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Oxygen production from lunar regolith: thermochemical equilibrium, pyrolysis kinetics, and electrochemical pump modeling

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Abstract: The production of oxygen from lunar regolith is essential for sustaining long-term human presence on the Moon. While thermal pyrolysis can effectively release oxygen from the regolith, the resulting gas stream contains impurities that must be removed to obtain high-purity oxygen. This study investigates the use of an electrochemical oxygen pump to concentrate and purify oxygen from the dilute pyrolysis product gas. A two-dimensional multiphysics model was developed in COMSOL to simulate the transport and electrochemical phenomena within the pump. The simulation results demonstrate effective oxygen capture even at low oxygen partial pressures and moderate current densities. At an inlet oxygen partial pressure of 0.04 Pa and an applied current density of 5000 A/m^2, the model predicts a capture rate of 42% and a Faradaic efficiency exceeding 98%. Transient analysis reveals that while the capture rate is sensitive to fluctuations in oxygen partial pressure, the cell voltage remains stable under varying conditions. These findings provide valuable guidance for the design and operation of integrated oxygen production systems for future lunar missions.

Keywords: in-situ resource utilization (ISRU); electrochemical oxygen pump; numerical simulation; oxygen capture; oxygen purification

1. Introduction

As deep-space exploration advances, the Moon has emerged as a primary target for long-term human habitation. Sustaining lunar bases requires reliable supplies of oxygen for life support and propulsion [1], but resupply from Earth is costly and logistically constrained [2,3]. This has driven growing interest in in-situ resource utilization (ISRU), with lunar regolith identified as a promising oxygen source due to its high oxygen content—approximately 40–45 wt%, primarily bound within silicates and metal oxides (see Figure 1) [4,5].

Several techniques have been developed to extract this oxygen, including hydrogen reduction, carbothermal reduction, molten electrolysis, and gas-phase pyrolysis [1]. Among these, gas-phase pyrolysis offers distinct advantages: it involves a relatively simple process and is well suited to the lunar

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environment, leveraging both the natural vacuum and available solar energy [6]. However, the gas stream produced by pyrolysis typically contains impurities such as SiO and TiO, which degrade oxygen purity and limit direct usability [7].

Electrochemical oxygen pumps (EOPs) based on solid oxide electrolytes provide a promising solution. These devices selectively transport oxygen ions, enabling efficient capture and purification of oxygen from mixed-gas streams [8–11]. Nevertheless, their performance under the low-pressure conditions characteristic of the lunar surface remains poorly understood. To address this gap, the present study develops a multiphysics model using COMSOL to evaluate EOP behavior under both steady-state and transient conditions. The findings aim to support the design and optimization of integrated lunar oxygen production systems based on regolith pyrolysis.

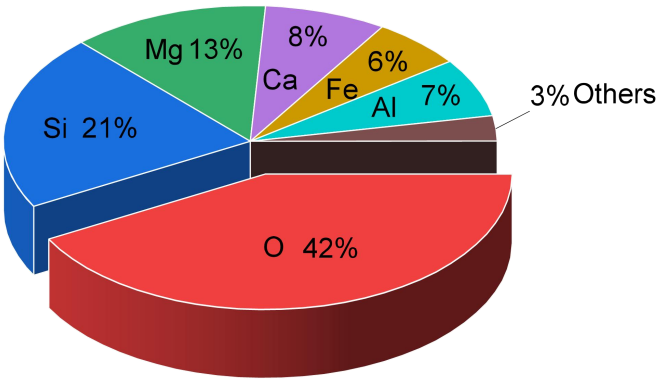


Figure 1 Elemental composition of lunar regolith.

2. Methods

This study combines thermochemical analysis, pyrolysis experiments, and multiphysics simulation to investigate the coupling of gas-phase pyrolysis with an EOP for in-situ lunar oxygen production. Thermochemical equilibrium calculations were performed using HSC Chemistry to identify key reaction pathways and gaseous species. Pyrolysis experiments on a lunar regolith simulant were conducted to characterize gas-release behavior, and a COMSOL Multiphysics model was developed to evaluate EOP performance under lunar-relevant conditions.

