

COMPUTATIONAL REANALYSIS OF THE PHOENIX LANDER WET CHEMISTRY LAB DATA

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Introduction: In 2008 NASA's Phoenix mission landed on the northern plains of Mars with the primary mission of understanding the history of water at the site and assessing the habitability of the region [1]. During this mission the first wet chemical analysis of the Martian regolith was conducted by the Wet Chemistry Laboratory (WCL) sensor array; to date, the measurements taken by WCL remain the only direct measurements of the soluble ions in the Martian regolith. The Phoenix WCL experiments measured Ca^{2+} , Mg^{2+} , Na^+ , K^+ , Cl^- , and ClO_4^- in the top 5 cm of the regolith [2, 4]. The identity and concentration of the soluble ions in the regolith serve as a basis for understanding many of the aqueous processes that have occurred on Mars.

The WCL sensor data contains significantly degraded and noisy signals. Some of the noise associated with the data can be attributed to specific software issues, and in these cases the noise was removed by deleting affected data points followed by Fourier filtering to remove the remaining high frequency noise [2]. However, uncertainties ranging from 25% to over 200% remained. Later attempts used Kalman smoothing techniques to reduce the noise without excluding additional data points [3]. This approach provided significant improvement, reducing the uncertainty to 10-50%, but included signals that are independent of the chemistry, resulting in a skewed data set.

Here we present a reanalysis of the WCL data through the application of a common factor algorithm, designed to eliminate these unknown systematic errors in a bias-free way, and the reinterpretation of the WCL data based on the newly processed data to a much higher degree of certainty. Using this method of error analysis and recalculating the ion concentrations based on the new potential values obtained using the common factor method, we present a more variable distribution of ions with a substantial reduction in uncertainty.

Methodology: We developed a new common-factor removal method that utilizes all ISE measurements simultaneously to find the hidden common factors that drive all measurements to vary simultaneously, but not as a result of the chemistry. These common factors

represent the errors and variations caused by the combined and complicated influence of varying temperature, pressure, stirring motion, device malfunction, sensor locations, and other common but unknown electronic interferences. We have cleaned the data by removing the effects of these common factors.

Let K denotes the number of common factors, F_{kt} the k^{th} common factor at time t . The observed data can be modeled as

$$E_t^{(i)} = \mu^{(i)} + \beta_1^{(i)} F_{1t} + \dots + \beta_K^{(i)} F_{Kt} + \varepsilon_t^{(i)}, \quad (1)$$

where $\beta_1^{(i)}, \dots, \beta_K^{(i)}$ are the coefficients of the K common factors for ISE signal i , and $\varepsilon_t^{(i)}$ are random white noise. Notice that the common factors are the same for all ion ISEs, but their influences on each ion may be different due to its different physical properties, and this is reflected in the coefficient $\beta_K^{(i)}$ for that ion. We want to use common factors to help us reduce the variations in the data without changing the base mean level of the data. So we require the base mean of factors to be zero.

The cleaned data to be calculated are

$$E_t^{*(i)} = E_t^{(i)} - \beta_1^{(i)} F_{1t} - \dots - \beta_K^{(i)} F_{Kt} = \mu^{(i)} + \varepsilon_t^{(i)}. \quad (2)$$

We assume that all the ISE sensors mounted on the inside walls of the same beaker that demonstrated similar patterns, were impacted by the same set of common factors. We iteratively estimate the common factors and coefficients of all ISE signals by minimizing the sum of squared errors of all the ions measured by the WCL. We then clean the data by removing the effects of these common factors.

