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Conceptual Design of Rocket Engines Using Regolith-Derived Propellants

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Abstract

Production of rocket propellants from lunar resources has the potential to significantly reduce the cost of space exploration. Recent research efforts in this area were focused on the extraction of water from icy regolith for conversion into hydrogen and oxygen, a highly efficient rocket bipropellant. However, water is available only in polar regions of the Moon, and its extraction is a challenge. The present paper aims to assess the feasibility of using propellant components that can be obtained from lunar regolith, specifically oxygen, metal alloys, and sulfur. Thermodynamic performance characteristics of rocket engines using these components were calculated over wide ranges of oxidizer-to-fuel mass ratios. It has been shown that the fuel obtained by extraction of oxygen from regolith, i.e., primarily a mixture of metal alloys, exhibits a relatively high specific impulse of up to 250 s. The use of fuel-lean propellants significantly decreases the temperatures, which facilitates cooling and potentially reduces the deposition of condensed products in the engine; at the same time, the expected decrease in the specific impulse is less pronounced. The use of sulfur in rocket engines is less promising from a thermodynamic point of view, but it enables engine designs without a need

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for feeding metal alloy powders. Among different designs of sulfur-based engines, a hybrid rocket (fuel: metal alloys mixed with sulfur, oxidizer: liquid oxygen) appears to be the most promising.

Keywords: Metal Combustion, Rocket Propulsion, In-Situ Resource Utilization, Lunar Regolith, Propellants

1. Introduction

It is commonly agreed that *in situ* resource utilization (ISRU) is an enabling technology for space exploration [1, 2]. The expected growth of Moon exploration activities increases interest in lunar ISRU, specifically for the production of rocket propellants on the lunar surface. The cost of shipping materials from Earth, over \$35,000 USD per kilogram [3], emphasizes the urgency of utilizing local material. Producing rocket propellants locally could facilitate transportation on the Moon and return to Earth.

The discovery of water ice in the polar regions of the Moon has drawn attention to the possibility of generating liquid hydrogen (LH_2) and liquid oxygen (LOX) on the lunar surface. LH_2/LOX engines are a mature technology with a high efficiency. However, some factors may limit the feasibility of LH_2/LOX ISRU. One challenge lies in the unverified quantity and uneven distribution of water ice concentrated in the polar regions of the lunar surface [4, 5]. As a result, propellant would have to be transported between production facilities on the Moon, where water ice is available, and bases where hoppers and return rockets are located. The infrastructure to sustain such an operation is difficult to establish. Alternatively, it has been suggested that hydrogen could be extracted from metal hydrides; this process would be energy intensive, and the quantities of hydrogen are low, at a maximum of 80 ppm [6]. In addition, long-term storage of LH₂ is challenging because of its low density (0.07 g/cc) and high boil-off rate (up to 11% per hour for the Space Shuttle on Earth and 2% per day on orbit for the PRSD subsystem [7]). Numerical studies for the lunar surface suggest boil-off can be reduced to 0.05% per day but might require large energy inputs; in a study 1500 W are required for cooling a tank with 9600 kg of LH₂ at 0.1 MPa and 160 K ambient temperature on the lunar surface [8]. Thus, hydrogen storage would require well-insulated, large tanks or, alternatively, high-productionrate facilities to supply sufficient amounts of LH_2 right before utilization. Finally, the sustainability of using valuable water resources, should they be confirmed, as a single-use, non-recyclable propellant is contentious.

An alternative ISRU solution involves the utilization of metal/LOX propellant mixtures. In this concept, both the oxidizer (LOX) and the fuel (metal alloy powder) are sourced from lunar regolith through a reduction process powered by solar energy. The lunar regolith primarily consists of oxides of silicon, aluminum, iron, calcium, titanium, and other trace elements [9]. These metals and their alloys can be conveniently stored for an extended period of time and subsequently used in rocket engines. Prior investigations have assessed the performance of such metal/LOX propulsion systems through experimental and theoretical analyses [4, 10, 11].

Hepp et al. performed thermodynamic calculations and proposed to burn metals with oxygen in a rocket engine [4]. They concluded that this propellant combination is attractive, but significant gaps remain in understanding how these metals would be extracted from regolith and integrated into an engine design. Linne and Meyer [12] compared different propulsion technologies and discussed Al/O_2 and Al/H_2O_2 propulsion systems with a similar conclusion. Meyer proposed different engine configurations and conducted laboratory scale tests of powder feeding systems as well as hot fire tests of the entire propulsion system [10]. The experiments demonstrated a performance level that hovered around 50% of the theoretical value, and multiple problems were identified in the design such as poor mixing and incomplete combustion. More concepts for rocket engines using metalized propellants and a liquid oxidizer were proposed in the context of Martian propulsion [13, 14, 15, 16, 17]. There are many planet-specific ISRU concepts that have been discussed in the literature; our work focuses on lunar applications, and the proposed concepts are also relevant to extraterrestrial bodies with similar regolith compositions to the Moon.

Since the propellants are regolith-derived, the regolith needs to be processed to obtain both the fuel and oxidizer for the rocket engine. In a recent study, the Technology Readiness Levels (TRLs) were estimated [18]. This nine-level scale ranges from 1 (basic principles observed and reported) to 9 (system is flight proven). Water mining and oxygen extraction from regolith are both reported at TRL 4/5 (required for a conventional bipropellant system), while the molten electrolysis process to obtain the metal components is estimated at TRL 3/4. Therefore, as of now, there is no significant technological advantage in terms of space mining technologies that would favor focusing on a bipropellant LH₂/LOX system.

All minerals within the lunar regolith need to be reduced to obtain metal

alloys and oxygen. There have been multiple studies on regolith reduction over the years with the primary goal of obtaining oxygen for a potential lunar habitat; they considered hydrogen reduction of ilmenite found within the regolith [19], carbothermal reduction processes [20], and molten fluoride electrolysis [21]. The two processes that have been most extensively studied are direct molten regolith electrolysis [22, 9] and an FFC-Cambridge process [23] using CaCl₂ as the electrolyte. Both processes have been verified on a laboratory scale; they achieved metal-alloy purities of > 95% and a similarly high oxygen extraction rate.

