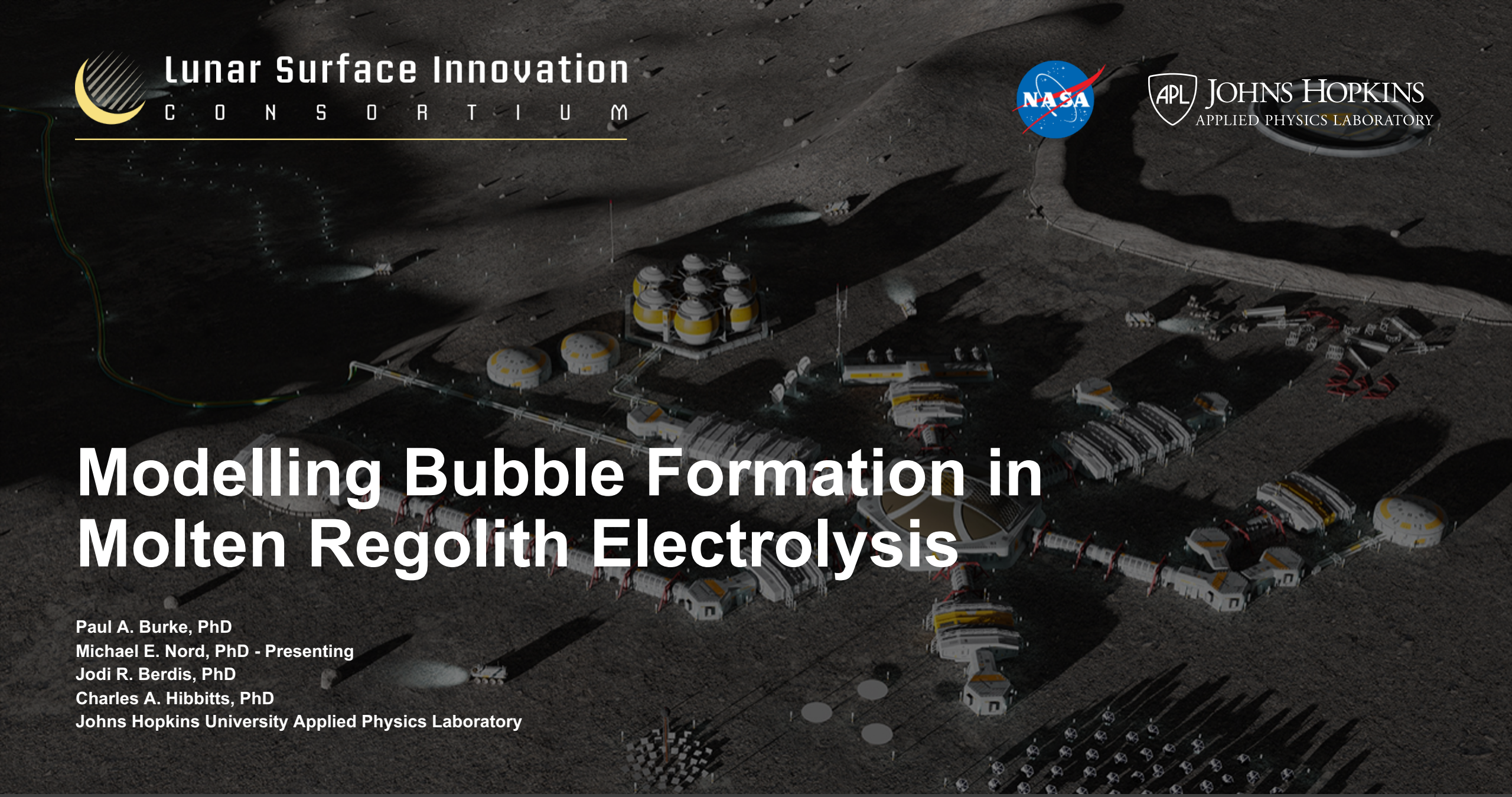

Lunar Surface Innovation CONSORTIUM

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Modelling Bubble Formation in Molten Regolith Electrolysis