The lunar regolith simulant HIT-LRS1 was used for all pyrolysis experiments. Approximately 200 mg of powder sample was heated to 1400℃ in an alumina crucible under flowing argon (200 mL/min). Heating rates of 5, 10, and 15 ℃/min were applied to assess kinetic effects. Mass loss was continuously recorded by thermogravimetry (TG), while evolved gases were monitored by mass spectrometry (MS). The main ionic fragments tracked included m/z =16 (O), 18 (H_2O), 28 (CO/Si), 32 (O_2), and 44 (CO_2), enabling identification of oxygen-containing species and potential impurities

A two-dimensional axisymmetric model of an EOP was developed in COMSOL to simulate oxygen capture under low-pressure lunar conditions. The model geometry comprises cathode and anode flow channels, porous electrodes, and a dense yttria-stabilized zirconia (YSZ) electrolyte. The following assumptions were adopted: ideal gas behavior, laminar and incompressible flow, and homogeneous and isotropic porous electrodes. Electrochemical kinetics at the three-phase boundaries were described by the Butler–Volmer equation. Gas transport within the channels and porous electrodes was modeled using convection–diffusion equations with Maxwell-Stefan diffusion and Knudsen corrections to account for

molecular and Knudsen diffusion regimes. Species source and sink terms due to electrochemical reactions were governed by Faraday's law.

The cathode inlet oxygen partial pressure was varied from 0.01 to 10 Pa, with inlet velocities ranging from 0.5 to 5 m/s. The anode side was continuously swept to maintain a low oxygen partial pressure, establishing a driving force for oxygen-ion transport. The cathode was grounded, and an applied voltage of 0.5–2.0 V was imposed at the anode. Both steady-state and transient simulations were solved using the finite element method. Faradaic efficiency was defined as the ratio of the actual oxygen flux through the electrolyte to the theoretical flux predicted by Faraday's law.

3. Results

This section combines thermochemical calculations, pyrolysis experiments, and multiphysics simulations to evaluate the coupled lunar regolith pyrolysis–EOP route. The main temperature range for oxygen release and impurity formation is first identified, the gas-evolution behavior is then verified by TG-MS, and the oxygen-capture performance of the EOP under low oxygen partial pressure is finally assessed.

The results show that lunar regolith can release oxygen at high temperature, but the product gas contains impurities and therefore requires subsequent capture and purification. The simulations further indicate that the EOP can achieve effective oxygen transport and separation, supporting the design of an integrated oxygen-production system.

3.1. Thermochemical equilibrium simulation

HSC thermochemical equilibrium calculations were performed for the lunar regolith simulant HIT-LRS1 to evaluate its oxygen-release behavior under high-temperature, low-pressure conditions, as shown in Figure 2. The input composition mainly included SiO_2, FeO, Al_2O_3, MgO, CaO, and TiO_2, and the calculations were conducted over 800–3000 K and 10^{-6}–10^{-2} bar to approximate the lunar vacuum environment. The results show that almost no significant gaseous products are generated below 1200 K. When the temperature increases to 1300–1500 K, FeO and TiO_2 begin to decompose, releasing O_2 together with small amounts of volatile impurities such as SiO and TiO. In the range of 1500–2000 K, oxygen evolution becomes significant and the oxygen partial pressure rises above 10^{-3} bar, indicating that this is the main oxygen-release window. However, the simultaneous generation of impurity gases limits the direct utilization of the product stream and highlights the need for subsequent oxygen capture and purification.

