A Transient Multiphysics Thermal/CFD Simulation Analysis of a Molten Regolith Electrolysis Reactor Within a Thermal Vacuum Chamber

Laurent Sibille,
ASTRION,
Exploration Systems, Swamp Works,
NASA Kennedy Space Center, FL

William Dziedzic,
Engineering Analysis Branch
NASA Kennedy Space Center, FL

Evan A Bell,
Exploration Systems, Swamp Works
NASA Kennedy Space Center, FL

Presented By

William Dziedzic

Presentation Outline

- Introduction
- Objectives and System Models
- ASSIST Chamber
- Analysis Methodology
- Lunar Regolith Simulant Material
- Modeling and Analysis
- Results
- Conclusion

- Background
  - Molten Regolith Electrolysis (MRE) is a technique for producing gaseous oxygen and various metals from unprocessed regolith (soil) in a single-step process reactor and can be operated at various planetary destinations including the moon and Mars.
    - It consists in melting a mass of regolith and performing direct electrolysis of the ionic electrolyte at high temperature to form gaseous oxygen at the anode and collect alloying metals in liquid state at the cathode.
    - The electrolysis process also provides internal heating of the melt mass by the Joule Heating effect.
    - The technology behind an MRE reactor has been under development for several years and is currently positioned to begin larger scale testing of a reactor.
    - The current MRE project led by NASA KSC will demonstrate and test a sub-scale and fully integrated reactor developed in collaboration with Lunar Resources, Inc. a commercial partner.
    - The results of the reactor test, plus lessons learned from executing this project, will help influence NASA's approach for investment and maturation of the MRE technology and better position the technology to be flown on a lunar demonstration mission.

- ## Background

  - The MRE test reactor is designed and built by LR in a modular way to be able to remove the molten materials (liquid metals and molten regolith), feed unprocessed regolith, collect oxygen, and perform regolith melting.

    - The reactor design also accommodates various regolith heating options (e.g., inductive, and resistive to form the molten mass prior to starting the electrolysis to enable flight forward technology tests by KSC.

  - The objective of the MRE project is to perform an integrated test of the MRE reactor under a vacuum environment in the Atmospherically Sealed Simulator for In-Situ System Testing (ASSIST) vacuum chamber at KSC's Swamp Works laboratory.

    - The test reactor will electrolyze a single batch of regolith while under vacuum to extract a targeted 10 wt.% of the regolith

- Background
  - The reactor will be tested at the NASA facility and will meet NASA safety and engineering requirements during development.
    - The work presented in this paper focuses on the thermal/CFD modeling and transient simulation of the reactor and the vacuum chamber that are performed to provide design guidance and ensure adequate protection of the chamber.
    - The illustrations omit detailed views of the reactor design to protect proprietary information.

Objectives

- The modeling and simulation task is aimed at providing a comprehensive description of the thermal environment of the combined system of the MRE reactor and the ASSIST chamber during selected phases of operations to assess the feasibility of conducting the test while ensuring that both the reactor and its subsystems and the ASSIST chamber remain within safe limits thermally.

- Pursuant of this goal, the effort was structured to achieve the following objectives:

  - Build a medium-fidelity 3-D analysis model of a MRE reactor in the ASSIST thermal vacuum chamber for thermal simulation in COMSOL.

  - Perform simulations of the transient thermal behavior of the reactor operating under vacuum conditions in the ASSIST for different analysis cases.

  - Validate the thermal model using data from subscale heating subsystem tests performed in the ASSIST at KSC.

  - Characterize the thermal environment of the ASSIST during expected reactor operations and identify protection options to maintain the temperatures of the internal walls of the chamber to below 150°C per the design limits of the ASSIST chamber.

System models and assumptions

Reactor Model

• The reactor is modeled in 3 dimensions with materials properties in agreement with the as-built reactor specifications. The gaseous atmosphere inside the reactor is modeled as originating from the anode surface and exiting at a targeted pressure to the VMOMS system as convection and heat loss from out-flow of gas is simulated. The reactor includes the following components and subsystems that are modeled using as-built CAD files:

1. Reactor structure
   a. Metal shell with ports for electrical input, sensors, material handling subsystems, etc.
   b. Reactor insulation subsystem
2. Regolith heating subsystem
3. Anode and cathode subsystems
4. Regolith addition subsystem
5. Reactor control system
6. Oxygen and Volatile measurement subsystem (VMOMS)

Reactor Heating Subsystem Model

- The internal structure of the heating system is not modeled to minimize meshing density while the heating model is focused on describing the heat transfer into the regolith and the surrounding reactor.

  - The interface between the heating system and the regolith is modeled as a refractory ceramic surface through which radiative and conductive heat transfer occurs. Heat conduction is modeled from the hot zone to the rest of the heating system, and the reactor.

Regolith Mass Model

- The properties of the lunar regolith assigned as a function of temperature; the properties of the regolith simulant selected for the test are used when they are known experimentally.

  - In the absence of the latter, published values of properties of highland regolith are used. Melt properties are assigned according to the same methodology as for regolith.

  - The circulation of electric current through the melt and the resulting Joule-heating effects during electrolysis is not modeled but will be part of future work. Surfaces of the anode and cathode within the melt mass are assigned a constant temperature of 1600°C to simulate thermal equilibrium at the targeted operational temperature during the electrolysis phase of the reactor that generates Joule heating.

- The Atmospherically Sealed Simulator for In-Situ System Testing (ASSIST) chamber model is a manufacturer's CAD file without the flanges and ports to simplify meshing for the intended simulations.
  - Water-cooled side walls are modeled by a heat extraction rate.
  - No atmosphere is assigned inside ASSIST (perfect vacuum).
  - Power cables, O_2 line and coolant lines are included to aid in finding their optimal placement with respect to thermal environment.
  - The expected heat extraction rate to the O_2 heat exchanger is modeled to verify expected temperature of outflowing O_2 to VMOMS.
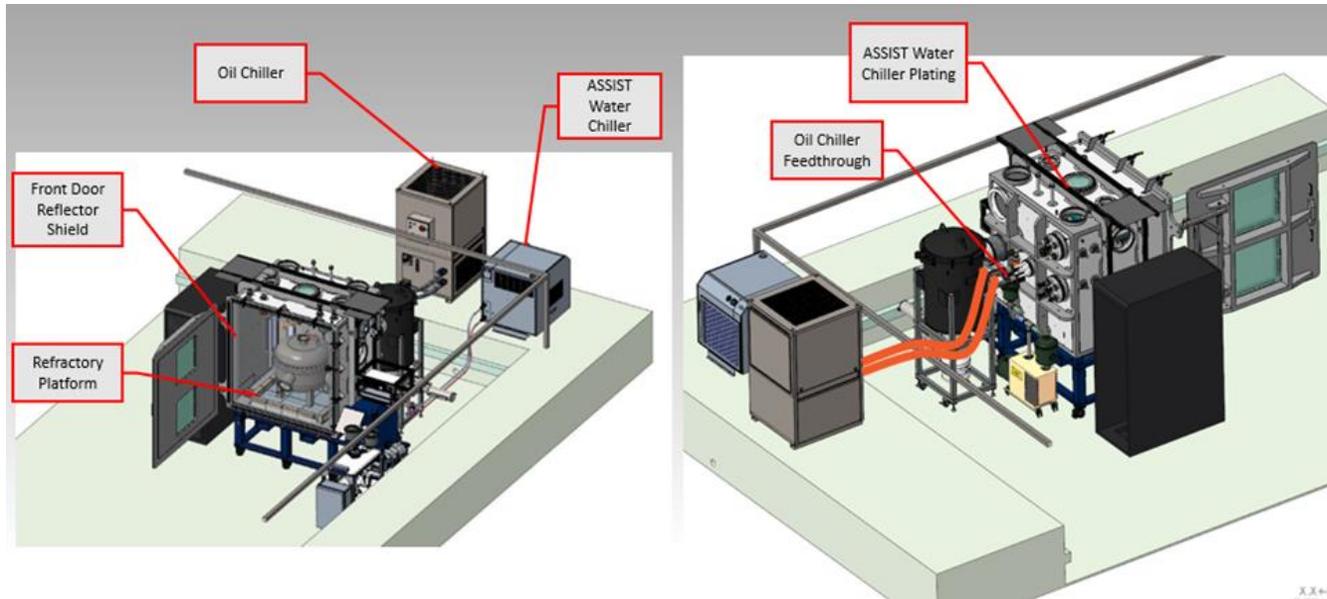
ASSIST thermal protection systems and reactor.

- ## Simplified Thermal Model

Front View

Front Door

Water Cooled (on 4 sides)

Windows

Fan Cooled

Side View
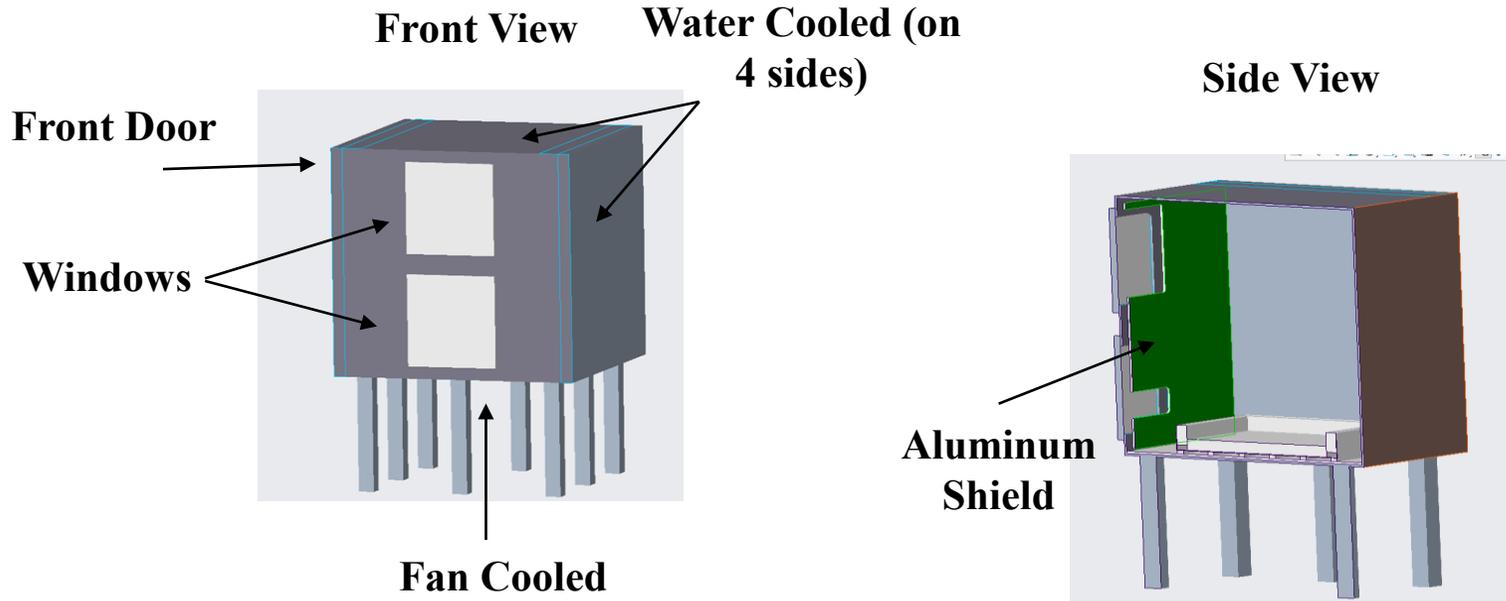
Aluminum Shield

ASSIST chamber model with front door windows (left). An aluminum plate (right, in green) fastened to the water-cooled walls serves as a radiative heat shield to protect door and windows.

