EPA United States Environmental Protection Agency

Atmospheric Chemistry, Fate and Transport of Air Toxics and Contaminants of Emerging Concern

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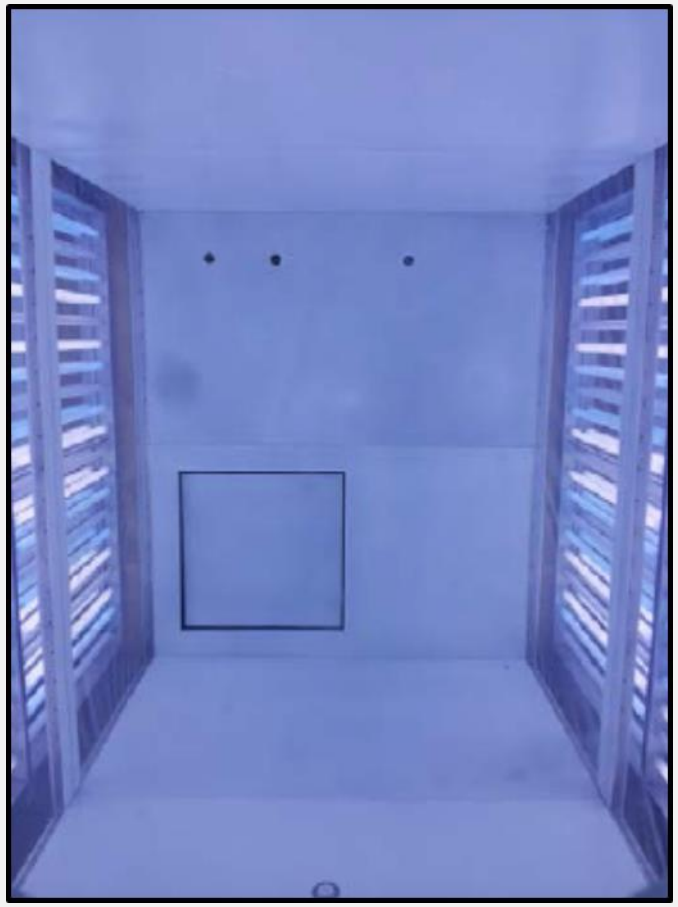
Modeling Air Toxics in CMAQ

- Capacity to simulate transport and fate of several Hazardous Air Pollutants (HAPs)
  - In both gas and aerosol phases
  - Predictions for air concentrations and deposition
- HAP simulations conducted while simulating Criteria Air Pollutants (CAPs).
  - Allows determining how emissions control strategies affect both CAPs and HAPs
- Two approaches used to predict HAPs
  - Chemical mechanism for CAPs, e.g. formaldehyde and acrolein
  - Reactive or inert tracers, e.g. ethyl benzene, particulate nickle
  - HAP treated explicitly if significant atmospheric chemistry
- Users can determine what HAPs to simulate at model runtime
  - Allow users flexibility based on their applications