Another element present on the lunar surface, though not as abundant as oxygen, silicon, and metals, is sulfur. The potential applications of sulfur in the context of ISRU have been examined [24], primarily with the idea of using it for construction purposes. Based on prior metal-sulfur combustion studies [25], it could serve as a rocket fuel in various configurations, including solid, hybrid, and potentially bipropellant engines. One configuration that has been studied uses sulfur-oxygen as the propellant, and it is known as a brimstone rocket [24].

The objectives of the present study are to determine the thermodynamic characteristics of rocket engines using regolith-derived metal fuels (RDFs), oxygen, and sulfur, and to analyze possible configurations of propulsion systems employing these propellants.

2. Methods

The thermodynamic calculations determining the theoretical performance of the rocket propellants were performed and verified using three different thermodynamic codes for highest fidelity. The standard approach in previous publications assessing ISRU rocket fuels has been to rely on NASA CEA [4, 26, 27]. However, this code is not optimized for metal fuels and sulfur as an oxidizer. Therefore, Thermo (a Russian thermodynamic code) and FactSage [28] (a commercial thermodynamic software) were also used. The methodology for the thermodynamic calculations is presented in the Supplemental Material.

3. Results and Discussion

3.1. Performance Characteristics of Rocket Engines Using Regolith-Derived Fuels

3.1.1. Selection of Regolith Compositions for Analysis

Different lunar compositions are considered to assess whether the theoretical performance of RDFs from various types of regolith is sufficient for the concept to be competitive. Figure 1 shows a map of regolith resources on the lunar surface and provides three typical regolith compositions [9]. The main elements that will be the constituents of the RDF after reduction (based on ten regolith samples from the Apollo missions [29]) are shown in Figure 2.



Figure 1: Different regolith compositions and their locations on the lunar surface. The majority of the regolith is similar to the highlands type with Al_2O_3 and SiO_2 as the main constituents. Reprinted from [9], with permission from Elsevier, copyright 2016.

Two exemplary compositions (A-11 and A-12, one Low-Ti and one High-Ti regolith) were considered in the thermodynamic calculations. Their compositions before and after reduction are shown in Tables 1 and 2. While Mare regoliths mainly differ in their titanium content, there is also a Highlands regolith which contains less iron and more aluminum. There are also differences regarding grain size and thermochemical properties between the different regoliths [30]. For a first analysis and simplicity's sake, we only focus on the two compositions and neglect trace elements (oxide < 5 wt%) with the exception of sulfur.



Figure 2: Composition of ten different regolith-derived fuels assuming all of the oxygen is electrolytically removed.

Table 1: Composition of two exemplary regolith samples before oxygen removal.

Region	Al_2O_3	CaO	FeO	MgO	${f SiO}_2$	TiO	Trace
A-11 (wt%)	13.8	12.1	15.8	8.2	42.2	7.7	0.3
A-12 (wt%)	13.7	10.6	15.4	9.9	46.2	3.1	1.2

3.1.2. Metal-Oxygen Rocket Engines

Specific impulse (I_{sp}) at perfect expansion and combustion chamber temperature (T_c) were calculated for oxidizer-to-fuel (O/F) mass ratios ranging

Region	Al	Ca	Fe	Mg	Si	Ti	S	O_2 ext.
A-11 (wt%)	12.5	14.8	20.9	8.4	33.9	7.9	0.2	41.4
A-12 (wt%)	12.6	13.1	20.9	10.4	37.6	3.2	0.2	42.6

Table 2: Composition of two exemplary regolith-derived fuels (RDF).

from 0.5 to 10 (in steps of 0.1 between 0.5 and 1, and after that in steps of 0.5) for all major metallic regolith components (Al, Si, Fe, Ti, Ca) with oxygen and for sulfur with oxygen. The initial temperature of the reactants was set to 298 K except for the calculation with LOX at 90 K (neither Thermo nor FactSage can run calculations with LOX). The difference between using LOX and gaseous oxygen at 298 K is negligible as shown for aluminum in Figure 3. To smooth the curves, a spline interpolation was utilized. The chamber pressure (P_c) was set to 20 atm, and the ratio of the chamber pressure to the exit pressure (P_e) was set to 1000 (P_c/P_e), which corresponds to $P_e = 0.02$ atm. On the lunar surface, the exhaust expands into a vacuum, and the $I_{\rm sp}$ will be slightly higher due to the pressure term as can be seen in equation

$$I_{\rm sp} = \frac{v_{\rm e} + \frac{(P_{\rm e} - P_{\rm a})A_{\rm e}}{\dot{m}}}{g_0} \tag{1}$$

where $v_{\rm e}$ is the exhaust velocity, $P_{\rm e}$ the exit pressure, $P_{\rm a}$ the ambient pressure, $A_{\rm e}$ the nozzle exhaust area, \dot{m} the propellant mass flow rate, and g_0 the standard acceleration of gravity.

CEA can calculate the specific impulse in vacuum, which is the case for the Moon, however Thermo does not have that capability. To ensure compatibility, the specific impulse at perfect expansion is calculated and shown in Figure 3. The deviation from the specific impulse in vacuum is about 5-10 s (see Figure S3 in the Supplemental Material). The results were computed using different codes, and a rationale regarding the selection of each code for specific calculations is provided in Table S1 in the Supplemental Material.