- The ASSIST model includes the chamber walls, two borosilicate glass windows in the door, and the chamber supporting pillars as shown in the image.
- The ceiling and side walls are water cooled with a recirculating chiller set at 20 ℃.
- The door is not water cooled and it and the windows require protection from radiative heat transfer from the reactor.
- A door heat shield consists of an aluminum plate fastened to water-cooled side walls to cool the plate by conduction.

Material Overview

AISI 304	ASSIST Chamber walls
Brick	ASSIST Chamber Floor
Aluminosilicate Blanket	ASSIST Chamber Floor
Aluminum 5052	Radiation Shield for ASSIST Door
Borosilicate glass	ASSIST Windows
Fiberglass	Wire coatings

Simplified Thermal Model

- The image below shows the modeled elements that comprise the thermal protection of the floor directly underneath the reactor.

- A steel stand engineered to support the MRE reactor is placed on a refractory platform made of an assembly of high temperature refractory bricks layered on a steel platform.

- An aluminosilicate blanket adds protection below the platform and around it.

- A fan provides convective cooling underneath the ASSIST floor.
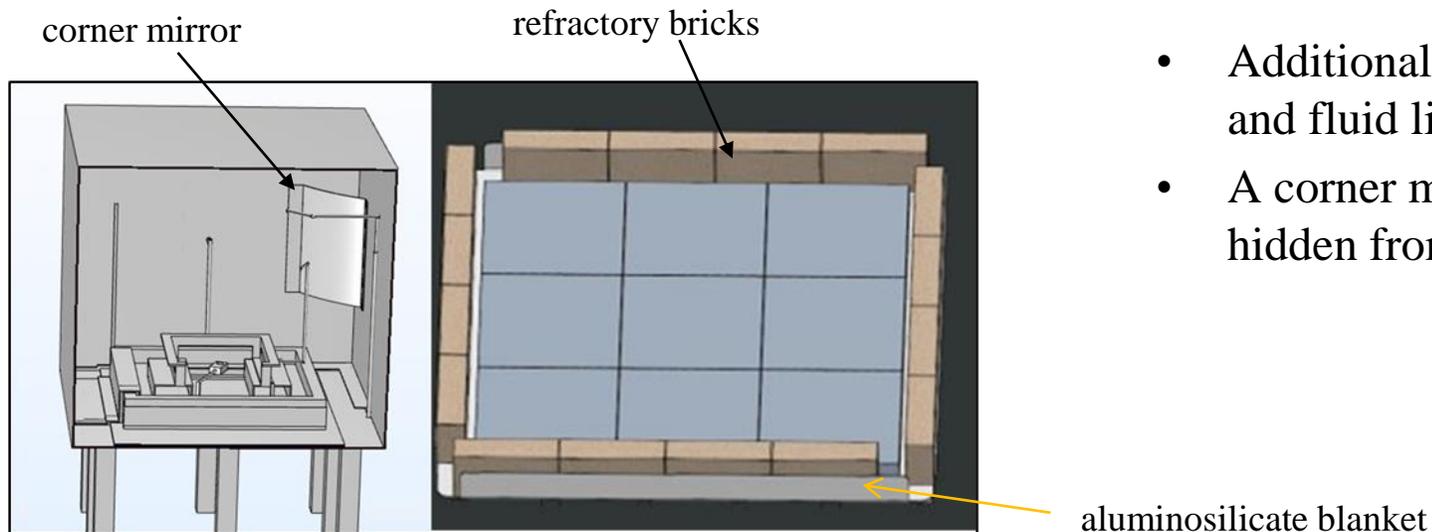
- Additional refractory blanket material protects wiring and fluid lines.

- A corner mirror allows viewing of reactor areas hidden from the door windows.

corner mirror

refractory bricks

aluminosilicate blanket

Thermal protection elements for the ASSIST chamber floor. The refractory platform (right) supports a steel stand on which the reactor is emplaced (left).

- The transient thermal/CFD analysis of the reactor and thermal vacuum chamber uses a commercial software package called COMSOL Multiphysics.
  - The multiphysics analysis includes heat transfer in solids and fluid analysis. Radiative heat transfer is included as both surface-to-surface radiation and radiation in a participating media represented by the regolith region.
  - Heat input into the system was modeled using experimental data acquired during subscale regolith melting tests using the same heating subsystem to determine the time-dependent heating power conditions for the analysis.
  - The results of the simulation include a time history plot of temperatures on the internal and external thermal vacuum chamber walls.

Approach

- The COMSOL model does not include electrolysis and Joule-heating caused by the electrolytic current through the melt that heats the reactor internally.

  - Consequently, the approach involves validating the heating model of the melt using thermal data collected during a separate subscale melt test in vacuum using the heating system.

  - The validated model is then applied to simulate the reactor heating phase until a regolith melt mass is formed between the electrodes. The heating phase simulation is then followed by an electrolytic phase simulated thermally by a constant and uniform melt temperature selected as the operating temperature for each simulation.

  - The heating system is assumed in a non-energized state during the electrolytic phase.

- ## Transient thermal/CFD Model

 - <u>MRE Thermal Process Steps for Simulation</u>

  1. Heating Phase:
     - The regolith is gradually heated to 1400 °C via heating system over the course of 17.5 hours.
     - The target temperature is selected to ensure the melt is fully formed and can pass electrical current for the subsequent electrolysis phase.

  2. Electrolysis Phase:
     - The electrodes are energized to pass current through the regolith melt pool for 20 hours.
     - The electrical physics are not part of the simulation.
     - Regolith heating is turned off during the electrolysis phase.
     - Joule-heating of regolith by electrolytic current is assumed to sustain the melt mass temperature at 1600 °C.
     - The melt mass is kept at this steady-state value in the simulation.

- The scale of the heating subsystem is proprietary and is not disclosed in this paper. The values in the figure are that of a subscale system to illustrate the heating rate only.
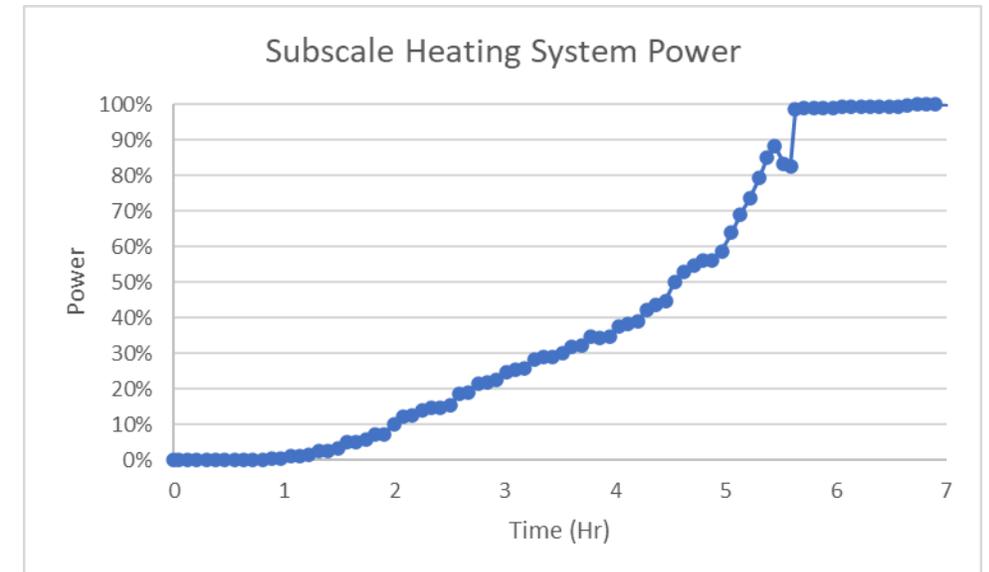
Subscale heating system power.

Selection of Lunar regolith simulant material

Samples of lunar regolith are not made available by NASA to perform experimental tests that would result in permanent alterations of the samples.

- Consequently, technology tests such as the one described in this work require the use of simulant materials of the regolith.
  - These materials are typically sourced from terrestrial natural rock and mineral mixtures that approximate the most relevant characteristics of the targeted lunar material.

- Lunar regolith is formed by breakage and comminution of lunar rocks under the combined forces of meteoritic impacts and thermal cycling between day and night temperatures.
  - This formation process produces a dry material typically described as a well-graded/poorly sorted, silty sand to sandy silt that corresponds to the Unified Soil Classification System categories "SW-SM" to "ML".
  - The median particle size is 40 to 130 μm, with an average of 70 μm.
  - It is distributed ubiquitously over the entire Moon to a depth of several meters with consistent physical characteristics and with mineralogical variations that depend on the region or location of interest.

- The lunar destinations currently targeted by NASA's Artemis program are in the south polar regions where highlands mineralogy dominates.
  - The selection of a suitable simulant material for the MRE process focused on a high weight percent of Anorthosite rock (with high anorthite content) and a high glass content (30-40 wt.%) of similar origin as the anorthosite to represent the chemical composition and the glass formed by meteoritic impact on the Moon.
  - In addition, the selection included a desired iron content of ~ 5-7 wt.% of FeO and low levels of impurity to reduce safety risks from hazardous volatiles and reduce unwanted electrochemical effects.
- The simulant selected for this work is CSM-LHT-1G produced from anorthosite and basalt that contains a high glass content to approximate the viscosity of polar lunar material as best as possible.

