# *Approaches for Addressing Scientific Challenges and Key Uncertainties in Characterizing Air Toxics and Contaminants of Emerging Concern*

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Office of Research and Development
Center for Environmental Measurement and Modeling (CEMM)

- Changes in measurement technologies

  - FRM/FEM (congressionally mandated) v. sensors

    - *Regulatory grade vs. screening level estimate*
    - *FRM/FEM are "gold standard" instrumentation, but sensors can be less expensive, more obtainable - comes with accuracy "costs"*

  - Time-integrated (can, cartridge, filter) sampling v. real-time, (semi) continuous measurement technologies

    - *Air pollution "events" from local sources not adequately captured when samples collected over multi-hour or multi-day period*
    - *High temporal frequency and large spatial coverage needed to support assessments, emission characterization, and model development/evaluation*

- Data/model fusion techniques can improve characterization of air toxics and pollutants of emerging concern
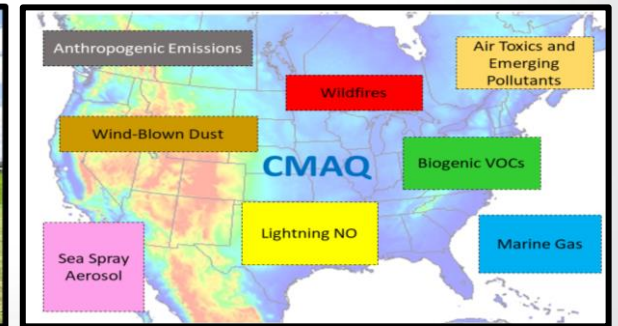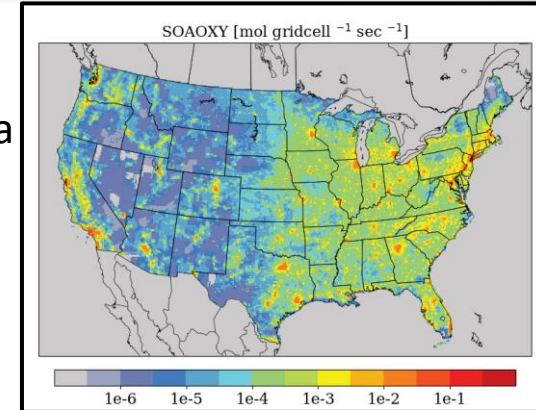


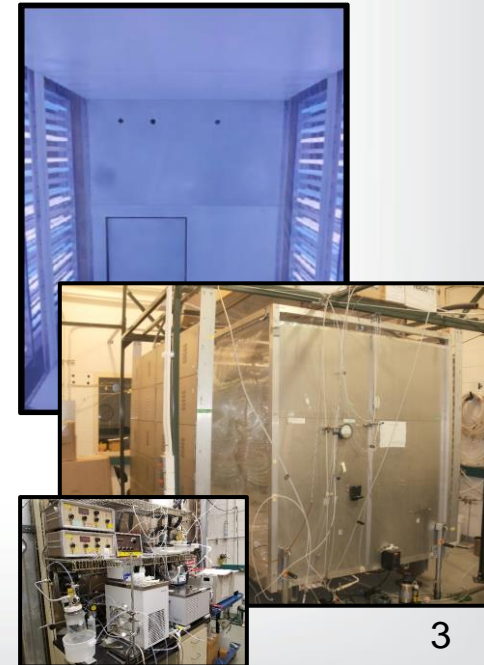**source**          **near-source/fenceline**          **ambient**          **modeling/emissions database**

- Air Quality Modeling and Air Toxics & Contaminants of Emerging Concern

  – Huge uncertainties in emissions estimates without sufficient (temporal, spatial) observational data

  – Need more data to build confidence in models and improve our understanding of emissions and chemistry/transformation and transport/fate processes

- Measurement and Characterization

  – Paradigm shifting for characterizing air pollutants and source emissions

    - *Need to capture lower ambient concentrations*

    - *Need speciated data*

    - *Need real-time measurement capabilities to capture local pollution "events"*

- Modeling, measurement and characterization can work together: Recent Atmospheric Chamber Intercomparison Test for EtO Instrument/Techniques

  – Chamber study with varying conditions and multiple instruments informs both the modeling and measurement methodology efforts

