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Simulating Oxygen Production on Mars for MOXIE (Mars Oxygen In-Situ Resource Utilization Experiment)

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The Mars Oxygen In-Situ Resource Utilization Experiment (MOXIE) represents the first time that NASA is demonstrating In-Situ Resource Utilization (ISRU) on the surface of another planetary body. MOXIE will produce oxygen from atmospheric CO_2 on Mars. It is being developed for NASA's 2020 Mars Rover and will produce greater than 99.6% pure oxygen through solid oxide electrolysis. MOXIE is roughly 0.5% of the scale that would be necessary to produce oxygen for breathing and use as a propellant for a human Mars mission.

Tests are being performed on MOXIE in the laboratory at NASA's Jet Propulsion Laboratory (JPL) and the Massachusetts Institute of Technology (MIT). At the same time, a model is being developed to simulate and predict the performance of MOXIE. The ability to predict the performance of MOXIE on Mars is a critical step in preparation for surface operations. Without the ability to estimate inefficient or unsafe operating conditions, MOXIE operations on Mars run a spectrum of risk ranging from loss of efficiency to the loss of the entire mission. Therefore, to predict performance and thus avoid subjecting flight hardware to unsafe conditions, a dynamic model has been developed that simulates MOXIE's operation. Simulink, a package contained within the MATLAB programming language, was chosen as a convenient way to build this dynamic representation of MOXIE. The model is a combination of theoretical and empirical values regarding the gas flows, thermal transfers, electrochemistry, and control loops that are representative of the true MOXIE system. The results of this model have been validated against data from JPL's MOXIE testbed laboratory. Continued model validation will occur as JPL acquires new data throughout 2018.

This paper gives an overview of how MOXIE works and how it is modeled. MOXIE is the first instrument of its kind to leave the Earth, and the modeling of this instrument is similarly unique. As the dynamic model continues to evolve with new data, it becomes a fast and inexpensive way to test MOXIE without subjecting expensive hardware to hazardous conditions.

*Note: This paper has not been presented at a previous meeting

Acronyms/Abbreviations

ASR	Area Specific Resistance
ISRU	In-Situ Resource Utilization
JPL	Jet Propulsion Laboratory
MAV	Mars Ascent Vehicle
MOXIE	Mars Oxygen ISRU Experiment
SOXE	Solid Oxide Electrolysis
YSZ	Yttria-Stabilized Zirconia

1. Introduction

There are many reasons to send humans to Mars. A clear example is for scientific exploration. Despite the wealth of information provided by robotic craft that humans have put on Mars or in Mars orbit, there is no denying that having humans present on the surface would significantly speed up the exploration process. The Curiosity rover's top speed, as an illustration, is just under 0.1 miles per hour (0.16 kilometers per hour). The Opportunity rover, which has been exploring Mars since 2004, has covered roughly 30 miles of terrain in its 15 years of operation: a distance conceivably able to be covered by humans in a vehicle in just a few hours or on foot in a few days. Another reason to send humans to Mars is to begin a permanent human outpost that could eventually lead to a civilization. And, of course, the fact that it would be an inspirational leap for humanity is a compelling reason on its own.

Despite the motivation and the fact that the first human step on the Moon was 49 years ago, humans have not been to Mars. One of the primary roadblocks to human Mars exploration is cost. A 1-tonne, Curiosity-size mission costs about 2 – 2.5 billion USD (1.7 – 2.2 billion euro). When factoring in the life support equipment, habitation, Mars Ascent Vehicle (MAV), consumables, return propellant, landing mechanisms and more that are needed to support humans, the mass and cost of the system bloom spectacularly.

The goal of the Mars Oxygen In-Situ Resource Utilization Experiment (MOXIE) is to substantially reduce one of these costs: the return propellant. MOXIE will demonstrate the ability of solid oxide electrolysis to convert the carbon dioxide atmosphere on Mars into oxygen. This oxygen can be burned with methane or hydrogen as rocket fuel to power a MAV and return the astronauts safely to Earth. By producing the propellant on the surface of Mars rather than carrying it from Earth, nearly 30 tonnes of mass can be saved[1]. This reduces costs on the order of hundreds of millions or even billions of dollars, putting humans one economical step closer to setting foot on Mars.

