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DOI

[10.1016/j.actaastro.2024.02.035](https://doi.org/10.1016/j.actaastro.2024.02.035)

Publication date

2024

Document Version

Final published version

Published in

Acta Astronautica

Citation (APA)

Gallbrecht, M. M., Cervone, A., & Vincent-Bonnieu, S. (2024). The Moon as an effective propellant source: A comprehensive exergy analysis from extraction to depot. *Acta Astronautica*, 218, 307-313.
<https://doi.org/10.1016/j.actaastro.2024.02.035>

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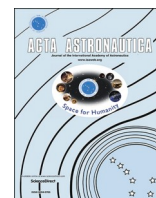
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The Moon as an effective propellant source: A comprehensive exergy analysis from extraction to depot

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ARTICLE INFO

Keywords:

Exergy
Moon
Propellant
Economic
Depot

ABSTRACT

Establishing a permanent lunar base has gained increasing attention since it offers opportunities for international cooperation and the commercialization of space, forming the foundation and testing ground for a human existence independent from Earth. Essential to future missions beyond cislunar space is the exploration and in situ processing of the Moon's resources, especially the sustainable production of energetic resources and propellants. Utilizing in situ generated propellants can dramatically reduce transportation costs by removing the need to source propellants from Earth. Resources on the Moon are limited, and the extraction of available resources are energy-intensive processes demanding advanced techniques and technologies. Consequently, one of the biggest challenges lies in developing process architectures with a positive energy balance, for which comprehensive analyses are still missing. The focus currently lies on the extraction of water ice from lunar regolith and the production of hydrogen and oxygen through water electrolysis. However, alternative fuel and process options may reduce the energy cost while providing equivalent energetic revenue. In the scope of this research, the infrastructure and technologies required for extraction, refining, and storing are assumed to exist in cislunar space; therefore, only the operating cost is considered. Exergy analyses of in situ extraction methods are conducted to investigate whether the required energetic budget allows sustainable implementation. The analysis includes extraction methods and propellant options to reveal the extent to which alternatives to hydrogen are feasible. Exergy analyses determine thermodynamic losses of energy flows giving the ground for process optimization. The exergy destructed represents the margin of improvement within the process architecture and thus reflects the process's thermodynamic and economic value while allowing a more distinct examination of energy use. Assuming the availability of water and carbon dioxide ice in permanently shadowed regions, the analysis shows that choosing methane instead of hydrogen in combination with oxygen as propellants can reduce the required exergy input by up to a third. An example mission allows to directly compare the operating cost of the extraction processes for the different propellant options. The mission entails a spacecraft propelled by a liquid bipropellant engine utilizing the extracted propellant and transporting a payload of the same propellant to a depot located in lunar near-rectilinear halo orbit (NRHO). Although abundant in space, the results suggest that hydrogen may not be the only or even energetically cost-effective resource for developing cislunar and Martian space infrastructures. Likewise, sustainable extraction of propellants suitable for current and future propulsion systems will foster humanity's reach further into the solar system.

1. Introduction

The human exploration of the Moon and Mars are receiving increasing interest in recent years. To sustain humanity's permanent reach beyond cislunar space, the exploration and in-situ utilization of lunar resources, i.e., sustainable extraction of energetic resources and

the generation of propellants, are imperative. Likewise, a permanent human lunar base implies the production of energy and materials for human activities and, if possible, the propellant required by interplanetary transfer vehicles to reach Mars and, in the future, other bodies of the solar system. In-situ generated propellants eliminate the need to source propellants from Earth and can significantly reduce transportation costs to locations beyond Earth and cislunar space. However,

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<https://doi.org/10.1016/j.actaastro.2024.02.035>

Received 13 December 2023; Received in revised form 14 February 2024; Accepted 23 February 2024

Available online 24 February 2024

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Nomenclature

c	concentration
Ex	exergy
ex	specific exergy
H	enthalpy
I_{sp}	specific impulse
l	number of atoms
M	molar mass
n	molar concentration
O/F	oxidizer to fuel ratio
p	pressure
Q	heat
R	universal gas constant
S	entropy
T	temperature
V	volume
v	velocity
W	work
w_v	effective exhaust velocity
x	mole fraction
y	mass fraction
Δ	change in
μ	chemical potential
τ	exergetic temperature factor

