Daniela Machnik is a graduating senior at Colorado School of Mines earning her B.S. in petroleum engineering with a minor in computer science and a McBride honors minor in public affairs in May 2019. Daniela's interest for drilling in extreme environments and the exploration of new horizons drew her to the opportunity of modeling water ice extraction from the lunar South Pole as an undergraduate researcher with Dr. Luis Zerpa, research professor in the Petroleum Engineering department at Mines. In May 2018, Daniela and her teammates won the NASA RASC-AL engineering competition presenting the lunar polar sample return architecture POSEIDON and an innovative approach to capturing icy regolith cores from lunar permanently shadowed craters. After earning her M.S. in computer science next year and obtaining valuable industry experience, Daniela wants to return to academia to pursue a PhD in data science and artificial intelligence.

Preliminary Modeling Evaluation of Water Ice Extraction from Lunar Permanently Shadowed Craters by Direct Heating of Icy Regolith

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Abstract

This work sets the foundation for preliminary modeling of water ice extraction from lunar permanently shadowed craters. Analysis of the research results indicates that (1) favorable phase changes at low temperatures and pressures (though not in-situ conditions) occur and lead to the upward migration of water vapor through the regolith and out of the crater surface, (2) the appearance of the liquid phase significantly reduces the timesteps in the simulation and limits predictive modeling capabilities, (3) adjusting the reservoir model to true lunar conditions requires specific modification of the Fortran base code of TOUGH+, (4) the lack of a void-like phase prevents realistic modeling of mass and energy balance in lunar permanently shadowed craters, (5) a stepwise heat source may yield greater water production for deeper ice reservoirs than a single heat element. The reservoir simulation investigated phase saturation changes of water iced buried in lunar regolith over a three-day period from a 25 W continuous heat source.

Background

In 2009, NASA launched its Lunar CRater Observation and Sensing Satellite (LCROSS) and identified the presence of hydrogen at the lunar South Pole via the impact of LCROSS's Centaur rocket inside Cabeus crater. The concentration of water ice was determined from infrared spectroscopy imaging of the vapor plume that followed the impact. Theories suggest that the deposition of water on the lunar surface results from the collision between hydrogen bearing asteroids and the moon approximately 3.9 billion years ago [1]. Today, water ice is solely found at the polar regions inside permanently shadowed craters where evaporation evaporation of the resource is inhibited. One year after LCROSS, the estimated total in-situ water volume in lunar permanently shadowed craters amounted to 1.3 trillion pounds [2].

The discovery of extraterrestrial water reserves in our solar system has motivated many studies on the possibility of using said reserves on future cislunar missions. Unencumbered by water restraints, human exploration could expand far beyond the reach of Earth's closest celestial neighbor.

Objective

Two extraction methods may be suitable for the retrieval of useable quantities of lunar water ice: the removal of bulk material followed by extensive rock processing, and the capture of gaseous water via heat induced in-situ phase changes and phase migration through regolith. The latter method takes a petroleum engineering approach to the problem leveraging extraction principles, whereas the former method involves methodologies from mining engineering. While both methods have merit, the latter approach presents the potential for greater efficiency as it does not require the transport of bulk material, facilitating remote controlled lunar operations. This study aims to test the viability of applying extraction principles to extracting gaseous water from icy lunar regolith.

Approach

In 2006, a study on thermally induced flow of water in Martian permafrost was explored using the simulator TOUGH+ by researchers George J. Moridis and Karsten Pruess of Lawrence Berkeley National Laboratory [3]. The practical similarities of this study to the issue of lunar water ice extraction inspired a similar approach in this paper. The TOUGH+ code environment consists of a base code, with methods characterizing the physiochemical properties of water and the geomechanical properties of reservoir rock, and a hydrate module describing the equation of state of the hydrate phase. TOUGH+ is written in Fortran 95/2003 and is run directly from the command line.

System Description

The reservoir characteristics in the model were developed from published geologic data [4], [5]. Research conducted by NASA and Honeybee Robotics indicate that the distribution of water ice in lunar permanently shadowed craters varies with depth. It is expected that the greatest ice saturations are located within the first 2.5 m of the crater subsurface and decrease significantly below the mixed ice and deep ice layers. Below a depth of 5 m, regolith has a negligible water saturation [6]. The geology of this work's reservoir model was designed to replicate lunar polar regolith with ice saturation estimates ranging from 23 % in lunar top soil to below one percent in deep regolith. The reservoir was split into five water ice bearing zones that are bounded by a high density breccia formation below. The upper zone consists of loose rock fragment and features low density, high porosity and high permeability. As regolith becomes more compacted at greater depths, rock density increases while matrix porosity and permeability decrease.