Applications of CMAQ Air Toxics Capacity

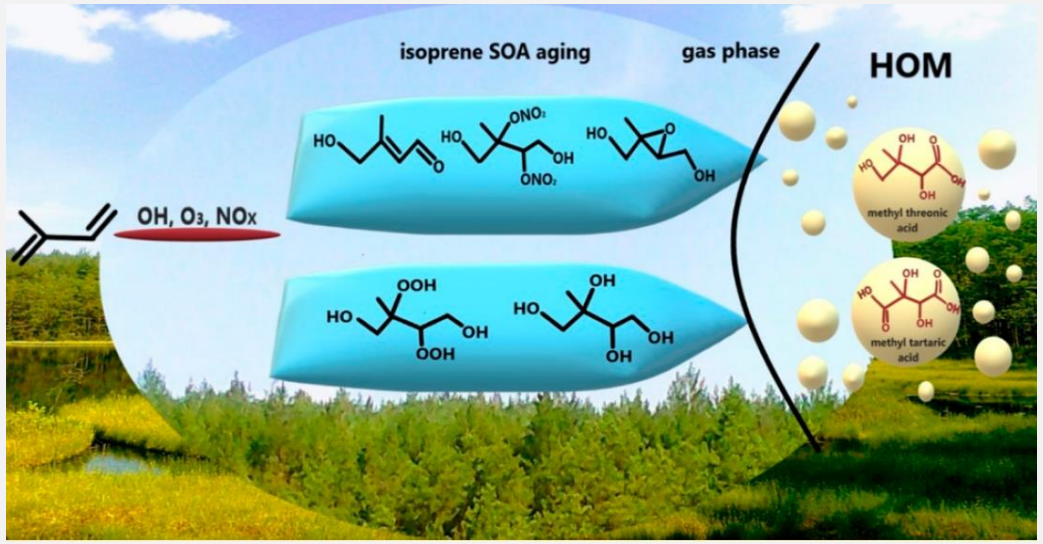
- Information provided by applications
  - Emissions determine concentrations versus atmospheric production
  - Deposition to watersheds
  - HAPs accounting for most of risk to human health
- Previous applications
  - US National Air Toxics Assessments for respiratory and cancer risks.
  - US EPA assessments on emission control strategies for motor vehicles
- Goals of future applications
  - Modeling semi-volatile HAPs such as benzo[a]pyrene
  - Runtime options allowing source apportionment for HAPs built on CMAQ-ISAM

Chemical Mechanisms & Kinetics



Jaoui et al. ES&T 2019

- Extensive analytical capabilities for gas and particle speciation
- Recent focus on secondary organic aerosol (SOA) formation
- Reaction rates, mechanisms and tracer identification
- Examining role of volatile chemical/consumer products (VCPs) on gas and aerosol formation
- Connections with STAR grant on chemical mechanisms
- Updating/revising chemical mechanism in CMAQ – Community Regional Atmospheric Chemical Multiphase Mechanism (CRACMM)



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Adding VCP chemistry to CMAQ

Havala Pye

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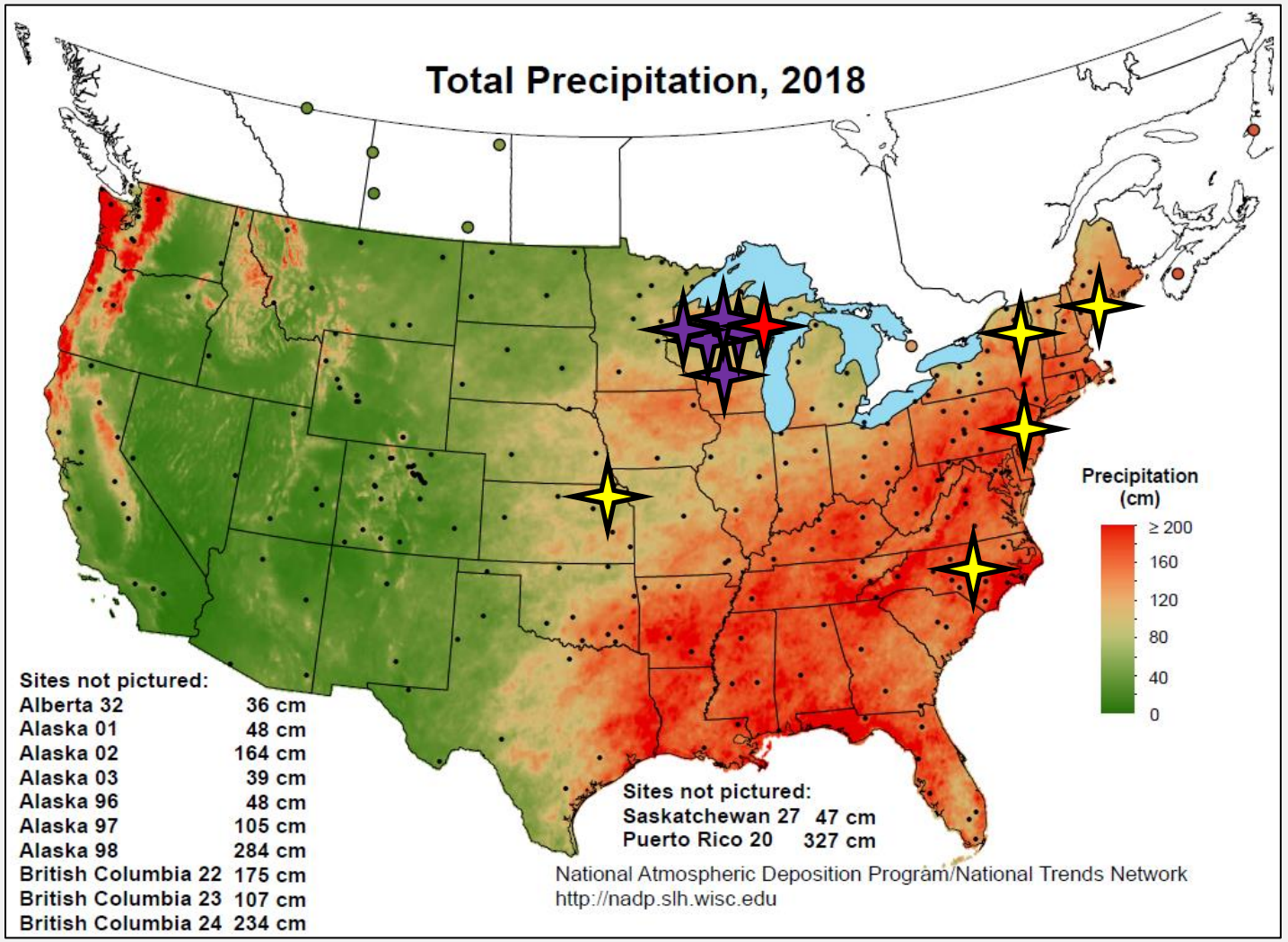
PFAS Wet Deposition Measurements