Subscripts

0	reference environment
---	-----------------------

ch	chemical
D	destruction
el	element
ex	exergetic
f	final
gen	generation
i	species i
i	initial
in	input
kin	kinetic
out	output
ph	physical
pot	potential
sh	shaft work
tot	total

Superscripts

0	standard
–	molar

Abbreviations

ISRU	in-situ resource utilization
NRHO	Near-Rectilinear Halo Orbit
O/F	oxidizer to fuel ratio
PSA	permanently shadowed area
wt%	by weight percent

lunar resources are scarce, and their extraction is energy intensive. Consequently, a significant challenge lies in developing energetically feasible process architectures incorporating advanced extraction and processing techniques and technologies. Here, comprehensive analyses of energy production and consumption processes on the Moon regarding the sustainability of ISRU processes and their energetic feasibility are still missing.

Volatile ices are expected to be present in PSAs in the Moon's polar regions [1–3]. Proposed extraction processes include the thermal mining of water ice from lunar regolith and the subsequent electrolysis into hydrogen and oxygen [4,5]. However, alternative fuels to hydrogen and process options may reduce extraction costs while providing equivalent energetic revenue.

Assuming the availability of water and carbon dioxide ice, the generation of hydrogen and methane as possible fuel options is investigated regarding their exergetic costs.

Exergy is a thermodynamic property that indicates the amount of useful work extractable from a system while it reaches equilibrium with its environment. A system has no exergy if it is in equilibrium with its reference environment, meaning when no difference in temperature, pressure, and chemical composition exists. Contrary to energy, exergy is only conserved for ideal and reversible processes, while exergy is destroyed in real processes [6]. Consequently, exergy analyses allow a more distinct examination of propellant generation processes within the lunar environment, indicating the expected economic cost of production.

For the subsequent exergy analysis, it is assumed that the infrastructure and technology for extraction, refining, and storing already exist on the lunar surface. Hence, the analysis only considers the operating cost of the extraction process. Additionally, an example mission is used to directly compare the operating cost of the extraction processes for both propellant options. The mission consists of a spacecraft propelled by a liquid bipropellant engine utilizing the extracted propellants and transporting a payload of the same propellant to a storage depot

Table 1

Reference environment parameters for PSAs in the polar region [8–11].

Property	Symbol	Value
Surface temperature	T_0	40 K
Surface pressure	p_0	3e-15 bar
Composition of atmosphere	y_{atm}	n/a
Composition of lithosphere		
Plagioclase	$y_{regolith}$	92.52 wt%
$CaAl_2Si_2O_8$	$y_{CaAl_2Si_2O_8}$	88.15 wt%
$NaAlSi_3O_8$	$y_{NaAlSi_3O_8}$	4.37 wt%
Volatiles/ices		
H_2O	y_{H_2O}	5.60 wt%
CO_2	y_{CO_2}	0.12 wt%
H_2S	y_{H_2S}	0.94 wt%
NH_3	y_{NH_3}	0.34 wt%
SO_2	y_{SO_2}	0.18 wt%
C_2H_4	$y_{C_2H_4}$	0.17 wt%
CH_3OH	y_{CH_3OH}	0.09 wt%
CH_4	y_{CH_4}	0.04 wt%

located in a lunar NRHO (see Table 1).

2. Material and methods

2.1. Reference environment

A system or stream's exergy depends not only on its inherent characteristics but also on the state of its reference environment. The reference environment affects the exergy analysis outcome and must be defined before conducting the analysis. The reference environment is defined to be in stable equilibrium for all parts of the environment. Only internal reversible processes may occur that still maintain the reference environment's state in which the temperature, pressure, and chemical