Above the crater surface, regolith is exposed to the lunar atmosphere (a thin layer of gas) and a water ice collection plate. Similar to the condensation of gaseous water on cold surfaces at standard conditions, gaseous lunar ice is expected to deposit on a cold collection plate above the regolith and grow to collectable ice chunks. In the simulation, the plate has a 15 cm clearance to the ground.

The flow of lunar water ice was modeled with an in-situ reservoir temperature of -90 C and a reservoir pressure of 2.89E+04 Pa (4.19 psi). The pressure of the atmosphere in the simulation was 2.89E+03 Pa (0.419 psi) which approximated the lowest pressure allowed with TOUGH+. The atmosphere was treated as a rock medium with 100% porosity (the permeability was low at one Darcy and calls for refinement in future simulations). A cylindrical 25 W heat source was buried in the rock and emitted heat at depths between 0.15 m and 0.65 m below the crater surface. The model consisted of 2500 grid blocks in the Cartesian XZ plane (2D model). The vertical axis encompassed z = +0.25 m to z = -4.65 m and the horizontal axis x = 0.1 m to x = 9.90 m. The mesh was altered throughout the study for XZ and YZ coordinate systems and visualized in MATLAB.

Results

The 25 W heat source continuously emitted thermal energy into the reservoir over a three-day period. The temperature difference between the outer reservoir and the heated rock in the vicinity of the source reached 340 C after three days. The ice phase disappeared entirely around the heat source within the first 24 hours of the simulation and the saturation continued to decrease over the course of the following two days. The gaseous phase spread spherically outward from the heat source, and liquid water was formed in the transition regions between ice and gas. The total ice mass inside the reservoir decreased by 8.913 kg, while the liquid and gas mass increased by 8.904 kg and 0.009 kg, respectively. Ice accumulated below the heat source and completely disappeared at the crater surface after three days. Simultaneously, the saturations of liquid water and water vapor assumed lower values below the heat source and greater values in the upper regolith. The spreading of water ice below the source derived from newly produced vapor that deposited as ice upon contact with cool regolith. The mobile liquid and gaseous phases horizontally beside or directly above the heat source thermally expanded and migrated upward towards the lunar atmosphere and were not cooled as quickly, thus reducing the saturation of ice in those regions. The endothermic phase change resulted in a slight lowering of the ambient temperature and could have facilitated the deposition of newly formed water vapor in regions far enough from the heat source. The liquid saturation after the third day indicates the spreading of liquid into the atmosphere, where z > 0 m. Under lunar conditions, these quantities would be gaseous and the collection plate above the reservoir could capture the escaped gas. The pressure around the heat source increased from 2.89E+04 Pa to 4.0E+04 Pa