Materials selected for ASSIST components

Mineralogical composition	wt.%
Anorthosite (rock suite)	55.2
Basalt / norite	15.15
Basaltic glass	11.7
Glass (basaltic, and synthetic)	15.2

Regolith Thermal Conductivity
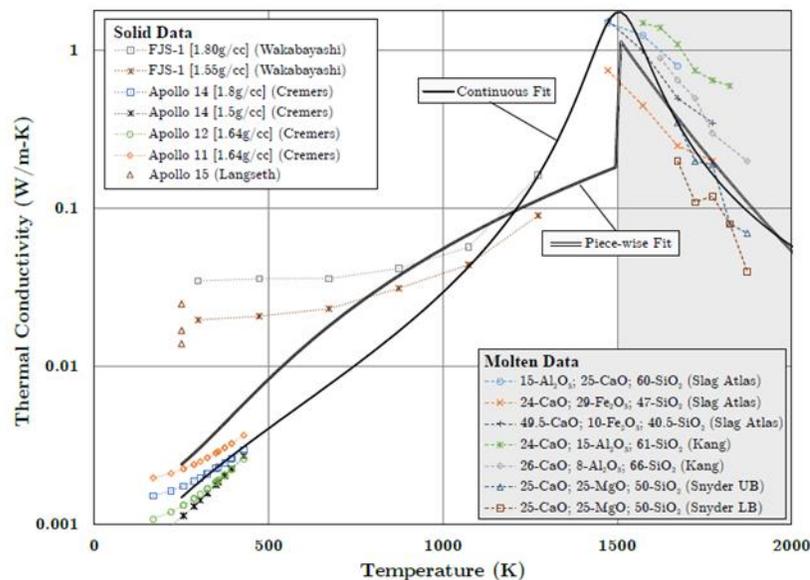
Schreiner, S.S., Dominguez, J.A., Sibille, L. and Hoffman, J.A., 2016. Thermophysical property models for lunar regolith. Advances in Space Research, 57(5), pp.1209-1222

Regolith Participating Media Absorption Curve

	Gauss 1	Gauss 2	Gauss 3	Gauss 4	Gauss 5
a_i	465	-0.650	163	0.325	1.45
b_i	-3670	200	528	175	150
c_i	5040	4.69	905	4.40	3.54
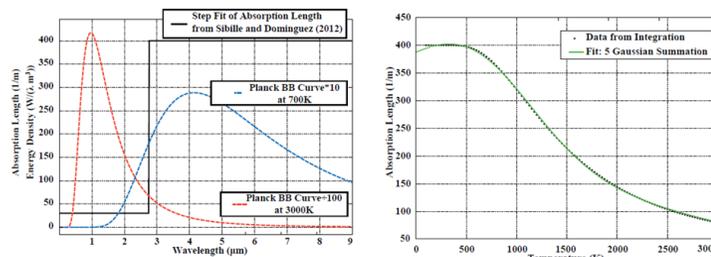
Regolith Density
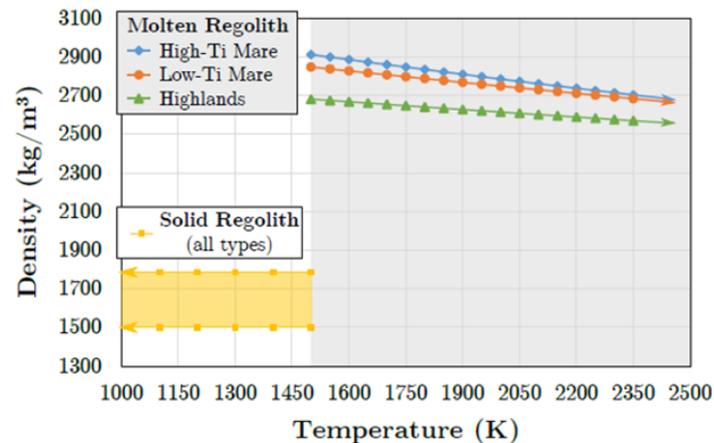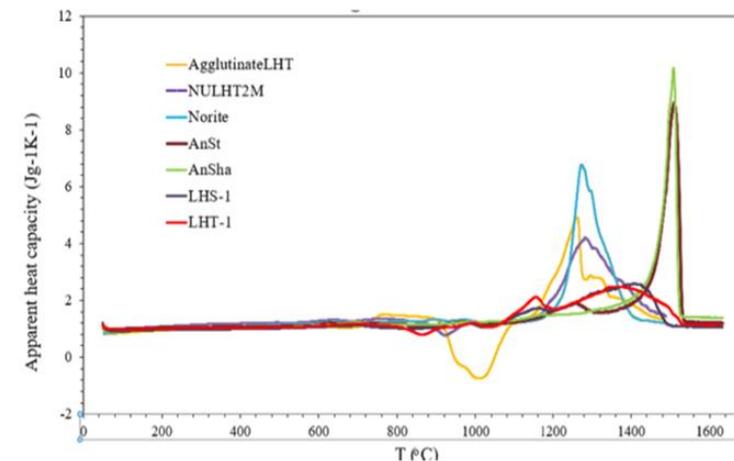
Regolith Specific Heat

Whittington, A.G., Morrison, A.A., Parspapoor, A., Patridge, A., (2023) Thermal and Rheological Properties of lunar Simulants from Ambient to Molten Glass, 54th Lunar and Planetary Science Conference 2023 (LPI Contrib. No. 2806). Available at: https://www.hou.usra.edu/meetings/lpsc2023/pdf/2811.pdf (Accessed: 27 July 2024).

- ## CFD Modeling

  - The heating phase of the regolith induces the thermal evolution of water from the mineral grains by desorption and dissociation of chemically bound hydroxyl and water molecules in the form of water vapor that dominates the total volatile production during this phase.

  - The modeled water vapor evolution includes two temperature-dependent phases.

  - During the initial heating of the regolith from 20°C to 500°C, an inlet steam flow rate boundary condition above the regolith is assigned a constant value of 4.78 x 10^{-5} kg/s.

  - After the regolith reaches a temperature of 500°C the flow rate is linearly decreased to about 10% of the maximum flow rate at the end of the heating phase (17.5 hours) when the regolith temperature at 2 cm from the heating system reaches 1400°C.
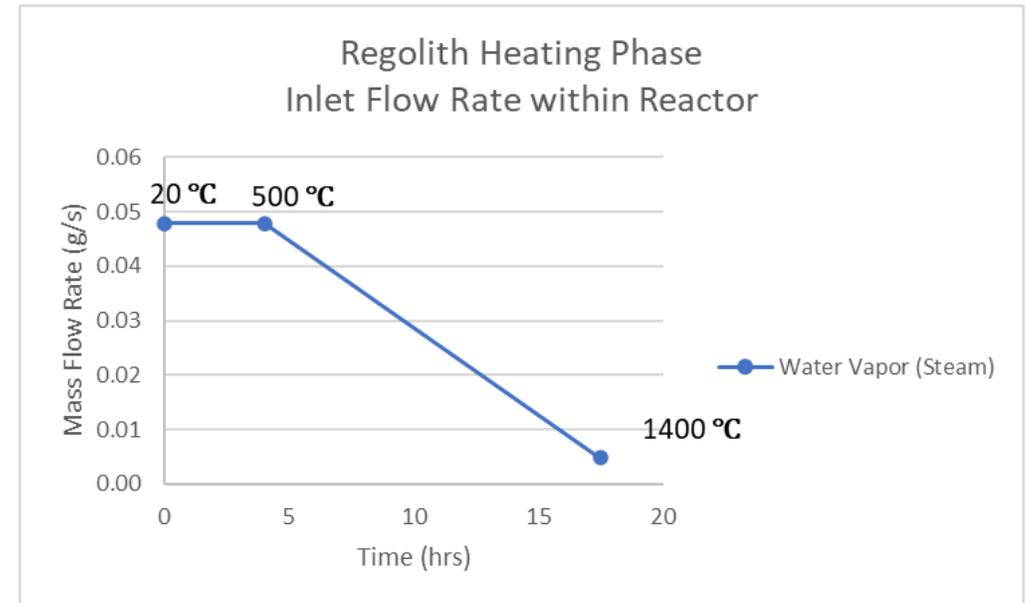
Water vapor flow rate from regolith.

- ## Transient thermal/CFD Model

  - The outlet pressure boundary condition for the water vapor (steam) is increased linearly within the same regolith temperature range to a maximum value.

  - Initially the pressure above the regolith is at vacuum pressure (approx. 1.3×10^{-3} Pa (10^{-5} Torr)).

  - As the heating system heats the regolith water vapor forms and the pressure outlet boundary condition increases linearly to 2.0 psia (13,789.5 Pa) at 17.5 hours when the regolith temperature at 2 cm from the heating system reaches 1400°C.

  - During the electrolysis phase, O_2 is assumed to be the only gas produced from the melt with a constant inlet mass flow rate of 6×10^{-5} kg/s.

  - The outlet pressure was set to a constant 2.0 psia. The surfaces within the regolith were set to 1600 °C.
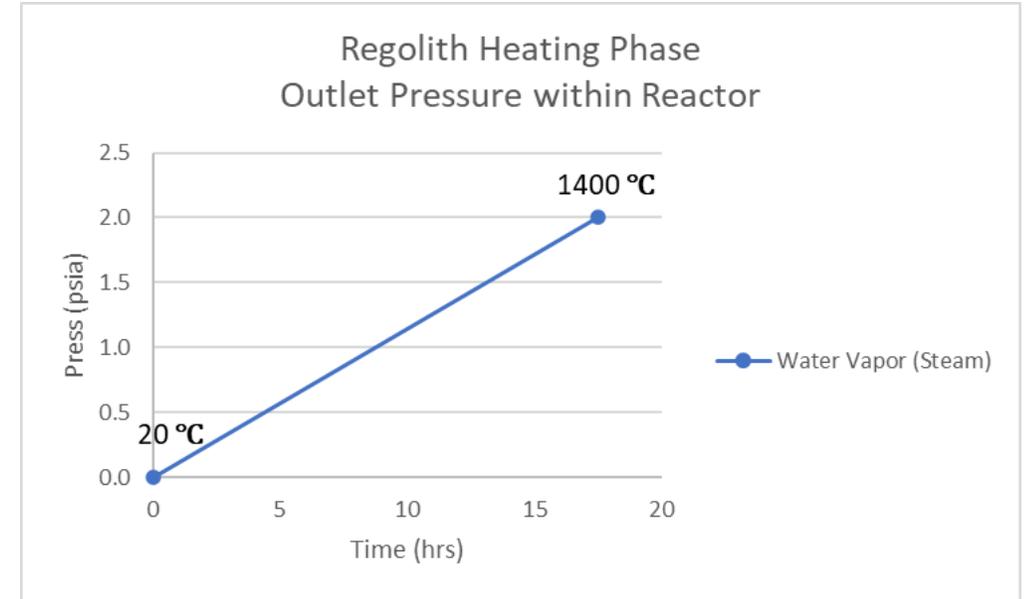
Assigned outlet pressure of water vapor.

Mesh

- User controlled mesh, with corner refinement.