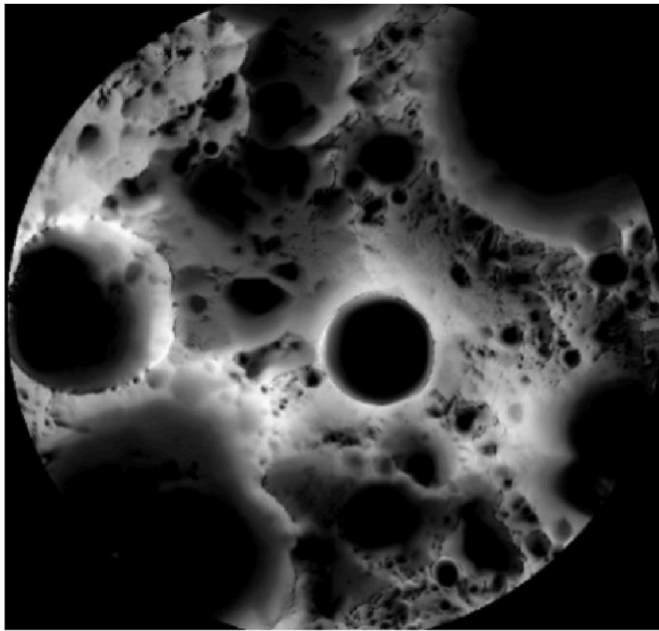


Fig. 1. Lunar south pole with the Shackleton crater (Diameter: 19 km) in the center (Image from NASA [12]).

Table 2

Specific standard chemical exergies for water, carbon dioxide, oxygen, hydrogen, and methane in relation to the PSA reference environment

Specific standard chemical exergy		
Species	\bar{ex}_{ch}^0 [kJ/kmol]	ex_{ch}^0 [kJ/kg]
H ₂ O	1232.7	68.4
CO ₂	4085.8	92.8
O ₂	1081.5	33.8
H ₂	2188.7	1085.7
CH ₄	4480.9	279.3

composition remain constant. The chosen reference environment for the extraction exergy analysis matches the surface conditions within permanently shadowed areas (PSAs). Craters at the lunar south pole, such as the Shackleton crater shown in Fig. 1, are possible locations suitable for ice mining [7]. The properties of the crater floor allow for the existence of volatile ices, e.g., H₂O and CO₂ [1,3], while the crater rim exhibits high solar visibility suitable for power generation. Table 2 lists the reference environment's parameters, assuming a lithosphere consisting of icy regolith composed of mainly plagioclase and condensed volatiles and a negligible lunar atmosphere [8–11].

2.2. Process architecture

Fig. 2 depicts the extraction and refinement subprocesses. The process architecture is based on the ice mining and propellant generation architecture introduced by Sowers and Dreyer [4]. For the methane production a Sabatier reactor is coupled with the electrolysis reactor to allow utilization of the exothermic heat of the Sabatier process to reduce the overall heating requirement and mined H₂O [13]. The resting ice deposits are assumed to be in equilibrium with the environment. A heating tent heats the regolith up to 110 K, allowing the ice deposits to sublime. The vapor collects and solidifies in passively cooled cold traps connected to the heating tent, radiating excessive heat to space. The extracted volatiles are reheated and further processed. Water is split through electrolysis into hydrogen and oxygen, while for the methane production, an additional Sabatier reactor generates methane and water. The during the Sabatier process generated water is subsequently