All propellants but iron have an $I_{\rm sp}$ peak range of 251 s (Ca) to 279 s (Al) over the considered range of O/F mass ratios. Chamber temperatures at peak ISP are predicted to range from 3720 K (Si) to 4900 K (Ti). Iron shows a rather low $I_{\rm sp}$ (max. 183 s) but also a significantly lower chamber



Figure 3: Thermodynamic calculations for the most important metals and metalloids found in regolith, and sulfur. The legend is ordered by peak temperature/peak $I_{\rm sp}$. A dashed line is used to indicate LOX as the oxidizer and a dot-dashed line is used for the nonmetallic element sulfur.

temperature with the peak being at slightly over 3300 K. As seen in Figure 3, the chamber temperatures decrease significantly for higher O/F ratios, which facilitates cooling. Sulfur burning with oxygen shows both a lower $I_{\rm sp}$ (peak at 243 s) and a lower chamber temperature (peak of approx. 3650 K) than the metals (excluding iron) over the considered O/F mass ratio range.

When a mixture of all these elemental metals and metalloids burns with oxygen, complex products of two or more metals will form, which may change the performance characteristics. We performed the same calculations for two RDFs derived from A-11 and A-12 regolith, shown in Table 2. The predicted performance indicates a peak $I_{\rm sp}$ of 256 s with a $T_{\rm c}$ of approximately 3450 K, and there is only a marginal difference between the two RDFs (see solid lines in the lower graph of Figure 4). As expected from the calculations with the single metals, the $I_{\rm sp}$ and chamber temperature for the alloy are lower than that of pure aluminum, the most commonly proposed ISRU fuel.

This calculation is, however, only an approximation of the actual compo-



Figure 4: Thermodynamic calculations for A-11 RDF and A-12 RDF burning with oxygen performed by Thermo. The calculations for aluminum–oxygen are shown as a reference. The RDF is considered as an elemental mixture and alloy.

sition of RDF. After the reduction process where the regolith is dissolved in an electrolyte and reduced at 900 °C [23], the product will be an alloy. Separation of its metallic components would require an additional step, which, depending on the process, is either energy intensive or requires chemicals not available *in situ*, or both.

Table 3: Equilibrium alloy composition calculated in near vacuum $(p = 10^{-6} \text{ atm})$ for reduced regolith A-11 (A-12 is very similar and therefore not shown).

Code	Al ₂ Ca	CaSi	FeSi	Mg_2Si	Si	Si_2Ti	TiSi	TAU2	FS2L
Thermo (mol%) FactSage (mol%)	18.9	$11.3 \\ 37.6$	$30.6 \\ 13.4$	14.1 17.8	8.4	16.8 -	- 12.2	- 9.5	- 9.6

FactSage and Thermo have been used to calculate the equilibrium compositions for the alloys that would be present in the regolith-derived fuel. The results are presented in Table 3. Partly, the same phases are predicted by both codes, while some phases differ; this is mainly due to FactSage predicting ternary solutions (TAU2, FS2L¹), which Thermo does not do. In general, this calculation is only an approximation of the actual alloy composition after reduction, which will depend on the reduction process, cooling of the liquid phases, and other factors. For the FFC-Cambridge process, the authors noted, for instance, a decrease in silicon concentration after the reduction process due to process related reduction losses for SiO₂ [23]. They found a ternary Ca/Si/Al phase (sometimes also containing magnesium), a binary Al/Fe phase (sometimes with silicon), and a binary Fe/Si phase (sometimes with Ti and/or Al) in the final composition, some of which neither solver predicts (this indicates the relevance of including ternary phases).

The composition obtained with Thermo is then used as a new RDF composition burning with oxygen, and the results for the chamber temperature showing the difference between alloy and elemental mixture as initial state of the RDF are presented in the upper graph of Figure 4. Slightly lower temperatures are predicted for the alloy than for the elemental mixture. As expected, the slightly lower chamber temperatures also lead to a small decrease in specific impulse as shown in the lower part of Figure 4.

Thermo was used for the calculations since FactSage is unable to calculate the $I_{\rm sp}$. However, chamber temperatures for compositions predicted by FactSage were verified, showing a similar temperature decrease for the alloy compared to Thermo (Figure S7 in the Supplemental Material). While there are limitations in either code's database when calculating multispecies equilibria, it does not affect the calculated performance characteristics significantly. Therefore, it is unlikely that the omission of more complex products (that none of the codes contain in their respective database) impacts the validity of these results. As will be discussed later, it is much more difficult to achieve the theoretical performance in practice, and minor differences in the theoretical $I_{\rm sp}$ are negligible.

The small effect of using alloys instead of individual elements is explained by small enthalpies of formation of the intermetallic compounds, shown in Table 4, compared to the enthalpies of formation of the produced oxides. Indeed, the standard enthalpies of formation (during combustion) for alumina (Al₂O₃), hematite (Fe₂O₃), calcium oxide (CaO), quartz (SiO₂), magnesium

¹TAU2 is a ternary solution $Al_5Fe_2Si_2-\gamma$ ($Al_5Fe_2Si(Al,Si)_2$) (almost identical for both A-11 and A-12 RDF calculations, enthalpies of formation differ by < 1%) from FSstel (solution #168); FS2L is a low-temperature ternary solid solution (Fe)₁(Si,Al)₂ from FSstel (solution #79) [31]

oxide (MgO), and rutile (TiO₂) are, in kJ/mol, -1620.6, -825.5, -634.6, -910.9, -601.5, and -938.7 respectively [32]. The calculations show that the enthalpy of combustion decreases only slightly if the individual elements are replaced by intermetallic compounds.

Table 4: Enthalpies of formation of the predicted intermetallic compounds from the Thermo and FactSage databases and partly verified with experimental data from [33, 34].

Compound	Al ₂ Ca	CaSi	FeSi	Mg_2Si	Si_2Ti	TAU2	FS2L
Enthalpy of Formation Thermo [kJ/mol]	-216.7^2	-150.9	-80.3	-77.8	-134.3	-	-
Enthalpy of Formation FactSage [kJ/mol]	-90.0	-87.0	-76.4	-65.1	-161.0	-266.1	-96.9

In conclusion, burning an alloy will lead to an insignificantly lower performance than a mixture or the metallic components. The decrease in performance is not significant enough to warrant the purification or separation of the RDF metal fuels.