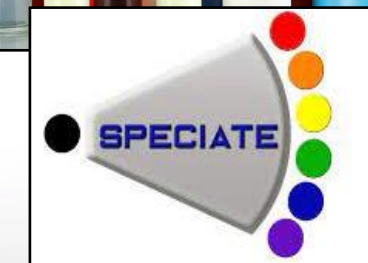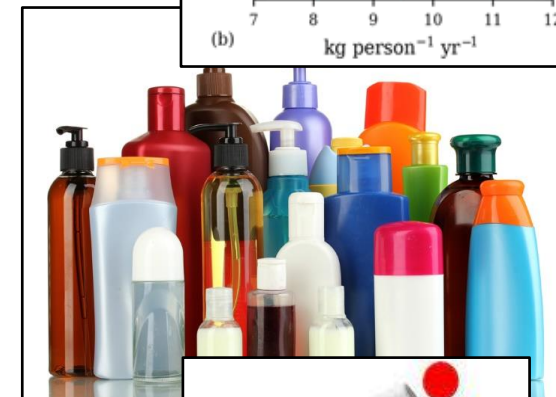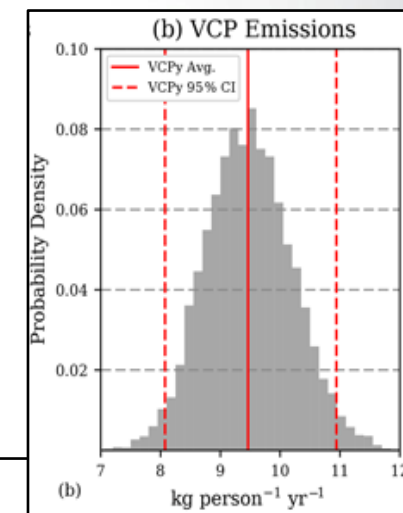  – Likewise, modeling and measurement results inform further chamber studies



SOAOXY [mol gridcell $^{-1}$ sec $^{-1}$]

Courtesy of Havala Pye

- Research Objective(s): develop, evaluate, and apply databases and multimedia models for air toxics and pollutants of emerging concern for research applications

- Associated Challenges: limited data available to develop databases and build modeling capabilities for air toxics and pollutants of emerging concern

- Research Implementation for Solutions:
  - **Determine secondary organic aerosols (SOA) and ozone formation from volatile chemical products (VCPs) through laboratory testing; VCP emissions inventory methodology and tools**
  - **Updates to SPECIATE database with new emissions profiles for air toxics and pollutants of emerging concern**
  - **Incorporate PFAS and EtO chemistry, transport, and deposition into Community Multiscale Air Quality (CMAQ) model**
  - **Leveraging air toxic and emerging pollutant measurement studies to inform fine-scale modeling and estimates of near-source deposition and concentrations**

- Research Objective(s): develop, evaluate, and utilize measurement methodologies and technologies, characterize ambient air toxics concentrations, determine fate and transport, incorporate into models, involve communities

- Associated Challenges: achieving real-time, continuous measurement across a wide-range of concentrations; ever-changing technologies that impact ambient pollutant concentrations; need for additional chemistry and deposition data to inform model development

- Research Implementation to Support Solutions:

  - **Advance FRM/FEMs and development of sensors to better characterize emissions and inform emission inventories and ongoing public health and environmental assessments**

  - **Improve characterizations for air toxics by improving existing, or developing new, measurement methods/technologies**



ODOR EXPLORE

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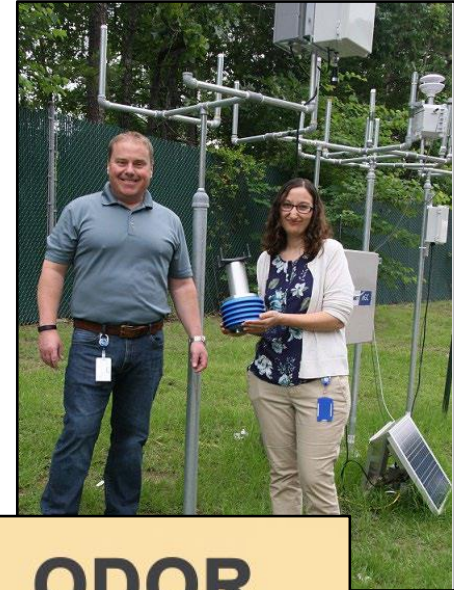
- Research Objective(s): improve, develop, evaluate, and utilize measurement methodologies and technologies to characterize emissions of air toxics from point and area sources, determine fate and transport, incorporate into emissions characterizations for incorporation into models and databases

- Associated Challenges: changing technologies and source uncertainties; developing methods, instrumentation, and technologies for characterizing difficult to measure compounds

- Research Implementation for Solutions:

  – **Improve emissions measurement methods and characterizations for air toxics and pollutants of emerging concern to inform control strategies, emissions inventories and databases used for regulatory guidance and modeling**

  – **Determine point and area sources of interest for testing and characterizing emissions**



Figure 1. Schematic of Condensable Particulate Sampling Train
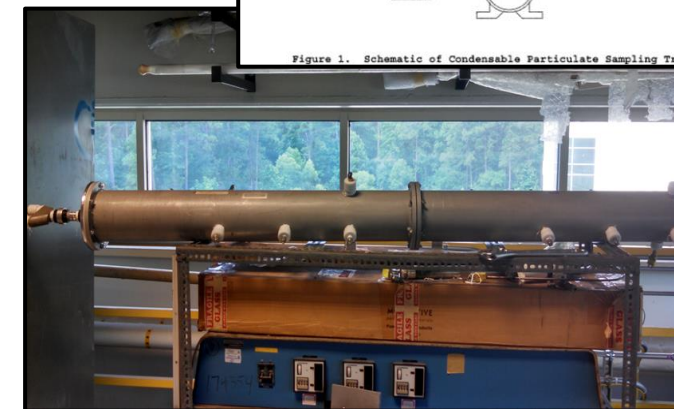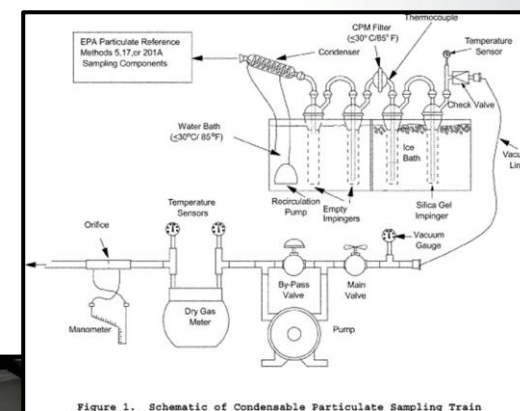
- <u>Research Objective(s)</u>: measurement methods improvements and development, characterize ambient concentrations (when/where elevated), fate and transport, incorporate into models