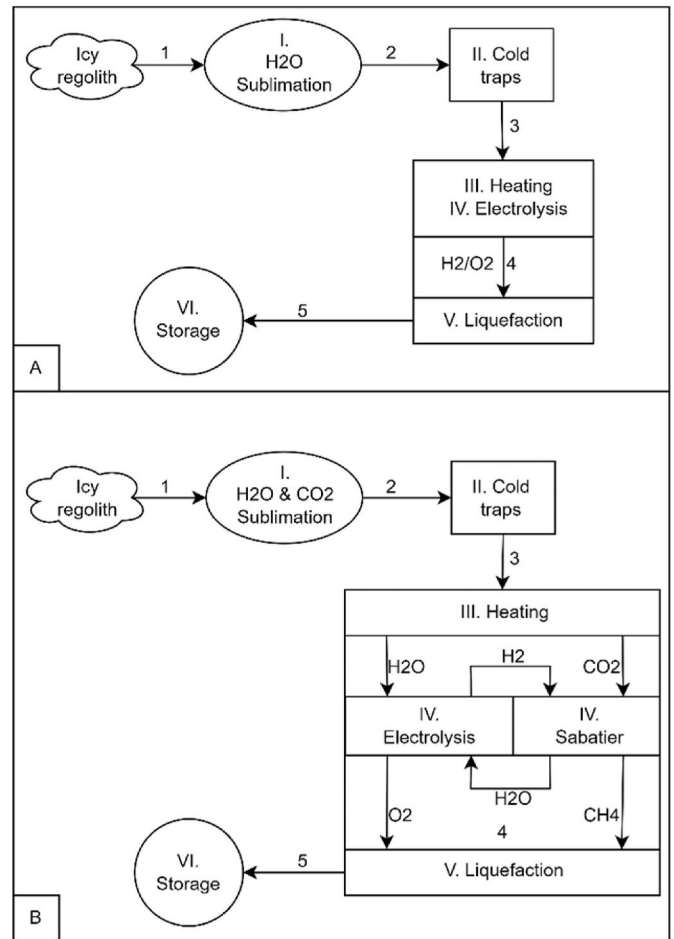


Fig. 2. Process architecture of lunar ice extraction and subsequent propellant generation (A: process chain for H₂ and O₂ generation from water ice; B: process chain for CH₄ and O₂ generation from water- and carbon dioxide ice).

reintroduced into the electrolysis cycle. During the fuel production, oxygen, used as the oxidizer, is extracted during the electrolysis process. The generated propellants are liquefied and stored under conditions aiming at low exergetic storage costs for an assumed storage time of six months. All post-extraction processes are performed near the extraction site within the same reference environment.

3. Theory and calculations

Exergy allows the evaluation of energetic and non-energetic resources, indicating their economic values. For instance, comparing high-energy-high-exergy fossil fuels to high-energy-low-exergy waste heat at environmental temperatures reveals their respective economic worth due to the exergy's indication of the available energy quality [6].

Further, exergy permits the same rating scale for non-energetic resources like mineral deposits. Deposits with a low mineral content hold comparably little exergy; thus, a higher amount of external exergy is necessary to make the minerals useful. When a deposit is mined, the contained exergy is sustained and increased during subsequent refinement processes [6].

3.1. Standard chemical exergy

The standard chemical exergies Ex_{ch}^0 for the lunar reference environment within the PSAs are calculated assuming an icy highland regolith lithosphere composed of plagioclase and volatile ices [9]. Rivero and Garfias [14] describe the following equations to estimate the

specific standard chemical exergy of species i contained within the reference environment's lithosphere:

$$\bar{Ex}_{ch,i}^0 = -RT_0 \ln x_{i0} \quad (13)$$

with

$$x_{i0} = \frac{1}{l_i} n_{0,el} c_{i,el} M_0 \quad (14)$$

l_i is the number of atoms of an element in the molecule of reference species i , c_i is the mass fraction of the element contained in species i , $n_{0,el}$ is the mean molar concentration of the element in the reference lithosphere, and M_0 is the mean molecular mass of the lithosphere and equal to 144.075 kg/kmol. Table 2 lists the standard chemical exergies for water, carbon dioxide, oxygen, hydrogen, and methane calculated with equations (13) and (14) with respect to the composition of the reference environment's lithosphere, analogous to the operations shown by Rivero and Garfias [14].

3.2. Exergy equations and balances

The total exergy Ex_{tot} of a system or stream is expressed through the physical, chemical, kinetic, and potential exergy components depending on the temperature, pressure, velocity, position, and chemical composition [6]:

$$Ex_{tot} = Ex_{ph} + Ex_{ch} + Ex_{kin} + Ex_{pot} \quad (1)$$

The kinetic and potential exergy components are considered negligible within industrial system analyses [15]. Therefore, only the physical and chemical exergy components remain to be considered. The physical exergy is expressed through [6]:

$$Ex_{ph} = (H - H_0) - T_0(S - S_0) \quad (2)$$

The enthalpy H , entropy S , depending on the process temperature T and pressure p , describe the physical exergy component, while the intensive properties of the reference environment are represented by H_0 , S_0 , and T_0 .

The chemical exergy of a mixture is composed of the standard chemical exergies of the contained species and its composition [6,16,17]:

$$Ex_{ch} = \sum_i y_i Ex_{ch,i}^0 + RT_0 \sum_i y_i \ln(y_i) \quad (3)$$

Exergy is a system characteristic, combining its intensive and extensive properties of the system with the intensive properties of the reference environment. For example, the inherent physical exergy of a system is equivalent to the maximum work obtainable from a system within its reference environment until it reaches thermal and mechanical equilibrium with the environment [6,15]. During the propellant generation, substantial amounts of energy are required. Within the exergy analysis, the external exergy transfer represents the required energy in relation to the reference environment. The exergy related to thermal, mechanical, and electrical energy transfers from or to a system are described in the following sections.

