TODOp

1. Find how garrett made charts in his manuscript
2. Make charts better or change input data
3. Do comparisons of Cl species with F species
    (a) Garrett seems to have started doing that in lagrangian hi res mass frac.ipynb, but he doesn't include measured Cl 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. Cantera increases time steps constantly, CFS has variable time steps
4. 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
        i. This is probably because the transient solution solves from the injection point and then tries to work backwards to the flame. Injecting at the flame may fix this.
5. CF3Or has 15 reactions, CF2s has 74, CF4 15, C2F6 6. C2F6 behavior in path diagrams may be caused by incomplete reactions
    (a) C2F6 may just not have that many reactions because it is a larger molecule, and the C-C bond is the most likely to break
6. Several reactions are "ambiguous" and cantera will use the designated default reaction
    (a) Default reaction may not be conducive for simulating C2F6
7. Some reactions are not parsed (they may just not be relevant)

Notes

1. CF4 will never be destroyed at temps below 1200K, 100% DE for temps ¿1600 C
2. Higher values of MAXIT seem to produce more residence time steps

Table 1: Files, Paths, and Descriptions

File	Path	Description
flow_convert.ipynb	PFAS_Modeling/	Converts liters per minute to kilograms per second for air and for CH4 using cantera
netj_generate.ipynb	PFAS_Modeling/	Takes a set of varying run conditions and produces netj files to do all iterations
cfs_batchrun.ipynb	PFAS_Modeling/	Uses CFS batch method to run generated netj files, prompts user for inputs to determine simulation duration
PFRTP-Garrett.ipynb	PFAS_Modeling/Pseudo_PFR	Uses a PFR simulation in Cantera to make similar results as CFS
cfs_post.ipynb	PFAS_Modeling/	Runs CFS in GUI mode to automate post-processing of vtk files to include species concentration
cfs2canteraPD.ipynb	PFAS_Modeling/	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	✓	✓	✓	✓					✓	✓	✓	✓