- The mesh operation creates an unstructured tetrahedral mesh.

- Total elements 787,188.

Solver

- The segregated solution approach was used.

  – This attribute makes it possible to split the solution process into substeps.

  – Each substep uses a damped version of Newton's method.

- The iterative linear system solver GMRES (Generalized Minimum RESidual) iterative method was used for the iterative linear system solver of the fluid variables.

- The Time-Dependent Solver used the implicit time-stepping BDF (backward differentiation formula) method for solving ordinary differential equations (ODEs).
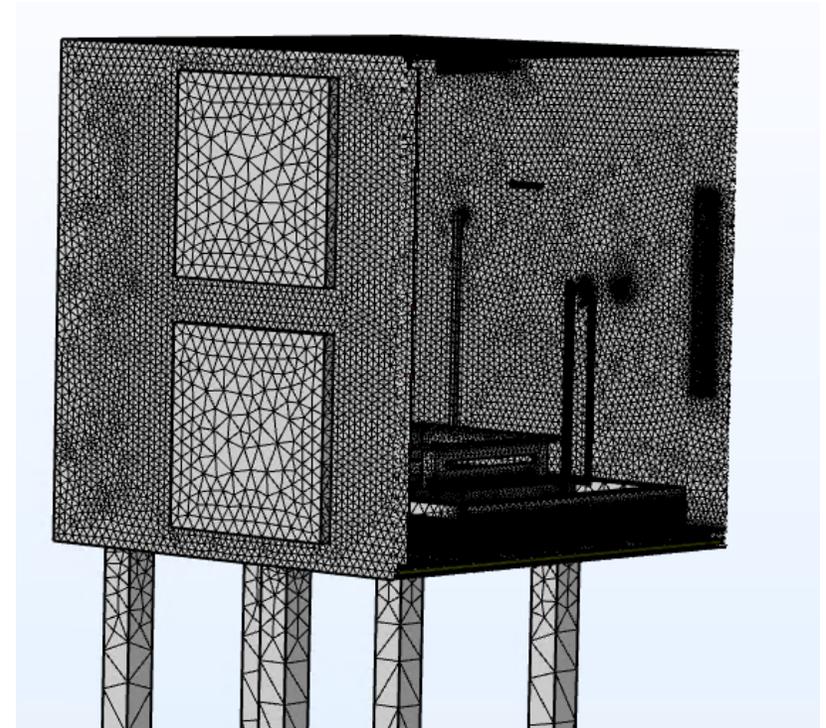
ASSIST chamber mesh.

- The contour temperature plot shows the temperatures on components above and below the reactor within the ASSIST chamber at the completion of the assumed test duration (37.5 h).
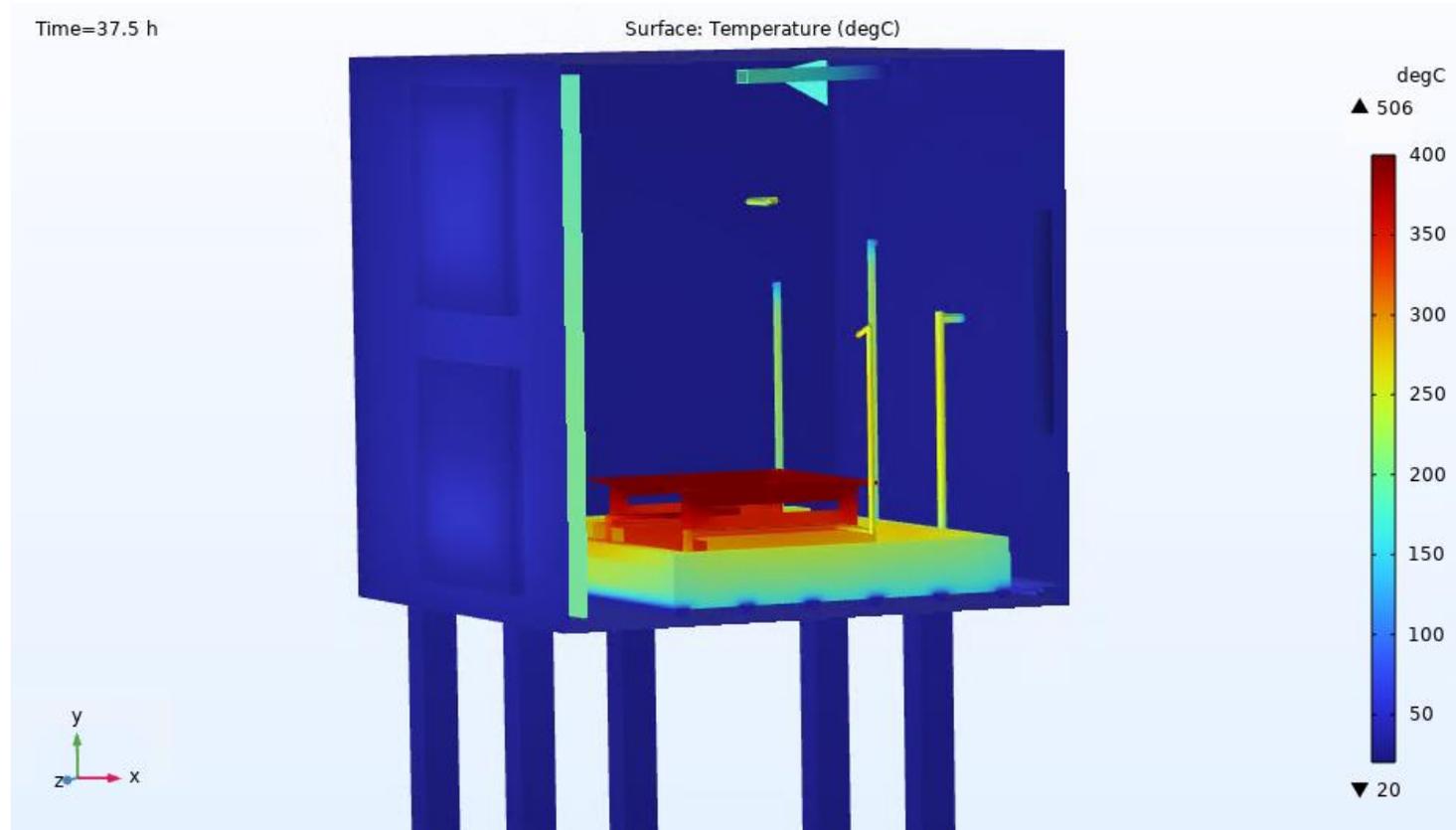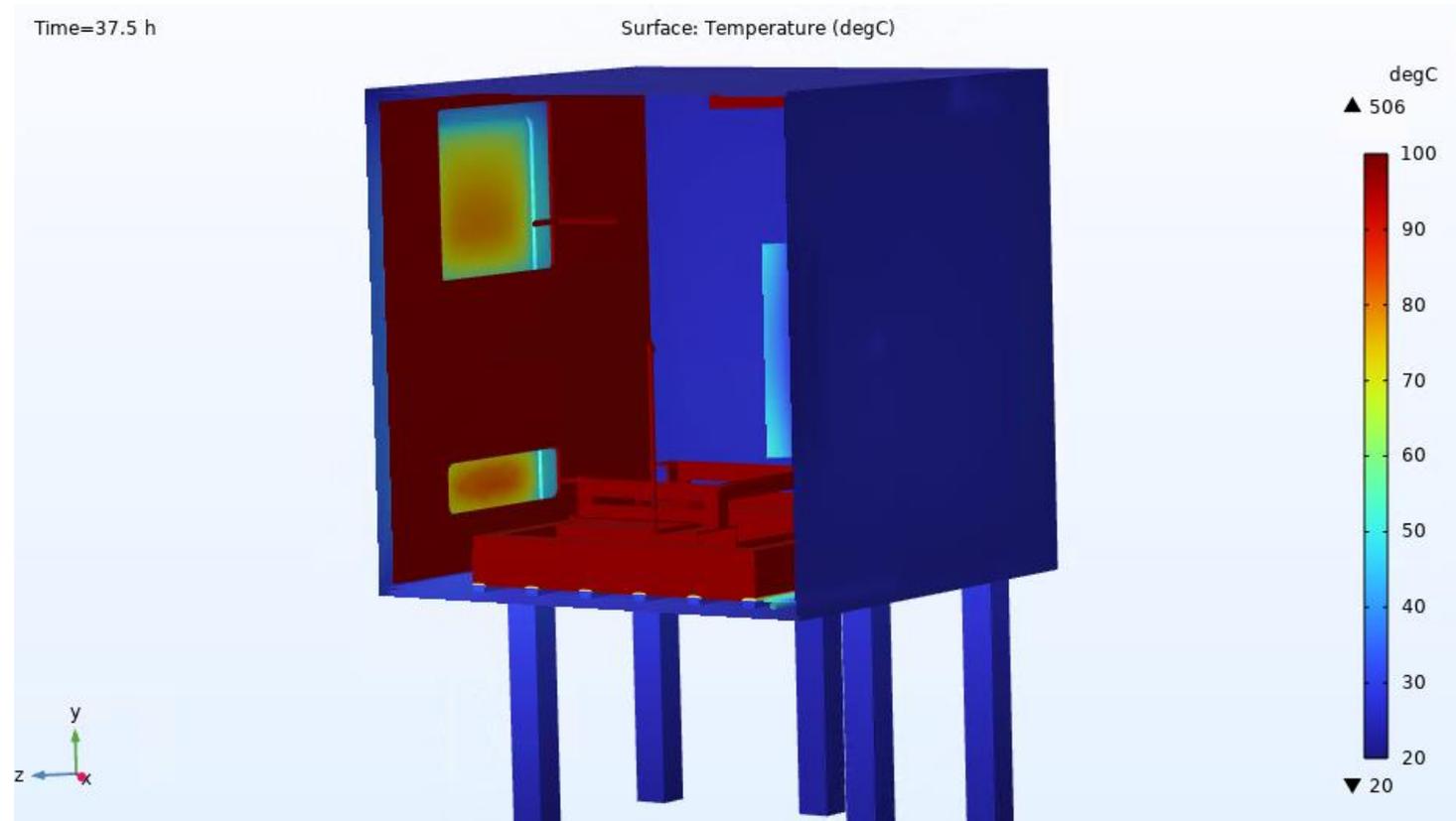

ASSIST chamber internal temperature contour plot.