3.2.1. Exergy of thermal energy

The heat transfer Q heats or cools a control mass at constant volume from its initial state i to its final state f . The exergy flow correlated to the heat transfer Q is then expressed as [6]:

$$Ex_Q = \int_i^f \left(1 - \frac{T_0}{T}\right) \delta Q \quad (4)$$

with T as the control mass's temperature and T_0 , as the environmental temperature. Further, the thermal exergy Ex_Q represents the minimum

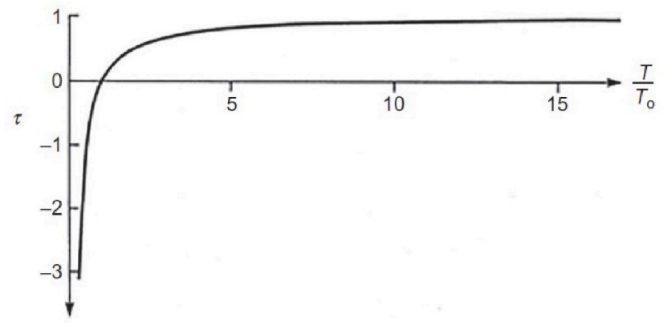


Fig. 3. Relation between the temperature ratio T/T_0 and the exergetic temperature factor τ (Figure from Dincer and Rosen [6]).

work required by the control mass and the environment to transfer the control mass from its initial to its final state. For a control mass at constant temperature T , the equation simplifies to:

$$Ex_Q = Q \cdot \left(1 - \frac{T_0}{T}\right) \quad (5)$$

The dimensionless exergetic temperature factor τ represents the ratio between the exergy Ex_Q and energy of the heat transferred Q and is defined as [18]:

$$\tau = 1 - \frac{T_0}{T} \quad (6)$$

Fig. 3 depicts the relation between τ and the absolute temperature ratio T/T_0 . If both temperatures, T and T_0 , are equal, the exergetic temperature factor is zero. For heat transfers above the environmental temperature, i.e., $T > T_0$, the exergetic temperature factor ranges between $0 < \tau < 1$. For heat transfers below the environmental temperature, i.e., $T < T_0$, τ is smaller than zero, indicating that exergy flows in the reversed direction of the energy flow. If $\tau < -1$, meaning $T < T_0/2$, the magnitude of the exergy flow surpasses the magnitude of the energy flow [6,18].

3.2.2. Exergy of work

Total work done by a system is the sum of the work caused by its volume change W and the shaft work W_{sh} done by the system. Shaft work refers to all work capable of raising weight, e.g., mechanical-, electrical-, or magnetic work. The exergy Ex_W corresponding to shaft work is equivalent to the shaft work W_{sh} itself [6]:

$$Ex_W = W_{sh} \quad (7)$$

The exergy transfer related to the work done by a system due to volume change is the net useable work W_{NET} caused by its volume change:

$$(W_{NET})_{1,2} = W_{1,2} - p_0(V_2 - V_1) \quad (8)$$

$W_{1,2}$ is the work caused by the change in volume from volume V_1 to V_2 . The term $p_0(V_2 - V_1)$ represents the relation to the reference environment and indicates the work required to change the volume against the environmental pressure p_0 . If the system's volume is fixed, W_{NET} equals zero [6].

3.2.3. Exergy of electricity

Analogous to shaft work, the exergy associated with electricity is equivalent to the corresponding energy [15].

