AFRL

PREDICTIVE APPROACH TO CHARACTERIZING HEALTH RISK FROM EXPOSURE TO THERMAL DEGRADATION BYPRODUCTS FROM HIGH TEMPERATURE PROCESSES

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Non-Disclosure

- Rebecca A Clewell, PhD has no conflict of interest to report

Disclaimers

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Combustion produces complex exposures

https://www.liveabout.com/3e7x1-fire-protection-air-force-job-description-3344332

- Benign aircraft relevant materials, when burned, can release toxic byproducts
  - Materials and chemicals found on board aircraft that could impact pilot breathing air
  - **Big 3: hydraulic fluid, turbine oil, and electronic coolant**
- Acute inhalation hazards are of primary concern
- Sensors and models can help inform decisions:
  - **Forensic attribution – where did the leak come from?**
  - **Site/mission risk assessment**
  - What type of response is needed? Do I need personal protective equipment (PPE)?
  - Which materials are safer when burned?
  - Which byproducts should be mitigated?

Trained Chemical Detectors for Field Forensic Attribution

Fieldable detector evaluation and enhancement with high-throughput combustion test fixture

Predictive chemistry modeling towards forensic attribution

Performance Goals

Reliable predictions

Quantified uncertainty

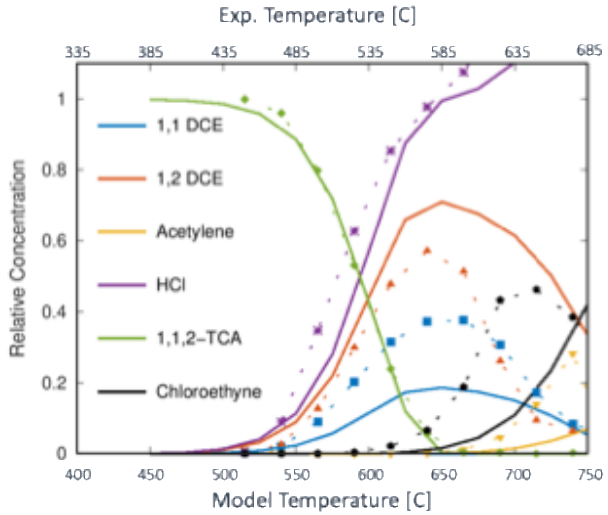
Forensic attribution

Challenges

Limited detector library

Limited detector sensitivity

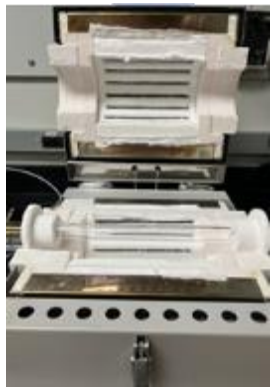
Unknown conditions

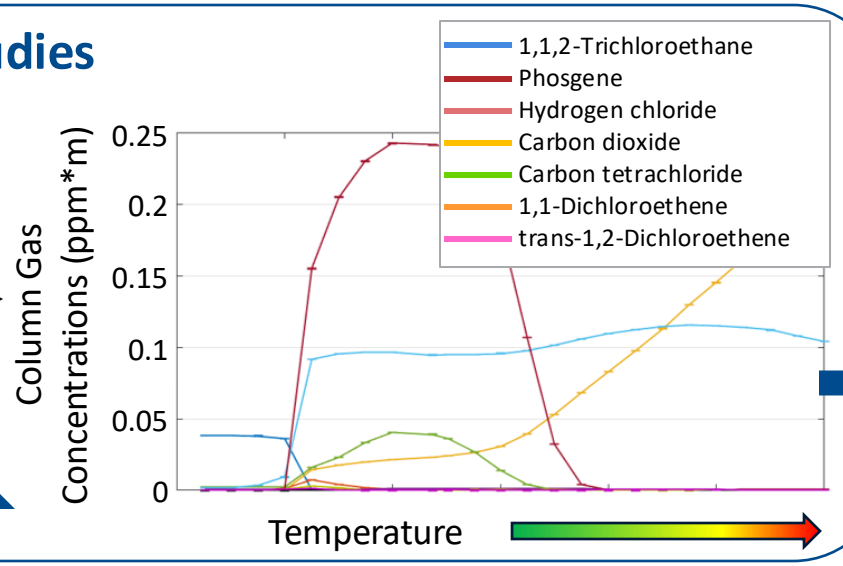


- Enhance chemical detector to make it tunable for forensic attribution

Thermal Degradation Studies

Pyrolysis & Combustion Test Unit





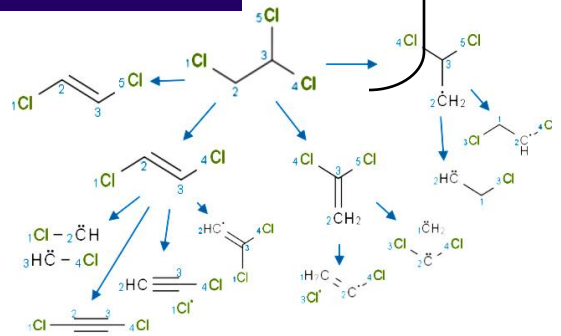
Identify Exposures

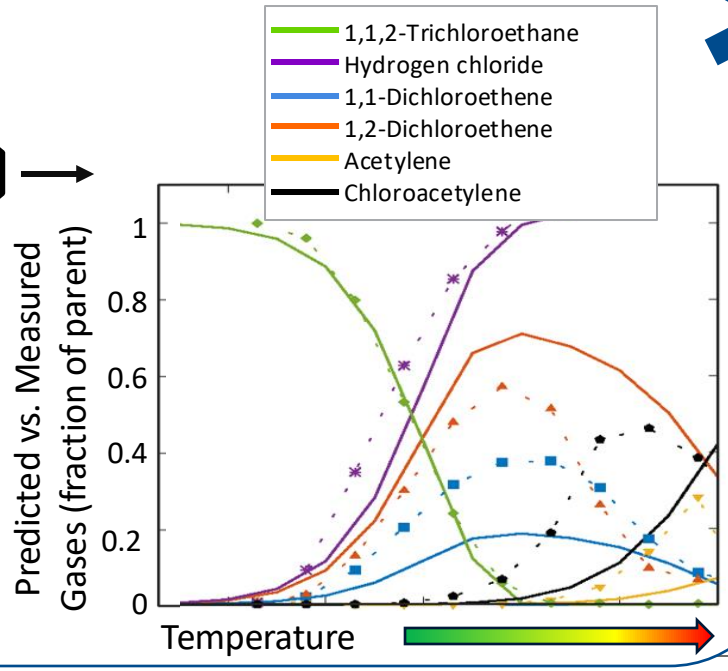
Combustion Models

Kinetics Database

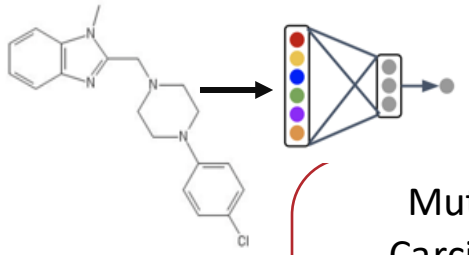
MISTRAL AI_

Argonne ATcT Active Thermochemical Tables





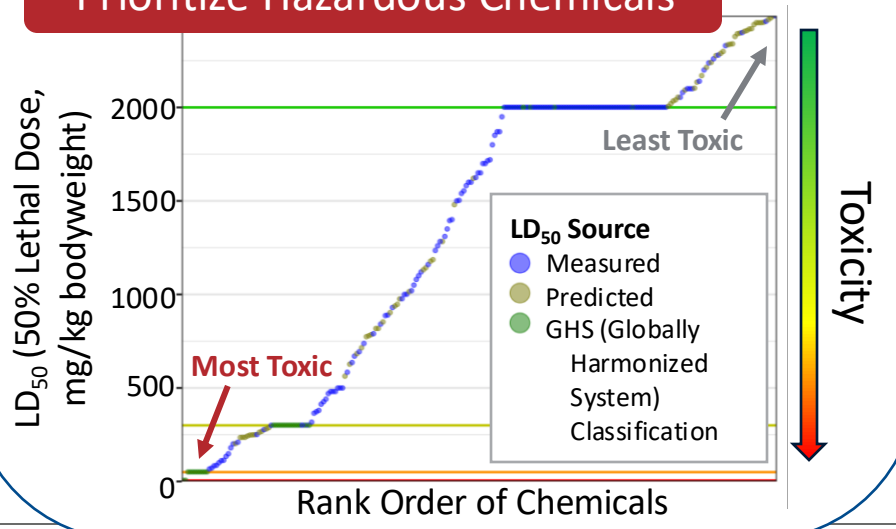
Health Risk Models



Predict Effects

Mutagenicity
Carcinogenicity
Acute Toxicity
Skin/eye Irritation
Lung Injury
Allergenicity

