Analysis of the Wet Chemistry Data from the Phoenix Mission Aided by Machine Learning

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The data for 4 WCL analysis events is posted at
http://www.cs.umb.edu/~ding/classes/470_670/homework/data/

You may read Sections 1 to 3 of the paper JGR 2009 - WCL data.pdf for more detailed explanation of the WCL operations.

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1: Introduction/Background

During the summer of 2008, the Wet Chemistry Laboratory (WCL) on board the Phoenix Lander performed the first comprehensive wet chemical analysis of the soil on Mars. Each WCL consisted of a lower cell whose walls were lined with an array of sensors and an upper assembly for adding water, reagents, soil, and stirring. The sensor array included ion selective electrodes (ISE) for K^+, Na^+, Mg^{2+}, Ca^{2+}, NH_4^+, Ba^{2+} (for SO_4^{2-}), Cl^-, Br^-, I^-, NO_3^-/ClO_4^-, H^+(pH), Li^+, and electrodes for conductivity, redox potential, cyclic voltammetry, chronopotentiometry, and an IrO pH electrode. The goal of the WCL ISEs was to analyze the chemistry of the soils at the surface and at depth in order to better understand, the history of the water, the biohabitability of the soil, the availability of chemical energy sources, and the general geochemistry of the site.

Figure 1. The Phoenix Lander Wet Chemistry Laboratory on Mars after the first analysis.

The WCL sensor data presents a significantly “clouded” and noisy picture produced by several types of interferences. Figure 2 and Table 1 show a synopsis of the 16 analyses run on Mars, 4 initial sample analyses on each cell, and the 12 subsequent analysis on the sample already in the cell or after more soil was added.

2: Project Goal--Fuzzy Sequence Mapping

For each cell, the first of the 2-sol analysis began with thawing and dispensing the leaching solution into the analysis beaker. After equilibration of sensors in the leaching solution, a second calibration point was obtained by adding a crucible of known salt content to the beaker. After calibration, the soil sample was delivered to the WCL sample drawer. The WCL analytical protocol is described in Figure 4.

It is evident that the changes of temperature not only affect the ISEs signal amplitude, but also offset in the time domain (Figure 2). Because of heat conduction through the cell wall and solution, the change of temperature measured by the beaker thermocouple is out of phase with that reflected by the voltage changes in the ISE signals. In order to apply a thermal correction, we will need to find the actual temperature affecting the ISE potentials.

In this project, we will design and implement a fuzzy sequence pattern matching algorithm. We will look for the optimal approximate alignment between temperature and ISE signals when an exact match is not possible.

