Test run instructions

Part 1)

Start uploading the data:

Go to the following folder: C:\Pyiast

Upload the following csv files: “IRMOF-1\_ethane\_isotherm\_298K” as gas 1 and “IRMOF-1\_methane\_isotherm\_298K” as gas 2 into the software.

Fit both isotherms with the interpolator function.

Enter the following pressures: 1,2,3

Enter the following mole fractions: 0.05, 0.1

Run the IAST calculation and save the file as an csv file. Your output should look like the “References\_Output.csv”.