SIMULATING THE SPECTRAL PROPERTIES OF IRON-BEARING REGIONS OF MARS USING THE SPLITS MODEL

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ABSTRACT

The mineralogy and environmental history of Mars are been extensively investigated through remote sensing observations paired with laboratory and *in situ* experiments. A significant portion of these experiments is being devoted to the identification and quantification of different iron oxides present in the Martian terrains. Although such experiments can provide valuable information regarding the presence of these minerals, the scope of the resulting observations may be hindered by logistics and cost-related constraints. We believe that predictive computer simulations can be employed to mitigate some of these constraints and contribute to the generation and validation of hypotheses in this area. Accordingly, we propose the use of SPLITS (*Sp*ectral *Li*ght *T*ransport Model for *S*and) in investigations involving the spectral signatures of iron-rich sand-textured soils found on Mars, and demonstrate its predictive capabilities in this context through comparisons of modeled results with actual measured data.

Index Terms**—** Mars, sand, regolith, iron oxide, spectral reflectance, simulation.

1. INTRODUCTION

Mars is covered by loose, particulate material, called regolith, characterized by the presence of iron oxides [1, 2, 3], such as hematite and goethite, whose spectral properties are directly associated with the overall reddish appearance of the Martian surface and the butterscotch color of the Martian sky (Figure 1). The identification and quantification of these iron-rich compounds is central in geoscientific studies of the "red planet". These minerals are indicators of environmental factors that are of relevance not only for the understanding of the origins of Martian terrains [4], but also for the search for potential environments that sustain life on Mars [5]. More specifically, iron oxides contain in their formula the ferrous (Fe^{2+}) and/or the ferric (Fe^{3+}) oxidation states of iron, which are considered to be associated with unweathered and weathered components of the Martian surface, respectively [1]. For example, the ferric iron-oxide goethite forms as a product of aqueous processes in natural environments, and it has the hydroxide anion (OH^-) as an essential part of its structure ($\approx$10% H_2O by weight) [4]. These characteristics of goethite have led its identification in certain Martian terrains to be interpreted as mineralogical evidence of aqueous activity on those areas [4].

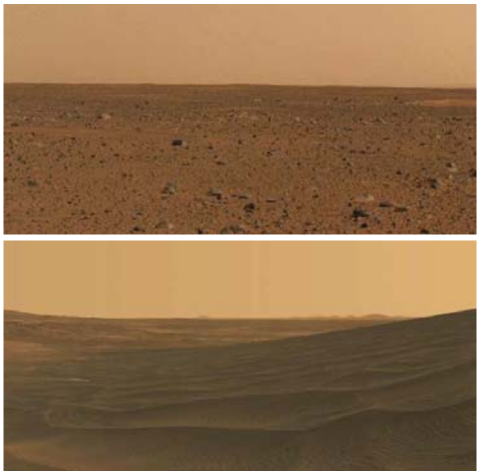

Fig. 1. Photos of the Gusev crater taken by the panoramic camera on board the Mars Exploration Rover Spirit (courtesy of NASA).

Arguably, the ferrous and ferric oxidation states of iron are the most spectrally-active cations in the visible to near-infrared (VNIR) remote sensing of planetary surfaces [1, 6]. Accordingly, valuable information about the mineralogy [4, 7], lithology [8], environmental history [1, 4] and astrobiology [5] of iron-bearing regions of Mars can be obtained through remote sensing observations of its surface coupled with laboratory experiments and simulations. Moreover, such combined efforts are crucial for the optimization of *in situ* explorations and measurements to be carried out by future missions to the "red planet" [3].

Laboratory experiments used in the investigation of Martian terrains usually employ soil analogues, or simulants [2, 9, 10], since true Martian regolith samples are either not available or too valuable to be modified and contaminated

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by experimental procedures [3]. However, although soil analogues have been extensively used in studies regarding the thermal, mechanical, morphological and chemical properties of Martian regolith, they have a limited applicability in spectral investigations involving these materials. This limitation is mostly due to the fact that certain mineralogical and physical properties (*e.g.*, iron oxide contents, density of parent material and grain shape) cannot be effectively mimicked or controlled in experiments involving regolith simulants [3].

