

BOSC: Meet the Scientist Panel Discussion

PFAS Modeling of Air Transport and Deposition

Emma L. D'Ambro

Ben Murphy

Havala Pye

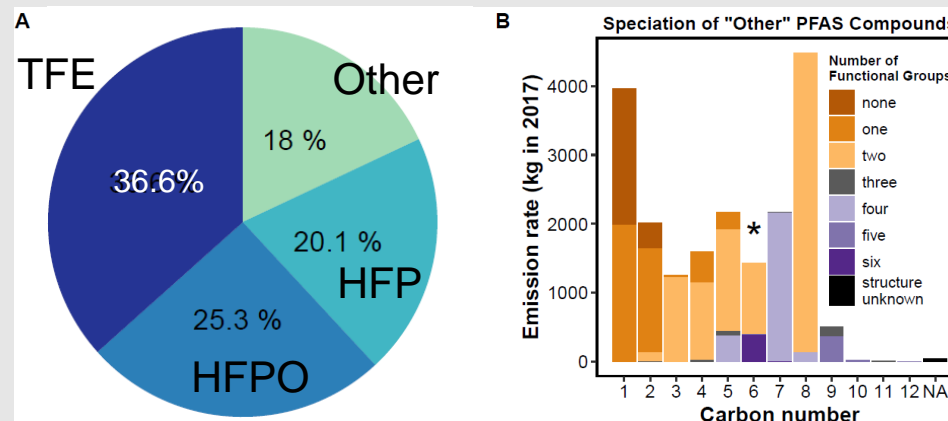
Atmospheric Chemistry and Aerosols Branch (ACAB)

Center for Environmental Measurement and Modeling (CEMM)

Case Study: North Carolina PFAS Manufacturer

- Partnered with North Carolina Department of Environmental Quality (NCDEQ).
- Simulated 26 explicit PFAS in CMAQ with state-of-the-art chemical property estimation.
- Full 2018 simulation. 1 km horizontal resolution
- Estimated impact at regional scale: air impacts extend further downwind than existing literature.

Emissions estimates (provided by The Chemours Company)

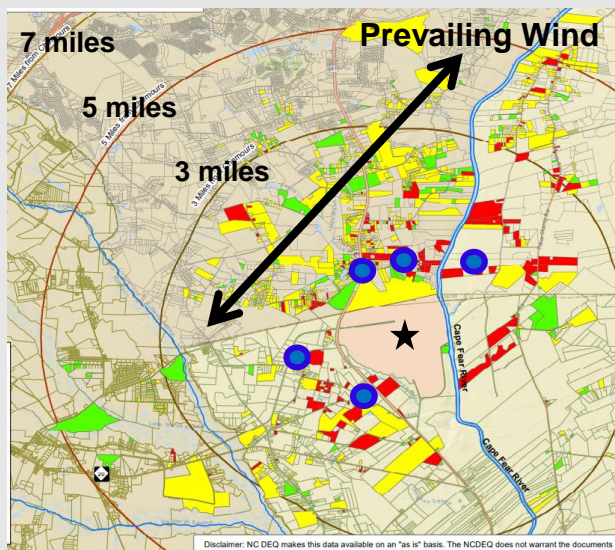


- ★ GenX compounds (956 kg yr⁻¹)
 - HFPO-DA (316 lbs yr⁻¹)
 - HFPO-DAF (725 lbs yr⁻¹)
- 49 PFAS compounds reported at total emission of ~109,000 kg in 2017