Prioritize Hazardous Chemicals



Chemicals and Mixtures to Burn

- 10 chemicals/mixtures chosen in collaboration with AFRL
  - TPP/TCP
  - Dodecane
  - Methyl methacrylate
  - 1-Decene
  - Naphthylamine/Aniline

  - Hydraulic fluid: RADCOLUBE FR282 *(MIL-PRF-83282)*
  - Hydraulic fluid: RADCOLUBE RHP5606 *(MIL-PRF-5606)*
  - Turbine Oil: TURBONYCOIL 160 *(MIL-PRF-7808)*
  - Turbine Oil: ROYCO 899 23699CI *(MIL-PRF-23699)*
  - Electronic Coolant: RADCOLUBE 500M *(MIL-PRF-87252)*

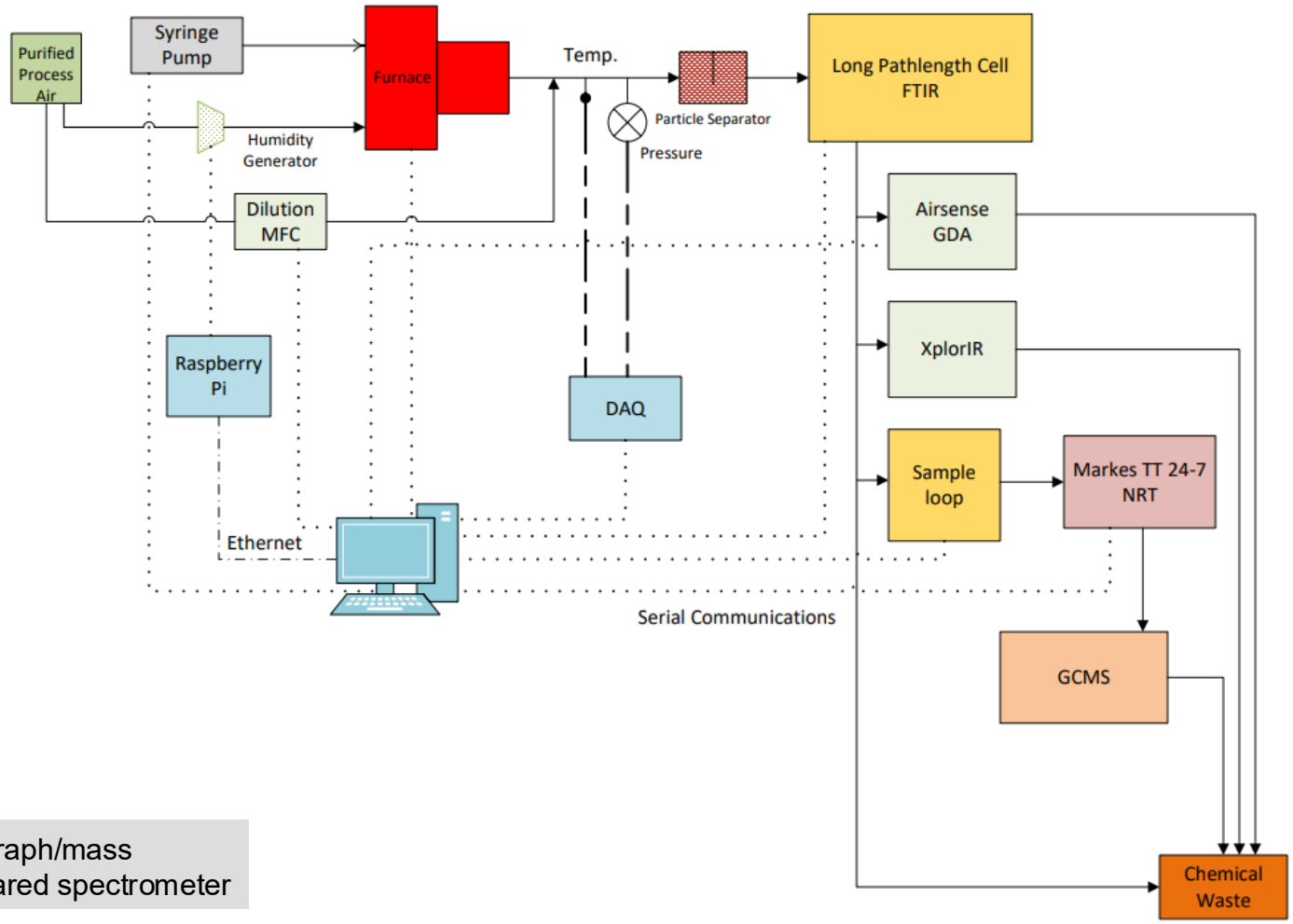
TCP: Tricresyl phosphate
TPP: Triphenyl phosphate

- Chosen with the following criteria:
  - Presence/use on the plane(s) of interest (by quantity purchased and availability, from Aircraft Contaminants Project report*)
  - Part of the “Big 3” – hydraulic fluid, turbine oil, electronic coolant
  - Chemical is toxic OR has reasonable expectation that degradation products might be toxic
  - Utility of chemical for forensic attribution – i.e., is it unique to one of the Big 3 or degrades differently based on mixture components
  - Experimental/modeling constraints

*Cowan et al. AFRL-RH-WP-TR-2026-0004, AD1357183

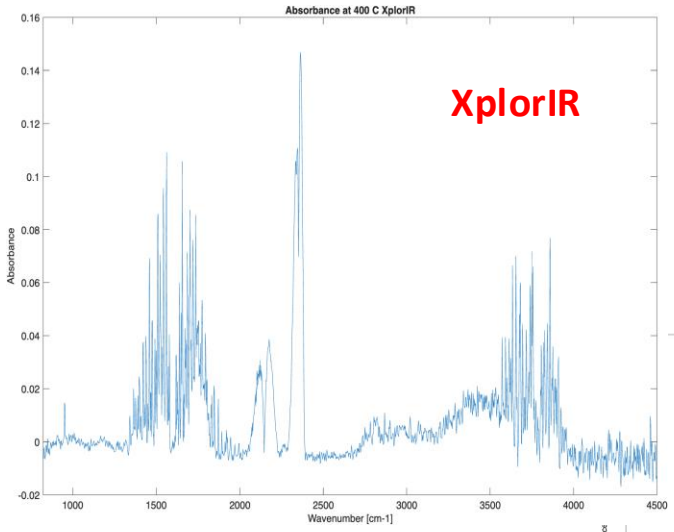
Schematic of Aircraft Fluid Combustion System with IR Devices

- Purified process air
- Syringe pump fluid injection
- Particle trap removes large particles
- Chemical analysis
  - FTIR
  - IMS
  - XplorIR®
  - GC/MS

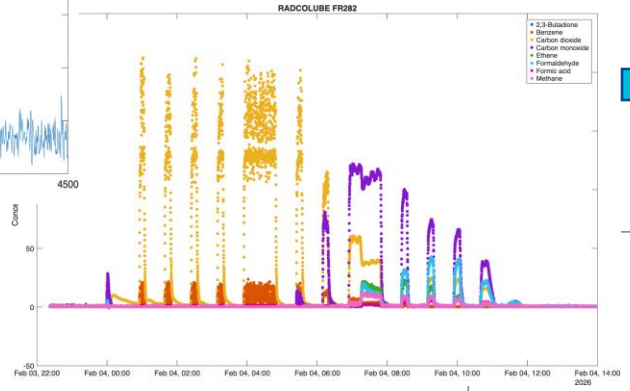


FTIR: Fourier-transform infrared spectrometer; GC/MS: gas chromatograph/mass spectrometer; IMS: ion mobility spectrometer; XplorIR®: hand-held infrared spectrometer