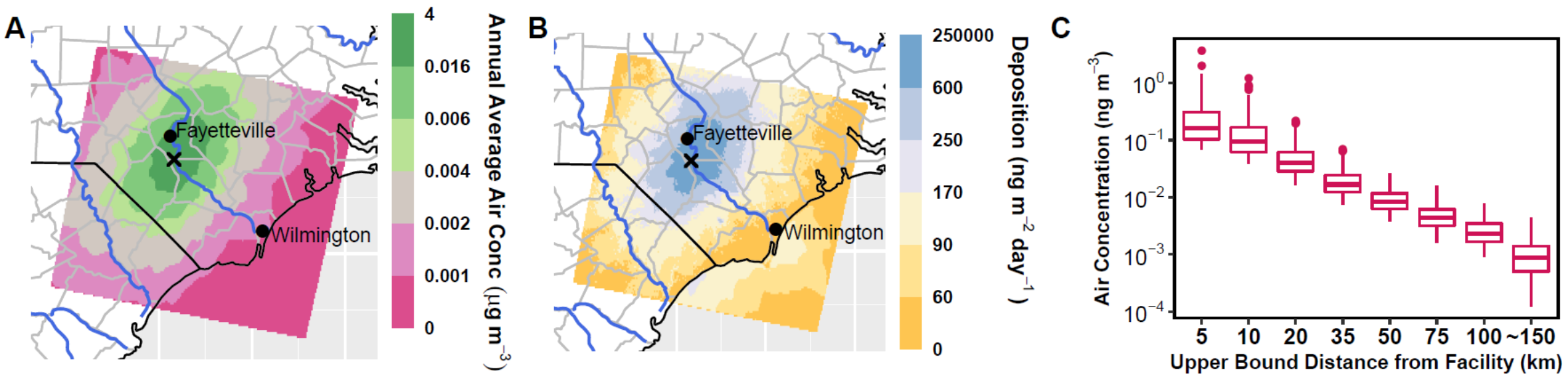
NADP/NTN Targeted PFAS
2 yrs @ 3 sites
Duke Forest: more detail & longer

Wisconsin Request: NTA

Source impacted & upwind sites: NTA?