2. The Importance of In-Situ Resource Utilization

MOXIE is an instrument that takes advantage of the principles of In-Situ Resource Utilization (ISRU). ISRU, often considered the science of "living off the land", is a concept that has been growing in momentum with humanity's push towards developing a space economy and enabling space exploration. ISRU involves the use of technology to convert materials present at the destination site into useful resources. Resources derived from ISRU can be used for life support, construction, propulsion, and energy for both manned and unmanned missions. By obtaining these functionalities with materials found in space, one no longer needs to bring the materials with them from Earth, thus significantly reducing the mass, cost, and risk associated with spaceflight. For these reasons, development of ISRU technology is critical to the enablement of manned missions into the solar system, including Mars.

ISRU for Mars has been a topic under discussion for decades. Analog experiments have been carried out on Earth to test various ISRU strategies for construction of dwellings, use of perchlorates, water purification, and production of oxygen, among others. This paper focuses on the last, as the current lack of oxygen on Mars is an important barrier that needs to be overcome to send humans to Mars. An example of an in-situ resource is the atmosphere of Mars, which is composed of 96% carbon dioxide. This can be converted into other useful chemicals, like oxygen, with appropriate ISRU equipment. MOXIE is being developed for NASA's Mars 2020 Rover to produce greater than 99.6% pure oxygen through solid oxide electrolysis. It is an ISRU instrument designed to reduce the cost of sending humans to Mars by using the planet's atmosphere as a resource.

3. How Does MOXIE Work?

MOXIE is an instrument that takes advantage of the large amounts of carbon dioxide present in the Mars atmosphere. As mentioned, the oxygen produced by a system like MOXIE could be used as the oxidizer for a Mars Ascent Vehicle (MAV) that would lift

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[1] Hoffman, J., Rapp, D., & Hecht, M. (2015). "The Mars Oxygen ISRU Experiment (MOXIE) on the Mars 2020 Rover". *AIAA Space 2015 Conference* (AIAA 2015-4561).

astronauts off the surface of Mars to begin their journey back to Earth. In addition, some of the oxygen could be used for breathing and for rover and habitation pressure. MOXIE is roughly 0.5% of the scale that would be necessary to produce oxygen for use as a propellant for a four-person mission to Mars, assuming that the empty oxygen tank on a Mars ascent vehicle would be filled in 14 months. For context, an image of the Mars 2020 Rover is shown below.

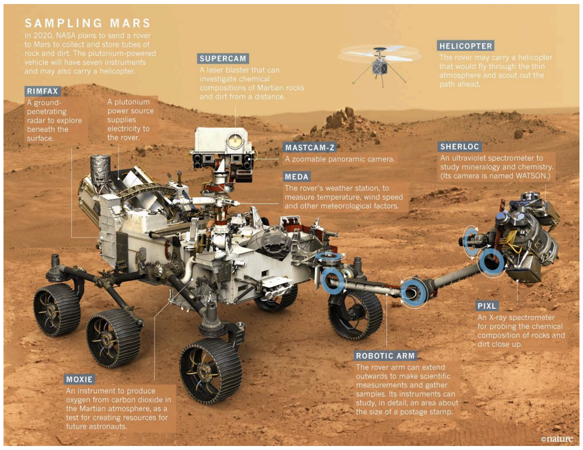

Figure 1: Mars 2020 Rover with payloads labeled. Image credit: NASA.

As Figure 1 indicates, there are many payloads being sent onboard the next Mars rover from NASA, including MOXIE. These payloads will attempt to tackle several science objectives, including the continued study of Martian geology and the search for life. MOXIE is shown in greater detail in Figure 2.

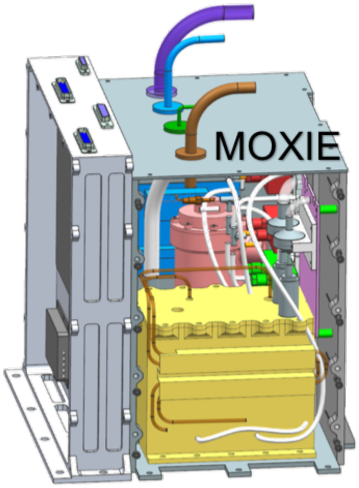

Figure 2: MOXIE Schematic.