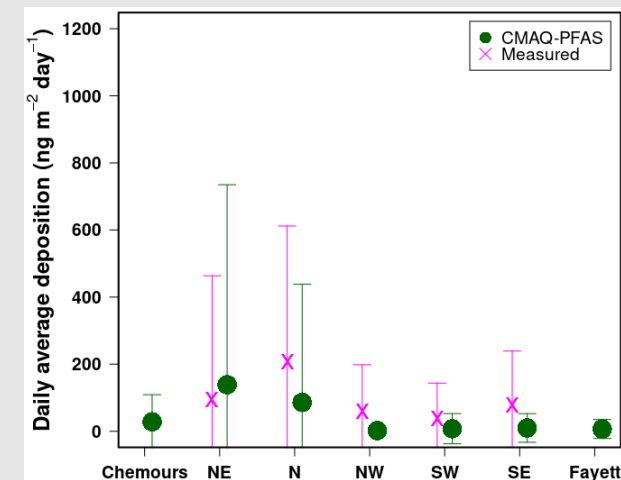
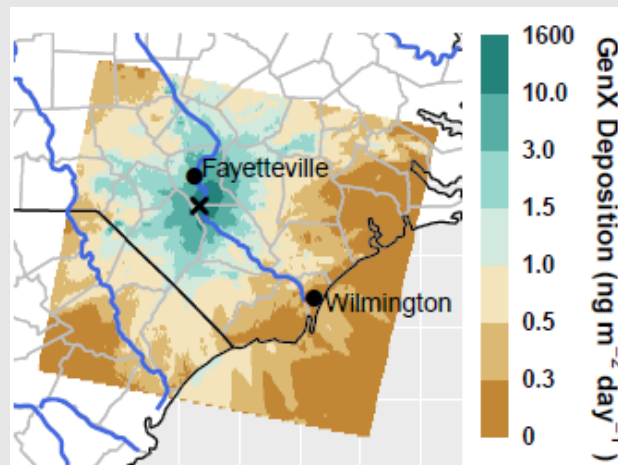
Observations

NC DEQ well sampling

- ★ The Chemours Company
- Deposition Measurement Site
- GenX ≥ 140 ppt
- Total PFAS ≥ 70 ppt, or Any PFAS ≥ 10 ppt
- Non-detect, or All PFAS < 10 ppt



CMAQ-PFAS Results

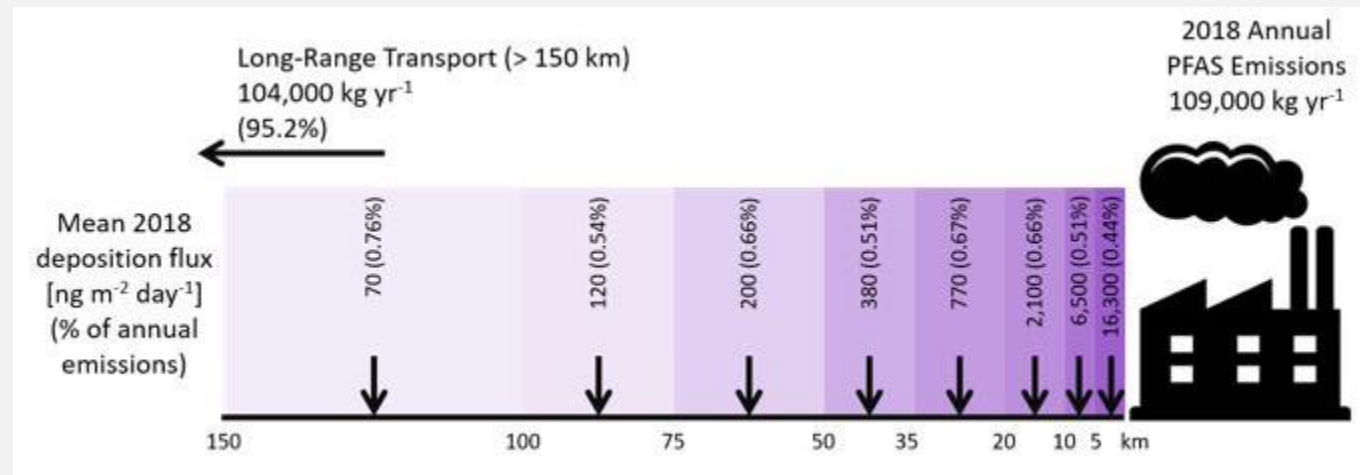


GenX Deposition is elevated near facility (max = 1,550 ng m⁻² yr⁻¹) and dispersed throughout the region (domain-wide mean = 1 ng m⁻² yr⁻¹)

Impact and Future Work

- **For North Carolina Case, CMAQ-PFAS predicts:**

- 95%+ of total PFAS air emissions are transported farther than 150 km downwind of this manufacturing facility (top right).
- 16.3 $\mu\text{g m}^{-2}$ deposition flux on an average day within 5 km of the facility
- Locations within 10 miles of the facility experience GenX air concentrations $> 1 \text{ ng m}^{-3}$ for a cumulative of more than 100 days of the year.