Thermodynamic calculations offer insight into potential operating conditions for rocket engines and their optimal theoretical performance. These conditions may vary slightly depending on the specific regolith mixtures. The calculations suggest operating at fuel-lean conditions, with an O/F mass ratio typically ranging between 2 and 4, contingent upon the regolith composition. Under these parameters, the specific impulse is projected to fall within the range of 240 to 250 s with chamber temperatures in the range of 3300 K to 3500 K, which is suitable for regenerative cooling.

The actual performance characteristics of the proposed engine can be affected by the relatively high amount of condensed products in the exhaust. They may cause deposition within the engine and lead to two-phase losses of specific impulse. Detailed calculated products are available in Figures S4, S5, and S6 in the Supplemental Material. For clarity, Figure 5 displays only the phase of the products. It is seen that the quantity of condensed species decreases at higher O/F ratios. Gaseous oxides are predominant up to an O/F ratio of 4, beyond which oxygen replaces them. Figure 6 shows the amount of condensed species at different cross sections of the rocket engine

²The FactSage values for the formation enthalpies are in close agreement with the literature. The values in the Thermo database for Al₂Ca and CaSi differ significantly, but the effect on combustion temperatures is marginal as seen in Figure S7 in the Supplemental Material. The Thermo results were further used due to its capability to calculate I_{sp} .





Figure 5: Products in the combustion chamber for A-11 RDF predicted by FactSage.

The deposition is known to be more significant when the condensed products are liquid. A study by Miller and Herr investigated deposition in aluminum–steam and magnesium–steam rocket engines, two metals that are also present in RDF [35]. There was much less deposition in the engine using magnesium fuel as the melting point of magnesia (3125 K) is much higher than that of alumina (2345 K). For RDF, given that adiabatic flame temperatures with oxygen significantly surpass the melting points of alumina and silica, there might be significant deposition. Indeed, the thermodynamic calculations indicate predominantly liquid phases within the combustion chamber. However, at the nozzle exit, where temperatures are much lower, there are much more solid products, which may decrease the deposition. With increasing the O/F mass ratio from 3 to 10, the solid fraction at the nozzle exit increases from 24% to 99% (Table 5).

The two-phase losses of specific impulse are also an important problem caused by condensed products. Should the formed particles reach a sufficient size, they will not maintain the same velocity as the gas, and the thermal equilibrium of the exhaust products is also disturbed. Both velocity and



Figure 6: Fraction of condensed products inside the combustion chamber, at the throat, and the nozzle exit for A-11 RDF.

Table 5: Phase of the condensed products at different cross sections for the A-11 RDF + $\rm O_2$ thermodynamic calculation.

Cross Section	Phase	O/F Mass Ratio							
	1 mase	0.5	1	2	3	5	10		
Chamber	Liquid	100.0%	100.0%	100.0%	100.0%	100.0%	80.0%		
	Solid	-0.0%	0.0%	0.0%	0.0%	0.0%	20.0%		
Nozzle	Liquid	48.0%	58.5%	70.0%	76.0%	34.0%	1.0%		
Exit	Solid	52.0%	41.5%	30.0%	24.0%	66.0%	99.0%		

thermal lags decrease specific impulse [36]. Often, the thermal lag is negligible, but the velocity lag is significant [37, 38]. If the product particles are smaller than $1 \,\mu$ m, the two-phase losses of $I_{\rm sp}$ do not exceed 2% [39]. As previously described, the final particle size after the reduction process will be in a range of $75-300 \,\mu$ m [23]. Therefore, to minimize two-phase losses, one should attempt to generate nanoscale combustion products.

When alloy particles burn, it is not easy to predict the combustion mode and the size of the condensed products. A simplified assessment could be based on the comparison of the RDF flame temperature with the boiling points of the individual metals at the same pressure. Table 6 shows such a comparison for a pressure of 20 atm. It is seen that at all O/F ratios, the $T_{\rm f}/T_{\rm b}$ ratio is more than 1 for Ca and Mg and less than 1 for Ti, Si, and Fe. Therefore, Ca and Mg would burn in vapor phase and generate nanoscale oxides, while Ti, Si, and Fe would burn heterogeneously. According to the literature, however, Ti particles always explode after a certain period of heterogeneous combustion, generating a lot of burning tiny fragments [40]. As a result, combustion of Ti particles produces much smaller oxide particles. Combustion of Si is known to involve the formation of intermediate gaseous product SiO, which leads to the production of nanoscale SiO_2 particles [41]. Therefore, combustion of Si, though occuring heterogeneously, also generates nanoscale products. For Al, the $T_{\rm f}/T_{\rm b}$ ratio is close to 1, which makes the assessment difficult. However, combustion of Al is known to include the formation of intermediate gaseous suboxides [42], so it is also promising from this point of view. Thus, the only metal that may not produce nanoscale oxides is Fe. Thermodynamic calculations for combustion of A-11 RDF at 20 atm have shown that the gaseous fraction of iron oxides is equal to 1, 0.90, 0.23, 0.16, and 0 at the O/F mass ratios of 0.5, 1, 2, 5, and 10, respectively. Small values indicate that most iron oxide particles will be of the same scale as the initial fuel particles.

Table 6: Boiling points $(T_{\rm b})$ of the individual metals at 20 atm compared to the adiabatic flame temperatures $(T_{\rm f})$ of A-11 RDF burning with O₂ at different O/F mass ratios and the same pressure.