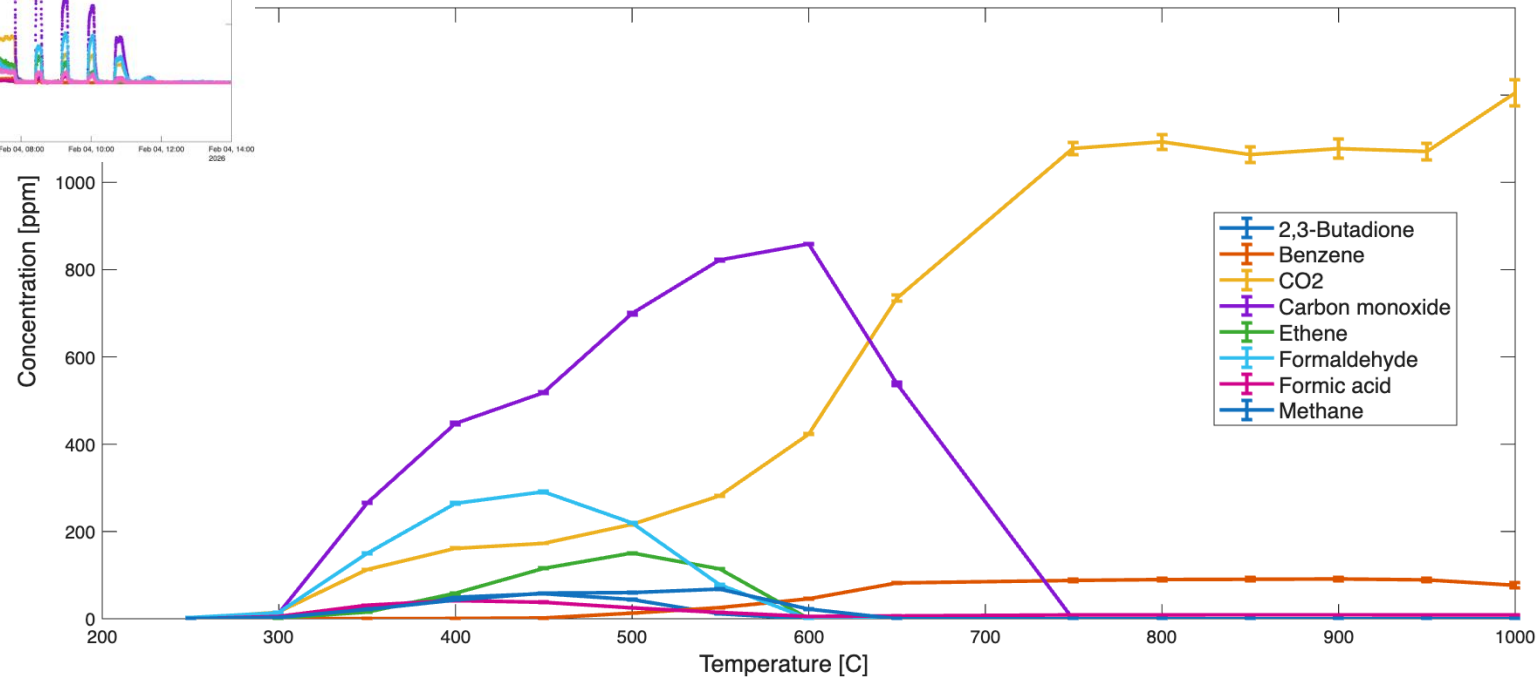
FTIR Data into Chemical Concentrations



XplorIR

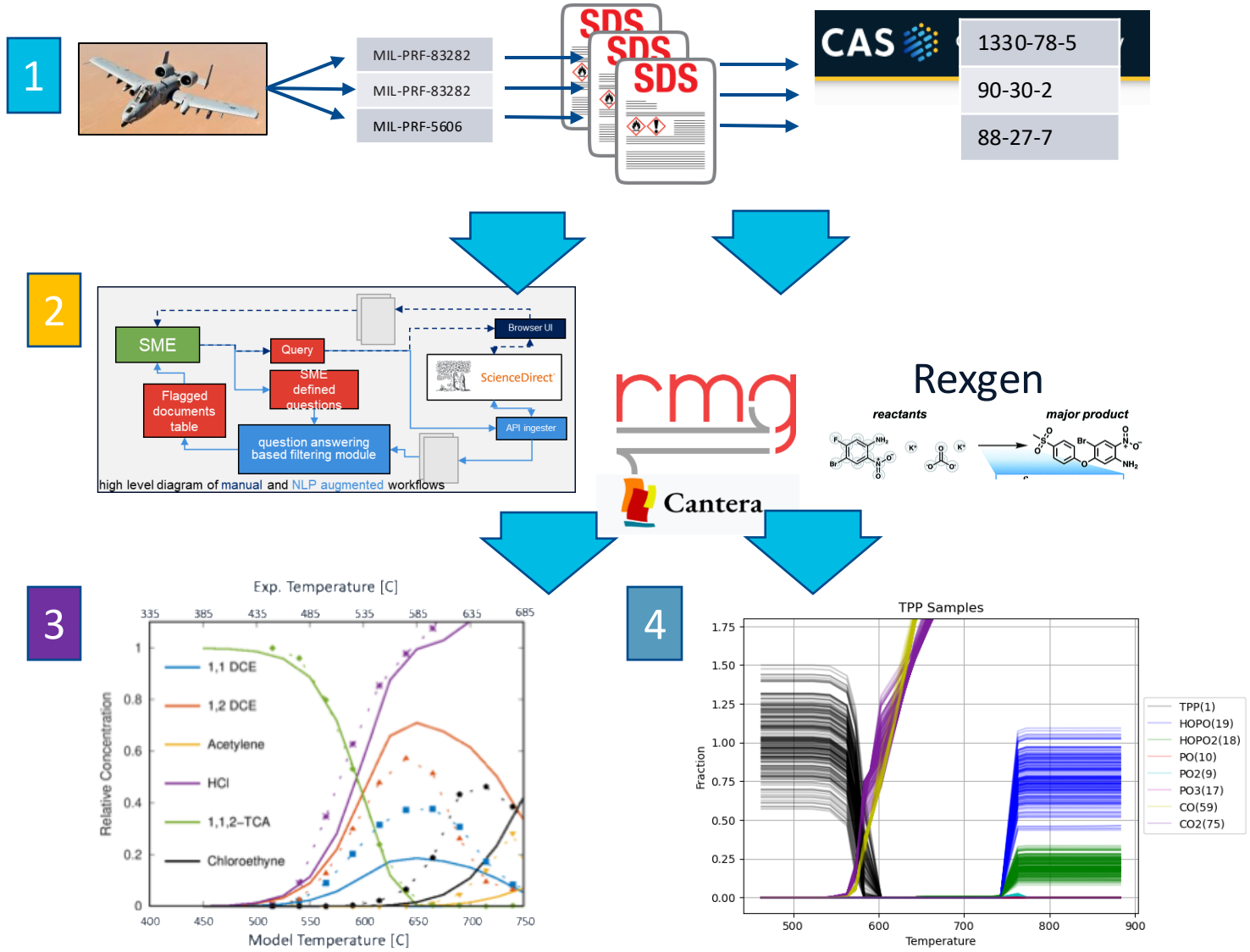


Formation of combustion byproducts versus temperature from combustion of RADCOLUBE FR282 hydraulic fluid



