**Introduction to CPDheat – the Matlab version**

The CPD\_heat Matlab version was translated from the original FORTRAN version of CPD\_heat found on Dr. Fletcher’s website. As it is a little different in its construction and usage, this guide is for use as a general introduction on how to use the program.

This version requires an input of a heating rate, end temperature, start temperature, hold time, and pressure, along with several coal-specific parameters and some kinetic parameters.

As it currently stands, there are 7 files associated with this code. All 7 files are necessary for the code to run, so make sure they are all in the same directory for Matlab to access them. The two files that you will be making changes to are titled: “cpd\_driver.m” and “cpdheat.m”.

The file “cpd\_driver.m” is also known as the input file. This is where you will make the majority of your changes. The first five parameters (NMR parameters: p0, c0, sigp1, mw1, and mdel) are all coal-specific parameters that describe the 13C NMR characteristics of the specific coal molecule. The next set of parameters are the temperature inputs. the parameter labeled heating0 is the first heating rate this “particle” is exposed to, with Tf0 being the final temperature. The hold time doesn’t mean anything when you have a heating rate, it signifies how long you will hold a constant temperature. The second set of temperature parameters indicate a second stage of temperature history. You can set a secondary heating rate or a quenching rate, or you can set a constant temperature for a specified hold time. The next set of parameters are the kinetic parameters used internally in the CPD program. DO NOT CHANGE THESE PARAMETERS, as they are optimized for use with the CPD program. The rest of this input file is just to set up internal matrices to make the program run more efficiently.

The next file is “cpdheat.m”. This is the main program that references the rest of the files. There are a few more parameters in this file that may need to be changed. Starting in line 81 of the body of the code, the parameters as follows are for nitrogen chemistry: fnit, fst, fhyd, fcar, and foxy. These should not be necessary to change, unless you are doing more specific nitrogen studies. Line 101 in the code is the pressure in atmospheres at which the code makes its calculations. This quantity will need to change as part of the assignment.

To make changes to any file, double-click on the correct file in the Current Folder window. This will bring up a tab in the Editor window that will allow you to make any changes to the file. Make sure to save any changes to your files in your directory, as Matlab only runs files that have been saved.

To run the code, make sure you have all 7 files in the same directory (cpd\_driver.m, cpdheat.m, flash.m, inverf.m, lightgas.m, perkp.m, and perks.m). These are all necessary for the code to run. Make the necessary changes to the input file or the main file and save the changes. For those unfamiliar with Matlab, there are two ways to execute the code. The first way is to type “cpd\_driver” in the Command Window (excluding quotations) and hit enter. The other way is to highlight the “cpd\_driver” tab in the editor window and click “run” in the upper toolbar (this is a big green triangular symbol in the editor tab of the toolbar).

After you have run the CPDheat code, move over to the Workspace window, where all the associated matrices are stored. The matrices of interest are titled “tar”, “temperature”, “time”, and “total\_volatiles”. These may be copied directly over to Excel, or you can plot them up in Matlab itself.

If you have any other questions, feel free to email Dr. Fletcher at [tom\_fletcher@byu.edu](mailto:tom_fletcher@byu.edu), or Andrew Richards at [andrewprichards1@gmail.com](mailto:andrewprichards1@gmail.com).