O/F	$\mathbf{T_{f}}$	$ m T_f/T_b$								
Mass	[K]	Ti Si		Fe	Fe Al		Mg			
Ratio		$T_b =$	$T_b =$	$T_b =$	$T_b =$	$T_b =$	$T_b =$			
		4702 K	4439 K	4066 K	3662 K	$2515~{ m K}$	1882 K			
0.5	3422	0.73	0.77	0.84	0.93	1.36	1.82			
1	3868	0.82	0.87	0.95	1.06	1.54	2.06			
2	3616	0.77	0.81	0.89	0.99	1.44	1.92			
5	3337	0.71	0.75	0.82	0.91	1.34	1.77			
10	2675	0.57	0.60	0.66	0.73	1.06	1.46			

3.1.3. Sulfur-Based Rocket Engines

Sulfur is not abundant on the lunar surface, but its utilization increases the possible design options for ISRU rocket engines. Early lunar samples indicated the existence of a low percentage of elemental sulfur in regolith [43] with regional variance in abundance (e.g., high in the Mare soil). The Indian probe Chandrayaan-3 recently confirmed the abundance of sulfur in lunar regolith [44]. The underlying assumption is that sulfur can be extracted separately from the alloys (using a simple heating process which has been tested on Apollo samples [45]), and it is available in its elemental form to cast/mix rocket propellants. There are ISRU applications for sulfur outside of rocket propellants, mainly using it as a cement alternative for construction purposes [24]. This make large-scale sulfur generation attractive, which could be integrated in regolith processing facilities that are set up for oxygen generation.

Just as with the metal–oxygen propellants, we calculated chamber temperature (T_c) and specific impulse (I_{sp}) at perfect expansion for O/F mass ratios ranging from 0.5 to 10 (in steps of 0.1 between 0.5 and 1, and after that in steps of 0.5) for all major metallic regolith components (Al, Si, Fe, Ti, Ca) separately reacting with sulfur (also in a solid state) as an oxidizer. The initial temperature of the reactants was set to 298 K. The chamber pressure (P_c) was set to 20 atm, and the ratio of the chamber pressure to the exit pressure (P_e) was set to 1000 (P_c/P_e), which corresponds to $P_e = 0.02$ atm.

The results, shown in Figure 7, predict combustion temperatures ranging from a peak of 4600 K for calcium–sulfur to very moderate temperatures of around 1460 K for iron–sulfur. The predicted peak $I_{\rm sp}$ ranges from 60 to 175 s for the metal–sulfur reaction, much lower than when oxygen is used as the oxidizer.

The utility of metal–sulfur propellant does not lie in its performance, which is significantly lower than that of a metal–oxygen system, but in its simplicity. Metal–sulfur can be cast into a solid propellant grain for a solid rocket motor.

To maximize performance, while still benefiting from easier propellant handling through casting metal–sulfur grains, a metal–sulfur–oxygen hybrid system is proposed. The hybrid system consists of a solid metal–sulfur propellant grain which reacts with liquid or gaseous oxygen as the oxidizer. This could be in the form of metal sulfide propellant or by using sulfur as "cement" to cast RDF powder into a solid form. There are only minimal quantities of naturally occurring metal sulfides on the lunar surface, and their predicted performance is lower than that of an RDF – S mixture since additional heat is generated through the metal–sulfur reaction before it reacts with the oxygen. Therefore, the thermodynamic calculations were only performed for metal–



Figure 7: Thermodynamic calculations for metal–sulfur reactions. Calculations for the $I_{\rm sp}$ of iron–sulfur do not converge for higher O/F mass ratios. The same applied for other metals at low O/F mass ratios. The legend is ordered with descending peak temperature and peak $I_{\rm sp}$, respectively.

sulfur–oxygen systems for all metals separately, and the results are shown in Figure 8.

The volumetric metal/sulfur mixture ratio corresponds to 70 vol% metal and 30 vol% sulfur, an intermediate value between the maximum (74 vol%) and random (63.5 vol%) packing density of equal spheres (assuming all metal particles are spheres). This assumption has to be modified depending on the particle size of the RDF (for an FFC-Cambridge process mainly > 300 μ m [23], which would require additional grinding for powder feeding but might be acceptable for casting a solid grain with sulfur) and the sulfur. Moreover, some reduction processes produce porous particles which would alter the calculations as well.

The mass fractions based on the volume ratio were calculated by:

$$Y_m = \frac{0.7\rho_m}{0.7\rho_m + 0.3\rho_S} \qquad Y_S = \frac{0.3\rho_S}{0.7\rho_m + 0.3\rho_S} \tag{2}$$



Figure 8: Thermodynamic calculations for different metal–sulfur–oxygen systems. Calculations for the $I_{\rm sp}$ of iron–sulfur–oxygen do not converge for higher O/F ratios. The calculations of aluminum–oxygen and sulfur–oxygen are also plotted in the graph as a reference.

where $Y_{\rm m}$ is the mass fraction of the metal, $Y_{\rm S}$ is the mass fraction of sulfur, and $\rho_{\rm m}$ and $\rho_{\rm S}$ are their respective densities. The mass fractions are shown in Table 7. We define the O/F mass ratio for the metal–sulfur–oxygen system as follows; the solid metal and sulfur grain (at the given volume ratio) is considered as the fuel and we use the molar mass of the grain to calculate the O/F mass ratio with oxygen, the oxidizer.

Table 7: Mass fractions of the metal and sulfur in a mixture of $70\,\mathrm{vol\%}$ metal and $30\,\mathrm{vol\%}$ sulfur.

	Al	Fe	Si	Mg	Ca	Ti
wt% metal	79	84	76	73	59	78
wt% sulfur	21	16	24	27	41	22

Figure 8 shows that the peak $I_{\rm sp}$ ranges from 180 to 270 s for the different

metals with chamber temperatures up to 4800 K. The performance is about 10% lower for a metal–sulfur–oxygen system compared to a pure metal–oxygen system (aluminum–oxygen is shown as a reference). However, all of the metal–sulfur–oxygen mixtures but iron show a higher $I_{\rm sp}$ than the brimstone rocket (S–O₂).