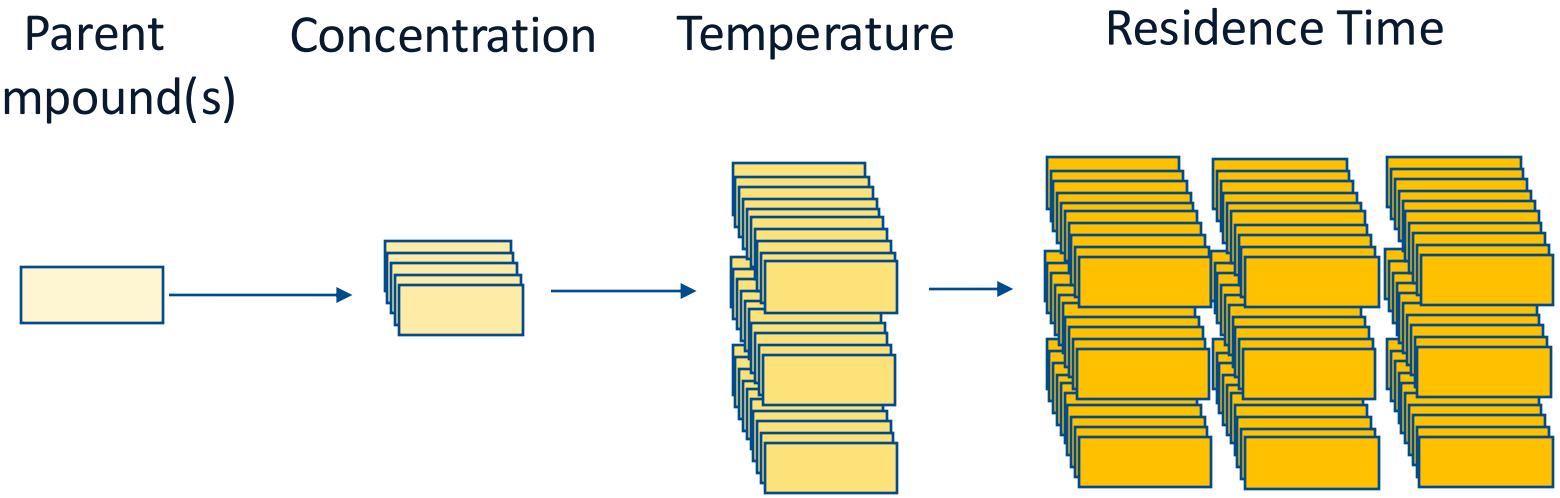
Enhance Computational Predictive Tools for Forensic Attribution

1. Identify relevant chemicals from Air Force platforms, MIL-STD and SDS
2. Apply computational tools to all relevant and related chemicals, and to mixtures of chemicals
3. Apply lab analysis and chemical kinetics models to selected chemicals from library in (1)
4. Generate modeled pathways for chemical reactions under a variety of conditions for comparison against experimental data



MIL-STD: military standard; SDS: safety data sheet

Generating Modeled Pathways



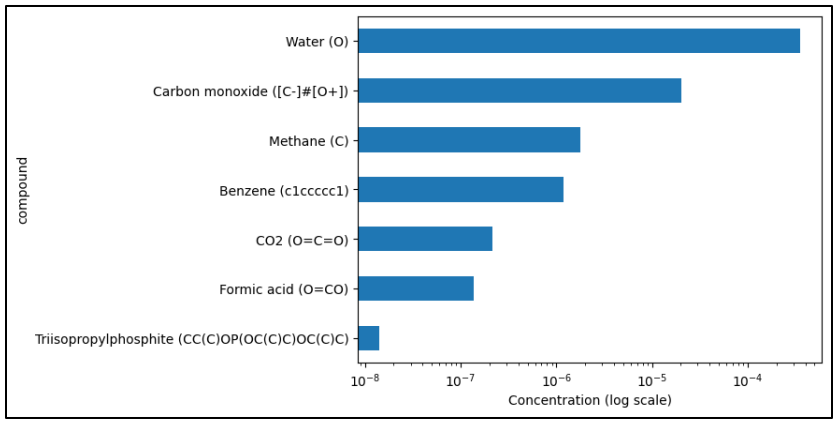
Scaling example: 6 parent compounds→ ~24K unique condition combinations and >400 distinct product compounds

Pathway: Final product compound concentrations given a specific parent compound mixture, temperature, and residence time

sec: second

How Do We Turn Experimental and Modeling Data into Forensic Attribution?

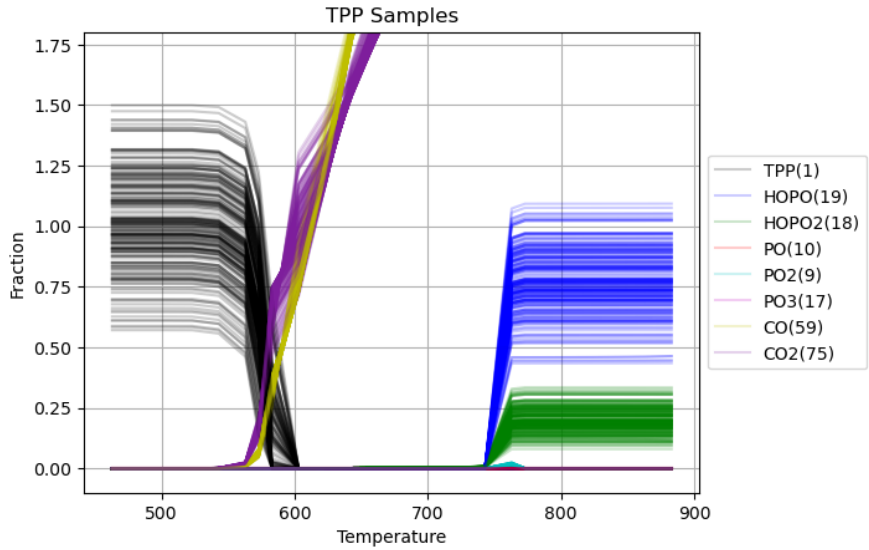
Experimental data from fieldable detectors



Modeled pathways are vast and don't take into account:

- What is plausible in the 'real world'
- What can actually be measured by any specific device

Modeled pathways of combustion reactions



- Statistical comparison tools map experimental results to modeled pathways

Combining Modeling, Detector Capabilities, and Measurements to Inform Forensic Attribution

Forensic attribution: identifying initial/parent compounds of reaction

Modeling produces 1,000s of final compound across 40K+ pathways from a set of initial compounds and conditions

Detector capabilities establish what can be detected

Modeling outputs are filtered to align with detector capabilities

A physical event is measured with the detector

Modeled final compounds of pathway N

Compound	A	B	C	…	Y	Z
Conc. (ppm)	25	10	.5	…	2	0

Measurable compounds

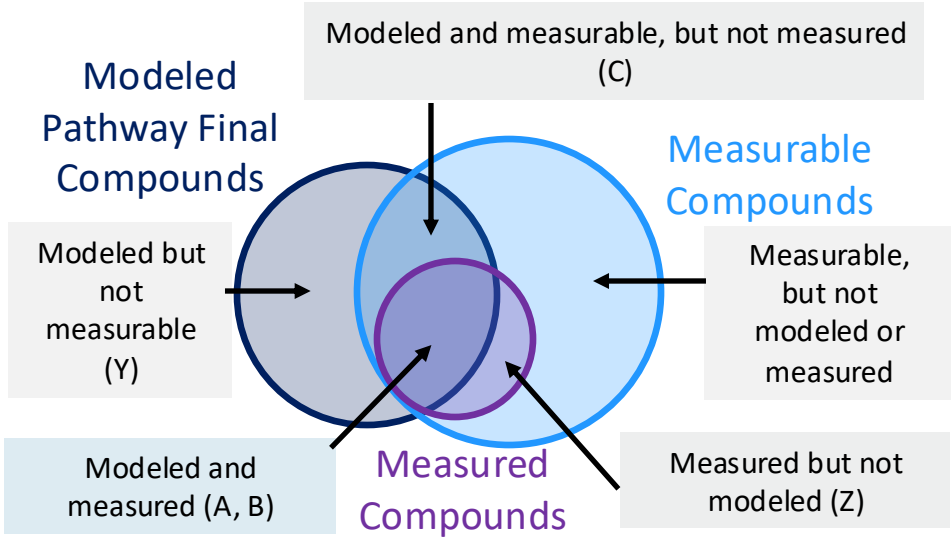
Compound	A	B	C	…	Y	Z
Min. Threshold (ppm)	1	5	.5	…	--	5

