

TODO

1. Find how garrett made charts in his manuscript
2. Make charts better or change input data

cfs2canteraPD

1. Get injected_species from netj_file
2. Get conc.cutoff from netj_file (inject conc)
3. Make it run PFRTP-Garrett and cfs_post if needed

cfs_post

1. Make trajectory selection faster
2. Make it run PFRTP-Garrett if needed

PFRTP-Garrett

1. Make interactive widget to choose run conditions
2. Fix thing with flame temperature estimate
3. Temperatures shouldn't go down then back up

Instructions

1. Run netj.generate.ipynb to generate input files from lists of run conditions
2. Run cfs.batchrun.ipynb to send the generated .netj files to CFS and run the simulations
3. Run PFRTP-Garrett.ipynb to use Cantera to perform the same simulations.
4. Run cfs.post.ipynb, and select .netj files.
5. Run cfs2canteraPD.ipynb to generate path diagrams using Cantera.

Problems

1. There are many many .ipynb files in Modeling.GPD, many of which are near duplicates of each other, scattered across folders. It is difficult to tell which ones are the most up to date and which ones are obsolete.
2. Residence Time column from cantera has no duplicate times. CFS will have 3-7 rows of identical times
3. Concentrations of non-major species in cantera are around 1e-100, in CFS they are around 1e-15
 - (a) Produces problems for reaction path diagrams because cantera can't tell which is the major species
 - (b) Concentrations are all 0 until injection, then they all instantly increase
 - (c) CFS spray settings may introduce significant concentrations from transient phase?
4. CF3Or has 15 reactions, CF2s has 74, CF4 15, C2F6 6. C2F6 behavior in path diagrams may be caused by incomplete reactions
5. Several reactions are "ambiguous" and cantera will use the designated default reaction
 - (a) Default reaction may not be conducive for simulating C2F6
6. Some reactions are not parsed (they may just not be relevant)

Table 1: Files, Paths, and Descriptions

File	Path	Description
netj-generate.ipynb	path	Takes a set of varying run conditions and produces netj files to do all iterations
cfs.batchrun.ipynb	path1	Uses CFS batch method to run generated netj files, prompts user for inputs to determine simulation duration
PF RTP-Garrett.ipynb	path2	Uses a PFR simulation in Cantera to make similar results as CFS
cfs_post.ipynb	path3	Runs CFS in GUI mode to automate post-processing of vtk files to include species concentration
cfs2canteraPD.ipynb	path4	Converts vtk to csv data, then produces a path diagram using Cantera for a specified trajectory, residence time, and threshold.
lagrangian hi res mass frac.ipynb	L:/Lab/AMCD.PFAS.Incineration/Modeling.GPD/Cantera/PFR DE S Curves/	Makes plots of multiple species DE% vs Temperature
eulerian <injectant>.ipynb	L:/Lab/AMCD.PFAS.Incineration/Modeling.GPD/Cantera/influent concentration/	Make multidimensional color plots for conc. vs Temperature vs DE%. Also absolute and relative yield vs conc.
paths <SR>.ipynb	L:/Lab/AMCD.PFAS.Incineration/Modeling.GPD/Cantera/paths/	Makes path diagrams for several species at specified SR
T99.ipynb	L:/Lab/AMCD.PFAS.Incineration/Modeling.GPD/Cantera/T99/	Makes T99 plots of multiple species
lagrangian.ipynb	L:/Lab/AMCD.PFAS.Incineration/Modeling.GPD/Cantera/PFR DE S Curves/archive/	Makes plots of species DE vs Temperature. Plots from this script don't look the same as plots in the doc, so it is probably outdated.

Table 2: Validated Path Diagrams - CFS

	CF4				CHF3				C2F6			
	Ports				Ports				Ports			
	1	4	6	8	1	4	6	8	1	4	6	8
27.5 kW									×			×
45 kW	×	✓							×	×		×

Table 3: Validated Path Diagrams - Cantera

	CF4				CHF3				C2F6			
	Ports				Ports				Ports			
	1	4	6	8	1	4	6	8	1	4	6	8
27.5 kW	×	×	×	×					✓	✓	✓	✓
45 kW	✓	✓	✓	✓					✓	✓	✓	✓

Table 4: CFS Executed Simulations

	CF4				CHF3				C2F6			
	Ports				Ports				Ports			
	1	4	6	8	1	4	6	8	1	4	6	8
27.5 kW		✓							✓	✓	✓	✓
45 kW	✓	✓			✓	✓	✓		✓	✓	✓	✓

Table 5: Cantera Executed Simulations

	CF4				CHF3				C2F6			
	Ports				Ports				Ports			
	1	4	6	8	1	4	6	8	1	4	6	8
27.5 kW	✓	✓	✓	✓					✓	✓	✓	✓
45 kW	✓	✓	✓	✓					✓	✓	✓	✓