- Completed year 1 of wet dep measurements
- Added KS site October 2021 in collaboration with Kickapoo Tribe
- Completed triplicate sampling in NC – shifting to examine throughfall

Developing CMAQ-PFAS for modeling air transport and fate of PFAS emissions

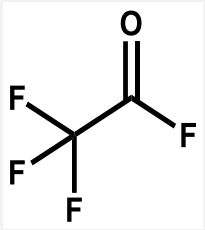


- 26 individual PFAS + 1 lumped species were added to CMAQ, the EPA's flagship air quality model
- Left: annual average air concentration of the total PFAS added to CMAQ
- Middle: daily average deposition of total PFAS.
- Right: air concentration of total PFAS as a function of distance from the facility

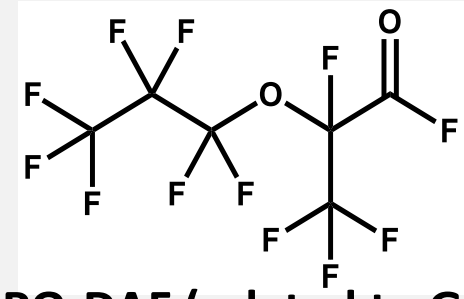
D'Ambro et al, ES&T 2021, 10.1021/acs.est.0c06580

Computational Chemistry of Per/polyfluorinated Alkyl Substances

Courtesy: D'Ambro, Murphy *et al.*



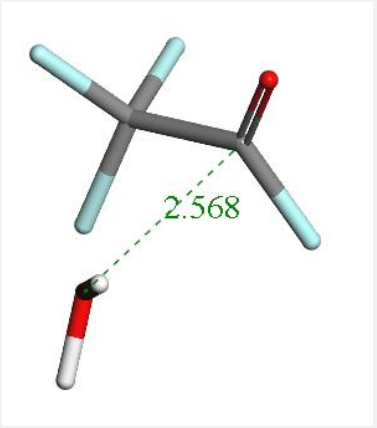
PAF



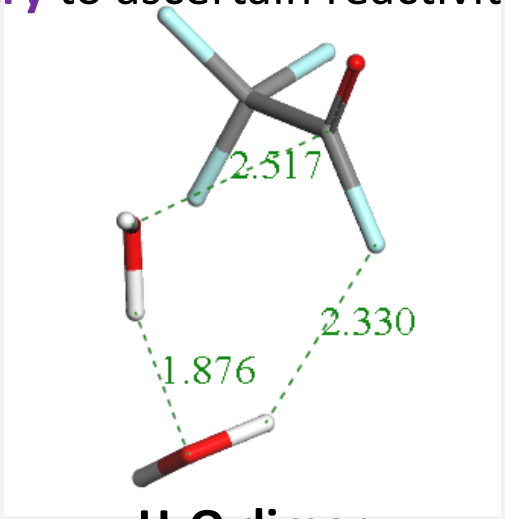
HFPO-DAF (related to GenX)

- acyl fluorides make up ~9000 pounds of emissions/yr from NC chemical facility
- they react quickly in water – what about air?
- use **computational chemistry** to ascertain reactivity

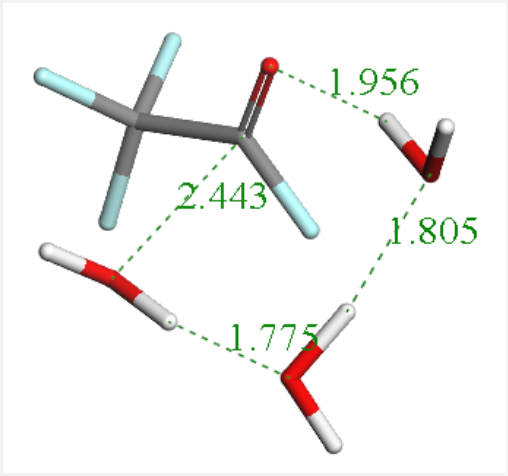
PAF Chemistry:



H_2O monomer



H_2O dimer



H_2O trimer

increasing reactivity

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Incorporating PFAS into CMAQ

Emma D'Ambro

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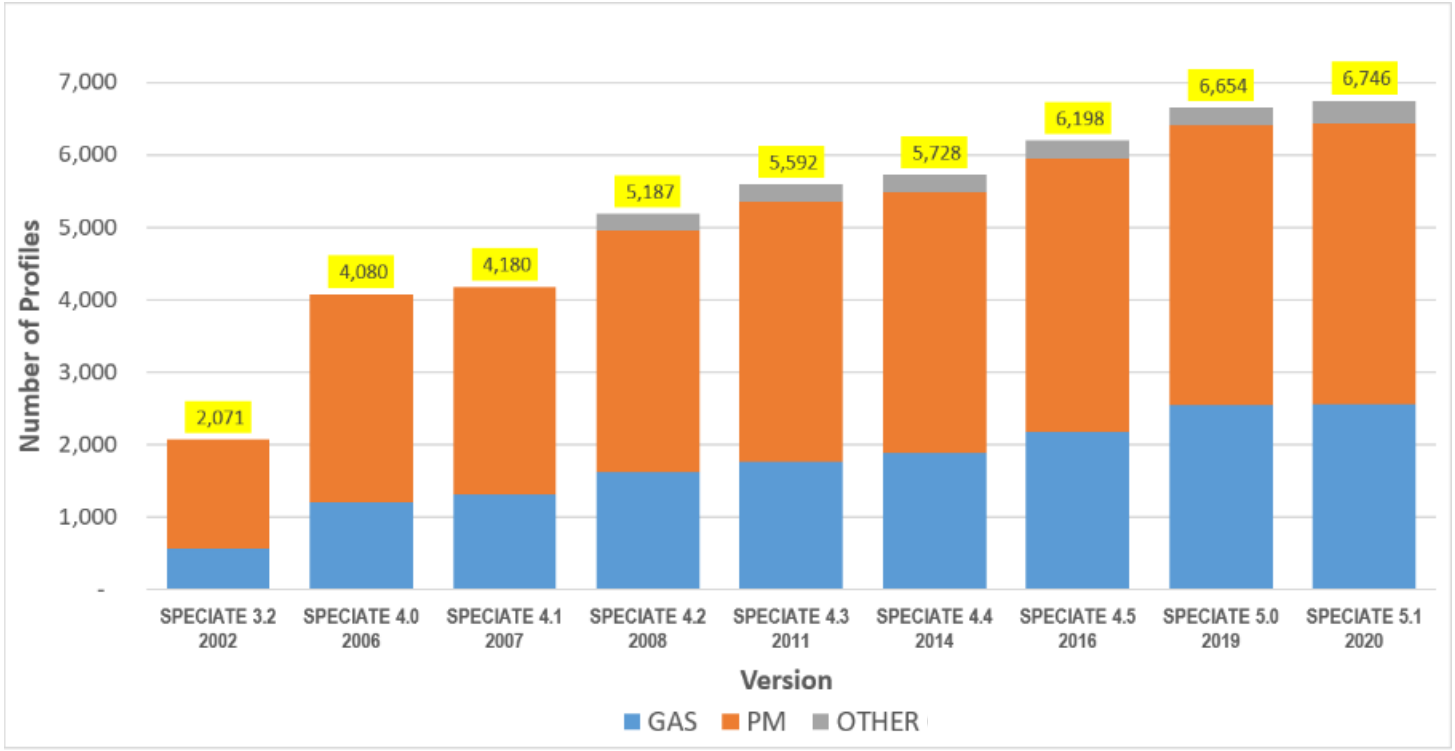
SPECIATE 5.1: Database Expansion

- Gas and PM speciated emissions profiles
- Research model development & regulatory applications



SPECIATE 5.1
6,746 profiles
# of Profiles Added:
16 Gas,
18 $PM_{2.5}$
58 mercury

Each version is a cumulative update of the previous version

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Updates to the SPECIATE Database

George Pouliot

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