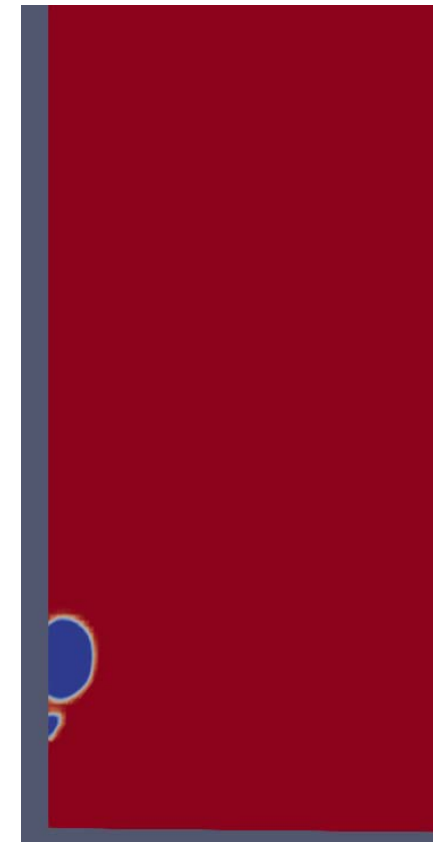
Gravity Level	Orientation of Electrode	Time to first bubble detachment (s)
1 g	Horizontal	0.125
1/6 g	Horizontal	0.475
1 g	Vertical	0.15
1/6 g	Vertical	0.625



Horizontal Electrode (Lunar g)



Vertical Electrode (Lunar g)



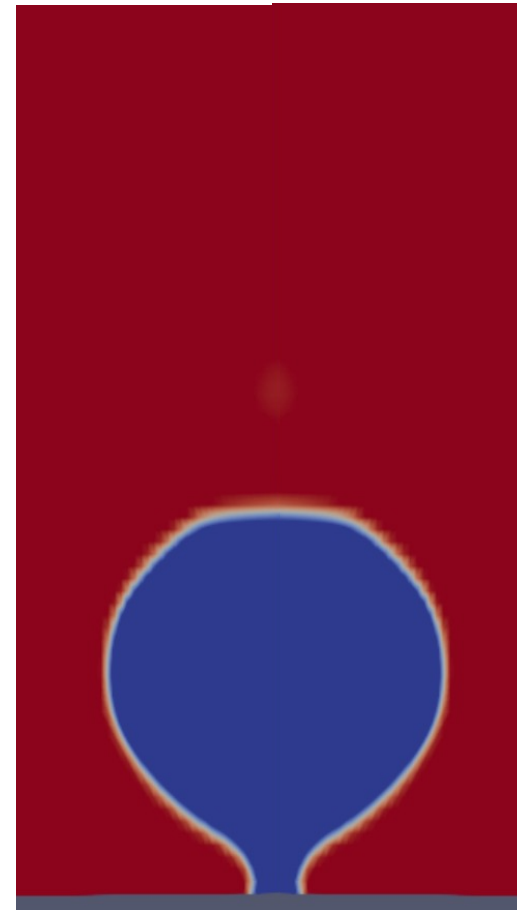
CFD Results – MRE

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

MRE Electrolysis CFD Results

Gravity Level	Orientation of Electrode	Time to first bubble detachment (s)
1 g	Horizontal	7.075
1/6 g	Horizontal	20.75
1 g	Vertical	Limited due to CFD computation time
1/6 g	Vertical	Limited due to CFD computation time

Horizontal Electrode (1 g)



Comparing MRE to Water Electrolysis

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

Water Electrolysis CFD Results

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1/6 g	Horizontal	0.475
1 g	Vertical	0.15
1/6 g	Vertical	0.625

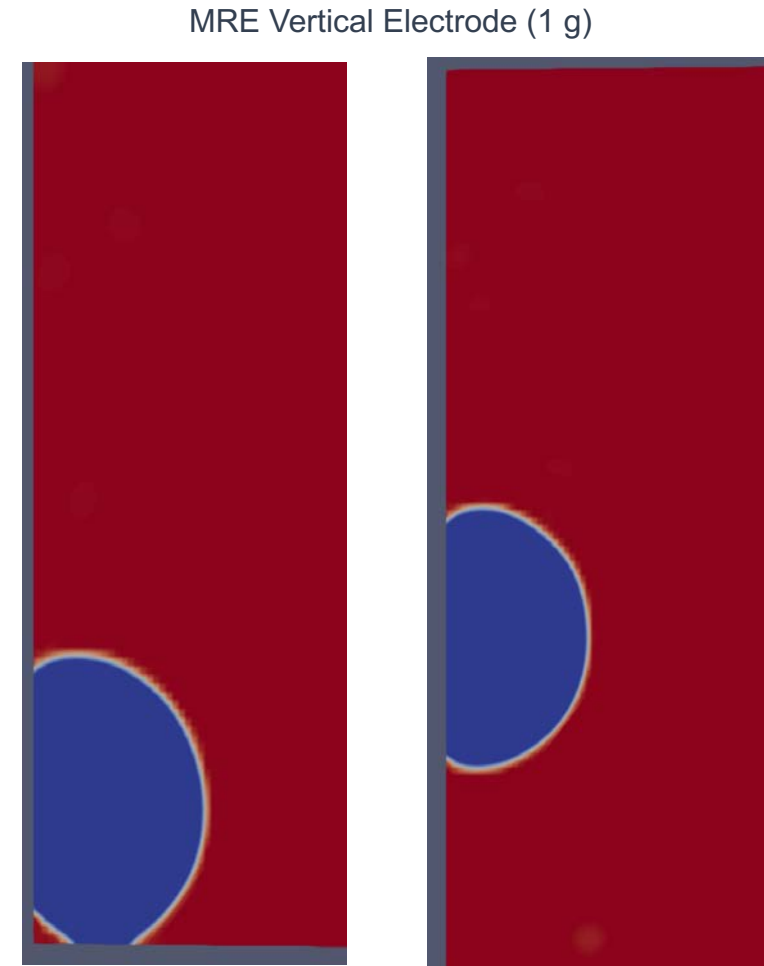
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Problems Encountered When Modeling MRE

