Compositional modelling of sediment formation at the surface of Mars

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Poster presentation

1 Introduction

Compositional modelling is performed on chemical compositions of Martian surface materials in order to understand weathering scenarios and the role of meteoritic accumulation. Compositional techniques are applied to elucidate the influence of remote weathering by combined analysis of several soil forming branches. The results foster evidence for the past activity of volcanic exhalation products along with that of liquid water.

One of the most exciting results of the Mars Exploration Rover (MER-A and MER-B, NASA) and Mars Express (ESA) mission is the clear indication for the presence of liquid water as an agent of chemical weathering on ancient Mars. A comprehensive interpretation of the available data is introduced in Kolb et al. (2006). In our compositional modelling we employ chemical data that were obtained in the course of the Mars Pathfinder and the MER missions to identify the processes involved in the degradation of primary planetary material and in sediment formation.

Aitchison (1986) defined a composition as a collection of D non-negative measurements, which sum to unity per weight, volume, or abundance. Such constraints are obeyed by the Simplex space geometry, which represents a D-dimensional analogue of a triangle, in contrast to the D-dimensional orthogonal Euclidean space geometry. Centered log ratio *clr* transformation translates compositional data from the constrained Simplex space to the Euclidean real space. The *clr* transformation of a compositional vector $\mathbf{C}$ with components c_i is defined as $clr(\mathbf{C}) = [\ln \frac{c_1}{g(\mathbf{C})}, \ldots, \ln \frac{c_D}{g(\mathbf{C})}]$, where $g(\mathbf{C})$ is the geometric mean of the vector $\mathbf{C}$. In this work we focus on visualization of data variability by means of biplot techniques (Aitchison and Greenacre, 2002). Based on the variability patterns, rock alteration and soil formation processes such as remote weathering are modelled.

2 Compositional modelling

If in the course of an alteration process a subset of elements is mobile and is added or lost from a given volume of rock, the concentrations of all components, the mobile ones but also the immobile ones, will change merely due to the closure condition. Aitchison (1986) proposed the so-called perturbation mechanism in order to model an exchange of chemical compositions by means of compositional vectors under consideration of the Simplex geometry. The application of a compositional vector $\mathbf{C}$ on the chemical composition $\mathbf{C}^*$ to yield the chemical composition $\mathbf{C}^{**}$ by means of the perturbation operation $\oplus$, is defined as $\mathbf{C}^{**} = \mathbf{C} \oplus \mathbf{C}^* = \left[\frac{c_1 c_1^*}{\sum c_k c_k^*}, \ldots, \frac{c_D c_D^*}{\sum c_k c_k^*}\right]$. The components of the alteration vector $\mathbf{C}$ must be a measure of change for the same parts of individual observations linked by this vector. An active change of compositions takes place if values of the corresponding vector entries are not equal to the geometric mean. Vector entries which are above this level are actively increasing, values which are below are actively decreasing. However, a passive change of compositional values could occur, although the corresponding values of vector entries equal the geometric mean.

Chemical compositions of Martian surface materials in terms of element wt% of 13 elements $(Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, Cr, Mn, Fe)$ were taken from the literature (Kolb et al., 2006). Figure 1 represents a *clr*-biplot on Pathfinder and Mars Exploration Rover data, which describes 74% of the variance. In the biplot the presumed source rocks have been projected. The lines denote the distribution of *clr* transformed variables across the chemical variability of Martian surface materials. Five classes of sample suites are discernable: Domain of soil, MER-B evaporites, MER-B basalts, MER-A basalts and Mars Pathfinder basalt-andesites. The soils plot close to the origin. The presumed source rocks are located in different more peripheral positions, illustrating the chemical uniformity among soils as opposed to the rather heterogeneous nature of rock compositions. The trends allow discrimination between coated and abraded rocks which are located proximal and distal to the region of soils, respectively. The magmatic rocks plot on the side of *clr*(Si) and the evaporites are located in the area spanned by *clr*(S), *clr*(Cl), and *clr*(Mg). MER-A basalts plot in the vicinity of *clr*(Mg) and *clr*(Cr); basalt-andesites are shifted toward majority of *clr*(K) and *clr*(Si); MER-B basalts are of intermediary character. Overall, these observations are consistent with petrological models of Martian rocks. The shift between brushed MER-A basalts and abraded MER-A basalts indicates the formation of chemical weathering crusts different from fresh rocks (Fig. 1).