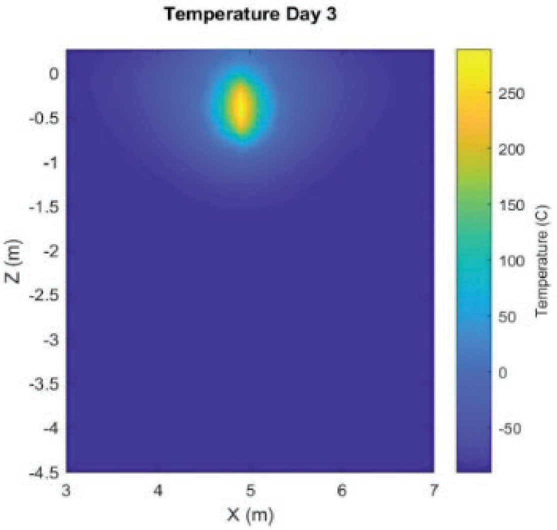

Figure 1 Temperature Distribution in Regolith Day 3, MATLAB

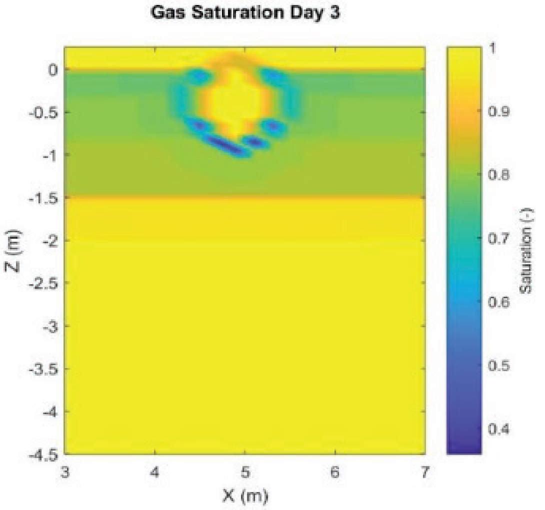

Figure 2 Gas Saturation in Regolith Day 3, MATLAB

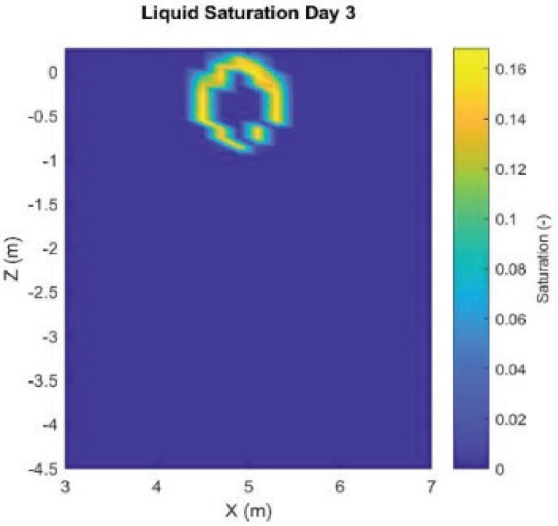

Figure 3 Liquid Saturation in Regolith Day 3, MATLAB

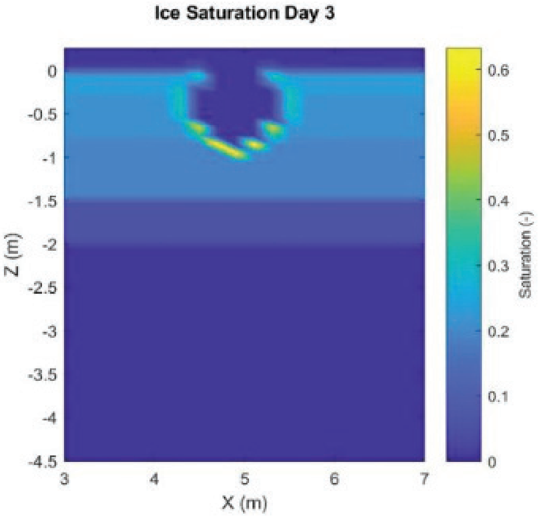

Figure 4 Ice Saturation in Regolith Day 3, MATLAB

following the thermal expansion of sublimed in-situ water ice. The following figures demonstrate the dynamic reservoir conditions of icy regolith during the three-day heat injection.

Discussion

The appearance of the liquid phase during the first day reduced the timestep of the simulation due to failed computational convergences. The instantaneous "thermal shock" of the reservoir from the introduction of the heat source at time zero significantly increased the complexity of the numerical model. Greater intensities reduce the simulation time but result in faster water recovery.

The accumulation of water ice below the heat source marks an important observation in the results (Fig. 4). The deposition of water ice around a single source could lead to a significant reduction of available pore space for outward water vapor movement. An elongated source, consisting of several independent heat stages, could potentially solve this problem via timed heat source operation. The source stack could carry water ice quantities upward sequentially and, thereby, increase the production yield in (deep) crater reservoirs.

The greatest limitation of the code for this specific application lies in the restrictions of reservoir temperature and pressure inputs. The numerical foundations of the hydrate module in TOUGH+ are based on the experimentally observed pressure and temperature behaviors of hydrate. The lowest tested temperature, -124 C, is the minimum allowable temperature for the Moridis correlations describing equilibrium hydration pressure and hydration dissociation heat. Reservoir simulation at - 124 C lead to the appearance of liquid water in lunar regolith, which does not reflect true phase behavior at cryogenic conditions in permanently shadowed craters. The allowable temperature range in TOUGH+ is encoded in while loops in the hydrate properties module. The base code should be modified (e.g. reduction of minimum temperature and pressure) such that water extraction can be correctly modeled with TOUGH+. Finally, to simulate water production from a high intensity heat source with TOUGH+, it is recommended to investigate the possibility for time-sensitive heat injection by means of continuous updating of the initial conditions during the simulation.

Conclusions

1. Heat injection into icy regolith creates favorable phase changes at low temperatures and pressures, subliming and melting water ice. Water vapor expands radially outward from the heat source and rises upward through media of greater porosity and permeability, and lower pressure. The accumulation of liquid water above the crater surface ($z > 0$ m) in the simulation indicates that production (with a collection plate) would be feasible.

2. The appearance of liquid water significantly reduces the maximum possible timestep of the simulation due to the increased modeling complexity associated with the phase change.

3. Lowering the ambient temperature to cryogenic conditions (approx. 50 K) requires modification of the Fortran base code of TOUGH+. The minimum allowable default temperature is -124 C (Moridis equation).

4. While indicating realistic phase changes under the specified input conditions for the simulation, TOUGH+ does not incorporate true conditions of lunar water ice reservoirs. The code requires an amplification to include a void-like phase.

5. To produce water ice from lower depths, a stepwise heat source, which injects heat at specific depths on a time schedule could be implemented.

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