In order to overcome the investigation constraints mentioned above, we propose the use of a computational simulation framework that allows for systematic *in silico* experiments involving the spectral properties of sandy landscapes and regolith-covered terrains found in Mars. Within this framework, the light interactions with the particulate materials forming these regions are simulated using a computer model, SPLITS (*Sp*ectral *Li*ght *T*ransport Model for *S*and) [11], that accounts for the morphological and mineralogical characteristics of the constituent grains of these materials and their distribution in the pore medium [12]. Employing this framework, researchers can change selected material parameters and analyse their effects on the spectral signature of these regions while keeping the other parameters constant. In fact, SPLITS can be run online [13] via a model distribution framework that enables researchers to specify experimental conditions (*e.g.*, angle of incidence and spectral range) and material parameters (*e.g.*, amount or iron oxides, soil texture and particle type distribution), and receive customized simulation results.

2. MATERIALS AND METHODS

In this paper, we demonstrate the predictive capabilities of the SPLITS model with respect to the investigation of Martian regolith through comparisons of measured data with modeled data computed for different iron-bearing regions of Mars, namely the Olympus-Amazonis [14], the Oxia Palus [14] and the Gusev crater [15]. It has been stated that the regolith materials found in these regions contain iron oxides such as hematite, goethite and magnetite, and have basalt as their primary parent material [4, 7, 15, 16]. Accordingly, in our simulations, we employed basalt (with a density of 3 kg/L [16]) as the parent material, and considered the iron oxides appearing as pure particles [1], as contaminants in the parent material [17], or as coatings within an illite matrix [18]. It is worth noting that we employed physical data obtained for Martian regolith whenever such data was available (*e.g.*, porosity (60%) [19]), and average data associated with terrestrial sandy soils otherwise (*e.g.*, grain roundness (0.482) [20] and sphericity (0.798) [21]). The dimensions for the sand-sized and silt-sized particles were obtained from data provided by Shirazi *et al.* [22], and the presence of clay-sized particles was assumed to be negligible. The remaining parameter values used to obtain the modeled reflectance curves are given in Table 1.

Set	r_{hg}	ϑ_{hg}	ϑ_m	sand	silt	μ_p	μ_m	μ_c
I	0.75	0.005	0.00	85	15	0	90	10
II	0.15	0.070	0.00	95	5	0	100	0
III	0.25	0.030	0.00	85	15	0	100	0
IV	0.20	0.030	0.00	95	5	0	100	0
V	0.50	0.030	0.01	85	15	10	80	10

Table 1. Input datasets I, II, III, IV and V used to obtain modeled reflectance curves for five sites on distinct regions of Mars: Olympus-Amazonis, Oxia Palus and Gusev crater (sites D-green, D-red and E-green), respectively. The parameter r_{hg} corresponds to the ratio between the mass fraction of hematite to the total mass fraction of hematite and goethite represented, which is given by ϑ_{hg}. The parameter ϑ_m represents the mass fraction of magnetite. The texture of the samples is described by the percentages (%) of sand and silt. The particle type distributions considered in the simulations are given in terms of the percentages (%) of pure (μ_p), mixed (μ_m) and coated (μ_g) grains. It is assumed that magnetite grains appear as pure particles [2, 23].

3. RESULTS AND DISCUSSION

Initially, we compared modeled results with measured spectra for the Olympus-Amazonis and Oxia Palus regions [14]. As it can be observed in the graphs presented in Figure 2, the modeled reflectance curves obtained using SPLITS capture the main qualitative trends depicted in the measured reflectance curves.

We note that the measured spectra depicted in Figure 2 correspond to composite spectra obtained by merging data captured using a scanning imaging spectrometer with a spatial resolution of 22 km/pixel with data acquired using ground-based telescopic observations. As a result, these composite spectra incorporate a certain degree of spatial and temporal variability that cannot be fully reproduced through simulations, either based on computer models (Figure 2) or regolith simulants (Figure 3), associated with discrete experimental conditions.

In order to further assess the predictive capabilities of the SPLITS model, we also compared modeled reflectance spectra with *in situ* measured spectra for different sites at the Gusev crater. These measured spectra were acquired through a multispectral imaging system on board the Mars Exploration Rover Spirit, and they were estimated to be within a 5 to 10% absolute accuracy [15]. The system was mounted on a mast assembly $\approx$1.5 m above the Martian surface. As it can observed in the graphs presented in Figure 4, the modeled curves show good quantitative and qualitative agreement with their measured counterparts. We note that this level of predictability was achieved despite the fact that not all minerals found in these regions could be accounted for in the simulations due to the lack of reliable supporting data such as spectral indices of refraction and extinction coefficients.