- The contour temperature plot below shows the temperatures on the front door of the ASSIST chamber and the two borosilicate glass windows.
- The thermal simulation indicates the maximum window temperatures is at 55 ℃ and the maximum door temperature is at 49 ℃ after 37.5 hours.
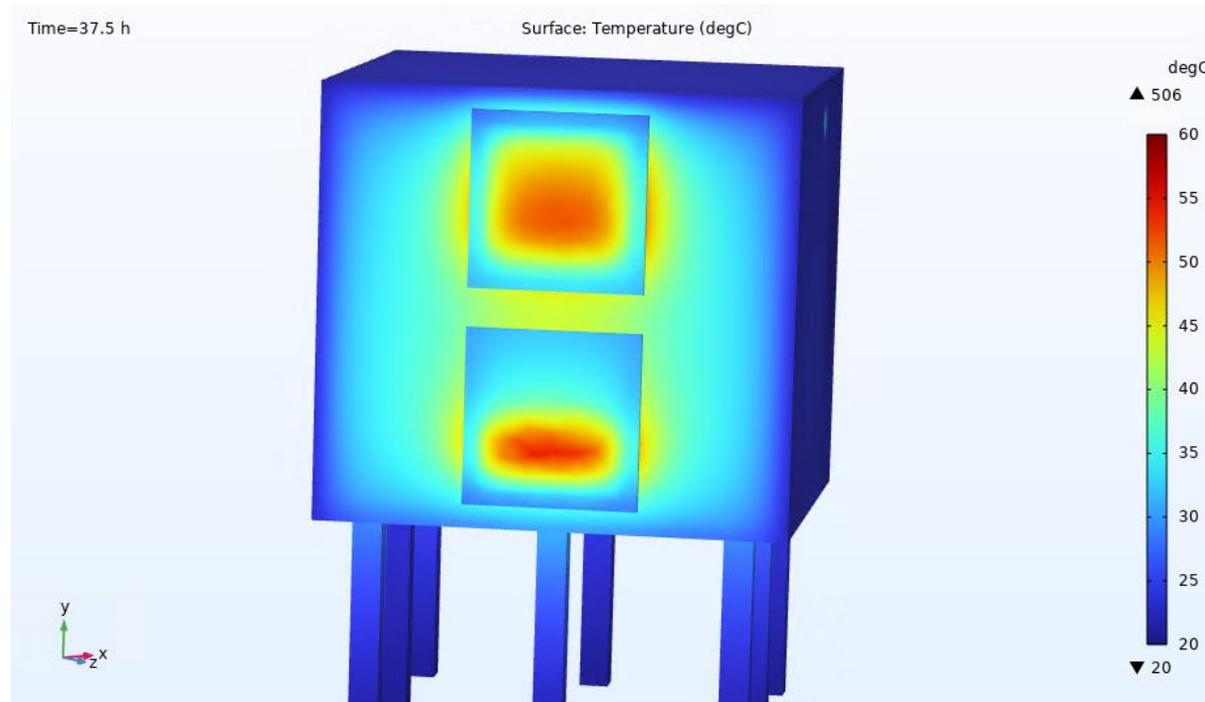
Internal temperature contour plot of ASSIST door elements.

- The contour temperature plot below shows the temperatures on the aluminum shield protecting the front door of the ASSIST chamber. The two cut outs show the front windows.

ASSIST chamber internal aluminum shield temperature contour plot.

- The graph shows the temperature history plot during the transient analysis at the heating system surface and in the regolith 2 cm from the heating system surface.
- The transition of boundary conditions at the end of the heating phase from 1400°C to 1600°C is shown as a step marking the beginning of the electrolysis phase.
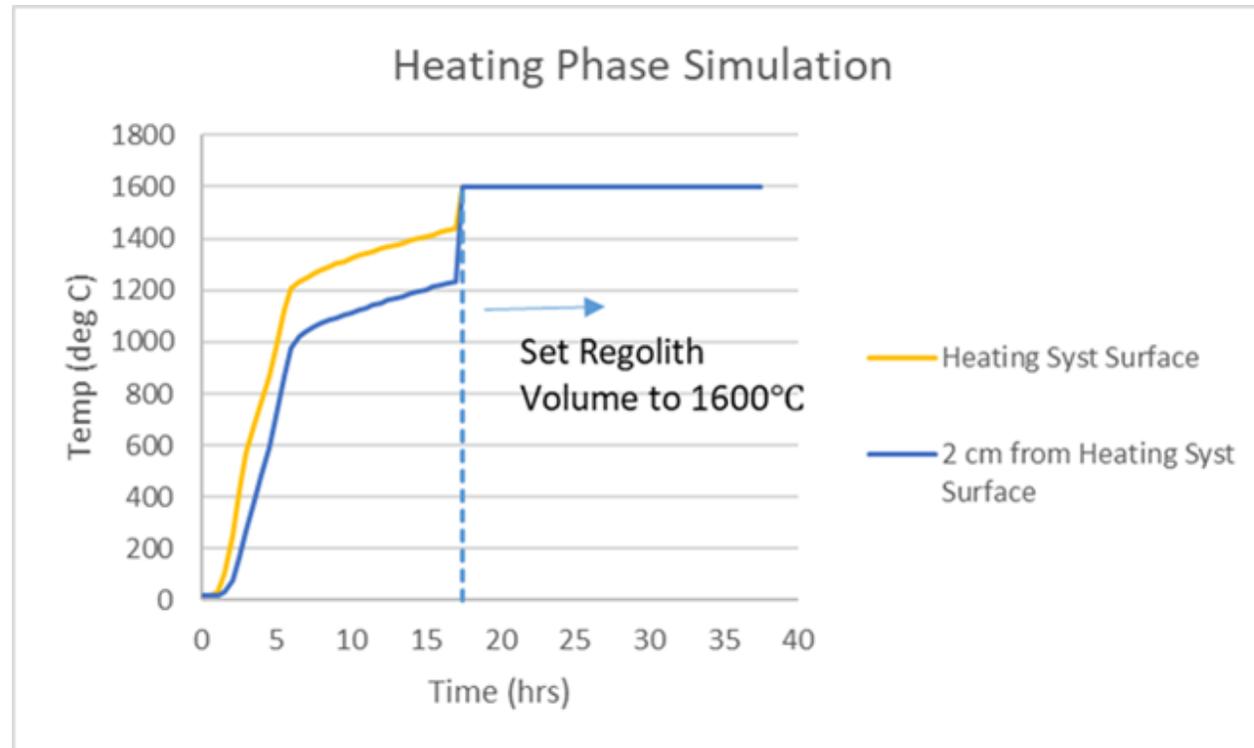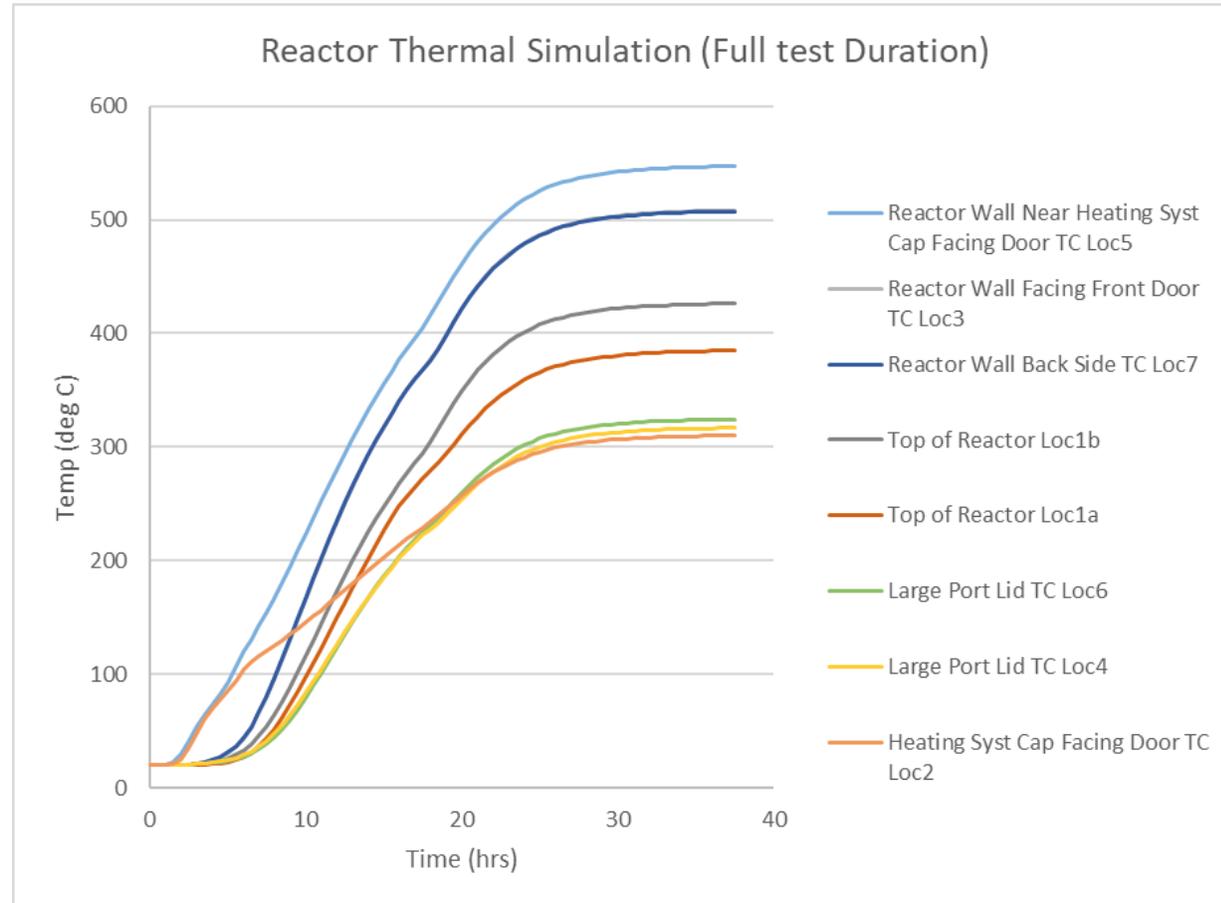

Heating phase to electrolysis phase: Temperature time history plot.