Measurable final compounds of pathway N

Compound	A	B	C	…	Y	Z
Conc. (ppm)	25	10	.5	…	--	0

Measured compounds

Compound	A	B	C	…	Y	Z
Conc. (ppm)	30	15	0	…	--	6



Pathway	1	2	…	N	…	40K
Score	.31	.15	…	.78	…	.60

Pathway N has initial/parent compounds α and β → Likely initial/parent compounds from physical event similar to α and β

Similarity score determined between every modeled pathway's measurable final compounds and detector measurement

High similarity between pathway and detected compounds = forensic attribution

*A pathway is a record of final compounds for a specific set of initial compounds and conditions

Conc.: concentration; Min: minimum; N: natural number variable; ppm: parts per million

Example: Evaluating Attribution with Modeling Data

AFRL

1. Known pathways

2. Select pathway

Pyrolysis of TFE (4%),
temp: 1350 K
residence time: .0625 sec

3. Select a few high-concentration chemicals from pathway to be "measured"

chemical label	modeled final concentration
CF4	5.6%
C8F10 (1)*	3.7%
C8F10 (2)*	1.6%
C7F8	.5%

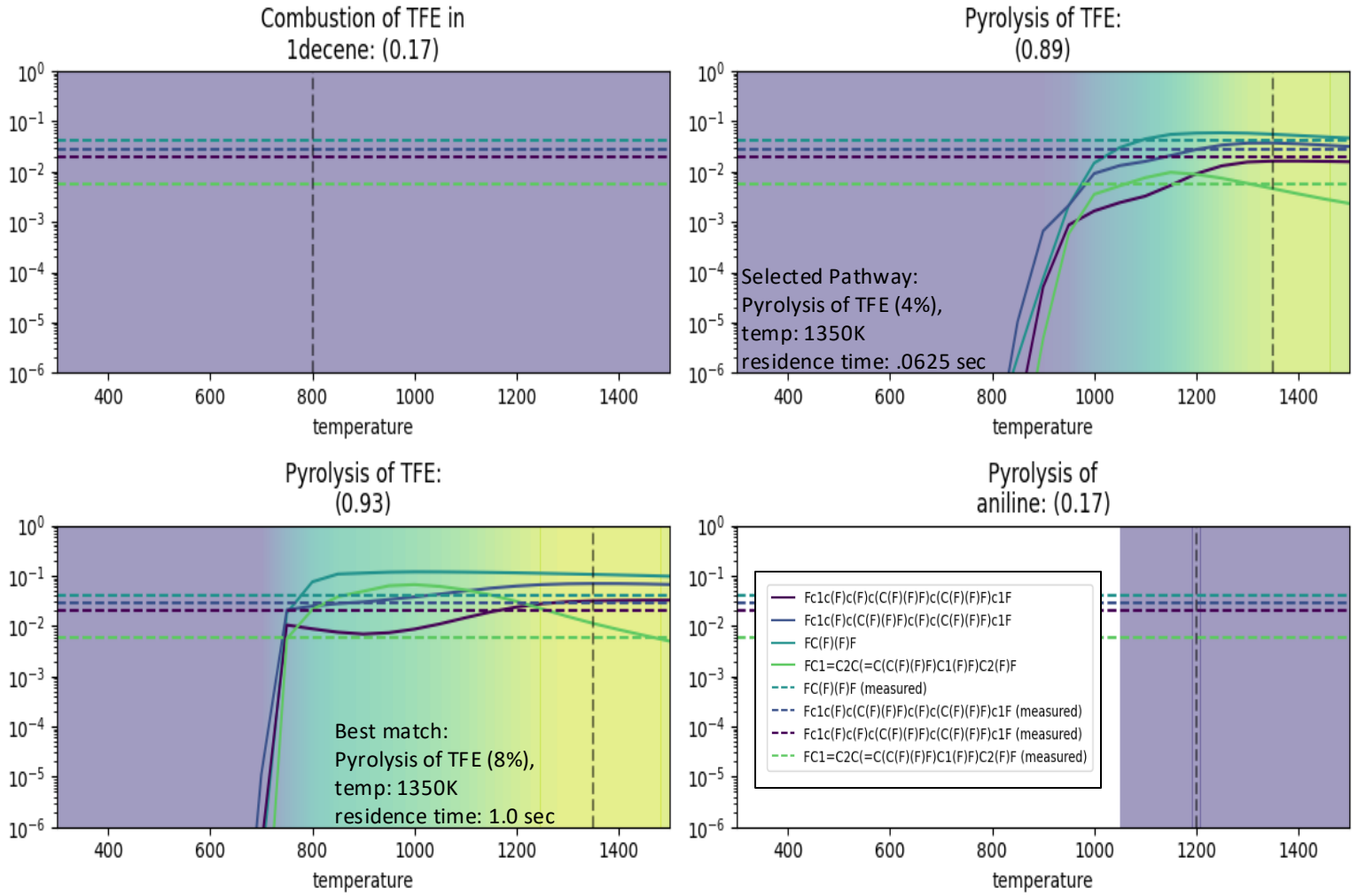
"measured" conc. with 25% error
4.2%
2.8%
2%
.6%

4. Compare pathways against measurements

pathway id	score	Category
1	92.9%	Pyrolysis of TFE
2	92.8%	Pyrolysis of TFE
3	92.8%	Pyrolysis of TFE
4	92.8%	Pyrolysis of TFE
5	92.8%	Pyrolysis of TFE

5. Estimate initial species

pathway id	score	Category	Initial compound	conc.
1	92.9%	Pyrolysis of TFE	TFE	8.0%
1	92.9%	Pyrolysis of TFE	N2	92.0%
... 100	16.7%	Combustion of TFE in 1decene	O2	15.8%
100	10.16.7 %	Combustion of TFE in 1decene	1decene	15.8%
101	16.7%	Pyrolysis of aniline	aniline	8.0%



Limited measurable compounds and concentration variance drive a different best match pathway, but parent compound prediction is unaffected

TFE: tetrafluoroethylene

Forensic Attribution Capability

RADCOLUBE FR282
(MIL-PRF-83282)

