Readme: for REALISTIC (REal Adsorption Langmuir Isotherms for Sorption Theory Implementing Chemical potentials)

To install:

Navigate inside install folder, open terminal or command prompt, and run

**pip install -r requirements.txt**

To run as default:

python isoMain.py

Main file is isoMain.py, user input is at the bottom (after line 122, if name == ‘main’). Examples for EH046, ET094, ET095 are included. Put excess data in the rawData folder (note: naming is important for these files! Name must be sampleExcess.csv where sample is the sample name. The script only uses the mmol/g column, so if weight percent is not included just leave a gap for that column)

The command to start the run is startRun(names=names,bulkDens=bulkDens,skelDens=skelDens,Vpore=Vpore,useFugacity=useFugacity,RECALC\_FITS=RECALC\_FITS,CLOSE\_FIGS=CLOSE\_FIGS,gasName=gasName,model=model,numThreads=72)

numThreads should be a multiple of the local computer’s thread (or core count if non-hyperthreaded) count, see example for available isotherm models

In step 3a, in isoMain.py (~line 60) can change the Xpore calculation being used

Isotherm models are in the isotherm.py file. The main thing to change here are the bounds for each model (especially if looking at different gases/non ZTC materials) or adding new models. To add a new model, the model must have a defined theta function as well as a dPdT function, and needs to define the fitting coefficients and bounds.

parseData.py handles file loading/saving code

analyzeData.py handles calculating excess,absolute, and isosteric heats of adsorption

plotData.py handles the code for plotting figures

EOS.py handles the density and fugacity calculations

nonLinearCor.py is not needed for the code, but is an example to determine how nonIdeal a gas is in a certain pressure temperature range