- The graph shows the temperature history plots during the transient analysis at various locations on the ASSIST walls.
- The three water-cooled ASSIST wall temperatures have a much smaller temperature rise and similar transient temperature curves compared to the ASSIST floor transient temperatures since the floor is not water cooled.
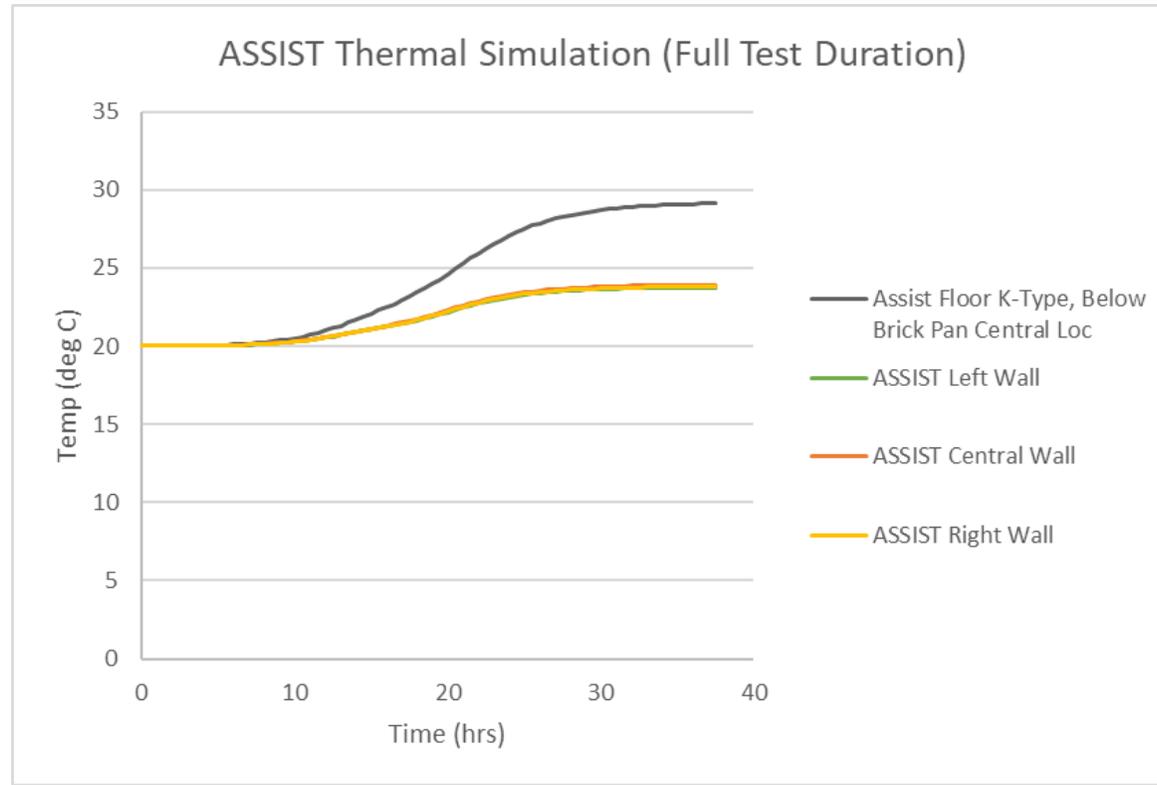

ASSIST chamber wall temperature time history.

- The graph shows the temperature time history plots during the transient analysis at various locations on the reactor.


Reactor temperature time history plot.

- The graph shows the temperature time history plot during the transient analysis at various locations of electrical connector and wires in the proximity of the reactor.
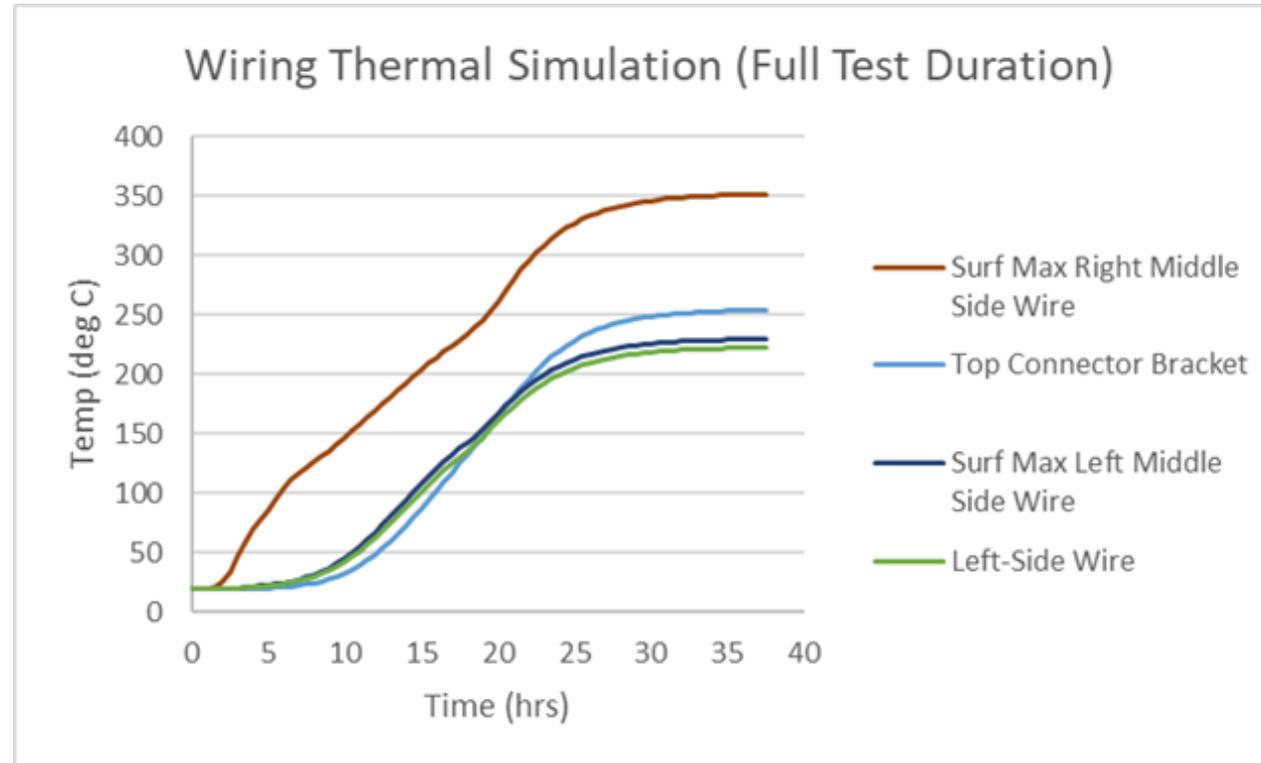

Wiring thermal simulation for full test duration.

- The figure on the left displays the dimensions of the regolith height and width along with the regolith temperature 2D contour plot at the end of the heating phase at 17.5 hours when the molten regolith reaches 1400°C at locations 2 cm from the active heating zone surface.

- The figure on the right shows a 3D iso-surface plot of the melt domain at the same time mark.

- The temperature of the surfaces contacting the melt domain is set at a constant 1600°C after 17.5 hours to simulate the electrolysis phase. This includes the anode, cathode and any surface of the heating system in contact with the melt area.
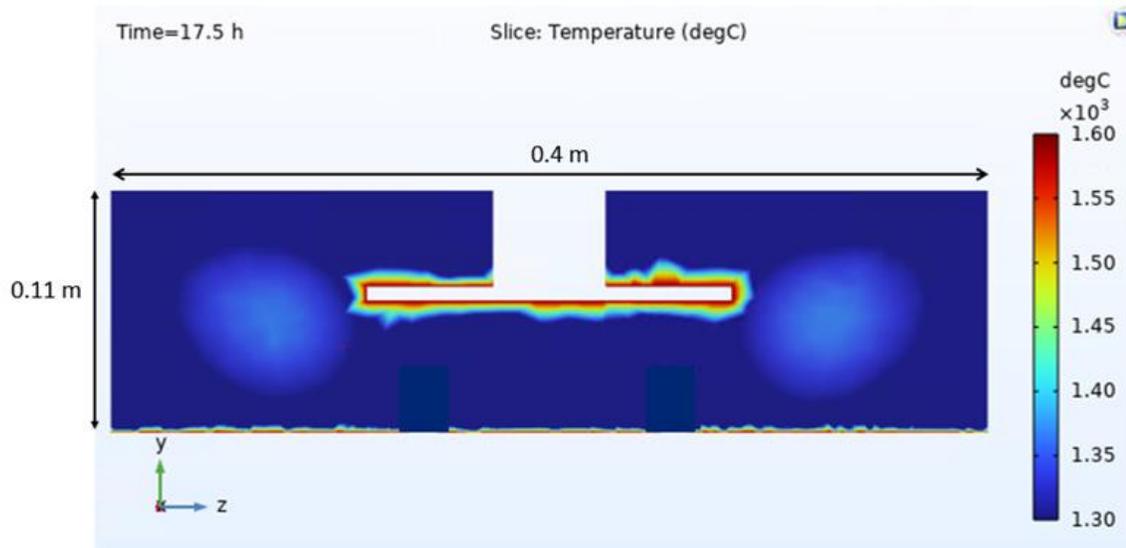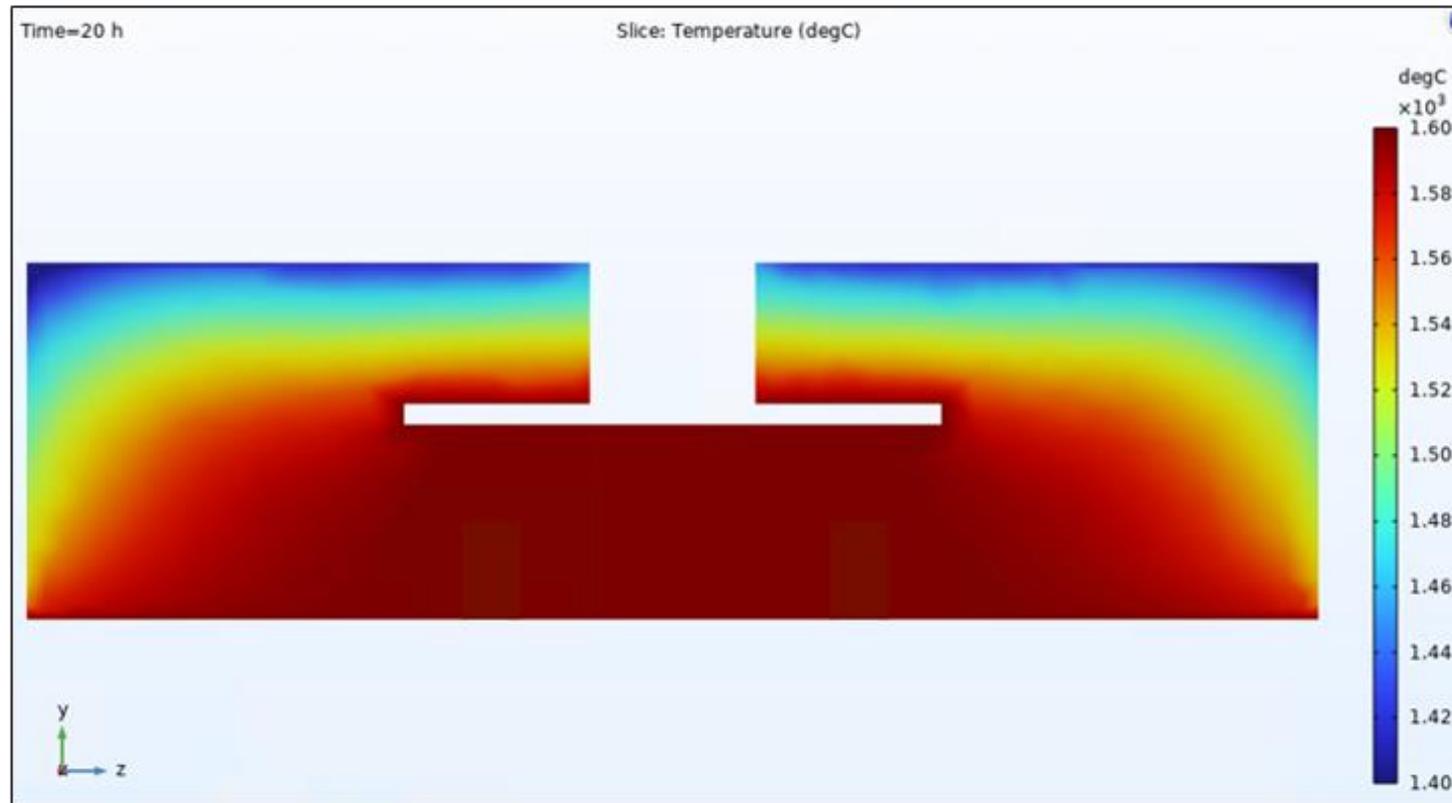