The alteration vector calculation is based on *clr* Principal Component Analysis (*clr*-PCA) of fresh basalts (abraded) and their crusts (brushed rocks). We transform back the first *clr*-PCA eigenvector to obtain the

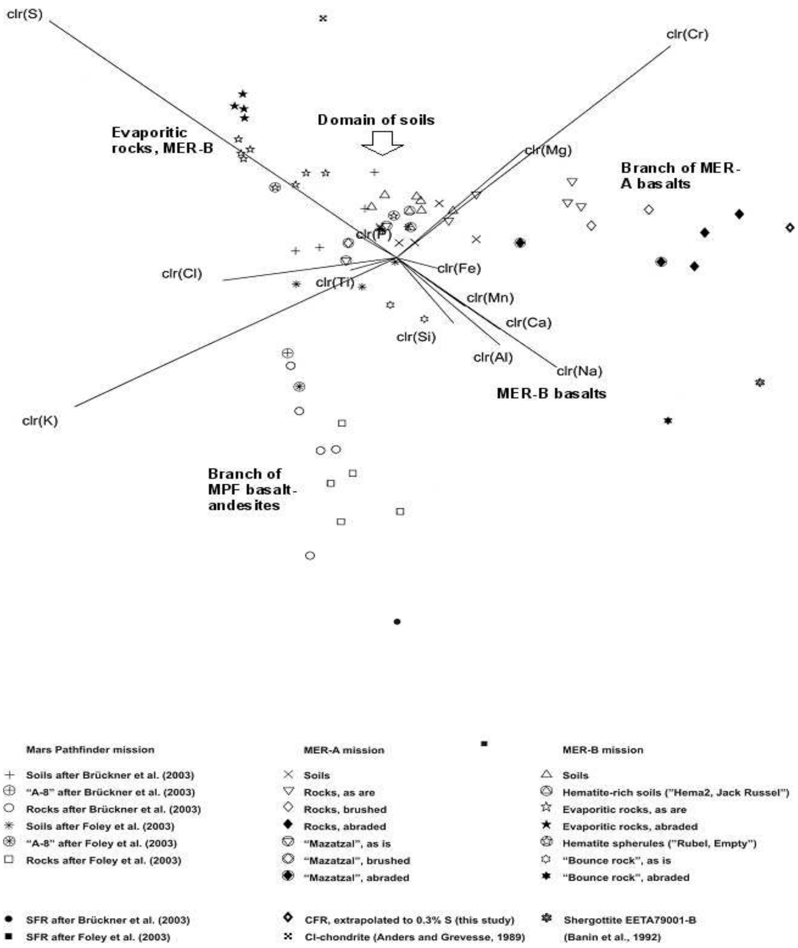

FIGURE 1. *clr*-biplot of Martian samples. The abbreviation SFR and CFR stands for Soil Free Rock and Crust Free Rock, respectively.

alteration vector $\mathbf{C} = (Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, Cr, Mn, Fe) = [7.2, 5.3, 6.4, 6.2, 6.8, 12.6, 12, 12.7, 6.2, 6.5, 6.2, 6, 5.9]$, which has geometric mean equal to $g(\mathbf{C}) = 7.3$. This vector explains 82% of variability. The relation of vector entries to the geometric mean is a measure for their degree of change. The element Na remains actively unchanged in the course of alteration, the others change to different degree. S and Cl are incorporated in crust, while Mg and Fe are removed from crust in relation to the fresh rock. This is consistent with the formation pathway of Mg-, Fe-bearing sulfates and ferric oxides upon dissolution of Mg-, Fe-bearing primary silicates.

The element K in crusts stems most probably from impurities, derived from remote weathering of basalt-andesitic or other K-bearing rocks. This procedure based on *clr*-PCA analysis is applied to the others branches (Fig. 1). Applied to the entire MER-A basalt and soil data complex to derive soil formation vectors, are capable to explain high levels of variability (94%). Application of *clr*-PCA to the Mars Pathfinder (MPF) basalt-andesitic rock and soil branch provided a vector with 92% explanation of variability. The vector along the MER-B basalt branch by means of *clr*-PCA covers 99% of variability. In Kolb et al. (2006) detailed interpretations are given. Compositional data analysis by means of *clr*-biplot visualization techniques provides a clear separation of Martian surface samples and allows to assign individual elements to specific principal component characteristics: basalt-andesites are related to K, Si; MER-A basalts are related to Mg, Cr; MER-B basalts are of intermediary nature and MER-B evaporites are related to S, Cl, Mg. Overall, these findings are consistent with existing petrological models of Martian rocks. Furthermore, chemical weathering rinds are observed to be significant differently composed in relation to soil and fresh rock, but appear as intermediate stage of soil formation.

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