MOXIE is primarily composed of three subsystems: the compressor system, the solid oxide electrolysis (SOXE) system, and the process monitoring and control system. These systems, when functioning together, combine to pull in atmospheric gas on Mars, compress it, convert it to oxygen, measure its composition and production rate, and release the products back into the atmosphere. An expanded view of MOXIE highlighting these subsystems is shown in Figure 3.

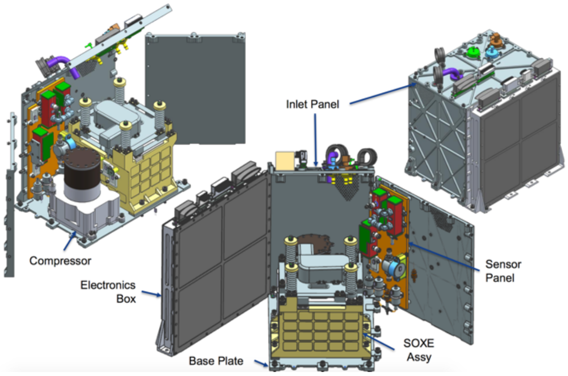

Figure 3: MOXIE Exploded View

Compressor Subsystem

The compressor system acquires and compresses the Martian atmosphere by way of a scroll pump. A scroll pump is composed of two spiral-like structures superimposed on top of one another. In the case of MOXIE, one of the scrolls is fixed while the other orbits within it. This orbiting motion results in small pockets of air being compressed and pumped into the system. A cut-away view of a scroll pump is shown in Figure 4.

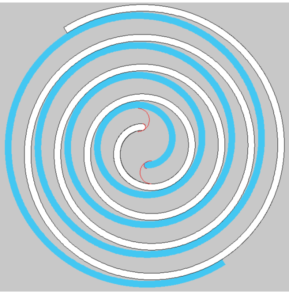

Figure 4: Scroll compressor sectional view. Credit: JPL

The Martian atmosphere is drawn first through a HEPA filter by the scroll compressor in order to remove dust and particulates that could damage the internals of MOXIE. As the atmosphere passes through the scroll pump, it is compressed from around 7 mbar - the ambient pressure on Mars - to 0.7 bar. SOXE is designed to operate at 0.7 bar, and as such, the majority of testing and characterization work has been done at this pressure.

SOXE Subsystem

Solid oxide electrolysis (SOXE) is a heritage chemical engineering technology. It has been used in the nuclear industry, for example, to generate hydrogen gas from water[2]. However, the SOXE used on MOXIE takes a relatively new and unexplored approach: creating oxygen from carbon dioxide without the assistance of water. This is called “dry” electrolysis, and has been studied and developed for MOXIE in recent years.

SOXE is the key technology that drives oxygen production in MOXIE. A SOXE cell consists of an Yttria-Stabilized Zirconia (YSZ) electrolyte membrane that is sandwiched between a cathode and an anode. This is seen in more detail in Figure 5.

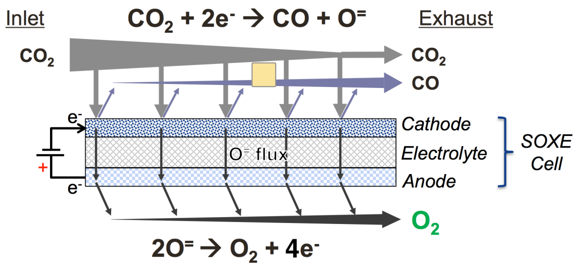

Figure 5: Schematic of SOXE cell and the chemical reaction that it drives

The cathode has a nickel coating that initiates the electrochemical reaction by providing a conductive avenue for electrons. Both the cathode and the anode are porous materials that establish a three-phase contact surface and allow diffusion of oxygen ions to occur through the electrolyte. When a voltage is applied to the system and carbon dioxide is flowed over the cathode, the following net reaction takes place.

$$2CO_2 \rightarrow 2CO + O_2$$

This reaction takes place over the entire surface of the cathode, as demonstrated in Figure 5. To improve oxygen production rate beyond that of a single cell, the SOXE system on MOXIE consists of 10 cells arranged in two stacks of 5 cells each.

Process, Monitoring, and Control Subsystem

The process, monitoring, and control (PMC) subsystem consists of a suite of sensors that measure pressure, temperature, voltage, and composition throughout MOXIE. Of particular interest are the four composition sensors, as they measure whether or not oxygen is being produced.