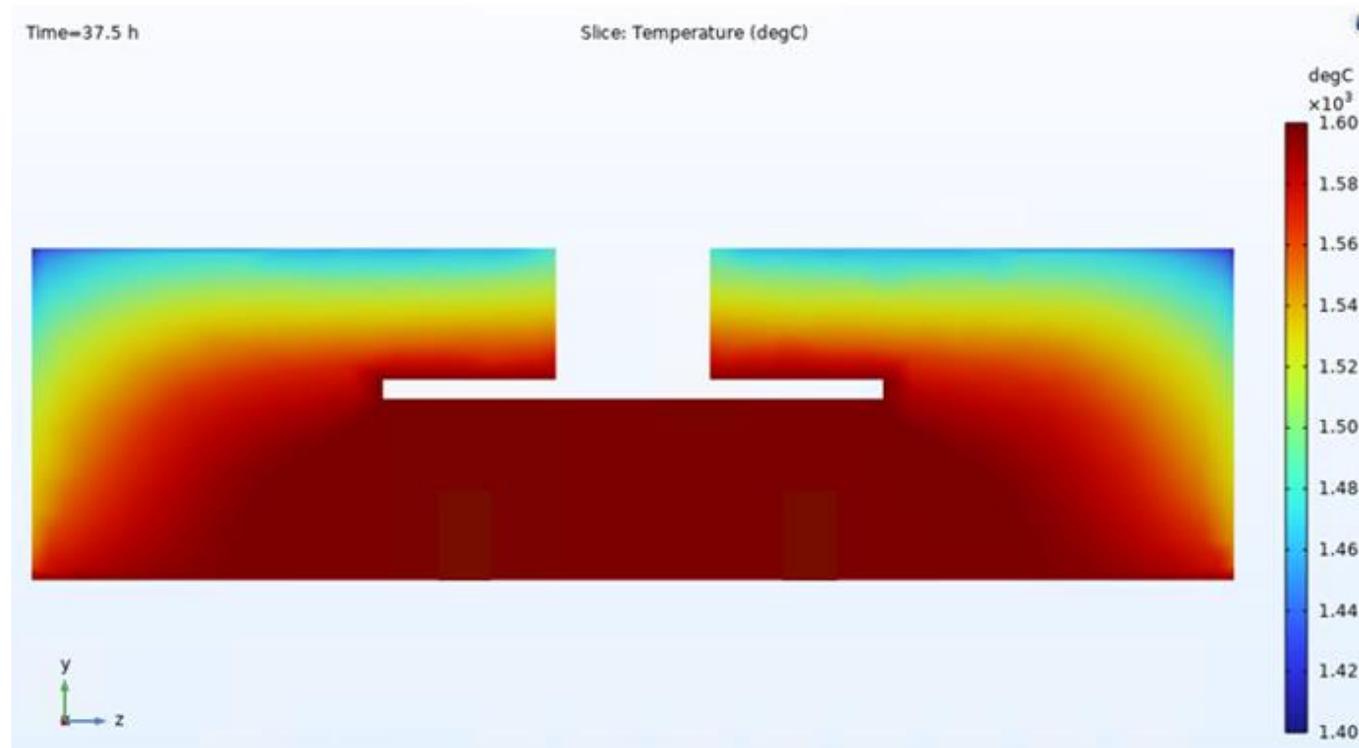2D contour temperature plot of the regolith volume at 17.5 hours
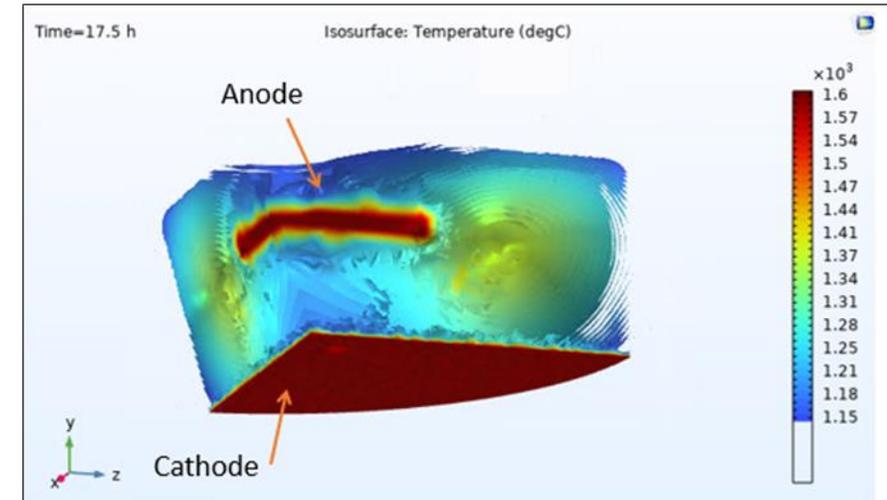
Temperature iso-surface cross-sectional plot of the regolith volume at the end of the heating phase (17.5 hours) .

- The image below shows the regolith temperature 2D contour plot at 20 hours at which point the melt domain surfaces have been maintained at 1600°C for 2.5 hours following the transition from the heating phase to the electrolysis phase.
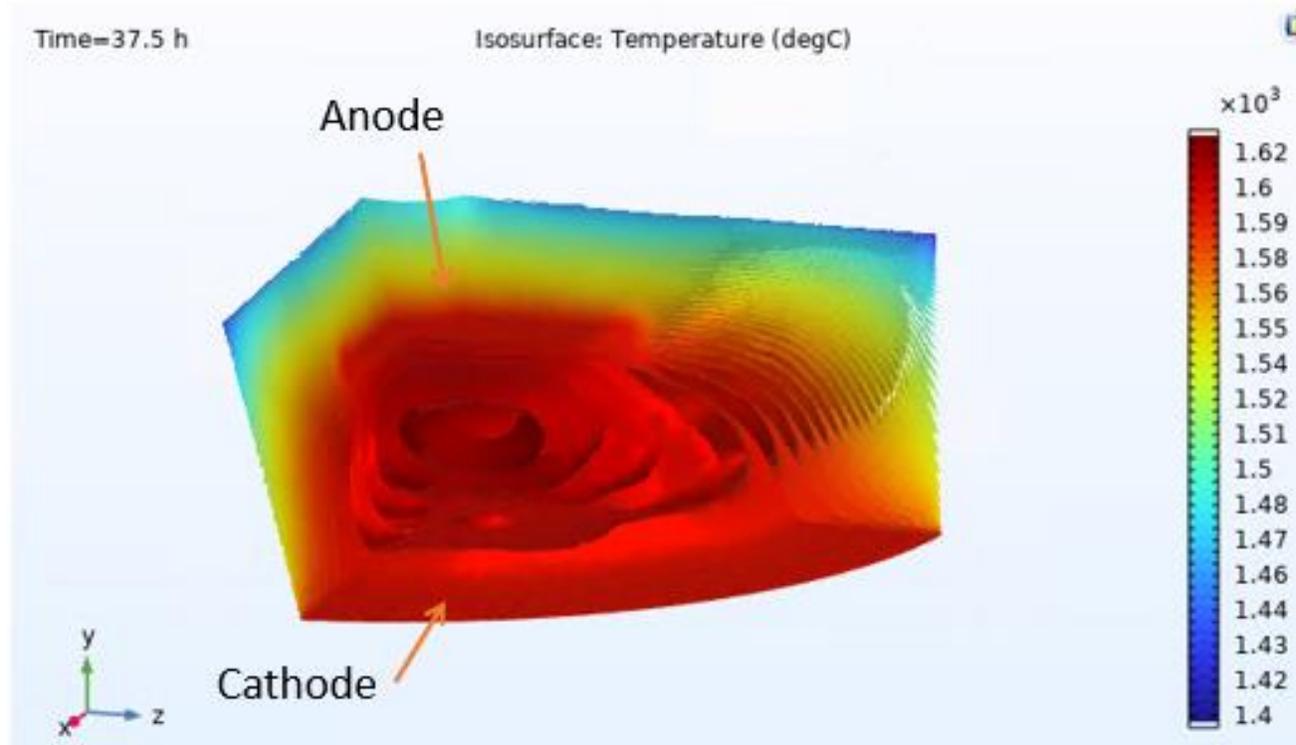

2D contour temperature plot of the regolith volume at 20 hours.

- The figure shows the regolith temperature 2D contour plot at the completion of the electrolysis phase (37.5 hours).

- The volume of molten regolith between the anode and the cathode remains at the desired operating temperature 1600°C thus validating the surface boundary conditions.


2D contour temperature plot of the regolith volume at 37.5 hour.

- The figure shows an 3D iso-surface cross-sectional plot at 37.5 hours displaying details of the temperature gradient throughout the molten phase with a top surface at a temperature lower by 100°C.
- The top surface is cooled by the flow of water vapor and O_2 exiting from it.


Temperature iso-surface cross-sectional plot of the regolith volume at the end of the electrolysis phase (37.5 hours).

- The rate of heat loss associated with water vapor (steam) as a function of time is displayed during the heating phase (first 17.5 hours).

- The COMSOL CFD analysis modeled the region above the melt pool and simulated the flow of water vapor.

- The inlet and outlet temperature were monitored to calculate the rate of heat lost due to the convection of heated water vapor leaving the top of the reactor shown in the graph below.