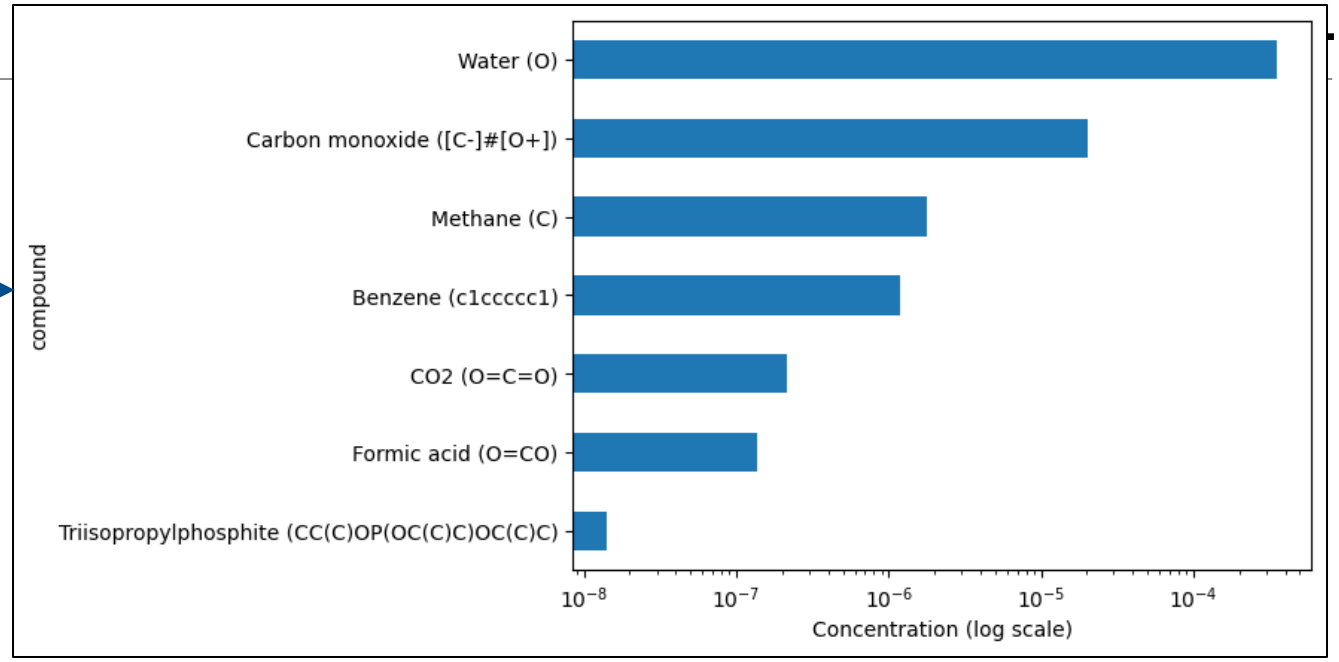
Initial compounds:
UNKNOWN

hydraulic fluid

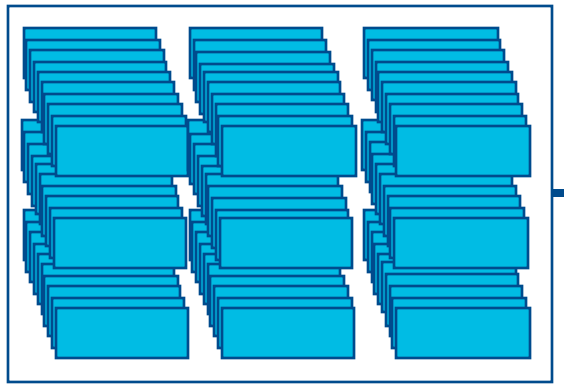
950 °C

XplorIR

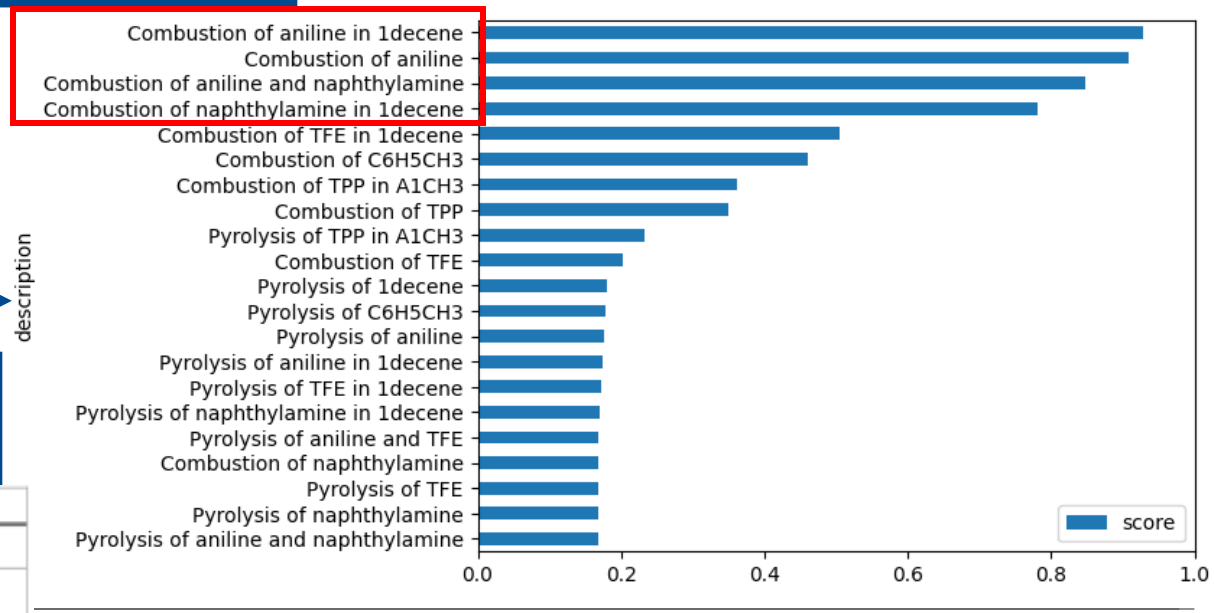
fieldable detector



Modeled Pathways
Final Compounds



Similarity Analysis



Similarity analysis ranks aniline high, and RADCOLUBE FR282's compounds are similar to aniline

Name	CAS-No.	%	GHS US classification
1-Dodecene, polymer with 1-decene, hydrogenated	151006-60-9	0 – 70	Asp. Tox. 1, H304
Alkylated amine*	Trade Secret	< 5	Repr. 2, H361 STOT RE 2, H373