Three of these composition sensors use the nondispersive infrared radiation (NDIR) method to detect concentration, where IR radiation is passed through the gas residing in the sensor’s chamber. By analyzing the frequency bands on the spectrum that were attenuated in the chamber, it is possible to determine the composition of the gas. These sensors are tuned for CO and CO_2 to determine the composition of gas leaving the cathode and to search for leaks to the anode. The fourth sensor is a luminescence sensor and detects oxygen composition on a scale of 0 – 100% at the anode.

4. How Does the Model Work?

Modeling of MOXIE is useful for a couple of reasons. The first is that it helps the team understand how MOXIE behaves without spending too much time and money on costly hardware testing. The second is that it will be a useful tool during surface operations to predict how MOXIE will react to flight software commands and to troubleshoot anomalies that arise from Mars.

Simulink, a package contained within the MATLAB programming language, is a convenient way to build a dynamic representation of MOXIE. It allows a user to place blocks corresponding to a range of things, including pumps, resistors, PID controllers, and more generically, variables defined in an associated MATLAB file. In addition, Simulink allows connections to be made between these blocks, which can represent electrical cables, thermal contacts, and general passage of information, among others. As such, a time-domain model of MOXIE can be built in Simulink that simulates how MOXIE might operate when turned on.

The dynamic model that has been built models the gas flows, electrochemistry, electrical loop, thermal transfers, and control loops that are representative of the true MOXIE system.

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[2] O’Brien, J., Stoots, M., Herring, J., & Hawkes, G. (2006). “Hydrogen Production From Nuclear Energy Via High Temperature Electrolysis.” *1st Energy Center Hydrogen Initiative Symposium.*

1. *Electrochemistry*

The electrochemistry in SOXE is driven by the following equation:

$$V_{op} = V_{Nernst} + V_{Act} + I * \frac{ASR_i}{A}$$

where V_{op} is the operating voltage that represents the voltage actually seen by the SOXE cell, V_{Nernst} is the Nernst voltage, V_{Act} is the activation voltage, I is the current in the cell, ASR_i is the intrinsic Area Specific Resistance (ASR) of each cell, and A is the area of each cell that is exposed to electrochemistry. While a full analysis of these variables will not be explored in this paper, a brief explanation of the Nernst Potential will serve to highlight an important aspect of electrochemistry in MOXIE.

The Nernst Potential

The Nernst potential is a quantity that represents the voltage at which a particular electrochemical reaction will take place. For a given set of input parameters (temperature, pressure, and chemical composition), each chemical reaction has its own particular Nernst potential. In order to achieve conversion of carbon dioxide to oxygen, for example, the Nernst potential of the following reaction must be surpassed.

$$2CO_2 \rightarrow 2CO + O_2$$

For the operating conditions of MOXIE, which are taken nominally to be 800 °C, 0.7 bar, and an initial composition of gas equal to that found on Mars, the Nernst potential turns out to be:

$$V_{Nernst} = 0.9208\,V$$

for each cell. Therefore, if the voltage applied to each cell surpasses 0.9208 V under these conditions, carbon dioxide will begin to decompose into carbon monoxide and oxygen ions. This is what MOXIE aims to do, as its goal is to produce oxygen.

Importantly, there is also a Nernst potential for an unwanted side reaction that can occur in MOXIE: the decomposition of carbon monoxide into solid carbon and oxygen ions. This is shown below:

$$2CO(gas) \rightarrow 2C\ (solid) + O_2(gas)$$

This reaction causes solid carbon deposition on the cathode of each SOXE cell, which increases its resistance and ultimately leads to performance-reducing degradation. Therefore, it is critical that SOXE is operated *above* the Nernst potential for CO_2 decomposition but *below* the Nernst potential for CO decomposition. By fitting into this voltage window, oxygen will be produced and the cell will not experience significant degradation from carbon deposition.

