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Multivariate approach for evaluating the composition of Meridiani spherules

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Introduction

One of the reasons for selecting Meridiani Planum as one of the two landing sites for the MER (Mars Exploration Rover) mission was the detection of a hematite signature by the TES (Thermal Emission Spectrometer) instrument onboard MGS (Mars Global surveyor) [1]. The presence of hematite at Meridiani has since been confirmed by instruments of the Athena Science Payload of the Opportunity MER rover [2,3]. Meridiani plains appear to be sulphur-rich sedimentary layered rocks covered by basaltic soils (outcrops being exposed within impact craters) [3,4]. Ubiquitous mm-sized spherules, nicknamed 'blueberries', have been observed in both the rocks and the soils. Opportunity's mini-TES and Mössbauer spectrometer (MB) have shown that hematite is present both in the matrix of the layered rocks and in the spherules [2,3].

Despite various suggestions accounting for some characteristics of the spherules, no fully convincing terrestrial analogue has been proposed yet and their formation process remains controversial [5,6,7,8] especially as their composition is not fully constrained by the measurements of the Athena Science Payload. Estimating the composition of the blueberries is indeed a challenging question mainly because their diameter is smaller than the fields of view (FOV) of the APXS (Alpha-Particle X-ray Spectrometer) and the MB (Fig. 1) [9,10]. Some constraints have nevertheless been established, suggesting that they contain at least 50% (in mass) of hematite [3]. Some attempts to determine their chemical compositions were also performed using mass-balance mixing models [11]. Here we propose a statistical approach based on Blind Source Separation (BSS) to estimate their chemical composition.

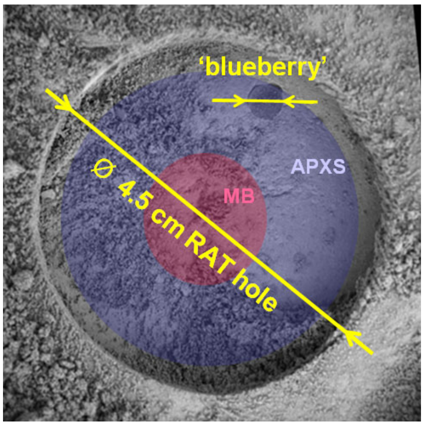

Figure 1: Micro-Imager mosaic of 'Tennessee' abraded rock target, in Endurance Crater, showing the relative sizes of a typical spherule (with a diameter of several mm) and surfaces sampled by the contact instruments (Ø 38 mm for APXS, Ø 15 mm for MB). This figure illustrates the sub-FOV mixing of different materials.

Method

Elemental compositions from APXS are approximated by a linear mixing of pure rock and soil constituents (Fig. 1): Y=A.S (Y: compositions for Meridiani samples measured by APXS [12], A: proportions of constituents, S: compositions of constituents). We propose to estimate the matrices A and S under two main constraints to ensure physical interpretation. A strong constraint is the positivity of the elements in both matrices A and S. The second constraint that may be imposed is additivity of the elements of A, as the constituent proportions should sum to unity for each sample. The constrained estimation of A and S can be considered as a source separation problem and can be addressed in a Bayesian framework. An algorithm to perform an unsupervised joint estimation under positivity and additivity constraints has been used [13,14]. This algorithm

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is based on hierarchical Bayesian models to encode prior information regarding the parameters of interest and include the additivity and sum-to-one constraints. The estimation from the posterior distribution is performed using Markov Chain Monte Carlo methods.

Input data Y were expressed in mass oxide compositions, implying a 'closing relation' as they are normalized at 100% (mass oxide) for the usual APXS-detected elements. This condition should also be verified for the S vectors. The number of sources (one of the two dimensions of matrix S, the other being the number of APXS-detected elements) is an unconstrained parameter. We tested several possibilities and selected the best result based on two criteria: (i) S vectors are all normalized and therefore interpretable in terms of oxide composition (ii) best solution with the maximum number of sources (to improve data fitting).

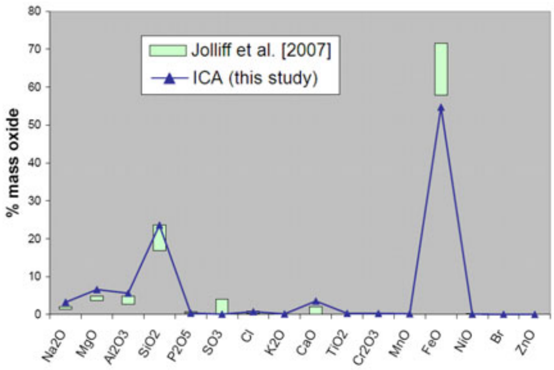

Figure 2: Comparison of the composition of the Fe-rich source obtained through ICA with the ranges of values for the spherules' compositions computed through mass-balance mixing models, under various hypotheses [11].

Results and implications

In the analyses performed on the Meridiani dataset (both rocks and soils), an iron-rich source was easily identifiable (unambiguously having the highest Fe-content of all determined sources). The samples with the most important contributions of this source were the spherule-rich targets (according to imagery). Assuming that spherules and their fragments are homogeneous in composition, both individually (no internal zonation) and spatially (along the several km-long traverse of Opportunity), it suggests that this source may represent their composition. We compared it (Fig. 2) with the spherule compositions inferred using mass-balance mixing models [11]. Despite some discrepancies between both methods, our analysis also appears in favour of non-purely hematite blueberries, containing a certain fraction of a silicate component. Our source contains slightly more CaO, Al_2O_3 and MgO, but less FeO and SO_3. The weak SO_3 content (~0.09%) that we obtain might be explained by the fact that our statistical approach similarly takes into account mixing in both surface proportions and (thin) depth, and should be less affected by effects relative to thin dust layers [11]. We obtain a ~55% FeO content (if all Fe is listed as FeO) which is equivalent to a ~58% Fe_2O_3 content (if all Fe is listed as Fe_2O_3). According to our method, this value would represent an upper limit for the hematite content of the spherules, as some APXS-blind low Z elements could also be present. If these spherules are sedimentary concretions, as assumed in most formation models, a hematite content below 70% is then consistent with a growth by replacive process rather than displacive [5].

These preliminary results are encouraging, and further work should allow chemical interpretation of the other sources identified by this unsupervised method. This can help characterizing other rock or soil components at both Gusev and Meridiani, thereby contributing to the understanding of these sites' geological history.

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