- When modeling a vertical electrode for MRE, bubble detachment has not yet been observed
 - In the first case ran, the bubble grew so large about the nucleation site that it attached itself to an adjacent tank wall
 - In second case ran, 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

C O N S O R T I U M

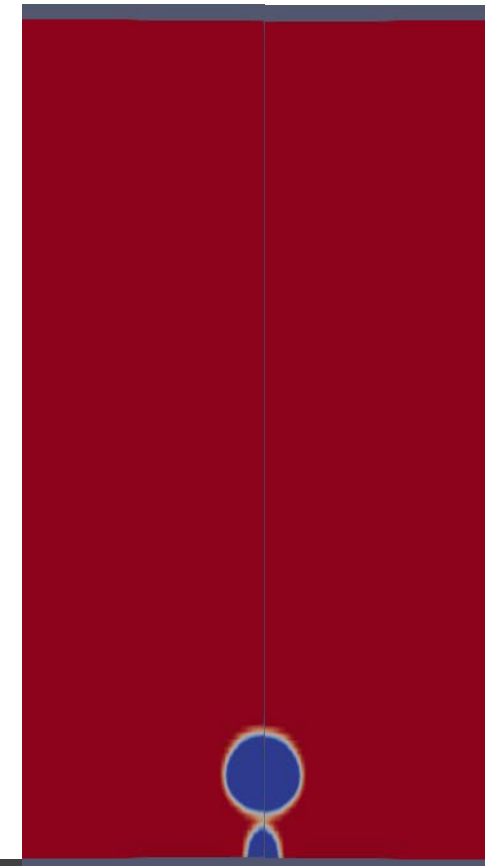


Water Electrolysis CFD Results

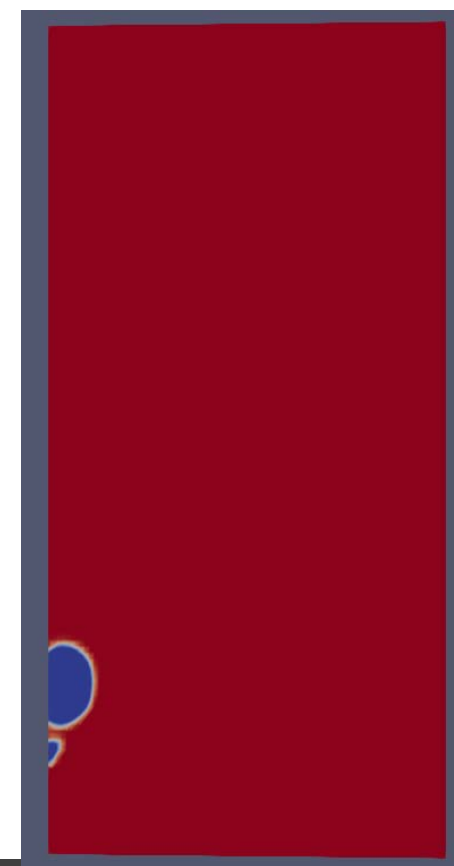
- When scaling from 1 g to Lunar gravity, the time to bubble detachment increases by over 3 times
- An increase in bubble size is seen when the electrode is vertical, due to increased bubble spread
- When electrode is vertical, bubble tends to stay attached to the electrode – could possibly be used to induce other bubble detachment

Gravity Level	Orientation of Electrode	Time to first bubble detachment (s)	Bubble volume at detachment (μL)
1 g	Horizontal	0.125	15.32
1/6 g	Horizontal	0.475	36.427
1 g	Vertical	0.15	XX
1/6 g	Vertical	0.625	XX

Horizontal Electrode (Lunar g)



Vertical Electrode (Lunar g)



MRE Electrolysis CFD Results

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

MRE Electrolysis CFD Results

Gravity Level	Orientation of Electrode	Time to first bubble detachment (s)	Bubble volume at detachment (μL)
1 g	Horizontal	7.075	204.23
1/6 g	Horizontal	20.75	284.636
1 g	Vertical	XX	XX
1/6 g	Vertical	Limited due to CFD computation time	Limited due to CFD computation time