3.2. Thermal decomposition experiments

Pyrolysis experiments were conducted to verify the thermochemical predictions and to characterize the actual gas-release behavior of the lunar regolith simulant. As shown in Figure 3 (a-c), the TG curves exhibit a three-stage mass-loss behavior. The initial stage is mainly associated with the release of adsorbed water and weakly bound volatiles, followed by a pronounced mass-loss region corresponding to the main oxide decomposition stage, after which the curves gradually stabilize. With increasing heating rate, the major mass-loss region shifts to higher temperature/time and becomes sharper, indicating thermal lag and kinetic limitations.

The MS results in Figure 3 (d-f) further reveal the gas evolution characteristics. O_2 (m/z = 32) is the dominant gaseous product and mainly appears in the range of 1100–1350 ℃, in good agreement with the HSC prediction. The signal at m/z = 28 suggests the co-release of SiO and CO, whereas the CO_2 signal (m/z = 44) remains weak. In addition, lower heating rates lead to smoother oxygen release, which is favorable for continuous downstream capture, while higher heating rates produce sharper transient oxygen peaks and thus impose stricter control requirements on the purification stage.

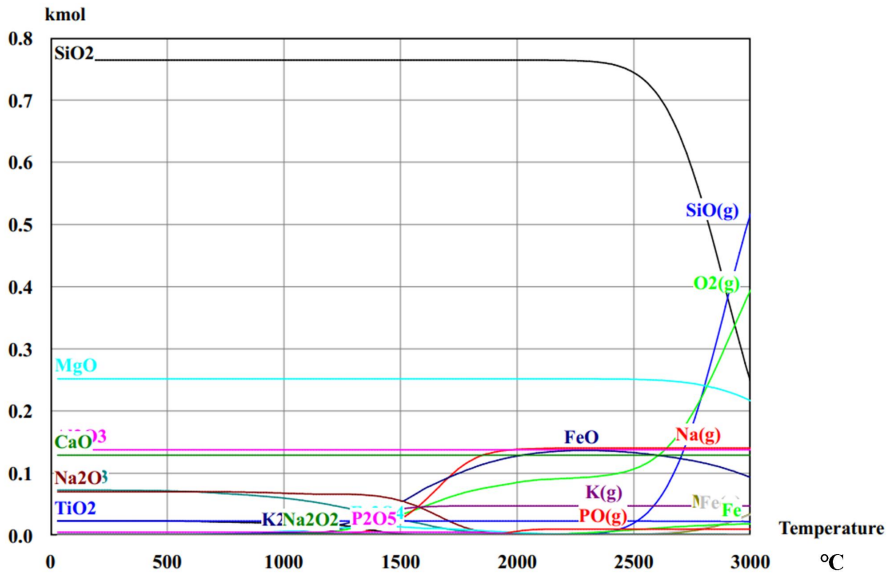


Figure 2 Thermochemical equilibrium results of the lunar regolith simulant calculated by HSC Chemistry.