3.2.4. Exergy balance

The general exergy balance is defined as follows [6,19]:

Table 3

The required exergy input for the process stages of H₂/O₂ and CH₄/O₂ generation with regards to 1 kg of the respective extracted fuel

Subprocess	Exergy input [MJ/kg]	
	H ₂	CH ₄
I Sublimation	20.85	11.40
III Heating	6.18	3.62
IV Electrolysis	47.09	–
IV Electrolysis + Sabatier	–	9.63
V Liquefaction	3.38	2.17
VI Storage (6 Months)	0.07	0.32
Total	77.57	27.13

$$\text{Exergy input} - \text{Exergy output} - \text{Exergy consumption} = \text{Exergy accumulation.} \quad (9)$$

For a non-steady flow process from a system's initial i to its final f state, Equation (9) can be expressed as [6]:

$$\sum ex_{\text{flow,in}} m_{\text{in}} - \sum ex_{\text{flow,out}} m_{\text{out}} + (Ex_Q)_{i,f} \quad (10)$$

$$- (Ex_w)_{i,f} (W_{\text{NET}})_{i,f} - (Ex_D)_{i,f} = Ex_f - Ex_i$$

During the process, exergy is consumed due to irreversibilities, resulting in the proportionality of exergy destruction Ex_D and entropy generation S_{gen} [6]. The exergy destruction is expressed as:

$$Ex_D = T_0 S_{\text{gen}} \quad (11)$$

Exergy analyses determine thermodynamic losses in the form of exergy destruction and reveal locations within the process architecture where process optimization may be possible. Here, the destroyed exergy represents the theoretical margin of improvement.

For a closed system, the exergy balance Equation (10) simplifies to:

$$(Ex_Q)_{i,f} - (Ex_w)_{i,f} (W_{\text{NET}})_{i,f} \quad (12)$$

$$= Ex_f - Ex_i$$

If the initial and final states of the system are equal, then the right sides of the exergy balances (10) and (12) are equal to zero.

4. Results

4.1. Exergy analysis results

The concept of exergy is applied to evaluate the efficiency and energetic cost of lunar in-situ resource extraction and propellant production. The exergy analysis focuses on hydrogen and methane extraction from ice deposits located in PSAs in the polar regions. Thermophysical properties employed in the calculations are extracted from the National Institute of Standards and Technology [20] and Schreiner et al. [21]. The electrolysis and Sabatier reactors are assumed to operate at 10 bars, and 323.15 K and 473.15 K, respectively [4,13,22]. Storage tank conditions for the liquid O₂, H₂, and CH₄ are 10 bar and 55 K, 31 K, and 91 K, respectively. The assumed temperatures are the lowest for which sufficient data is available while allowing the storage of liquid propellants close to environmental temperatures to minimize the required exergy input.

Table 3 lists the estimated exergy input for the subprocesses of the hydrogen and methane extraction processes and the total amount of required exergy input. For the methane extraction, thermal coupling between the electrolysis and Sabatier reactor is assumed, utilizing the Sabatier reactions generated heat to decrease the thermal demand of the electrolysis process.

Table 4

Required propellant masses and exergetic cost for the two example missions for a Δv of 2.75 km/s and a total payload mass of 50 t

	H ₂ & O ₂	CH ₄ & O ₂
O/F ratio	5.57	3.72
Payload		
Fuel [t]	7.61	10.59
Oxidizer [t]	42.39	39.41
Depot transfer vehicle		
Fuel [t]	11.23	23.73
Oxidizer [t]	62.54	88.29
Extraction		
Total propellant [t]	123.77	162.02
Total fuel [t]	18.84	34.32
Extracted O ₂ [t]	149.52	136.94
Required O ₂ [t]	104.93	127.70
Surplus O ₂ [t]	44.56	9.24
Exergetic cost		
Per kg fuel [MJ/kg]	77.57	27.13
Total [GJ/kg]	1461	931

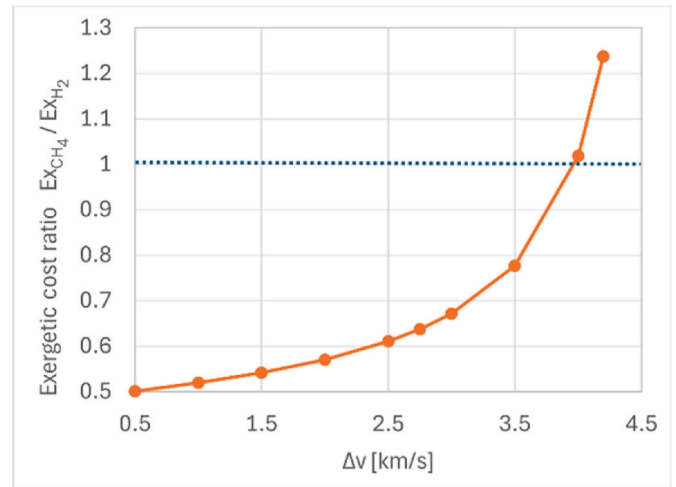


Fig. 4. Total exergetic cost ratio (Ex_{CH_4} / Ex_{H_2}) depending on the Δv required to reach the storage depot orbit.