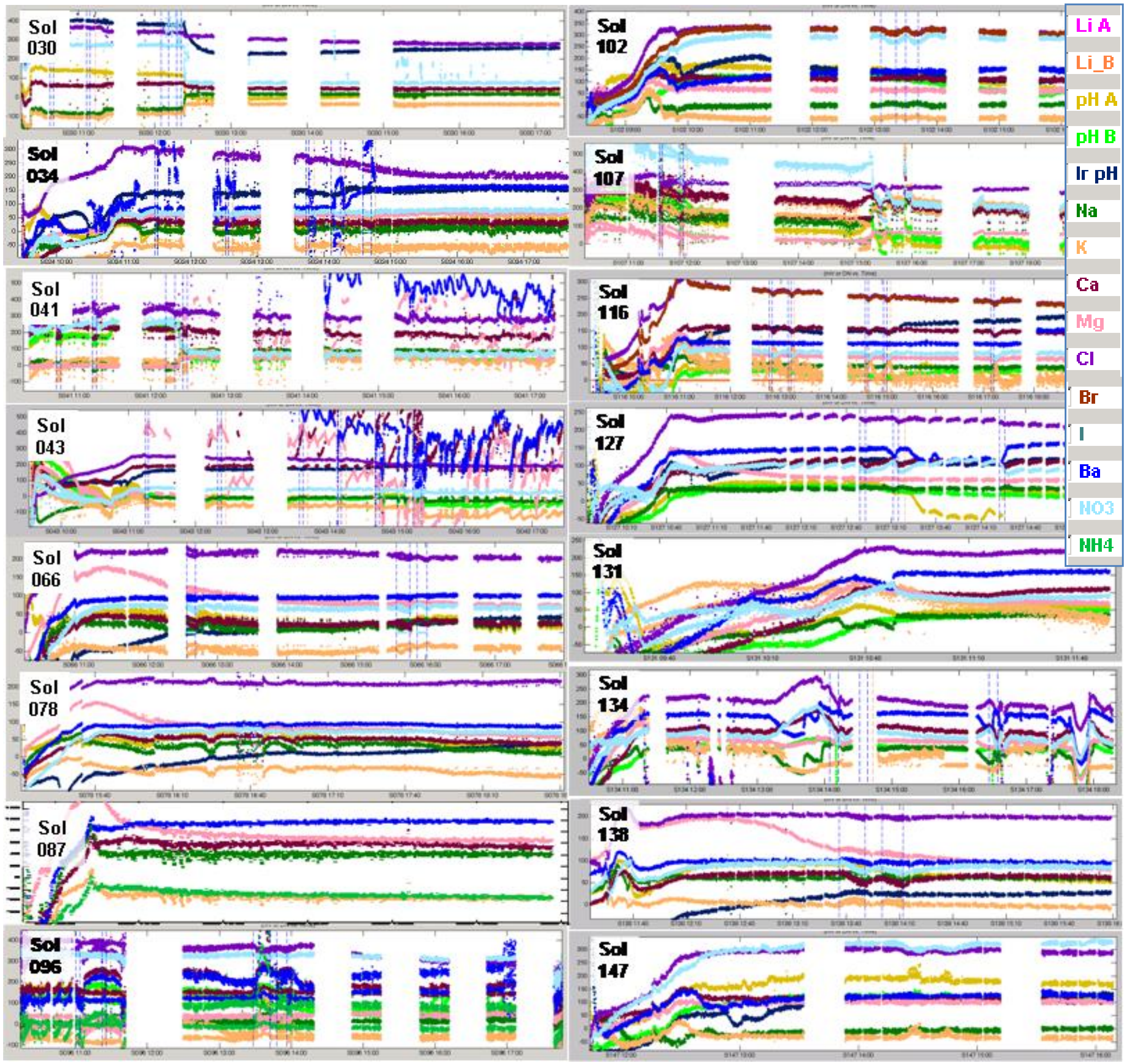

Figure 2. Raw WCL ISE sensor data collected for the entire sol for each cell during the entire mission (See Table 1).

Table 1. WCL analysis events for entire surface mission.

Run*	CELL-0 Rosy Red	CELL-1 Sorceress 1	CELL-2 Sorceress 2	CELL-3 Golden Goose
Run 1	Sol 030 - First Sample	Sol 041 - "First Sample"	Sol 107 - "First Sample"	Sol 096 - "First Sample "
Run 2	Sol 032 - Beaker Thaw	Sol 043 -- Acid & Barium	Sol 116 - Acid & First Barium	Sol 102 -Second Sample
Run 3	Sol 034 - Acid & Barium		Sol 127 - "Second Barium	Sol 147 - Third Sample
Run 4	Sol 066 - Second Sample		Sol 131 - Beaker Thaw	
Run 5	Sol 078 - Thermal Diagnostic		Sol 134 - Third Barium	
Run 6	Sol 087 - Diagnostic			
Run 7	Sol 138 - Third Sample			