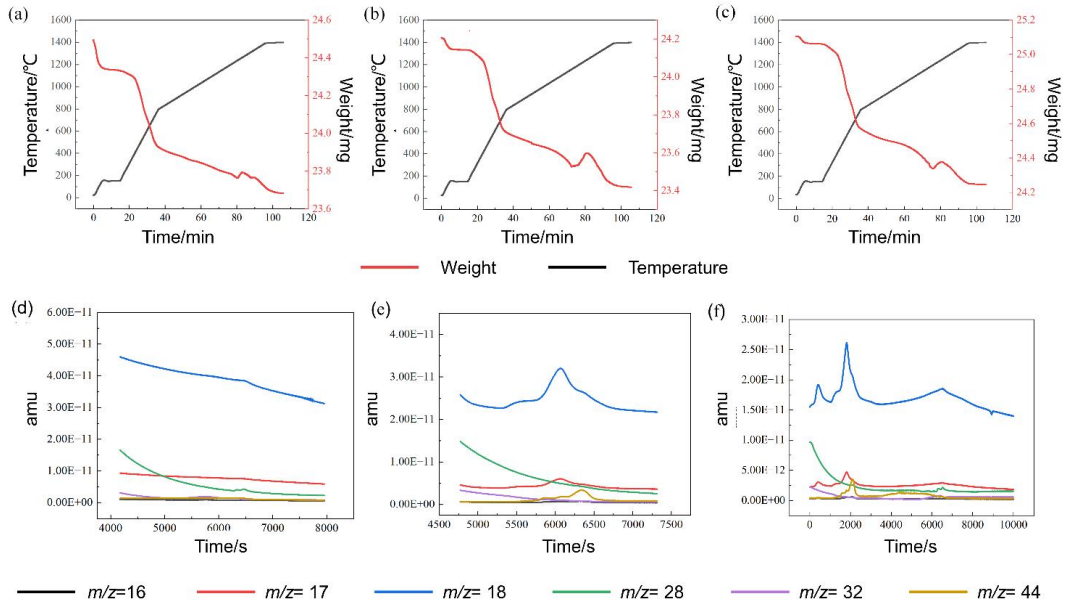


Figure 3 Temperature and sample mass as a function of time for the simulated lunar regolith at different heating rates: **(a)** 5 °C/min, **(b)** 10 °C/min, **(c)** 15 °C/min; Time-dependent profiles of monitored mass fragments at different heating rates: **(d)** 5 °C/min, **(e)** 10 °C/min, **(f)** 15 °C/min.

3.3. Multiphysics simulation of EOP

The reliability of the EOP model was confirmed by grid-independence analysis and literature-based current-voltage validation, as shown in Figure 4. The predicted oxygen capture rate becomes nearly unchanged when the mesh number exceeds 1000, indicating adequate numerical convergence. In addition, the simulated current-voltage curves agree well with literature data, with deviations below 5%. Under most operating conditions, the predicted Faradaic efficiency remains within 97%–99%, demonstrating that the model can reliably describe oxygen transport and capture behavior.

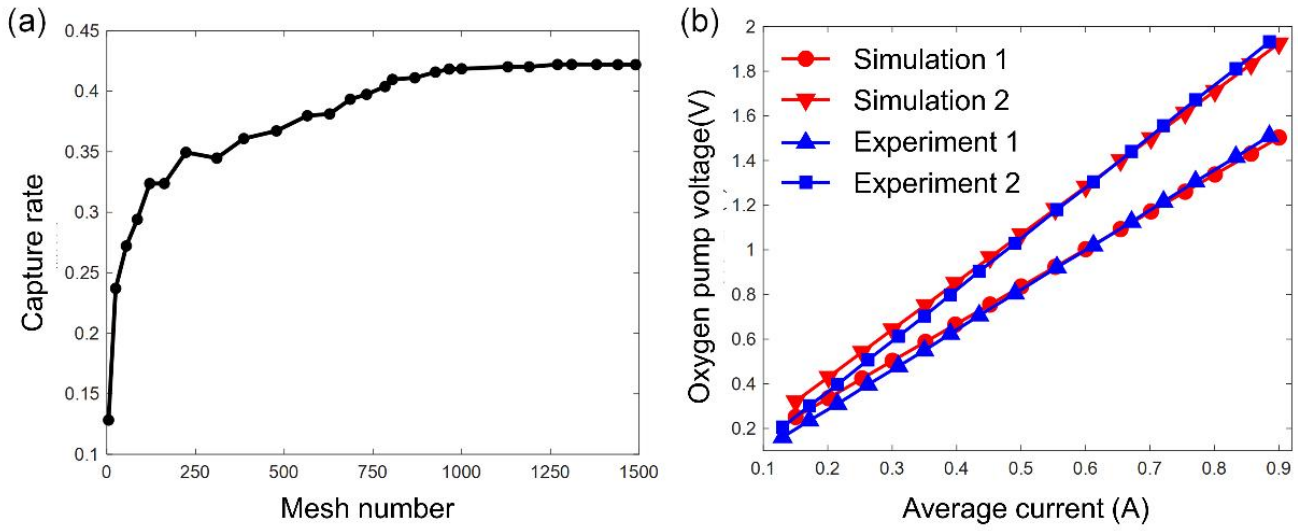


Figure 4 Numerical verification and validation of the EOP model. **(a)** Grid independence verification of the developed multiphysics model; **(b)** Current-voltage curve for validating the numerical model by comparing with experimental results.