2. *Electrical Loop*

One of the recent updates to the model was the inclusion of a fully functional electrical loop. MOXIE's core function – producing oxygen – is enabled by the electrical circuit that runs through SOXE. First, a voltage is commanded to MOXIE. The voltage level is chosen on the basis of enabling production of at least 6 g/hr of oxygen while staying under the Nernst potential for carbon formation. As the voltage is applied to the stack, it passes through the individual cells, which have their own resistance specified by their intrinsic ASR. The current that results from this circuit is representative of the flow of oxygen ions through the cells. This current is measured and fed back through a PI controller, which compares its signal to a target current and adjusts the commanded voltage accordingly for each stack.

Simscape is a tool that allows for the rapid development of physical systems within Simulink. It was chosen as a means to represent the electrical system of MOXIE because of its visual appeal. The process described above is modeled via Simscape. A view of the electrical system as a whole is detailed in Figure 6.

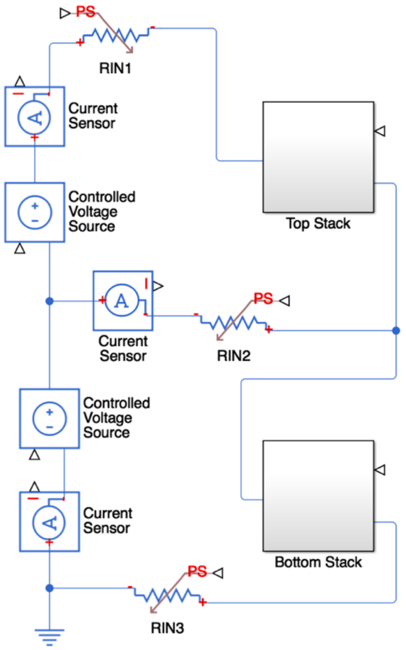


Figure 6: Simscape Electrical Loop of MOXIE

As can be seen from the image, the electrical loop model on the top half begins with a controlled voltage source and passes through a current sensor and a resistor before entering the stack of SOXE cells. It then either passes to the bottom stack or through the middle wire that exists between stacks, which is represented as an additional resistor. The bottom stack has a similar loop, which is shown in the bottom half of the image. It is important to note that the voltage commanded to the top and bottom voltage sources, referred to throughout this paper as VT_OUT and VB_OUT, are commanded by two identical PI controllers.

3. *Thermal Transfers*

In addition to the electrical loop, a thermal loop was also added in order to model the heat flow throughout the system as well as the temperature controller. The profile of heat exchange within the stack is critical to model accuracy, as the temperature of the cells affect a wide range of operating parameters, such as the Nernst potential and activation potential. The thermal modeling of cell #1 of the SOXE stack is in Figure 7.

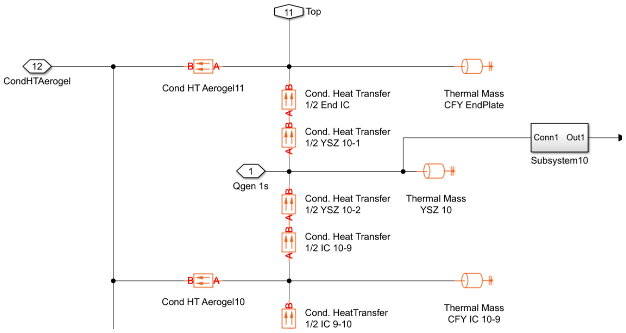


Figure 7: Section of Simulink thermal loop that represents the heat conduction around Cell #1 in the SOXE stack

In order to understand the figure, begin with the “Qgen 1s” block. This is an input parameter that represents the heat generated or consumed by the electrochemical reaction itself. From there, heat will spread upwards and downwards to the Yttria-Stabilized Zirconia (YSZ) electrode material, through the interconnect (IC) material that separates each cell, and either out the top of the stack or down to the next cell in line (not shown). This is modeled for all cells, and was added to the Simulink model as part of a greater thermal modeling loop.

4. *Control Loops*

Three control loops exist in MOXIE: the pressure controller, the temperature controller, and the voltage controller. The pressure controller utilizes a downstream pressure sensor to control the compressor rotation rate; if the pressure is below its setpoint, it will increase the RPMs of the compressor in order to increase compression and therefore internal pressure. The temperature controller uses temperature feedback to bring the stack up to temperature and maintain it at 800 °C during the electrolysis operation. The temperature is controlled by two heaters, one on the top and one on the bottom of the SOXE stack. A small heat gradient has been observed from the stack ends to its middle, but it is not expected to significantly impact performance. Finally, the voltage controller uses a current reading from the stack to determine what voltage to command to the stacks. All controllers are PI controlled.