- Once the electrolysis begins the fluid domain above the melt pool was updated to O_2. The COMSOL CFD analysis modeled the flow of O_2 similarly to that of steam.

- The inlet and outlet temperature were monitored to calculate the rate of heat loss due to the convection of heated O_2 leaving the top of the reactor.
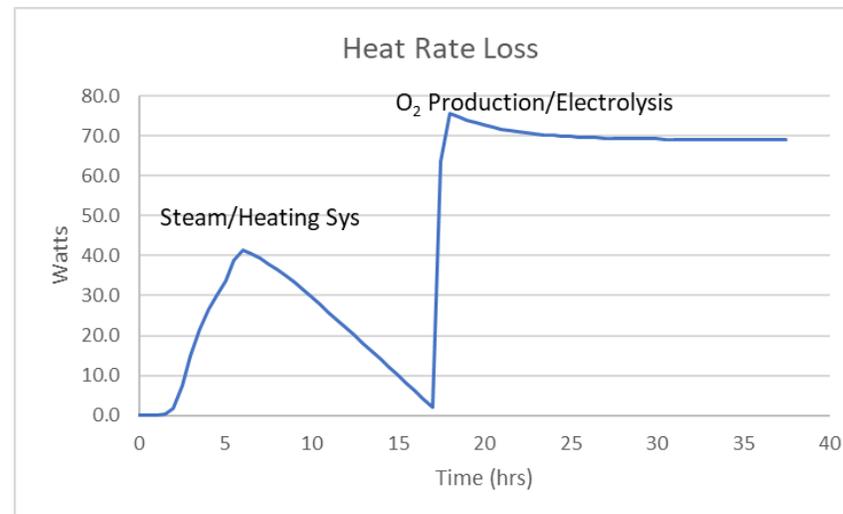
Rate of heat loss due to steam and O_2.
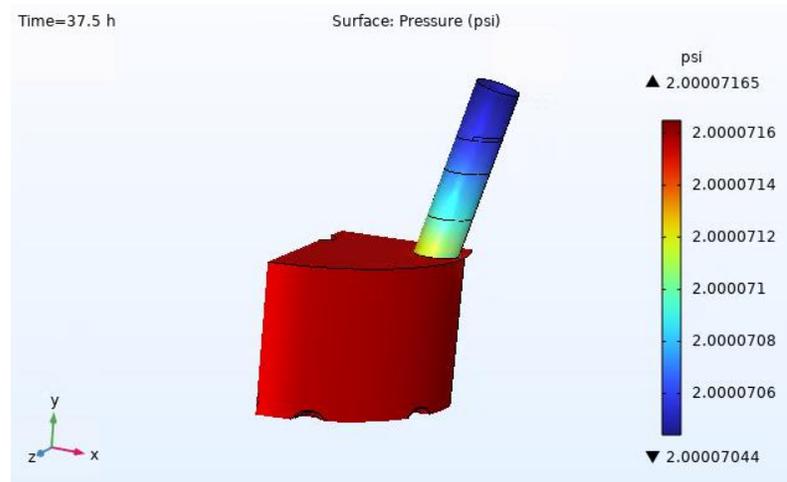
- The velocity contours of the O_2 leaving the reactor are displayed in the volume above the melt pool at the end of the test (37.5 hours).
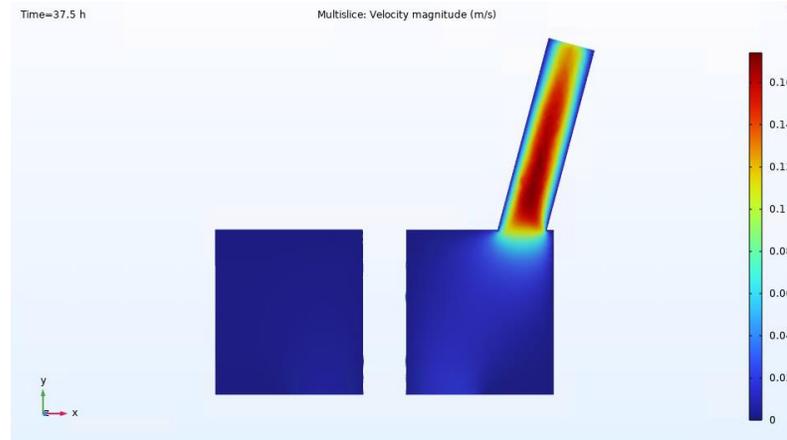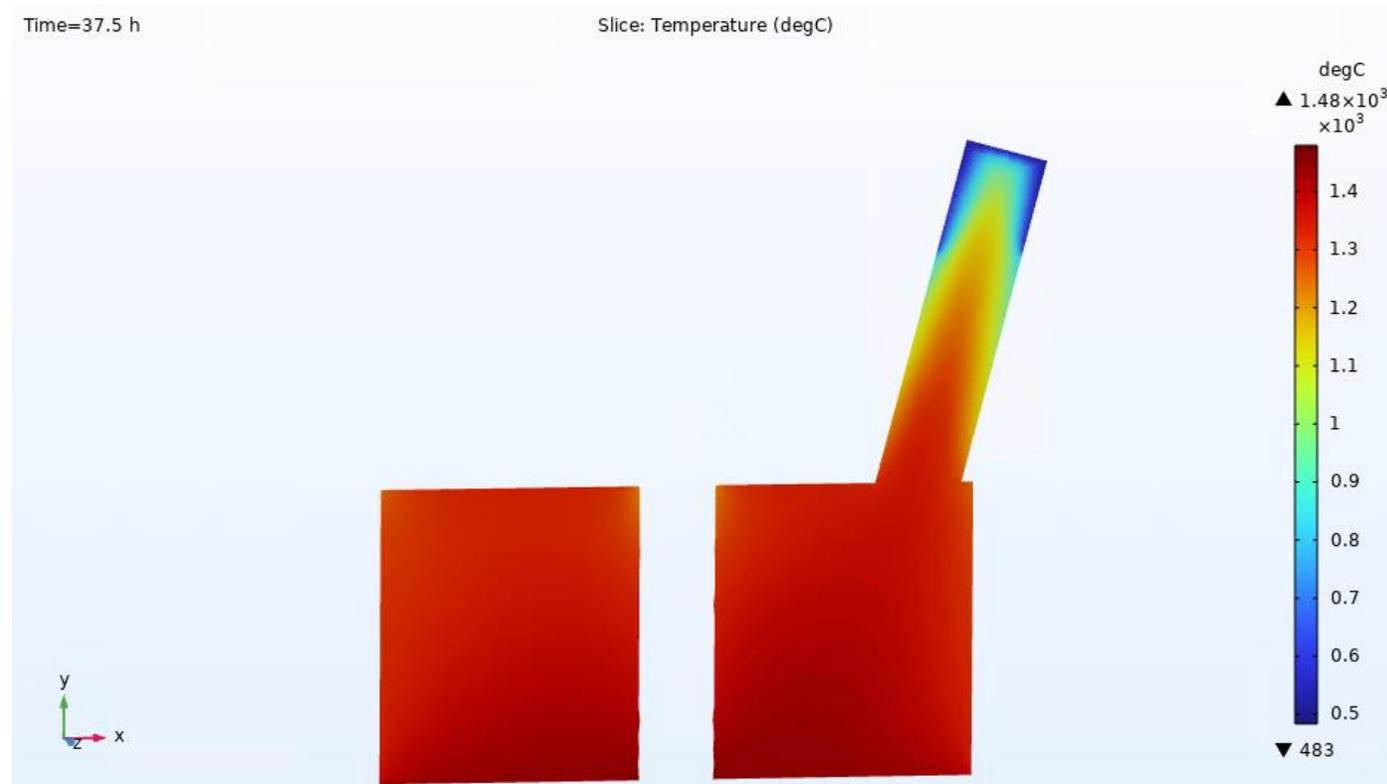

Velocity contour plot of O_2 exiting the reactor.

- The 3D contour plot shows the pressure contours of the O_2 above the melt pool and the outlet channel at the end of the test (37.5 hours).

Pressure contour plot of O_2.

- The contour plot shows the temperature contours of the O_2 above the melt pool and through the outlet channel at the end of the test (37.5 hours).

- A transient thermal/CFD analysis of the reactor and thermal vacuum chamber was created to simulate the thermal behavior of the reactor in the ASSIST chamber for different analysis cases. The thermal simulation model was used to characterize the thermal environment of the ASSIST during reactor operations and identify protection options for internal walls as needed to limit internal temperatures to below 150 **°C** on the internal walls of the ASSIST chamber.

- **ACKNOWLEDGEMENTS**
  - The author would like to thank Kennedy Space Center Molten Regolith Electrolysis team for their support of this work and Lunar Resources, Inc. for their assistance with MRE reactor specifics.

- **Future Work**
  - The circulation of electric current through the melt and the resulting Joule-heating effects during electrolysis is not modeled but will be part of future work.

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REFERENCES

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3. Whittington, A.G., Morrison, A.A., Parspapoor, A., Patridge, A., (2023) Thermal and Rheological Properties of lunar Simulants from Ambient to Molten Glass, 54th Lunar and Planetary Science Conference 2023 (LPI Contrib. No. 2806). Available at: https://www.hou.usra.edu/meetings/lpsc2023/pdf/2811.pdf (Accessed: 27 July 2024).

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Backup Slides

- Transient thermal/CFD Model

  – The transient thermal/CFD analysis of the reactor and thermal vacuum chamber uses a commercial software package called COMSOL Multiphysics.

  – The multiphysics analysis includes heat transfer in solids and fluid analysis.

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Approach

- The COMSOL model does not include electrolysis and Joule-heating caused by the electrolytic current through the melt that heats the reactor internally.

  - Consequently, the approach involves validating the heating model of the melt using thermal data collected during a separate subscale melt test in vacuum using the heating system.

  - The validated model is then applied to simulate the reactor heating phase until a regolith melt mass is formed between the electrodes.

  - The heating phase simulation is then followed by an electrolytic phase simulated thermally by a constant and uniform melt temperature selected as the operating temperature for each simulation.

  - The heating system is assumed in a non-energized state during the electrolytic phase.

- The Multiphysics simulation of the MRE reactor operations is designed to accept a range of values as user inputs for the subscale heating system power and duration, target temperatures for the melt, duration of the test at target temperature, and water and oxygen mass flow rate from the anode.

- The work presented here is a representative example of many potential operational settings for an actual MRE reactor test with a target duration of 37.5 hours.

  - The target melt temperatures listed below are selected based on the thermophysical properties of the regolith simulant CSM-LHT-1G selected for this test (see later section on regolith simulant properties).

  - In this case, 1400°C represents the liquidus temperature at which all components of the regolith are molten.

  - The simulation example is described below in two separate operations that are performed sequentially in COMSOL.