The steady-state and transient simulation results are summarized in Figure 5. Under steady-state conditions, oxygen capture is strongly affected by cathode oxygen partial pressure, anode pressure, current density, and inlet velocity. Lower cathode oxygen partial pressure significantly improves capture performance; for example, the capture rate reaches 42% at = 0.04 Pa and 5000 A/m^2. The Faradaic efficiency remains high over most operating conditions, indicating that nearly all of the current contributes to oxygen-ion transport. By contrast, increasing anode oxygen partial pressure strongly suppresses capture, and the capture rate decreases rapidly when it exceeds about 3.5 Pa. Inlet velocity also affects performance: lower velocity favors oxygen residence and diffusion, whereas higher velocity causes oxygen slip and reduces capture efficiency.

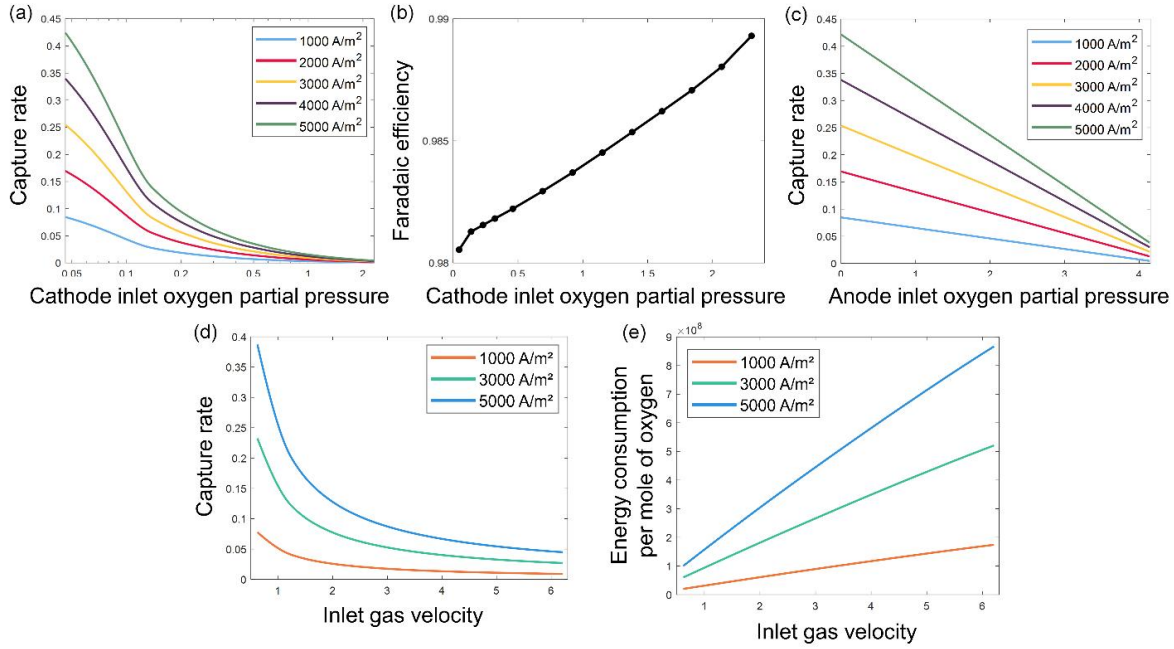


Figure 5 At different current densities: **(a)** Oxygen capture rate *versus* cathode inlet oxygen partial pressure; **(b)** Faradaic efficiency *versus* cathode inlet oxygen partial pressure; **(c)** Oxygen capture rate *versus* anode inlet oxygen partial pressure; **(d)** Oxygen capture rate *versus* inlet gas velocity; **(e)** Energy consumption per mole of oxygen *versus* inlet gas velocity.