The influence of the sulfur content in Al–S fuel (oxidizer: oxygen) on $I_{\rm sp}$ was investigated. The results are shown in form of a 2D-map in Figure 9 where the sulfur content was varied between 0 vol% (i.e., pure aluminum) to 100 vol% (i.e., pure sulfur) over the O/F mass ratio range of 0.5–10. The proposed composition is indicated by the vertical line in the figure, and four iso- $I_{\rm sp}$ lines are shown as contours.



Figure 9: Influence of the sulfur content on specific impulse for varying volume ratios of the Al–S mixture over different O/F mass ratios.

As expected, the addition of sulfur decreases the $I_{\rm sp}$ for any given O/F mass ratio. This underscores the idea to use the minimum required amount of sulfur for casting the propellant grain. However, the $I_{\rm sp}$ is relatively constant (> 250 s) for sulfur contents of up to 50 vol% when operating within the proposed O/F mass ratio range of 2 to 4, suggesting that the value of $\approx 30\%$, based on filling the space between spherical particles, is a reasonable

engineering choice. Similar results can be obtained when doing the same calculations for chamber temperature (the 2D-map is provided in the Supplemental Material in Figure S8).

Since the products are complex and the convergence of the three solvers is insufficient for some of the metal–sulfur systems, no calculations of an RDF-S system were performed. It is reasonable to expect that the the I_{sp} and chamber temperatures would fall in between the values for the metallic components separately.

For the metal–sulfur–oxygen system, the calculation was performed for both RDFs (A-11 and A-12) as an elemental mixture. Since there is virtually no difference between the results for A-11 and A-12, only one of them (A-11) is shown in Figure 10. It is seen that both $I_{\rm sp}$ and chamber temperature are within the expected range based on the calculations for the pure metals. The temperatures for the propellant mixture with sulfur are lower than when burning with oxygen, while the specific impulse is slightly higher for O/F mass ratios up to 3 and slightly lower for high O/F mass ratios >3. The RDF–sulfur–oxygen system provides a higher specific impulse than sulfur– oxygen over the whole O/F mass ratio range. It can be expected that an alloy, as previously seen for RDF–oxygen, would also exhibit a slightly lower specific impulse and chamber temperature than the mixture of metals.

3.2. Configuration of Rocket Engines Using Regolith-Derived Fuels 3.2.1. Metal-Oxygen Rocket Engines

Based on prior work, two configurations can be considered for a RDF–LOX rocket engine: a premixed "slurry" design and a binary propellant design using a fluidized piston bed to feed the powder into the combustion chamber.

A slurry of RDF and LOX, which can be pump-fed and sprayed into the combustion chamber like a monopropellant [26, 46], would be an inherently simple system, but the concept is disqualified for multiple reasons: first, sedimentation will occur when storing the premixed propellant (especially if it is fuel-lean) because of gravity. One commonly proposed solution is using gelled metalized propellants such as Al/RP-1/O₂ or H₂/Al [47]. However, both rely on either an organic fuel or H₂. Al–LOX mixtures have been used since the 1930s as explosives and are known to be a safety hazard, often resulting in a deflagration-to-detonation transition, even with a gelling agent [48, 49]. The proposed gellant was SiO₂, which is available on the



Figure 10: Thermodynamic calculation for an A-11 regolith-derived mixture, sulfur, and oxygen system. The A-11 calculations with oxygen as well as sulfur–oxygen are shown for reference.

lunar surface. Organic polymers are also used as gellants, but they cannot be found in-situ [50].

These problems could be mitigated by using a fuel-rich slurry, which minimizes the explosion risk. LOX is added through porous nozzle walls in order to improve combustion performance while avoiding nozzle cooling issues. Even with these improvements, the concept has never been tested, and it is questionable if it can be operated safely. Therefore, we propose a bipropellant design for the RDF-LOX engine. This system mimics the functioning of a liquid bipropellant engine: the fuel and most of the oxidizer are fed into the combustion chamber separately. A schematic of the concept and its proposed components is shown in Figure 11.

To feed the RDF, we propose to use the so-called positive displacement fluidized bed system, which uses a permeable piston. In this approach, the fuel is stored in a cylindrical pressure vessel (in powdered form) and backfilled with a carrier gas. When the valve is opened, the carrier gas (an inert or the oxidizer) entrains the fuel as it penetrates through the piston. Then the



Figure 11: Schematic of the RDF/LOX hybrid bipropellant rocket design.

fuel can flow into the combustion chamber as a dense mixture of carrier gas and metal particles. Such a system has been successfully tested for aluminum and air [11] and for aluminum/magnesium and water [35]. This system has also been proposed for magnesium and CO_2 [51] and successfully tested for these reactants [52, 53]. A study was conducted on aluminum-fueled ramjet engines also using a fluidized bed and piston system [39]. Their system does not use an inert dispersion gas but the oxidizer directly.

A study [54] also tested both the fluidized piston and a motorized piston, proposed earlier in [55]. The paper concludes that the fluidized system is more suitable than the motorized piston. One important difference is that regolith powder consists of an alloy of multiple metals, and laboratory experiments have indicated that silicon is very difficult to disperse. The dispersion of regolith mixtures has not been studied, and experiments will have to be conducted to identify which modifications on the dispersion system might be required.

Supplying cryogenic LOX is commonly done in rocket engines. However, most of these engines use an engine cycle (such as staged combustion, expander cycle, etc.), and the pressurization of the oxidizer is turbopump driven. For the RDF – LOX concept, a cycle could be used or LOX could be supplied through a pressurized tank. Another option would be an H_2O_2 gas generator to drive the pump or a battery-powered system like in the Electron rockets. A study [56] shows that, especially for lower thrust engines, the electric cycles are competitive to a gas-generator cycle. The batteries would be transported from Earth with the engine itself but could be charged using solar panels on the lunar surface.

LOX can either be pressure fed or delivered by a turbopump. It might also be possible to drive a turbopump with the oxygen after it has absorbed the heat from the primary combustion chamber, which is commonly done in expander cycles with the fuel. For a low thrust level, a pressure-fed system or an electric pump can be implemented instead of a turbopump; for a high thrust level, a turbopump will be required. To start up the engine and achieve a sufficient temperature for ignition, either a small amount of a hypergolic propellant or a pyrotechnic mixture could be used.