The two-common-factor model ($K=2$) was applied to clean the data during the same time intervals as the original analysis by Kounaves et al. [2]. These time intervals were maintained as they represent the most stable regions of the data, thereby minimizing the effect of sensor drift on the overall results. The uncertainty was generated from the standard deviations for the newly cleaned data and the error values given by

the original interpretation using the standard error propagation equation

$$\sigma^2(f) = \left(\frac{\partial f}{\partial x}\sigma_x\right)^2 + \left(\frac{\partial f}{\partial y}\sigma_y\right)^2 + \dots \quad (3)$$

Results: The Original interpretation of the WCL chemistry experiments based on this data suggested a uniform vertical and horizontal distribution of the measured ions within the top 5 cm at the Phoenix landing site. While the mean concentration of ions in solution varied somewhat between samples, the large degree of uncertainty associated with each measurement resulted in an interpretation of uniformity.

The application of our common factor algorithm, designed to eliminate these unknown systematic errors in a bias-free way, enabled the reinterpretation of the WCL data to a much higher degree of certainty. By replacing their potential mean and error estimates with our common factor cleaned mean and standard error, we are able to reduce the uncertainty, and therefore increase the validity of the WCL data.

Figure 1: Ion concentrations of WCL solutions as reported by Kounaves et al [2]

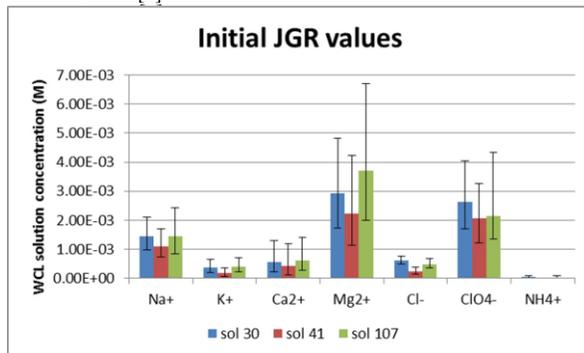
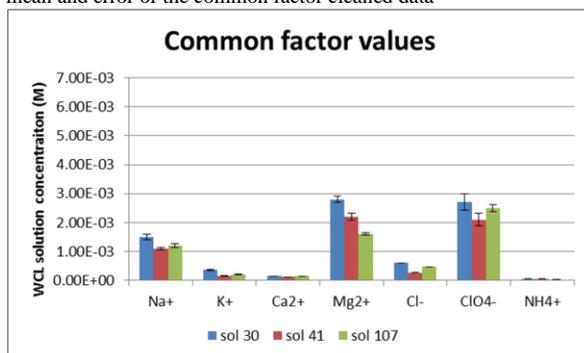


Figure 2: Ion concentrations of WCL solutions using the standard mean and error of the common factor cleaned data



Using the common factor values we were able to reduce the uncertainty in the measured ion concen-

trations to between 0.5% - 10%. This reduction in uncertainty revealed a heterogeneous distribution of ions both vertically and horizontally at the Phoenix landing site with a tendency toward concentration in the surface, sol 30, and sample. Similar redistributions have been observed in the hyper arid environment of Antarctica in connection with limited availability of liquid water [5] suggesting infrequent and minimal interaction of the Phoenix landing site with liquid water.

Table 1: Percent difference between original ion averages and common factor averages

	sol 30	sol 41	sol 107
Na ⁺	3.7%	0.0%	17.9%
K ⁺	0.8%	10.5%	60.4%
Ca ²⁺	118.2%	115.2%	119.7%
Mg ²⁺	4.5%	1.7%	79.3%
Cl ⁻	0.9%	9.6%	0.2%
ClO ₄ ⁻	2.2%	1.7%	15.0%
NH ₄ ⁺	15.4%	ND	13.9%

Table 2: Percent difference between sols using common factor averages

	sol 30_41	sol 30_107	sol 41_107
Na ⁺	8.7%	22.2%	13.6%
K ⁺	63.2%	53.2%	10.8%
Ca ²⁺	1.2%	6.3%	5.1%
Mg ²⁺	1.8%	54.5%	52.9%
Cl ⁻	57.4%	25.5%	33.2%
ClO ₄ ⁻	2.8%	7.7%	4.9%
NH ₄ ⁺	35.5%	50.8%	82.5%

Acknowledgements: This work was supported by NASA under Grant NNX13AJ69G.

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