4.2. Transportation to propellant depot

Both propellant options, H₂/O₂ and CH₄/O₂, and their exergetic extraction cost is compared through an example mission transporting in-situ generated propellants to a storage depot in cislunar space. The depot is located in NRHO requiring a Δv of 2.75 km/s to reach orbit from the lunar surface. A single-stage-to-orbit spacecraft operated by a liquid bipropellant rocket engine is assumed to transport a payload of 50 t of propellants to the storage depot while utilizing the same propellant combination for its engine. The estimated delivered vacuum performances and O/F ratios of the H₂/O₂ and CH₄/O₂ engines are calculated using the rocket propulsion analysis tool RPA Lite [23]. The engines operate with O/F ratios of 5.57 and 3.72, reaching an assumed I_{sp} of 467 s and 386 s and w_v of 4583.48 m/s and 3788.98 m/s, respectively. To estimate the necessary propellant masses for the two propellant combinations and Δv requirements, the following system of equations was solved:

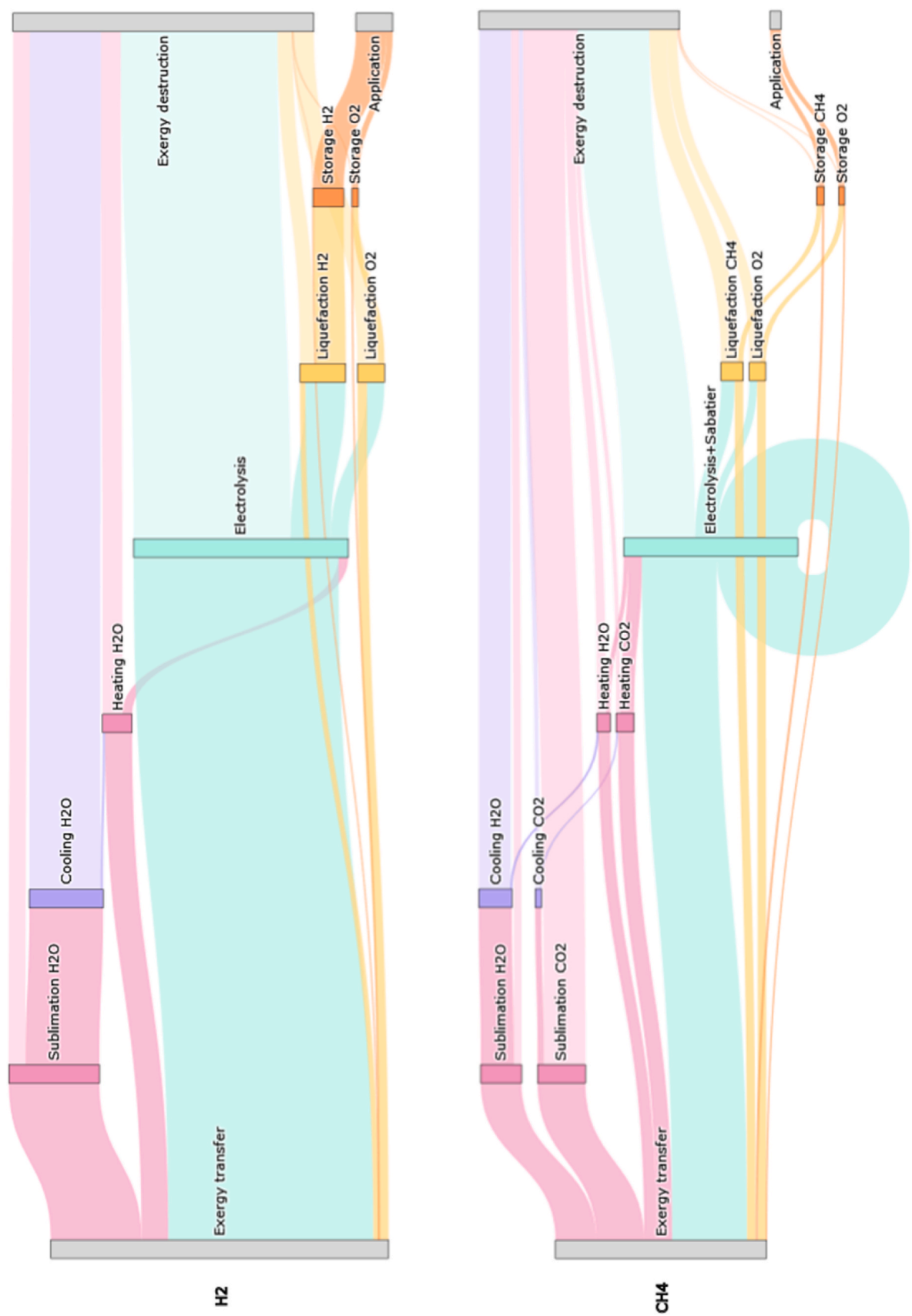


Fig. 5. Exergy flow diagram of the propellant generation process (H_2 : H_2/O_2 extraction, CH_4 : CH_4/O_2 extraction).

$$\begin{aligned}
m_i &= e_{\text{sv}} \bullet m_f \\
m_f &= m_{\text{payload}} + m_s + m_{p,\text{rest}} \\
m_{p,\text{used}} &= m_i - m_f \\
m_p &= m_{p,\text{used}} + m_{p,\text{rest}} \\
m_{p,\text{rest}} &= \frac{m_p}{\eta} - m_p \\
m_s &= \frac{\varepsilon}{1 - \varepsilon} - m_p
\end{aligned} \tag{15}$$

with an assumed structural factor ε of 0.14, and a propellant usage factor η of 0.855.

Table 4 lists the estimated required propellant masses and total exergetic cost of the propellant production for the two example missions. During the extraction process, more oxygen is generated than needed to satisfy the O/F requirement. The excess oxygen, especially in the case of hydrogen production, may be utilized in life-support systems or similar applications on-site. Fig. 4 depicts the total exergetic cost ratio between the two propellant combinations, depending on the distance between the depot and the Moon, represented by the Δv .

5. Discussion

The results indicate that servicing a depot in a lunar NRHO can reduce the required exergetic cost by a third if methane is utilized as the propellant instead of hydrogen. Increasing depot distances reduce the positive effect of methane, and it becomes a less favorable propellant option due to higher mass demands caused by its lower engine performance compared to hydrogen and distinct O/F ratios. More fuel is required compared to hydrogen overturning the benefit of the reduced exergetic extraction cost.