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Credit

- Paul Burke did most of this work, but was unable to attend.
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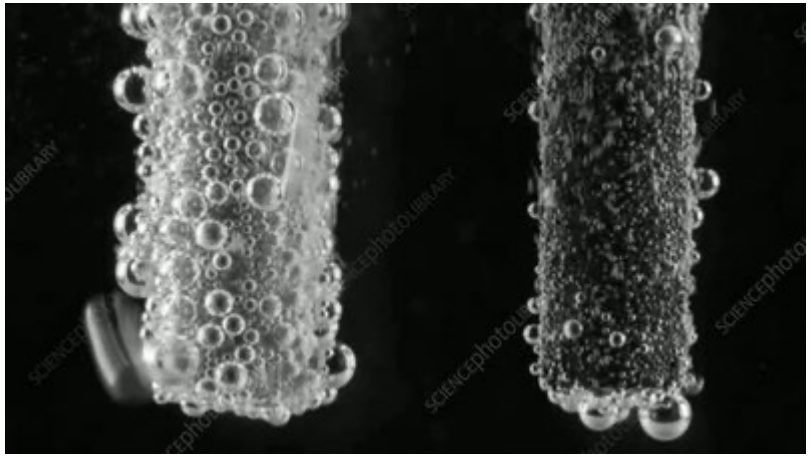
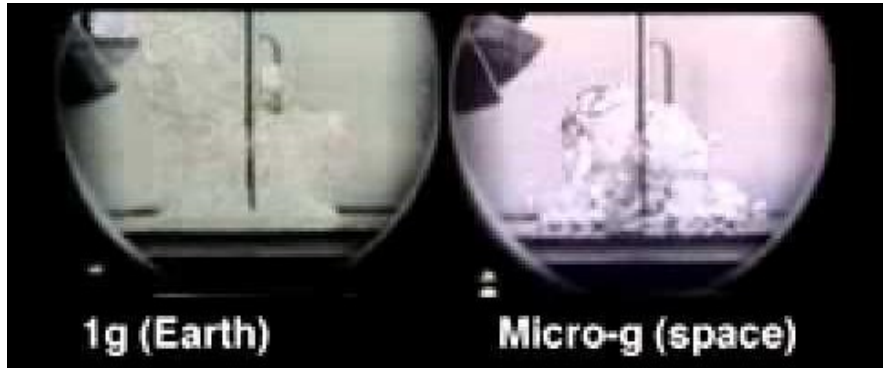
Molten Regolith Electrolysis (MRE)

- 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
  - Why does this matter?
    - Fluid phenomena have been discovered to scale nonlinearly (and sometimes discontinuously) with gravity
    - **In Lunar gravity, will O_2 bubbles detach from the electrode, or stall the electrolytic process?**



