Table 6: C1, C2, and C3 Chlorinated and Fluorinated Species

Formula	Species Name	Incinerability Index
CNCl	Cyanogen Chloride	17-18
CH_3Cl	Chloromethane	29-30
$COCl_2$	Phosgene	39-40
$C_2H_3ClO_2$	Methyl Chloroformate	46-50
$C_2H_2Cl_2$	Dichloroethene	54
C_2H_4FNO	Fluoroacetamide	55-56
C_2H_3Cl	Vinyl Chloride	60-64
CH_2Cl_2	Dichloromethane	65-66
$C_3H_4Cl_2$	1,2-Dichloropropene	89-91
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
$C_3H_6Cl_2$	1,3-Dichloropropane	165
$C_3H_5Cl_3$	1,2,3-Trichloropropane	168-173
$C_2H_4Cl_2$	1,1-Dichloroethane	175-178
C_3H_5ClO	1-Chloro-2,3-epoxypropane	183-186
$CHCl_3S$	Trichloromethanethiol	189-192
C_2Cl_6	Hexachloroethane	202-203
C_2H_5ClO	Chloromethyl Methyl Ether	218-220
$C_2H_4Cl_2O$	bis(Chloromethyl) Ether	222-223
C_3Cl_6	Hexachloropropene	234

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									$\times$			$\times$
45 kW	$\times$	$\checkmark$							$\times$	$\times$		$\times$

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	$\times$	$\times$	$\times$	$\times$					$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$
45 kW	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$					$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$

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		$\checkmark$							$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$
45 kW	$\checkmark$	$\checkmark$			$\checkmark$	$\checkmark$	$\checkmark$		$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$

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	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$					$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$
45 kW	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$					$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$

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 ($\checkmark$, 136-140), CHCl3($\checkmark$, 195-196), C2Cl6($\checkmark$, 202-203), CF4($\times$), CHF3($\times$), C2F6($\times$)) 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.