AIR FORC

Forensic Attribution Capability

AFRL

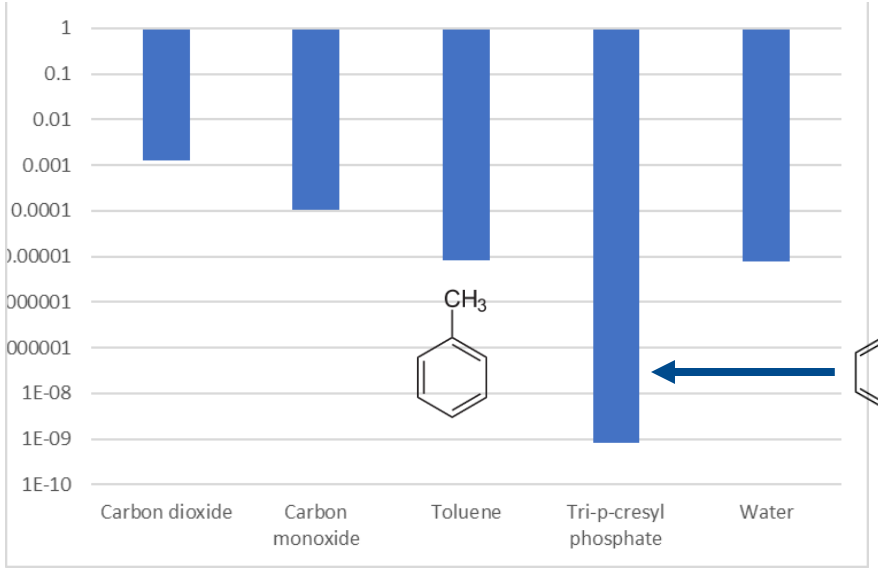
TPP in Toluene

Initial compounds: UNKNOWN

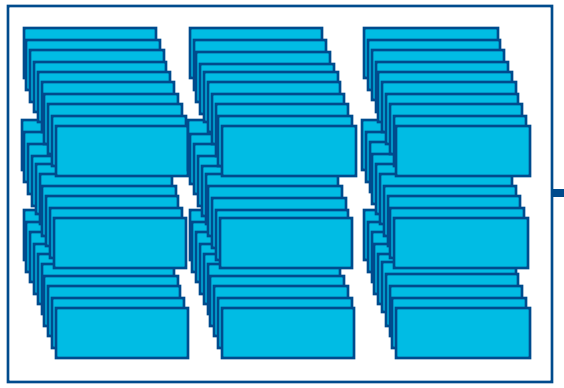
700 °C

XplorIR

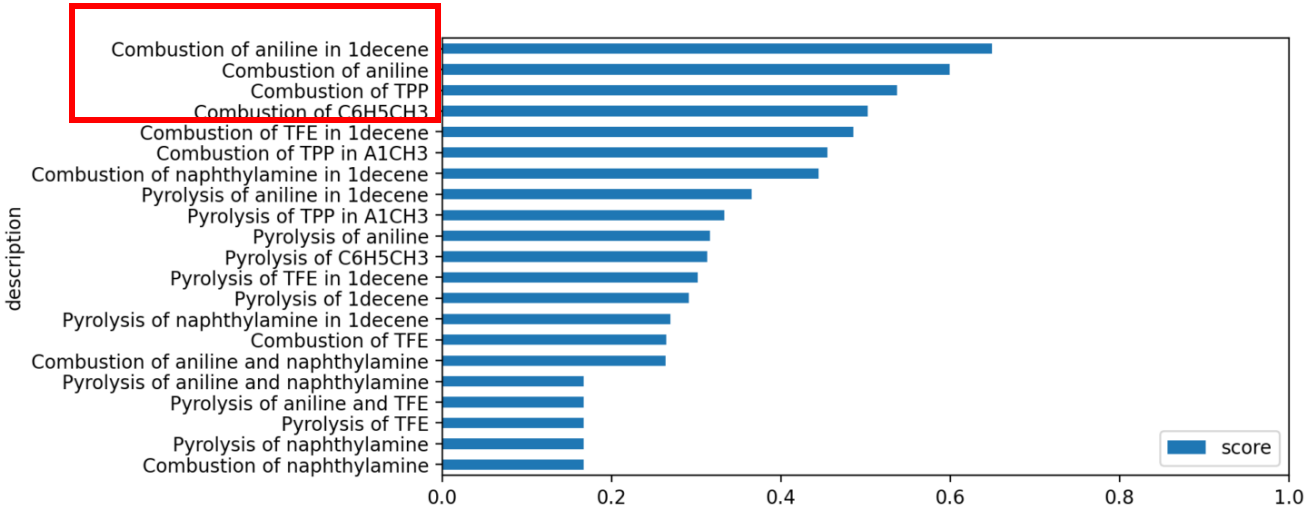
fieldable detector



Modeled Pathways
Final Compounds



Similarity Analysis



Forensic Attribution Capability

AFRL

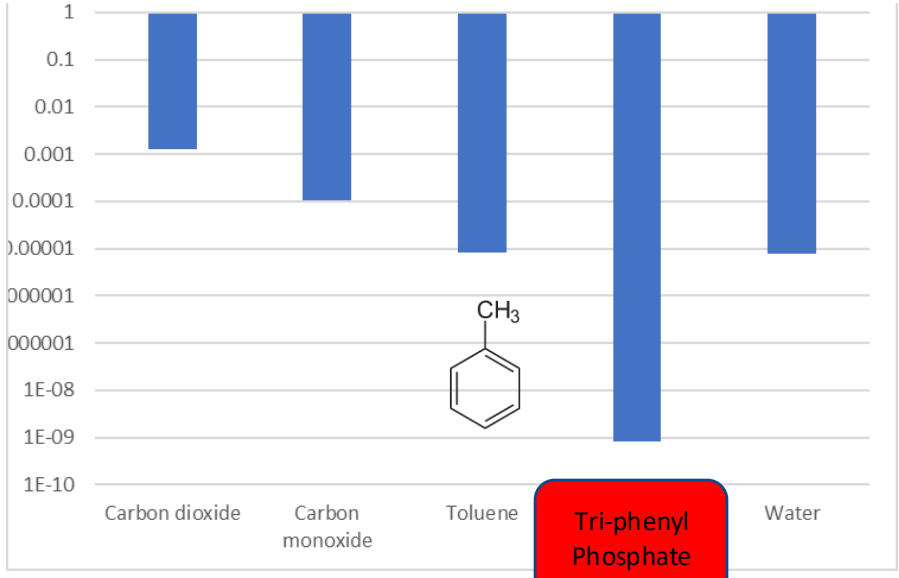
TPP in Toluene

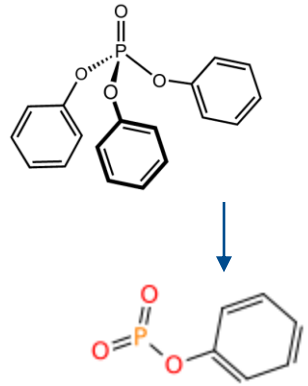
Initial compounds: UNKNOWN

700 °C

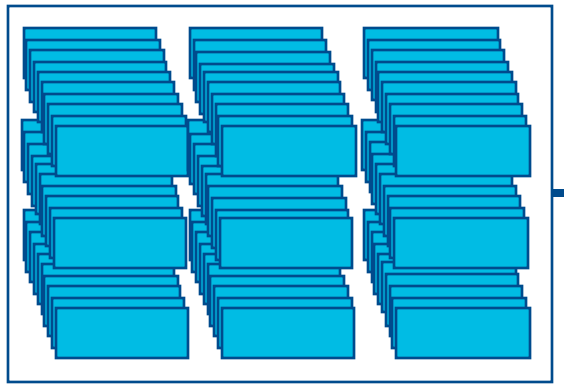
XplorIR

fieldable detector

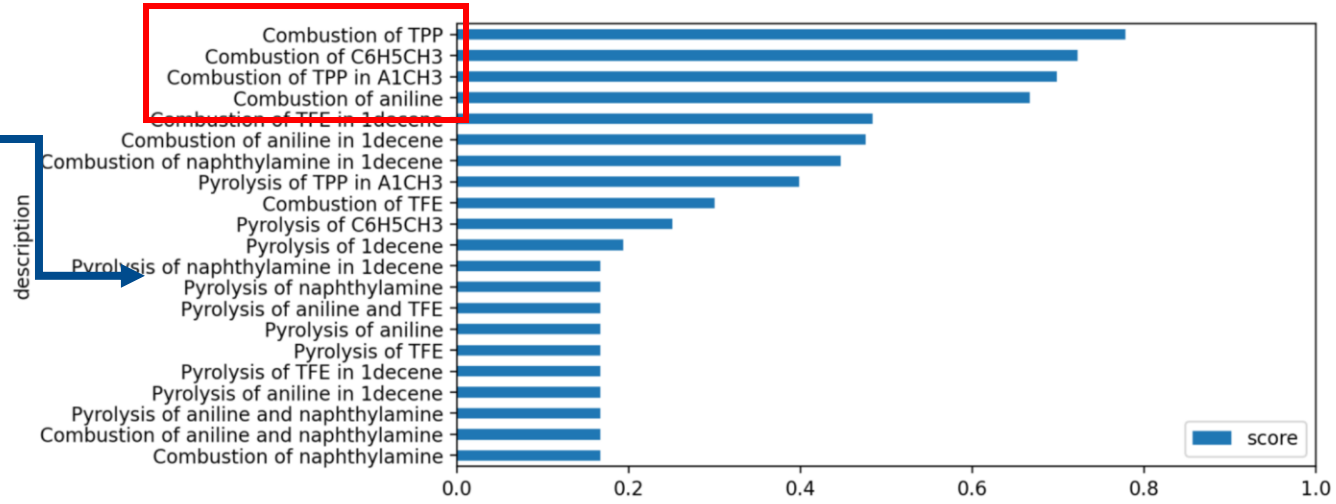




Modeled Pathways
Final Compounds



Similarity Analysis



Forensic Attribution Capability

AFRL

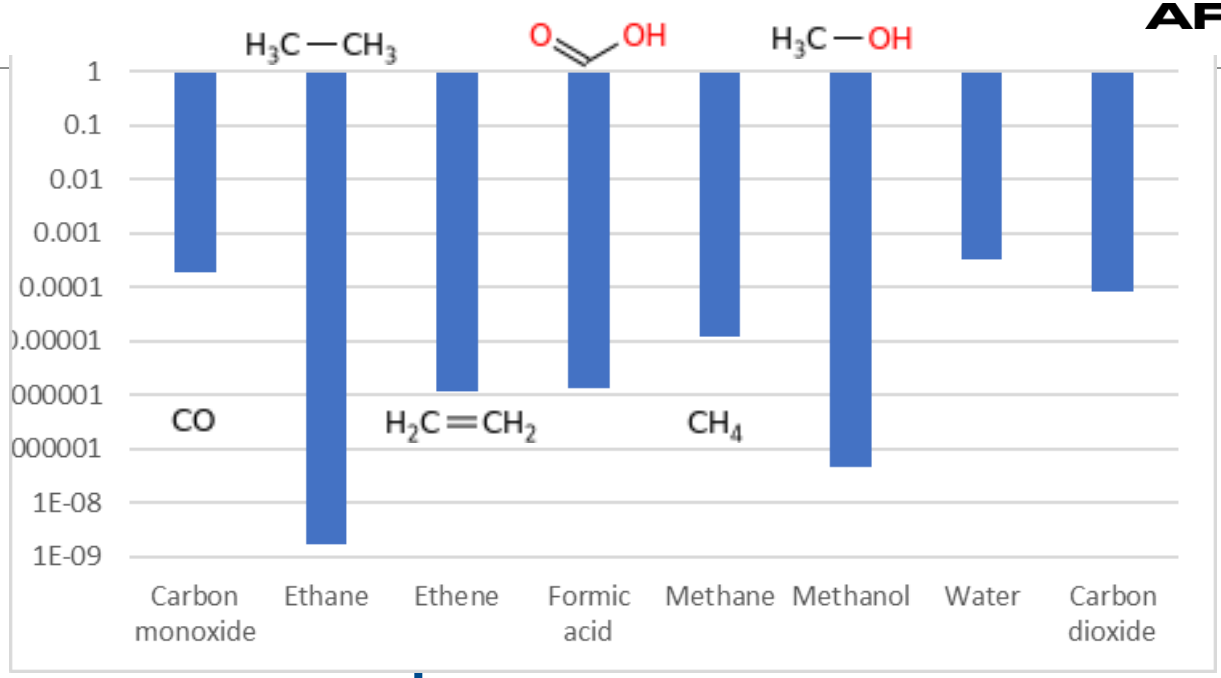
Dodecane

Initial compounds: UNKNOWN

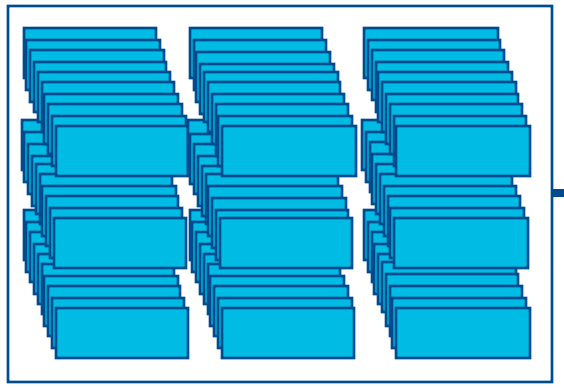
700 °C

XplorIR

fieldable detector



Modeled Pathways
Final Compounds



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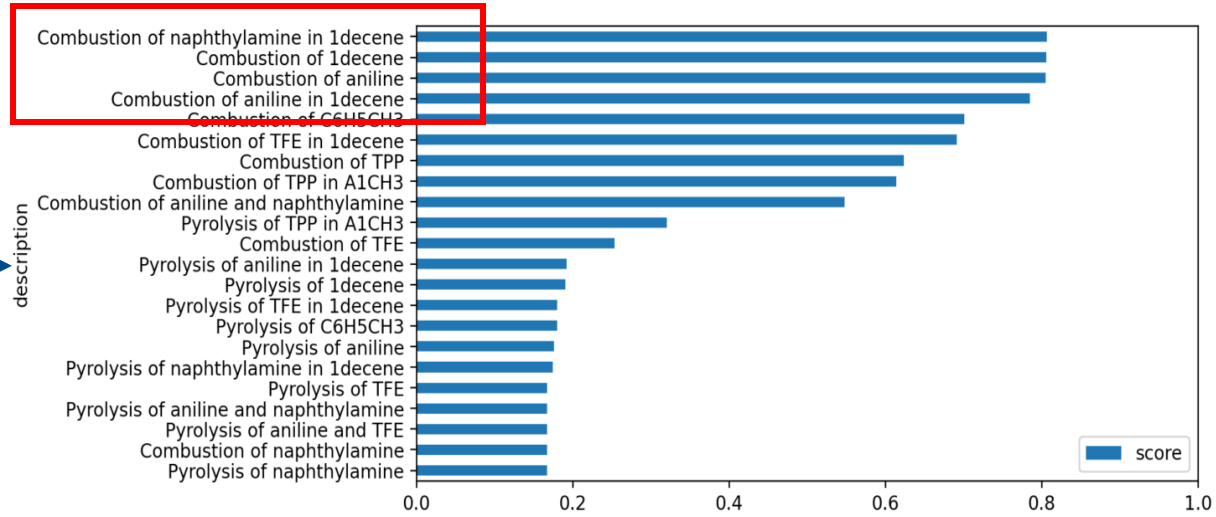


Results Trends

- Pure compounds are easier to distinguish
  - Triphenyl Phosphate (TPP) in toluene
  - Dodecane
- Mixtures have some unique products
  - Turbonycoil 160 – ethyl formate
  - Radco Lube 500M – acetic acid & octane
  - FR282 - ?
- Identification is easier at lower temperature
  - More unique products exist at 300 °C versus 1000 °C
  - Water and carbon dioxide can swamp the infrared detector
- Pathways reflect these trends, but are “rigid”
  - Never expect to get 100% agreement between modeled pathways and field measurements
- Can experimental data be added to pathways?

300 °C

Measured Compounds at 300C	TPP	Dodecane	TC160	RADCOLUBE500M	FR282
Acetic acid				X	
Carbon dioxide	X	X	X	X	X
Carbon monoxide	X	X		X	X
Ethane		X			
Ethene		X	X	X	X
Ethyl formate			X		
Formaldehyde		X	X	X	X
Formic acid		X	X	X	X
Methane		X	X	X	X
Methanol		X			
Octane				X	
Toluene	X				
Tri-p-cresyl phosphate	X				
Water		X	X	X	X

1000 °C

Measured Compounds at 1000 C	TPP	Dodecane	TC160	RADCOLUBE500M	FR282
Acetic acid				X	
Carbon dioxide	X	X	X	X	X
Carbon monoxide	X	X			
Ethane		X			
Ethene		X			
Ethyl formate					
Formaldehyde		X			
Formic acid		X	X	X	X
Methane		X			
Methanol		X			
Octane					
Toluene	X				
Tri-p-cresyl phosphate	X				
Water	X	X	X	X	X