From Figures 3, 4, 7, and 8, it is observed that the reasonable chamber temperature occurs for O/F mass ratios of > 2; however, to stabilize a flame, a fuel-rich environment is required [57]. Therefore, a primary combustion chamber is integrated into the system. This primary chamber is cooled, and the heat from this process is used to evaporate part of the LOX for the dispersion process. The rest of the LOX is injected into the secondary combustion chamber so that the combustion becomes fuel-lean and additionally through the porous nozzle for cooling with a boundary layer of oxygen.

Combustion of metals creates very high temperatures in the combustion chamber. Many rocket engines use regenerative cooling by the fuel [58]. Standard regenerative and film cooling strategies are also proposed for engines using LOX as the coolant. Despite the high reactivity of oxygen with any material at high temperatures, it is possible using specific copper alloys [59] and demonstrated in successful tests of engines with LOX cooling [60]. Multiple companies are working on innovative copper alloys that are 3D-printable and function well with LOX at high temperatures as shown in preliminary tests [61]. Different cooling solutions will be required for the different concepts. In a first step, the temperatures at different cross sections were analyzed over the O/F mass ratio range for the RDF-LOX concept and are presented in Figure 12. An increase in the O/F mass ratio decreases temperatures significantly, at the nozzle exit by almost 1000 K when going from a O/F mass ratio of 2 to 5, with an even larger decrease when approaching a ratio of 10. This is another indication that such an engine should be operated fuel-lean, where it is much easier to cool while only a moderate loss in $I_{\rm sp}$ is observed.

3.2.2. Sulfur-Based Rocket Engines

Possible configurations of metal–sulfur engines are presented in Figure 13. The S-LOX ("brimstone") rocket can either be configured as a bipropellant



Figure 12: Temperatures of the flow at different cross sections for the A-11 $\rm RDF-O_2$ thermodynamic calculations.

liquid system or as a hybrid. The two designs are shown in Figures 13a and 13b.

The melting point of sulfur is relatively low, $112.8 \,^{\circ}$ C, and the configuration in Figure 13a would resemble that of a standard liquid bipropellant engine using spray injection. The sulfur would be preheated to $150-160 \,^{\circ}$ C, where its viscosity is lowest [62], and then introduced as atomized droplets to react with either gaseous or liquid oxygen in the combustion chamber. A more detailed discussion can be found in [24].

Figure 13b shows a hybrid engine with a solid sulfur propellant grain and LOX as the oxidizer. Orthorhombic sulfur (its most stable phase) is very brittle and will be difficult to cast into a fuel grain without another component such as a metal. For a brimstone rocket without additives, the bipropellant design is more promising.

The enthalpy of formation of metal sulfides is considerably lower than that of corresponding oxides, which results in a relatively low $I_{\rm sp}$ of Me–S propellants as demonstrated by the thermodynamic calculations presented above. However, the non-cryogenic solid metal–sulfur fuels possess one im-



(a) Brimstone rocket in a liquid (spray injection) configuration.



(d) RDF, sulfur, and oxygen in a hybrid configuration.

Figure 13: Different possible engine configurations for sulfur, metal–sulfur, and metal–sulfur–oxygen rocket engines.

portant advantage: they have virtually unlimited storage life. Depots of stored metal-sulfur solid boosters would ensure guaranteed ascend capabilities to planetary orbits for mating with nuclear thermal or electric transportation tugs [63] and will permit fast on-planet emergency transportation via suborbital flights. Pressed zinc-sulfur powders have been used as a safe propellant in amateur rocketry since the 1950s. Beside their low $I_{\rm sp}$, the other undesirable property of Zn-S propellant is its very fast burning rate [64]. The sulfur in the metal-sulfur mixture can be melted by heating the Me-S powder blend above the sulfur melting point $(115 \,^{\circ}\text{C})$ [65]. which is 200-400 °C below the mixture ignition temperature. The resulting slurry can be cast as a propellant grain with a combustion channel of arbitrary shape. The burning rate of cast metal-sulfur compositions is much lower than of the pressed metal-sulfur powder grain and is in the $4-8 \,\mathrm{mm/s}$ range [25, 65, 66, 67], approaching the combustion rate of standard composite solid propellant. To increase the combustion rate, the metal-sulfur slurry can also be cast as small droplets in the manner of artillery propellant grains. The calculations indicate that 15 metals are capable of self-sustaining combustion with sulfur. Combustion of the cast Al, Ti, Si, Fe, Mn, -sulfur blends was observed experimentally [25].

The advantage of metal–sulfur boosters as shown in Figure 13c are their inherent simplicity allowing practically all-solid booster parts to be manufactured in-situ. For example, refractory nozzles that require heat resistivity can be net-shape manufactured using Self-Propagating High-Temperature Synthesis (SHS) of Cr-S cermets [67, 68]. To protect the wall of the combustion chamber from deposition of melted sulfide droplets, the propellant grain can be cast with a thin outside layer of pure sulfur whose gasification (boiling) at about 445 °C will provide outflow preventing deposition of the sulfide particles.

The most promising engine configuration using sulfur is a metal–sulfur– oxygen hybrid rocket engine whose schematic is shown in Figure 13d. While sulfur decreases the specific impulse of the system compared to pure metals, it enables the much simpler hybrid configuration in contrast to the configuration presented in Section 3.2.1. Therefore, it is recommended to minimize the sulfur content in the solid fuel grain to achieve maximum specific impulse (as presented in Figure 9). The minimum sulfur content is set to fill the gaps between spherical metal particles at maximum packing density, thus allowing for the solidification of the fuel grain.