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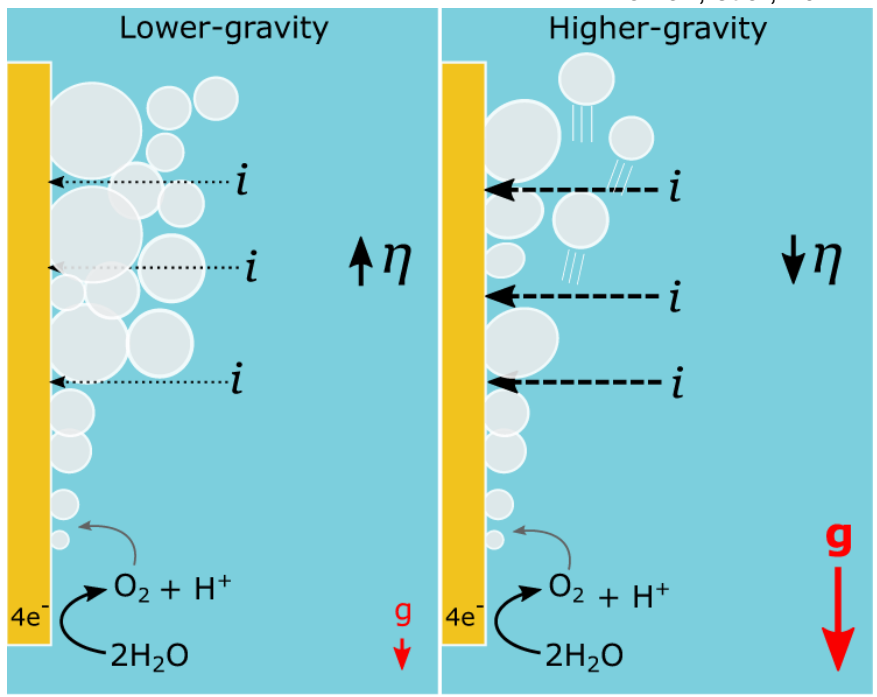
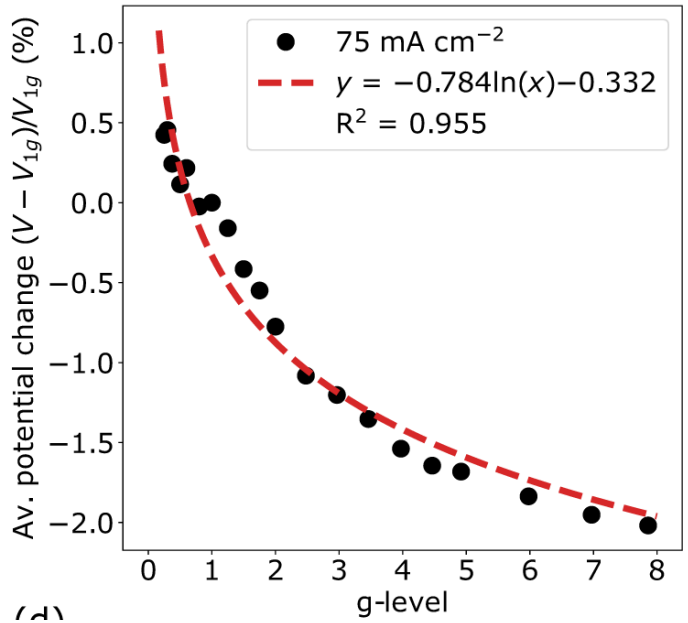
Lomax, et al, 2022

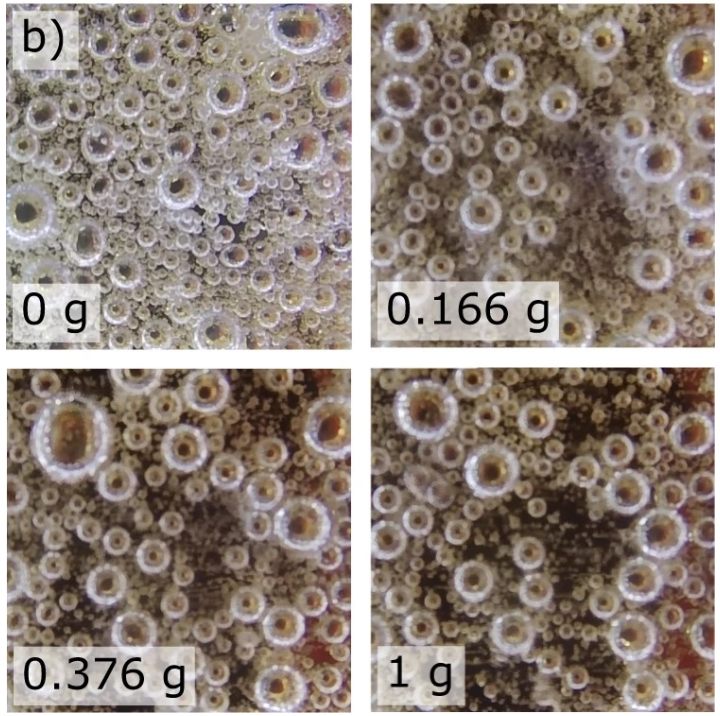


Experimental Findings of Water Electrolysis Runs

(Lomax, et al, 2022)

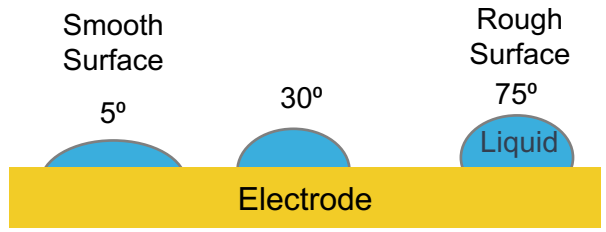
- Stalling of electrolysis due to decreased bubble detachment
- Bubble detachment scales nonlinearly with gravity
- 11% reduction in efficiency at Lunar gravity



