Calhoun CZO Data

1 on 1 data consult

27 October 2015

Jay Austin

Mineralogical Data (XRD): Level 0 or “raw”

The raw data that is collected by the XRD consists of two variables, degrees 2 theta and counts. This data is saved in a proprietary .raw format.

It is possible to convert this data to a .csv that can comply with YODA formatting, but it is not very useful in this format. Almost all programs that are used to analyze this data prefer to import some form of the .raw file. There are tools readily accessible on the internet that will convert these files into any number of proprietary files for use with which ever program the user chooses.

Intermediate “products” (XRD): (maybe level 1)

In addition to raw data files, there are a variety of data sets that can be generated including:

1) Crystallinity Indexes
2) Peak height and area ratios
3) Peak positions of specific mineral hkl reflections

Modeling related files (XRD): (maybe level 1)

Quantitative mineralogy is often accomplished by Reitveld modeling, or whole pattern fitting. There are a variety of programs available and each will produce a save file unique to it. These generally cannot be converted and will not be easily made to comply with the YODA format. In addition, there are other files that define the atomic structure of the minerals being modeled. They are available in online databases, but the characteristics are generally modified during the modeling process. Uploading the modified structure files will allow for recreating the models results reported in the Level 2 data.

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Mineralogical data (XRD): (Level 2, or "final")

Expected final products will be either qualitative, in the form of a list of minerals present, or quantitative, in the form of a table with % of each phase present or an operationally defined index.

These files can be easily made to comply with the YODA standards.

Mineralogical data : Other than XRD

There are a variety of other common forms of mineralogical data that should be considered (though we will not be creating any). Each of these examples will also have some form of intermediate or semi-quantitative data.

- Infrared Spectra
- Raman Spectra
- Mossbauer Spectra (Aaron Thompson)
- Thermal Analyses
- Energy/Wavelength dispersive spectroscopy
- X-ray fluorescence
- Optical microscopy
- Nuclear Magnetic Resonance
- Electron spin resonance
- Electron diffraction

Kathy O'Neill

Education and Outreach

Product	Anticipated Format
Educational modules and Virtual Field Experiences	iBooks Author
Educational materials	Powerpoint Word PDF
Datasets for classroom	Excel (static files) activities Ideally, would like ability to access some data (e.g., weather, soil temp.) in real time
Video & audio	Format uncertain; Evaluating WeVideo or Camtasia

Other Datasets Include:

- hydrology (John Mallard)
- historical hydrological data (Jingfeng Wang)
- water grab samples (Maryam Foroughi)
- EMI, resistivity, water chemistry, redox (Caitlin Hodges)
- litterfall (K. O'Neill, Will Cook)
- tree surveys (species, dbh, ht, coring data) (Will C., Dan R.)
- organic C, bioassays, isotopes (Sharon B., Christoph L.)
- soil chemistry (Paul Heine)
- soil profile data (Dan Richter)
- soil gases (Zach Brecheisen)
- macro inverts/eco-porosity (Zach Brecheisen)
- LiDAR derived data (Titta M., Zach B.)
- 1933 photos (Zach B., Will Cook)
- various historic maps & data (Don N., Jim G. & Mike C.)
- 14C in gas & solids (Alex Cherkinsky)

- modeling - basic model info posted at http://criticalzone.org/calhoun/models/numerical-models-calhoun/ but do we also need to post full details somewhere?