Although the utilization of methane requires more trips to the depot location to provide equivalent amounts of available propellant, it permits more accessible storage and handling. If the propellant storage depot is located near the Moon, methane may be a suitable alternative to hydrogen.

Additionally, utilizing methane as a propellant may be favorable when anticipating a growing space infrastructure, including lunar and Martian settlements and propellant generation facilities on Mars. Methane is regarded as the primary fuel option for ISRU on Mars, generated from its abundant atmospheric CO₂. Here, lunar methane production could advance the integration of both infrastructures.

The discussed extraction processes are complex systems that still require in-situ testing. However, lunar ISRU may benefit from not just applying one process but adapting process architectures, interlinking methods, and process chains to the extraction site conditions and feed-stock availability and composition. A multi-dimensional approach could increase the efficiency, sustainability, and independence of lunar resource extraction operations. For instance, moving the refinement facilities outside the crater would reduce the distance between the power source and the facilities if solar energy is used. Additionally, extracting an array of resources simultaneously through a suitable process architecture could decrease costs and increase overall process efficiencies.

Declaration of competing interest

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.

Acknowledgements

M. M. Gallbrecht thanks ESA for supporting the internship.

Appendix A. (Sankey diagram)

Fig. 5 displays the Sankey diagram of the hydrogen and methane extraction process. The diagram visualizes the exergy flows between the subprocesses and the required external exergy transfer, i.e., the external exergy input. The exergy destruction, moreover, represents the external waste emissions and internal irreversibilities within the process, indicating the theoretical margin of process improvement. The mapped exergy flows are based on the total fuel mass required by the example mission.

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