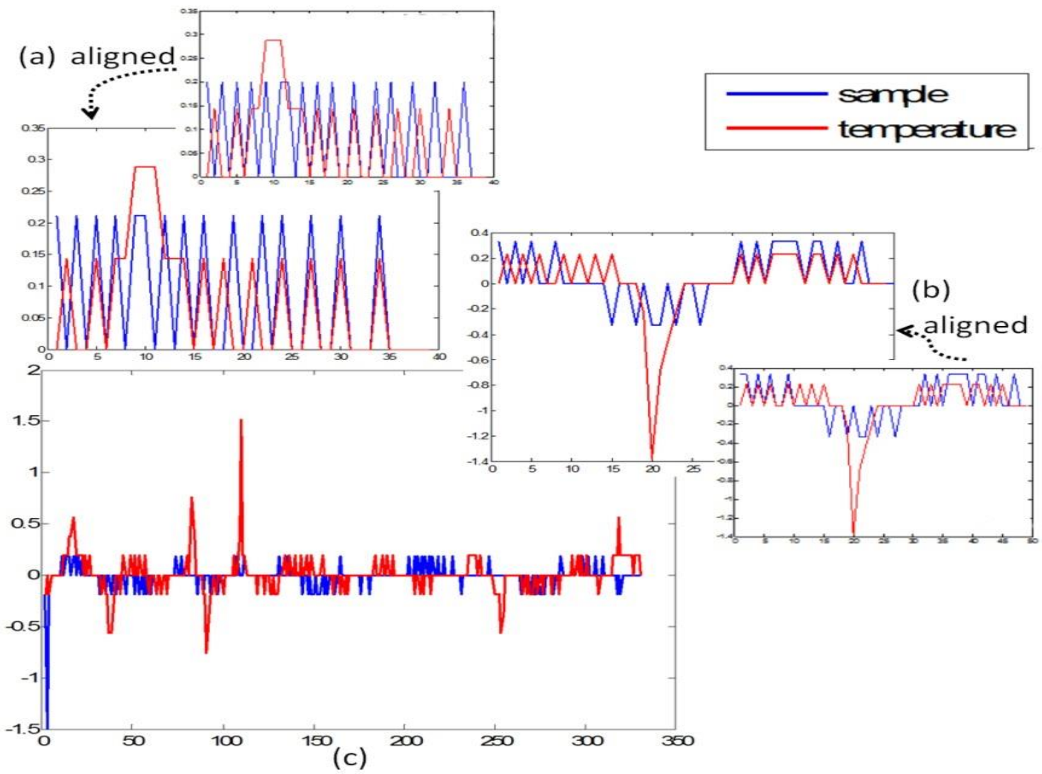

Figure 3. Normalized first derivatives of denoised temperature (red) and denoised Cl- ISE voltage (blue) in different phases of WCL experiments on sol 41 from Cell-1; changes of temperature not only affect the ISE signals, but also offset in time domain. (a) Equilibration Phase: leaching solution release. (b) Calibration Phase: calibrant crucible release. (c) Sample Delivery and Verification Phase: soil was delivered into the cell. Larger figures in (a) and (b) depict manually aligned temperature and voltage signals.

3: Data Description

There two data files for the first-sample analysis events on Sol30, Sol41, Sol96, and Sol107, respectively. For example, under the folder Sol030, the first data file ise_cell0_sol30.csv provides the ISE voltage readings, and the second data file pt_cell0_sol30 provides the temperature readings.

ise_cell#_sol#.csv:
Water Release: The timestamp of leaching solution (25mL) into the analysis beaker
Regent Release: The timestamp of 1st Crucible Calibrant into the analysis beaker
Drawer Open: The timestamp of the drawer of the analysis beaker was opened
Drawer Close: The timestamp of the drawer of the analysis beaker was closed
The column Li(B) is the reference column to all the other ISE readings. The true ISE reading should be subtracted from the column Li(B). For example, the Na+ ISE reading = Na-Column – Li(B)-Column