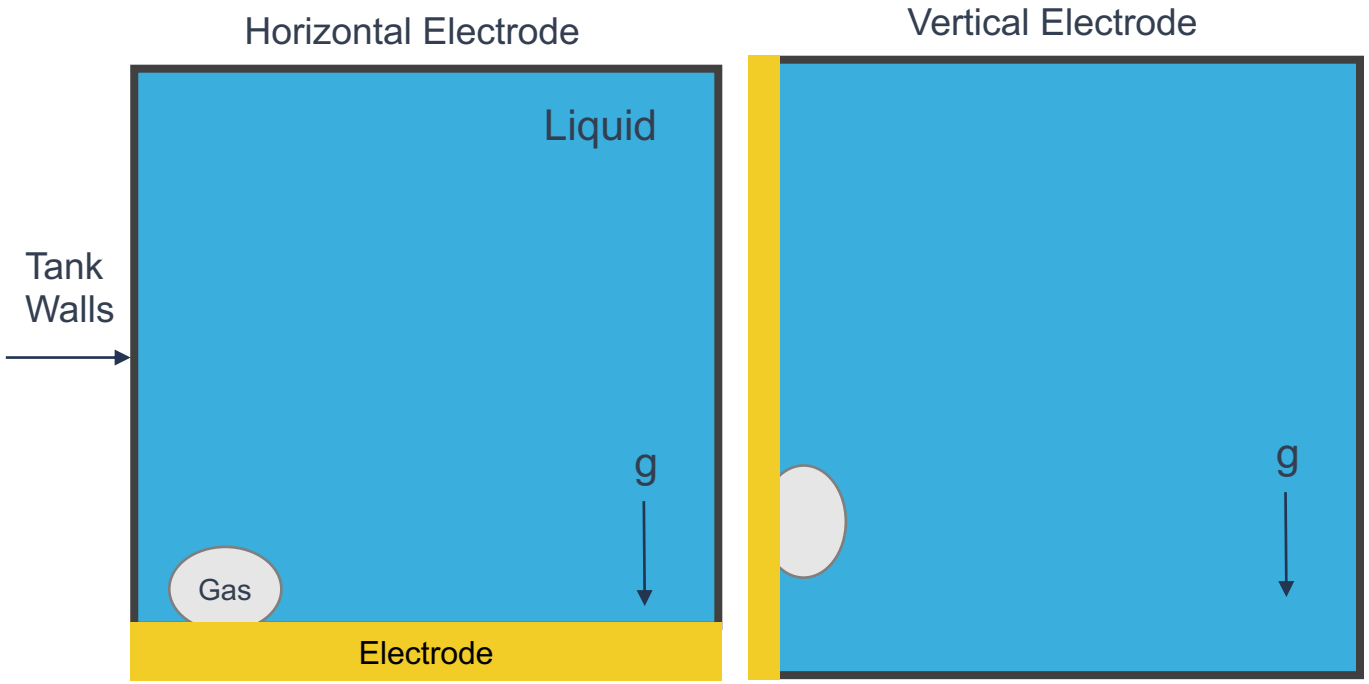


CFD Modeling Methodology

- OpenFOAM's InterFoam solver
- 2 mm radius single nucleation site (from which the bubble would nucleate and grow)
- 10 cm by 15 cm tank of liquid
- Constant, quiescent gas inject to simulate bubble growth



- Variables Tested:
  - Types of Electrolysis:
    - Water
    - Molten Lunar Regolith
  - Gravitational Acceleration:
    - 1 g
    - Lunar Gravity (1/6th g)
  - Orientation of Electrode:
    - Horizontal
    - Vertical
  - Surface finish of electrode:
    - Liquid Sessile Drop Contact Angle of:
      - 5º, 30º, and 75º



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 [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	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