In practice, hybrid engines have suffered from many problems that prevent

them from reaching their predicted performance and stable operation. Two main problems are the formation of a turbulent layer in the combustion zone and inconsistent regression rate [69]. The proposed propellant will lead to two separate combustion reactions: first, between the alloy and sulfur, which then further reacts with LOX. This could decrease the formation of a turbulent boundary layer and lead to a more consistent propellant burn rate. Studies on this innovative concept are required.

3.2.3. Comparison

The RDF-LOX bipropellant rocket engine is predicted to have the highest performance with a peak $I_{\rm sp}$ of 256s at an O/F mass ratio of 4 and chamber temperature of 3458 K. Additionally, it offers restarting capabilities, but the design is complex from an engineering perspective with the need to develop a reliable powder feeding system.

While powder feeding is the main engineering problem that has hindered the implementation of the proposed technology, there have been a lot of efforts and advances made in the field in the last few years. It has been shown that the developed powder feeding systems are very sensitive to particle shape and size of the powder. This means that such a system would have to be specifically tailored to work with RDF. Deposition problems can be mitigated by operating at conditions where liquid products are minimized and ablative, removable throat inserts can reduce problems with erosion. Cooling can be implemented using LOX, and high chamber temperatures can be avoided through operating at an appropriate O/F ratio. Flame stabilization issues can be solved by utilizing a primary and secondary combustion chamber, and incomplete combustion of the particles can be improved by lowering the particle size. Lastly, two-phase losses of I_{sp} may be a significant problem as the products contain a significant amount of condensed phase. If one were to decrease the RDF particle size to nanoscale to minimize two-phase losses, they may agglomerate more, possibly resulting in an even larger product particle size. It may be difficult to decrease the particle size and, at the same time, avoid/decrease the agglomeration. The combustion mode and combustion behavior will have to be verified in laboratory experiments with RDF powder. This is essential before attempting to develop and test a practical design for the rocket engine.

The RDF-S-LOX hybrid rocket engine has a simple design compared to the RDF-LOX concept, with a slightly reduced peak $I_{\rm sp}$ of 252 s at an O/F mass ratio of 4 and a marginally lower chamber temperature of 3447 K. Throttling and restarting is not inherently possible with the hybrid system as metal and sulfur can self-sustain combustion. However, one can deliberately choose a Me-S mixture ratio that will not support self-sustained flame propagation, though it will also fail to achieve peak performance. Then, the system can be quenched by cutting the oxygen flow and restarted.

S–LOX is a suitable rocket engine design when access to sulfur is abundant. The performance, with a $I_{\rm sp}$ of 243 s at an O/F ratio of 1.1 is sufficient for missions to Low Lunar Orbit (LLO) or hopper missions. The combustion temperature reaches a peak of 3633 K at the optimal O/F fuel mass ratio. As with all bipropellant concepts, it is more complex than a hybrid or solid engine but offers restarting capabilities.

RDF-S as a solid rocket engine is predicted to have the lowest performance with an $I_{\rm sp}$ of 100-120 s at a combustion temperature of 2000-3000 K. Solid rocket motors are simple to design but can usually neither be throttled nor restarted. The primary drawback of any system using sulfur is that its extraction necessitates a separate process from the rest of the RDF. The reduction process for RDF is required for oxygen generation on the lunar surface, with RDF serving as a convenient byproduct. However, this convenience does not extend to sulfur extraction. While exhibiting a much lower performance, the solid system excels in one aspect: propellant storability. The cast RDF-S propellant grain could be stored for nearly indefinite periods and would be well-suited as an emergency system, eliminating the need for propellant production close to the mission launch date.

4. Conclusions

Thermodynamic calculations have been conducted for regolith-derived fuels with oxygen. These calculations predict that RDF A-11 (a mixture of metal alloys) achieves a maximum specific impulse of 256 s at an O/F mass ratio of approximately 4. It has been shown that an alloy composition, which will be the fuel after the reduction process, exhibits a slightly lower ISP than an elemental mixture and aluminum, which was previously proposed as an ISRU fuel.

The high combustion chamber temperatures predicted by the thermodynamic calculations also indicate that such an engine would have to be operated fuel-lean to decrease deposition and allow for a simpler cooling system. With increasing O/F mass ratio, the $I_{\rm sp}$ decreases significantly less than chamber temperature. For O/F mass ratios between 4–8, chamber temperatures drop by 975 K while the $I_{\rm sp}$ decreases from its peak of 255 s to 230 s.

As the design of an RDF–LOX engine requires a powder feeding system, sulfur was considered as another ISRU fuel. It can act as a binder, an oxidizer for metals, or even as a fuel itself, enabling a wider range of propulsion options. Thermodynamic calculations were performed for different configurations. A key result is that the sulfur content in the fuel should be minimized while still allowing for the RDF to be cast into a solid fuel grain. This can be achieved at approximately 70 vol% RDF and 30 vol% sulfur. The decrease in peak $I_{\rm sp}$ through the inclusion of sulfur is predicted to be approximately 2%, while chamber temperatures are similar. At higher O/F mass ratios, the decrease in $I_{\rm sp}$ reaches up to 10%.

The brimstone rocket is calculated to have a lower performance than the systems including RDF and does not offer any other advantages over these systems. The last proposed design of a RDF – S solid rocket engine design is attractive because of its simplicity but exhibits low performance.

The RDF-S-LOX hybrid rocket engine is a promising design, which has not been previously proposed. Advancing the development of this concept, as well as the RDF-LOX concept, to the next stage necessitates addressing several open research questions and conducting experimental studies. In particular, the combustion mechanism of a Me-S grain in an oxygen environment should be investigated.

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Data Availability

The source data for the thermodynamic calculations is available upon request.

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Highlights

- Rocket propellants can be directly sourced from lunar regolith.
- Such regolith-derived fuels can produce a peak specific impulse of up to 250 s.
- Sulfur can be used as either an oxidizer or additive to the regolithderived fuel.
- Different configurations for rocket engines using these fuels are presented.

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Declaration of interests

 \boxtimes 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.

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