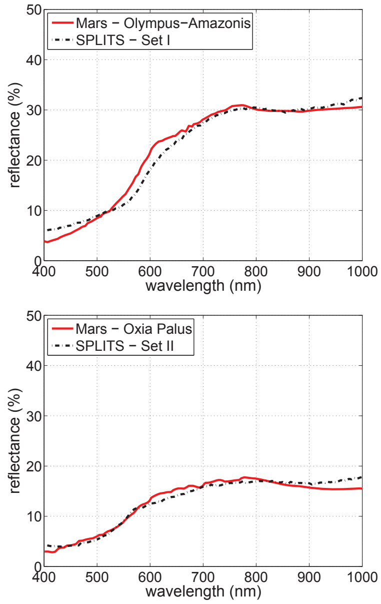

Fig. 2. Comparisons of measured and modeled spectra for bright (Olympus-Amazonis) and dark (Oxia Palus) regions of Mars. The measured composite spectra provided by Mustard and Bell [14] was obtained by merging data acquired through the ISM (Imaging Spectrometer for Mars) experiment on the 1989 Soviet Phobos-2 mission with ground-based telescopic observations of Mars, and removing atmospheric absorptions. The modeled data was obtained employing the SPLITS model [11, 13] and using the input datasets I and II given in Table 1. Top: Olympus-Amazonis region. Bottom: Oxia Palus region.

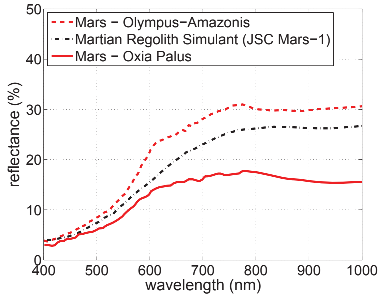

Fig. 3. Comparisons of measured spectra for bright (Olympus-Amazonis) and dark (Oxia Palus) regions of Mars provided by Mustard and Bell [14] with the measured spectrum of a Martian regolith simulant (JSC Mars-1) provided by Allen *et al.* [9].

4. CONCLUSION AND FUTURE WORK

We believe that the integration of remote sensing data with predictive modeling can play an important role in investigations involving the spectral properties, mineralogy, lithology and environmental history of Martian landscapes. The simulations reported in this work show that the proposed *in silico* experimental framework based on the SPLITS model has the flexibility and predictive capabilities required to support such investigations. As future work, we intend to employ the proposed framework in the study of different hypotheses related to weathering processes involved in the formation of Martian terrains. We also intend to extend our research to other planetary bodies, such as Venus and Titan, as more supporting morphological and spectral data becomes available.

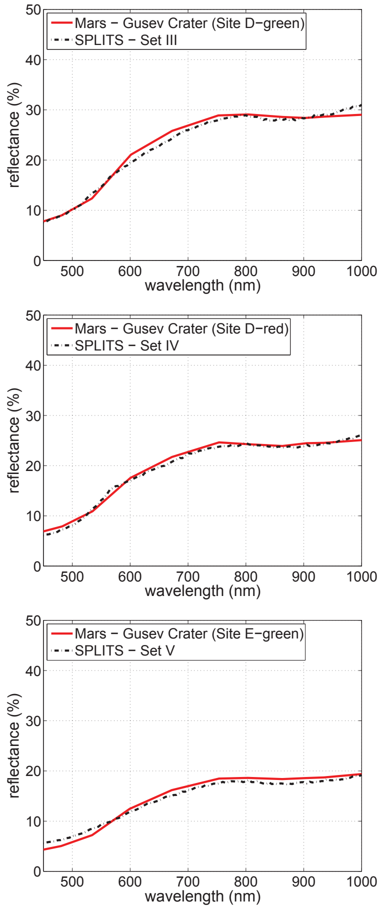

Fig. 4. Comparisons of measured and modeled spectra for different sites at the Gusev crater on Mars. The measured spectra provided by Bell *et al.* [15] was obtained from multispectral images acquired using a digital imaging system (panoramic camera) on board the Mars exploration rover Spirit. The modeled data was obtained employing the SPLITS model [11, 13] and using the input datasets III, IV and V given in Table 1. Top: site D-green. Middle: site D-red. Bottom: site E-green.

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