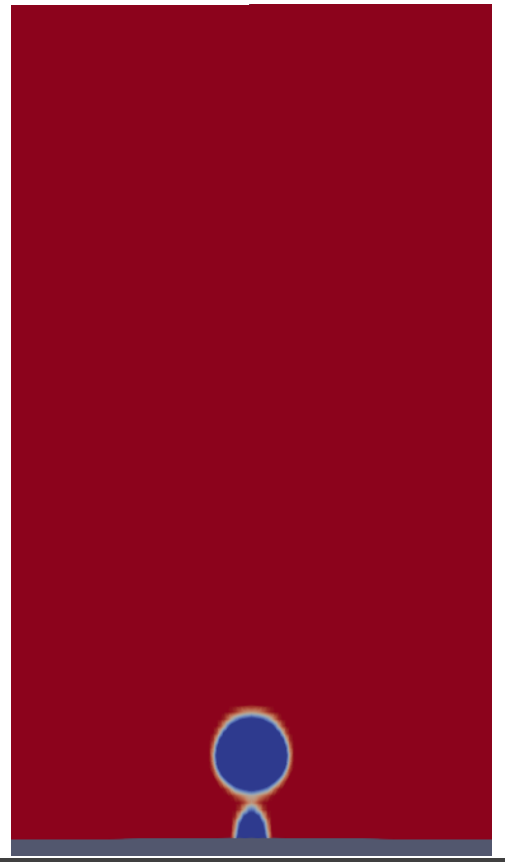
Major contributing differences

CFD Results – Water Electrolysis

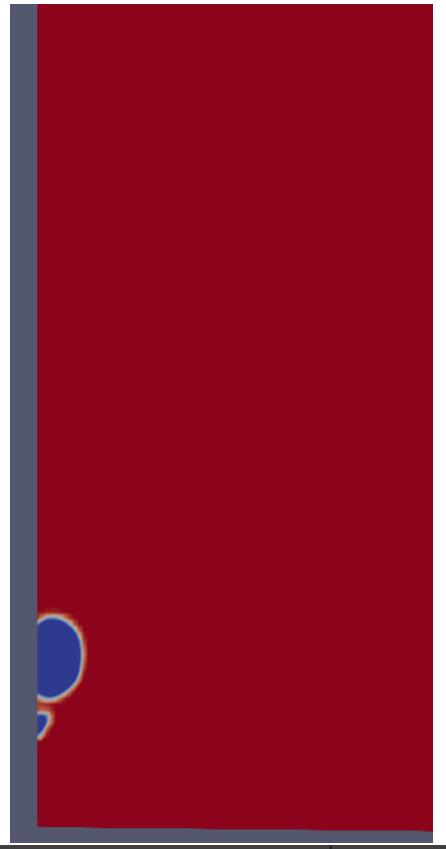
- When scaling from 1 g to Lunar gravity, the time to bubble detachment increases by ~4 times
- An increase in bubble size is seen when the electrode is vertical, due to increased bubble spread
- When electrode is vertical, bubble tends to stay attached to the electrode for part of its rise – could possibly be used to induce other bubble detachment

Gravity Level	Orientation of Electrode	Electrode Contact Angle (Deg)	Time to first bubble detachment (s)	Volume of bubble at detachment (mL)
1 g	Horizontal	30	0.125	0.0895
Martian	Horizontal	30	0.25	0.1791
Lunar	Horizontal	30	0.475	0.3402
1 g	Vertical	30	0.15	0.1074
Martian	Vertical	30	0.3	0.2149
Lunar	Vertical	30	0.625	0.4477

Horizontal Electrode (Lunar g)



Vertical Electrode (Lunar g)



