Data management plan

Publication and other products

We will share significant findings with the community through regional, national, and international conference participation and publication in respected, peer-reviewed journals as promptly as is consistent with high-quality, reproducible data.

Data types and products of the work

This research will generate numerous types of data and products. Products generated include synthesized iron sulfides, Mo-sorbed iron sulfides, and samples that have been transformed to pyrite. Data includes aqueous phase concentrations and solid phase characterization completed at the conclusion of each experiment. All raw data and images will be archived in usable formats at BCO-DMO within two years of collection. Although most of the generated sample material will be used in subsequent experiments and characterization, when possible, material will be preserved and made available to other researchers upon request. Samples and data will be shared with interested parties although most samples will be consumed during the characterization process.

Access and sharing

All synthesis, adsorption, and experimental procedures for producing these samples are described in detail in laboratory notebooks (see below) so samples can be recreated as necessary and detailed procedures can be readily shared. Spectra, diffraction patterns, and other computer-processed data are saved in both proprietary and ASCII formats to allow general access. Micrographs are stored as .tif files. While the need for outside parties to access data is unlikely, requests for sample material may be received. Such requests will be accommodated when sample material is available.

Plans for archiving, preservation, and data retention

Given the rapid turnover of undergraduate student researchers, clear and rigorous guidelines for note-taking and data archiving are essential to enable the consistent generation of accurate and precise data generation, timely publication, and to respond to questions about published data. A process in which all data is uploaded to F&M's Google Education Drive and further backed up with Spanning Backup is in place. Below are the instructions provided to students at the start of every research experience and posted in the laboratory. Team and individual meetings are used to emphasize these guidelines and check for compliance. When completing academic year research, student grades are partially based on their careful adherence to these policies.

Lab Note-Taking and Data Organization Guidelines

If we cannot tell exactly how you carried out an experiment, how data was obtained, and where the data files are, then it was a waste of time and money!

Your laboratory notebook should be...

1. A daily record of every experiment you do, think of doing, or plan to do.
2. A daily record of *your thoughts* about each experiment and the results thereof.
3. The basis of every paper, presentation, and thesis we prepare.
4. A record that would enable other researchers to pick up where you left off or reproduce your results.

Prof. Plass and Morford, future students, or any of your lab mates should be able to read your notebook associated with an experiment and know EXACTLY what was done, what was observed, and what you thought about it. We should be able to get all raw and worked-up data associated with the experiment. We should be able to get all of this information as soon as possible after it is carried out.

Note-taking organization

You will have a designated notebook for this project.

- For each experiment, you will likely have multiple samples. Each sample should be named as follows: your initials-experiment number with 3 digits
    - Experiment number starts at 1 then counts upward.
    - Will look something like this: kp-120
- If some of the samples are replicates of other experiments, they should each have a unique designation (kp-120, kp-121). However, make sure you note which samples should be similar or replicates.
- Describe each experiment COMPLETELY!
    - Include the date, experimental title and all necessary experimental details.
    - The description should encompass the entire experimental procedure to allow exact reproduction and publication. If you are following a previous procedure, note the page of the previous experiment and highlight any changes or differences. Include relevant calculations with attention to including units.
    - Keep careful notes regarding your observations and thoughts about the experiment.
    - Identify and describe all sample characterization, including what file names are associated with what conditions and what methods were used to generate the data. Include printed images and highlight data that supports specific arguments.
- Include a summary at the end of the experiment where you reflect on what you learned from this experiment. Copy particularly useful figures here.

Data organization and sharing

- You will have a named Google File Folder within the “Morford Research Lab” folder. Within your named folder, each experiment should be an individual folder. Upload all Excel spreadsheets, graphs, and documents related to a particular experiment to the same folder. Make sure each sample within an experiment is accurately labeled with the sample name and number and correlates with the information in your lab notebook.
- On all instrument computers there is a common folder for data storage named “Morford Lab Data”. Make a folder with your name in the Morford Lab Data folder.
- Name data files with the experiment name in the title (kp-120.txt, for example). If the file naming needs to be more complex (kp-120-beforeexchange.txt), be sure to write descriptions associated with each filename in your notebook.
- Never remove, rename, or erase data files!
- Upload a copy of all data files, including both **the raw and exported** data (for example upload the raw .XRD and the Highscore files in addition to the .PDF and .JPG that are created after you have analyzed the data from the PXRD) to the appropriate Google Drive folder.
- Ensure each uploaded file has a unique name and note these names in your notebook.