pt_cell#_sol#.csv:
T_beaker: the temperature (in Celsius) of the analysis beaker

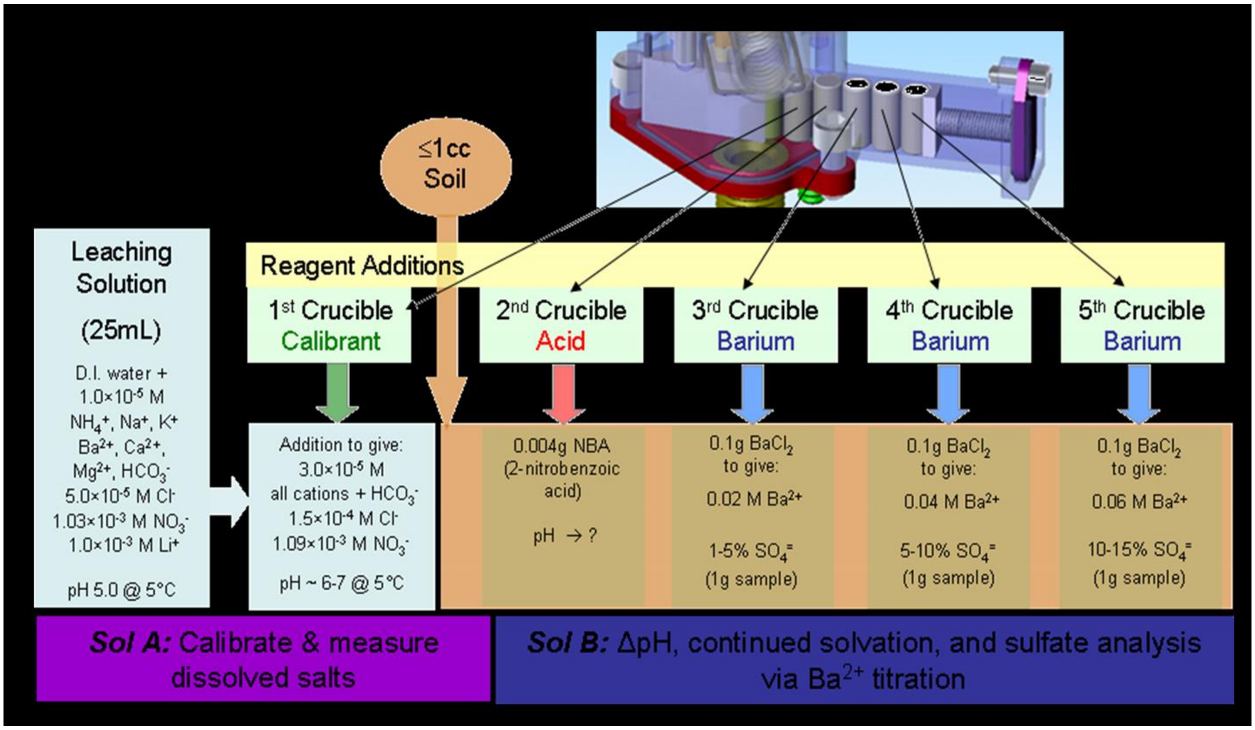

Figure 4 WCL analytical protocol.

4: Discussion

The WCL sensor data presents a significantly "clouded" and noisy picture produced by several types of interferences. The theoretical response of an ISE sensor to an ionic species in solution can be described in simple terms by the equation:

$$y=f(c)+\varepsilon,$$

where y is the analytical signal, c is the concentration of the analyte, $f(\cdot)$ is the response function of the sensor, and ε is the additive error in the measuring system response values. The error ε consists of random errors and systematic errors. There are three predominate types of errors in WCL caused by: (1) the fluctuation of the temperature due to the WCL heater activation; (2) spikes in the sensor electronics that appear during opening of the WCL drawer; and (3) "white noise" due to the sensor's high impedance and spacecraft electronics. The random "white noise" in the sensors signals is presumed to be, at minimum, a combination of inherent high impedance noise introduced by the sensor transduction mechanism, and spacecraft electronics noise.

In this project, you are not required to deal with Error 1, the fluctuation of the temperature due to the WCL heater activation. You can also simply remove the ISE readings during the phase of Error 2, spikes in the sensor electronics that appear during opening of the WCL drawer. However, you will have to deal with Error 3, "white noise" due to the sensor's high impedance and spacecraft electronics, in order to efficiently perform fuzzy sequence mapping.