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, Folders, and Descriptions

File	Folder	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.
pfr.ipynb	PFAS_Modeling/	Example PFR that came with Cantera
pfr2.ipynb	PFAS_Modeling/	Example Cantera PFR that includes heat loss
vtk2csv.py	PFAS_Modeling/	Stand alone script for converting a specific vtk to a csv
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 6: C1, C2, and C3 Chlorinated and Fluorinated Species

Formula	Species Name	Incinerability Index	Formula	Species Name	Incinerability Index
CNCl	Cyanogen Chloride	17-18	$C_3H_6Cl_2$	1,3-Dichloropropane	165
CH_3Cl	Chloromethane	29-30	$C_3H_5Cl_3$	1,2,3-Trichloropropane	168-173
$COCl_2$	Phosgene	39-40	$C_2H_4Cl_2$	1,1-Dichloroethane	175-178
$C_2H_3ClO_2$	Methyl Chloroformate	46-50	C_3H_5ClO	1-Chloro-2,3-epoxypropane	183-186
$C_2H_2Cl_2$	Dichloroethene	54	$CHCl_3S$	Trichloromethanethiol	189-192
C_2H_4FNO	Fluoroacetamide	55-56	C_2Cl_6	Hexachloroethane	202-203
C_2H_3Cl	Vinyl Chloride	60-64	C_2H_5ClO	Chloromethyl Methyl Ether	218-220
CH_2Cl_2	Dichloromethane	65-66	$C_2H_4Cl_2O$	bis(Chloromethyl) Ether	222-223
$C_3H_4Cl_2$	1,2-Dichloropropene	89-91	C_3Cl_6	Hexachloropropene	234
CH_3COCl	Acetyl Chloride	92-97			
$C_2H_2Cl_4$	Tetrachloroethane	121-125			
C_2H_5Cl	Chloroethane	126			
$C_2H_4Cl_2$	Dichloroethane	131			
C_3H_4ClN	3-Chloropropionitrile	143-144			
$C_3H_6Cl_2O$	1,3-Dichloropropan-2-ol	145-146			
$CHClF_2$	Chlorodifluoromethane	151-153			
$CHCl_2F$	Dichlorofluoromethane	154-157			
C_2HCl_5	Pentachloroethane	154-157			
$C_2H_3Cl_3$	Trichloroethane	158-161			
$CHCl_3$	Chloroform	158-161			

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	✓	✓	✓	✓					✓	✓	✓	✓

Notes from Bill

1. go through these lists and identify any C1, C2, and possibly C3 F and Cl species and their ranking
2. (CCl4 (✓, 136-140), CHCl3(✓, 195-196), C2Cl6(✓, 202-203), CF4(×), CHF3(×), C2F6(×)) listed?
3. other C1, C2, and C3 chloro or fluorocarbons
4. mixed Cl-F species?
   - mainly CFCs
5. analyze the fraction of chlorinated species, and number of fluorinated species included
   - Does this mean *all* chlorinated species, or only those with 1-3 C?
   - There are 320 total species in the list.

- Chlorinated species account for 113 species. Chlorinated C1-C3 species account for 40 of them.
- Fluorinated species account for 8 species. Only twe do not contain 1 to 3 carbons (Sulfur Hexafluoride and Fluoroacetic Acid)

6. anything you think notable.
   - It's interesting how the only fluorinated species on the list that aren't CFCs are SF_6 and $C_2H_3FO_2$
7. Find incinerability index for species

I'd like to begin the introduction of our Cl/F paper with a discussion of the Incinerability Index, and why we chose to study these 6 compounds. The main reasons are their combinations of different molecular structures, bond types, and their available/published kinetics.

Talk about why the incinerability index is used instead of other measures.

Talk about properties of these compounds.

Heat of combustion was used for a while, but it wasnt accurate because:

Why, specifically, is the thermal stability used instead of other measures?

Why are these compounds chosen? What makes them good candidates for this study?

What is it about the molecular structures that makes these representative compounds?

CCl4 has tetrahedral, single covalent bonds. CHCl3 is tetrahedral, like methane but with 3 Hs replaced with Cls. C2Cl6 is two carbons connected linearly, with each carbon bonded to three chlorine atoms in a trigonal planar arrangement. CF4 is tetrahedral, like methane but with all Hs replaced with Fs. CHF3 is tetrahedral, like methane but with 2 Hs replaced with Fs. C2F6 is two carbons connected linearly, with each carbon bonded to three fluorine atoms in a trigonal planar arrangement. The fluorine compounds all have higher bond energies than the chlorinated compounds.

What is it about the bond types that makes these representative compounds?

Not sure if he means that having the fluorinated and chlorinated compounds allows for comparing the behavior of the bond energies of the C-F and C-Cl bonds, or if he means that the bond types of the compounds themselves are important.

Having the chlorinated analogues of the fluorinated compounds could allow for establishing a routine to compare the two?

What is it about the kinetics that makes these representative compounds?

I think it's because the mechanisms of destruction of these compounds are expected to be used in more complex compounds. Basically, larger PFAS probably break apart into these compounds.

Make comparisons of fluorinated and chlorinated compounds

All the fluorinated compounds have higher bond energies, and usually slightly denser molecules.

As you will see many of the Class 1 species are PAHs with ring structures.

- Most of the PAHs have many carbons, so I'm not sure if they're relevant for the discussion of C1-C3 species

I'm thinking a discussion of these species and bond energies might be a good place to start.