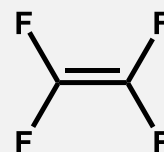


D'Ambro et al., ES&T 2021, <https://doi.org/10.1021/acs.est.0c06580>

- **Next Steps:**

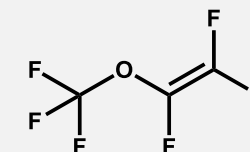
- Assessing the impact of model resolution in terms of chemical detail, spatial resolution, and temporal resolution of emissions.
- Examining atmospheric chemistry of abundant novel PFAS (bottom right).
- Developing a platform to quantify intra- and interstate transport and deposition of emissions from facilities in New Jersey.

PFAS + OH reactivity



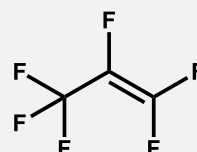
TFE:

11 days
40,082 kg yr⁻¹
V. Orkin, JPCA, 1997.
G. Acerboni, JPCL, 1999.
V. Orkin, JPCA, 2002.
V. Orkin, JPCA, 2011.



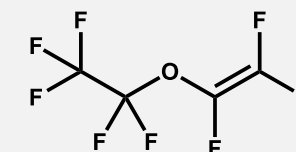
PMVE:

4 days
1,215 kg yr⁻¹
Z. Li, JGR, 2000
K. Tokuhashi, CPL, 2000
M. Mashino, JPCA, 2000
L. Vereecken, PCCP 2015



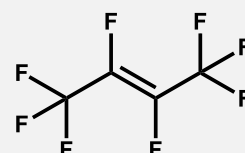
HFP:

5 days
22,018 kg yr⁻¹
A. McLroy, JPC, 2003
M. Dubey, GRL, 1996
V. Orkin, JPCA, 1997
M. Machino, JPCA 2000
K. Tokuhashi, CPL, 2000
V. Orkin, JPCA, 2011



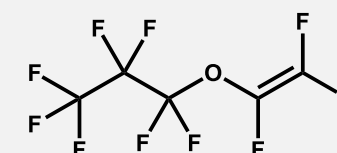
PEVE:

4 days
697 kg yr⁻¹
G. Srinivasulu, PCCP, 2018
A. Bunkan, PCCP, 2018



PFB:

24 days
447 kg yr⁻¹
C. Young, Atm En, 2009
V. Orkin, JPCA, 2011



PPVE:

3.5 days
1,291 kg yr⁻¹
D. Amedro, PCCP, 2015

Publication in Environmental Science and Technology:

D'Ambro, E.L., Pye, H.O., Bash, J.O., Bowyer, J., Allen, C., Efstathiou, C., Gilliam, R.C., Reynolds, L., Talgo, K. and Murphy, B.N., 2021. **Characterizing the Air Emissions, Transport, and Deposition of Per-and Polyfluoroalkyl Substances from a Fluoropolymer Manufacturing Facility.** *Environmental Science & Technology*, 55(2), pp.862-870.

<https://pubs.acs.org/doi/10.1021/acs.est.0c06580?fig=abs1&ref=pdf>

EPA Contacts:

Emma D'Ambro: dambro.emma@epa.gov

Ben Murphy: murphy.ben@epa.gov

Havala Pye: pye.Havala@epa.gov

Collaborators:

North Carolina Department of Environmental Quality
New Jersey Department of Environmental Protection
EPA Regions 1, 2, and 4
Office of Air Quality Planning and Standards
University of North Carolina
North Carolina State University
The Chemours Company