4. Conclusion

The purpose is to interpret and compare results and point out the features and limitation of the work. Relate the research to current knowledge in the field.

In this study, thermochemical calculations, TG-MS experiments, and multiphysics simulations were combined to investigate the coupled lunar regolith pyrolysis—EOP route for in-situ oxygen production under lunar-relevant conditions. HSC equilibrium analysis and pyrolysis experiments were used to characterize oxygen release and impurity evolution from lunar regolith simulant, while a two-dimensional axisymmetric COMSOL model was developed to evaluate oxygen capture and purification by the EOP under both steady-state and transient conditions. The main conclusions are as follows:

- High-temperature pyrolysis enables oxygen release from lunar regolith. HSC calculations and TG-MS experiments consistently show that oxygen can be released under high-temperature and low-pressure conditions, with the main oxygen-evolution window located at 1300–2000 K and accompanied by trace impurities such as SiO and TiO.
- Heating rate strongly influences the oxygen-release behavior. The TG-MS results indicate that heating rate affects the onset, intensity, and stability of gas evolution. Lower heating rates are more favorable for smoother oxygen release, while higher heating rates produce sharper transient peaks and impose stricter requirements on downstream purification.
- EOP performance is mainly governed by gas-pressure and transport-related parameters. The two-dimensional axisymmetric model shows that oxygen capture is primarily controlled by cathode oxygen partial pressure, anode pressure, current density, and inlet velocity. Under low oxygen partial-pressure conditions, the Faradaic efficiency can remain at a high level, approaching 99%.

- Low anode pressure is critical for efficient oxygen capture. Both steady-state and transient simulations demonstrate that maintaining a low anode-side oxygen partial pressure is essential for sustaining the driving force for oxygen-ion transport, while coordinated regulation of inlet flow and current density helps improve system stability under fluctuating operating conditions.
- The coupled pyrolysis—EOP route is feasible for integrated lunar oxygen production. These results provide both theoretical and experimental support for the design and optimization of integrated lunar regolith pyrolysis—EOP systems, and offer useful guidance for future in-situ oxygen production on the Moon.

Overall, the combined thermochemical, experimental, and simulation results demonstrate that the lunar regolith pyrolysis—EOP route is a feasible and promising strategy for integrated oxygen production and purification under lunar-relevant conditions. The present work provides theoretical and experimental support for the design and optimization of compact in-situ lunar oxygen production systems.

Declaration of Generative AI and AI-assisted Technologies

During the preparation of this manuscript, the authors used generative AI and AI-assisted technologies solely to improve the language, grammar, and readability of the manuscript. These tools were not used to generate research data, results, scientific interpretations, or conclusions. After using these tools, the authors carefully reviewed and edited the content as needed and take full responsibility for the accuracy, integrity, and originality of the manuscript.

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Authors' contribution

Conceptualization, Y.S., L.L. and B.W.; methodology, D.L. and L.J.; software, L.J.; validation, D.L., L.J. and P.W.; formal analysis, D.L. and L.J.; investigation, D.L.; resources, Y.S., L.L. and B.W.; data curation, D.L. and P.W.; writing—original draft preparation, D.L.; writing—review and editing, D.L., L.J., P.W., Y.S., L.L. and B.W.; visualization, D.L., L.J. and P.W.; supervision, Y.S., L.L. and B.W.; project administration, L.L. and B.W.; funding acquisition, Y.S., L.L. and B.W. All authors have read and agreed to the published version of the manuscript.

Conflicts of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Ethical statement

This study did not involve human participants, human data, human tissues, animals, or animal-derived materials. Therefore, ethical approval was not required.

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