5. Development of a GUI

The development of a Graphical User Interface (GUI) was necessary in order to allow people other than the model developers to run the simulation and gain useful information from it. The primary targets were the members of the MOXIE science and operations teams. The complexity of the Simulink model is demonstrated below in an image of its Level 0 configuration.

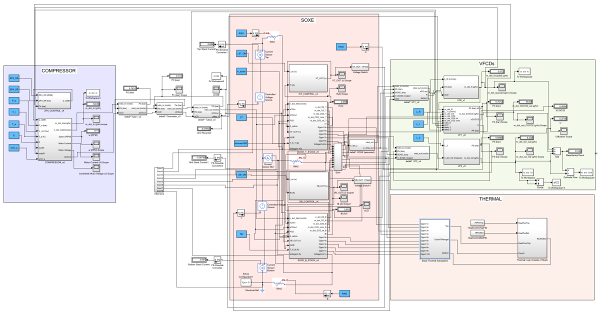
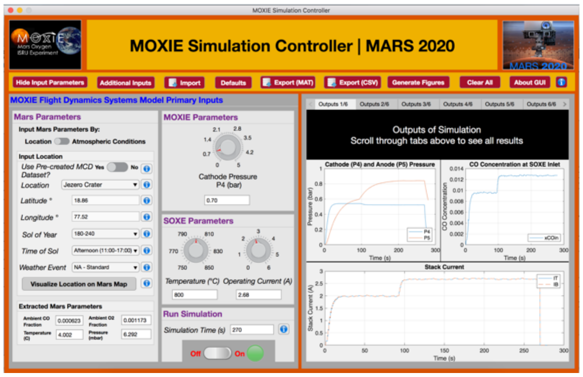


Figure 8: Level 0 view of the consolidated, dynamic model of MOXIE. Notice its complexity and perceived difficulty of use.

Note that within each gray box, another subsystem exists. This continues to partition up to five layers deep in some cases. While the model developers are comfortable altering variables and running simulations with this model, it would require significant training for others to do the same. This is what brought about the need for a simple-to-use GUI.

The GUI was created using MATLAB’s app developer. To use it, a user will select the appropriate inputs for the given scenario and click “run”. The GUI then exports those variables to the Simulink model and activates it. After the simulation completes, the GUI automatically loads in the results from the Simulink model and displays them on the GUI interface. An image of the final GUI is shown in Figure 9.



Use Pre-created MCD Dataset? Yes No
Location Jezero Crater
Latitude ° 18.86
Longitude ° 77.52
Sol of Year 180-240
Time of Sol Afternoon (11:00-17:00)
Weather Event NA - Standard
Ambient CO Fraction 0.000623
Ambient O2 Fraction 0.001173
Temperature (C) 4.002
Pressure (mbar) 6.292
Cathode Pressure P4 (bar) 0.70
Temperature (°C) 800
Operating Current (A) 2.68
Simulation Time (s) 270

Figure 9: GUI that is used to control the dynamic model of MOXIE. Inputs are on the left side and output plots are on the right.

On the left half of the GUI are the inputs that a user might want to change in order to see how they affect oxygen production performance of MOXIE. These include the physical location of MOXIE on Mars, whether or not there is a special weather event like a global dust storm, and the pressure and temperature setpoints of SOXE. The right half of the GUI contains several tabs of output figures that populate when the simulation is finished running. These show time-series plots of oxygen production, internal pressure, stack current, and gas composition, among others.

6. Summary

This paper is being submitted to detail the modeling efforts behind MOXIE. A dynamic model has been developed, tested, and validated against data taken at NASA's Jet Propulsion Laboratory. The model simulates MOXIE's performance under a range of input conditions, and includes modeling of MOXIE's control loops, oxygen production, and thermal behavior. In addition, a GUI was developed to allow members of the MOXIE science team to easily understand and operate the complex model.

MOXIE is an important step in the effort to put humans on Mars. It will demonstrate the usefulness of the Martian atmosphere in producing oxygen for rocket propellant. This application of ISRU on Mars is critical to reducing the cost of a human mission to the planet, one of the main barriers that is faced by human exploration of space today.

Acknowledgements

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