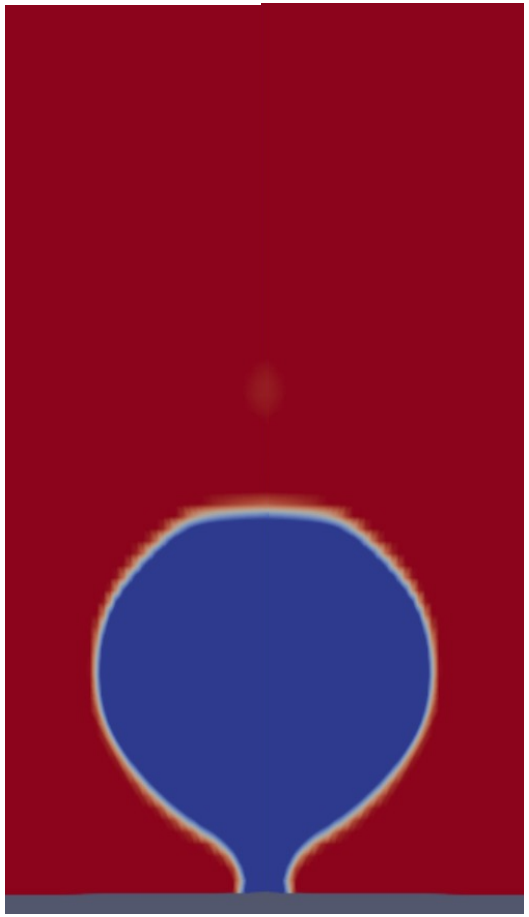
CFD Results – MRE

- 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	Electrode Contact Angle (Deg)	Time to first bubble detachment (s)	Volume of bubble at detachment (mL)
1 g	Horizontal	30	7.075	10.135
Martian	Horizontal	30	10.2	14.612
Lunar	Horizontal	30	20.75	29.725
1 g	Vertical	30	26.4	37.819
Martian	Vertical	30	23.7	33.952
1/6 g	Vertical	30	35.3	50.569

Horizontal Electrode (1 g)



Comparing MRE to Water Electrolysis

Water Electrolysis CFD Results

Gravity Level	Orientation of Electrode	Electrode Contact Angle (Deg)	Time to first bubble detachment (s)	Volume of bubble at detachment (mL)
1 g	Horizontal	30	0.125	0.0895
Martian	Horizontal	30	0.25	0.1791
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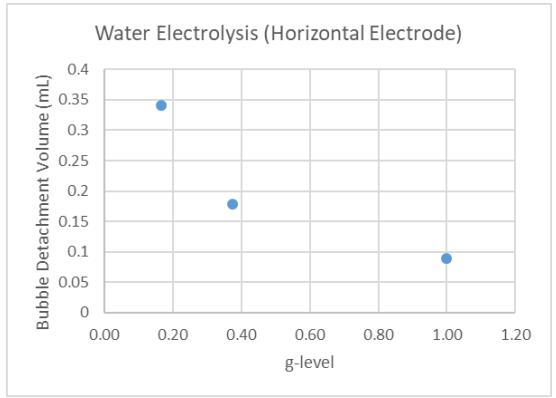
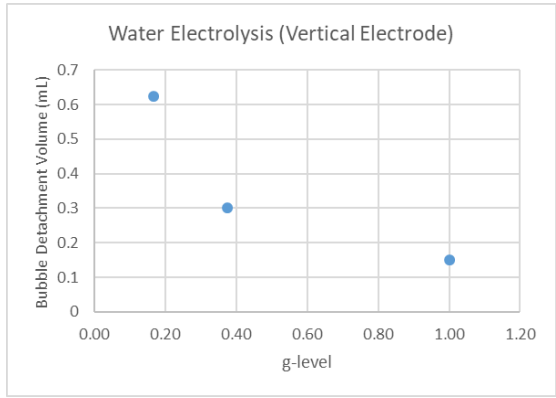
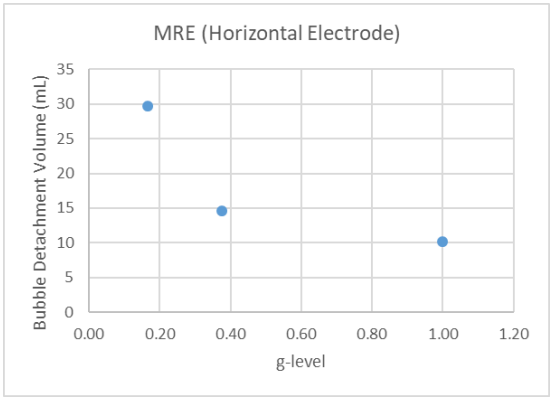
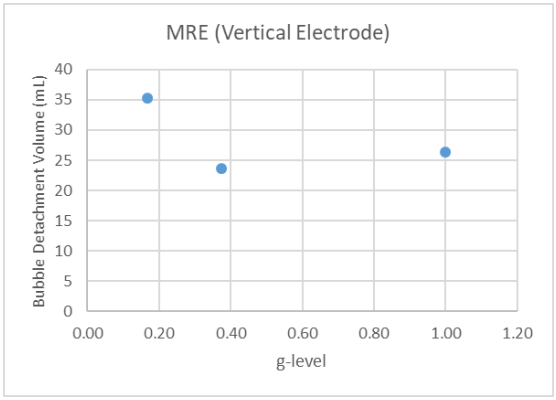




Water Electrolysis produces several bubbles per second in all gravity regimes.