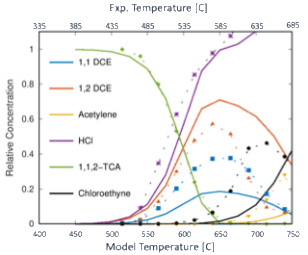
Next Steps

- Complete burns of all 10 chemicals/mixtures chosen
  - TPP/TCP ✅ - Hydraulic fluid: RADCOLUBE FR 282 *(MIL-PRF-83282)* ✅
  - Dodecane ✅ - Hydraulic fluid: RADCOLUBE RHP5606 *(MIL-PRF-5606)*
  - Methyl methacrylate - Turbine Oil: TURBONYCOIL 160 *(MIL-PRF-7808)* ✅
  - 1-Decene - Turbine Oil: ROYCO 899 23699Cl *(MIL-PRF-23699)*
  - Naphthylamine/aniline ✅ - Electronic Coolant: RADCOLUBE 500M *(MIL-PRF-87252)* ✅
- Perform forensic attribution framework on results from fieldable devices and ground-truth instruments to fully assess extent of performance enhancement
- Deliver forensic attribution modeling workflow and IR algorithm for AFRL field test of capability
  - Modeling workflow in use by Air Force; includes both input of alert data from fieldable device and capability to drawdown raw spectra, analyze, and input into forensic attribution workflow
  - Detailed instructions on using fieldable device during field tests and data analysis through forensic attribution workflow to results

Next Steps - Roadmap

July 2026

Next Step



Starting point:
- Basic standalone fieldable device
- Provides information on some acute exposures
- Limited by sensitivity, library
- No forensic attribution capability

Proof of concept forensic attribution with enhanced fieldable device:
- Standalone device and model – not yet fully integrated
- *Increased sensitivity and library* with APL spectral deconvolution
- *Forensic attribution capability* –
  - Alerts and raw data input into forensic attribution model to give results on parent compounds and combustion conditions

Proof of concept field test

Enhanced fieldable device with integrated forensic attribution model:
- Work with 908devices to integrate forensic attribution model
- Increased sensitivity and library tuned to AF relevant chem
- Field functional, ready for use by novice

QUESTIONS?

Predictive Risk Team AFRL/RHBAF

- Rebecca Clewell
- Daniel Cowan
- Slava Chushak
- Teri Sterner

Subcontracts

Johns Hopkins University

Applied Physics Laboratory

- Danielle Nachman
- Michael Salerno
- Thomas Buckley
- Mallory Solazzo

Government Collaborators and Advisors

- Christin Duran
- Mitch Rubenstein
- Sarah Pfahler
- Vince Falls
- Carolyn Prill
- Jerimiah Jackson