MRE requires several seconds to produce a single bubble across all gravity levels.





MRE Electrolysis CFD Results

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1 g	Vertical	30	26.4	37.819
Martian	Vertical	30	23.7	33.952
1/6 g	Vertical	30	35.3	50.569

Comparing Surface Roughness (Water)

Gravity Level	Orientation of Electrode	Electrode Contact Angle (Deg)	Time to first bubble detachment (s)	Volume of bubble at detachment (mL)
1 g	Horizontal	5	0.125	0.0895
Martian	Horizontal	5	0.25	0.1791
Lunar	Horizontal	5	0.475	0.3402
1 g	Vertical	5	0.175	0.1254
Martian	Vertical	5	0.325	0.2328
1/6 g	Vertical	5	0.575	0.4119
1 g	Horizontal	30	0.125	0.0895
Martian	Horizontal	30	0.25	0.1791
Lunar	Horizontal	30	0.475	0.3402
1 g	Vertical	30	0.15	0.1074
Martian	Vertical	30	0.3	0.2149
1/6 g	Vertical	30	0.625	0.4477
1 g	Horizontal	75	0.125	0.0895
Martian	Horizontal	75	0.25	0.1791
Lunar	Horizontal	75	0.75	0.5372
1 g	Vertical	75	0.1	0.0716
Martian	Vertical	75	0.225	0.1612
1/6 g	Vertical	75	0.4	0.2865

Increased bubble detachment times and volumes with increased Roughness

Comparing Surface Roughness (MRE)

Gravity Level	Orientation of Electrode	Electrode Contact Angle (Deg)	Time to first bubble detachment (s)	Volume of bubble at detachment (mL)
1 g	Horizontal	5	7.525	10.7800
Martian	Horizontal	5	8.175	11.7112
Lunar	Horizontal	5	19.5	27.9350
1 g	Vertical	5	30.4	43.5500
Martian	Vertical	5	30	42.9770
1/6 g	Vertical	5	38.45	55.0822
1 g	Horizontal	30	7.075	10.135
Martian	Horizontal	30	10.2	14.612
Lunar	Horizontal	30	20.75	29.725
1 g	Vertical	30	26.4	37.819
Martian	Vertical	30	23.7	33.952
1/6 g	Vertical	30	35.3	50.569
1 g	Horizontal	75	32+ Seconds (computationally limited)	
Martian	Horizontal	75	32+ Seconds (computationally limited)	
Lunar	Horizontal	75	32+ Seconds (computationally limited)	
1 g	Vertical	75	41+ Seconds (computationally limited)	
Martian	Vertical	75	88+ Seconds (computationally limited)	
1/6 g	Vertical	75	88+ Seconds (computationally limited)	

Increased bubble detachment times and volumes with increased Roughness

Significant Insights from CFD Models

- Vertical electrodes results in larger bubbles and longer time to detachment. This is due to the bubble spreading along the electrode surface, increasing contact area, increasing surface tension (attraction) force which opposes detachment.
  - Note: this model uses a simplified, single bubble nucleation site geometry. When multiple bubbles form on an electrode, the vertical electrode may be advantageous since the bubble could spread along the surface and encourage detachment of neighboring bubbles.
- MRE appears less dependent on gravity level, compared to water electrolysis.
  - Bubble volumes in Water Electrolysis increase by ~4x when scaling from 1 g to Lunar g
  - Bubble volumes in MRE increase in size by less than 3x when scaling from 1 g to Lunar g
- MRE is significantly dependent upon surface properties of the electrode, specifically surface roughness
  - For rough electrodes, the bubbles in MRE never detach from the electrode (for the length of model run).
  - This behavior is due to bubbles spreading along the electrode's surface, thus increasing contact area

Potential Future Work

- Investigate other ways to induce premature bubble detachment:
  - Model multiple nucleation sites (in progress)
  - Test various angles of electrode
  - Induce cross flow over nucleation sites
  - Model various surface finishes
    - Coatings
- Measure bubble rise velocity
- Test and model various gravity regimes to understand the full scaling effects

- What bubble models would you like to see run?

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

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 6-cores
- 2 mm radius single 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)

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 and rough electrodes 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)