- <u>Associated Challenges</u>: achieving real-time, continuous measurement of low-level concentrations; characterizing "background" concentrations and interferants; limited chemistry and deposition data to inform model development

- Research Implementation to Support Solutions:

  – **Improve and/or develop measurement techniques and methodologies to enable detection and measurement of lower-level concentrations for air toxics and pollutants of emerging concern (e.g., EtO)**

  – **Determine potential interferents and appropriate solution for data analysis considering elevated background concentrations**

  – **Determine fate and transport of PFAS and EtO to inform emissions inventories used for modeling; improving spatial and temporal resolution**

- <u>Research Objective(s)</u>: source identification, methods development, emissions characterizations, fate and transport, update emissions inventories, incorporate into models

- <u>Associated Challenge(s)</u>: defining compound(s) of interest; identifying potential sources; developing methods, instrumentation, and technologies for characterization of emissions; availability of quality gas standards

- Research Implementation to Support Solutions:

  - **Advance and/or develop measurement techniques and methodologies to enable better characterization of emissions from known sources; determine additional sources of interest**

  - **Determine sources of interest for testing, emissions characterizations**

  - **Determine fate and transport of these compounds of interest to inform emissions inventories used for modeling**



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- Q1: ORD is implementing research to develop new methods to quantify source and near-source emissions, as well as ambient levels, of toxic air pollutants and contaminants of emerging concern. These methods are needed to identify pollutant sources and levels of exposure for communities and individuals.

  – What suggestion(s) or recommendation(s) does the Subcommittee offer regarding progress to date of research activities related to air toxics and contaminants of emerging concern? How will our methods development efforts improve our understanding of pollution sources, emissions characterizations, and exposures?

- As the ACE BOSC works to address these Charge Questions, specific insights on the following would be helpful:

  – How might we best reduce uncertainty in sampling for PFAS and EtO in air?

  – What insights can you offer on the paradigm between use of FRM/FEM and sensors that we face as ORD supporting our internal regulatory partners?

# What's Up Next…

## Panel Discussions

- Panel 1: Research to Understand Source Emissions and Ambient Concentrations of Air Toxics and Contaminants of Emerging Concern
    - Air Methods and Characterization – Keeping Up with the Environmental Priorities (Richard Shores)
    - Atmospheric Chemistry, Fare, and Transport of Air Toxics and Contaminants of Emerging Concern (Alan Vette)
    - Insights from Partners/Users of ACE Research (Chet Wayland)

## Meet the Scientists Sessions

- Room A: Air Toxics – Source Measurement and Methods
    - PFAS Air Methods Development (Jeff Ryan)
    - Fugitive Sources and Fenceline Monitoring (Eben Thoma)
    - High Temperature Thermal Treatment of PFAS (Jonathan Krug)
- Room B: Air Toxics – Ambient Measurement and Methods
    - Odor Explore App and VOC Measurements (Rachelle Duvall)
    - Laboratory Evaluation of Fugitive and Ambient EtO Methods (Ingrid George)
    - Air Toxics: Methods Development & Ambient Measurement (Tamira Cousett)
- Room C: Air Toxics – Modeling and Databases
    - PFAS Modeling of Air Transport and Deposition (Emma D'Ambro)
    - The SPECIATE Database (George Pouliot)
    - Implications of Volatile Chemical Products (VCPs) for Criteria Pollutant Formation (Havala Pye)

# Supplemental Information

| | ACE Research Area | Example Research Products to Address NAAQS Scientific Challenges | Related Outputs |
|---|---|---|---|
| 1 | **Approaches to Support Air Quality Management for Multiple Pollutants at Multiple Scales** | • Analyze area-specific VOC compounds using passive samplers<br>• Develop VCP emission inventory methodology and tool<br>• Determine SOA and ozone production from VCPs<br>• Identify implications for VCP-driven nationwide criteria pollutant exceedances | 1.5, 1.6 |
| 2 | **Approaches for characterizing source emissions, air quality, exposure, and mitigation strategies** | • Develop and designate Federal Reference and Equivalent Methods (FRM/FEMs)<br>• Advance near-source measurements (fenceline, fugitive emissions)<br>• Improve source emissions characterization: on- and non-road mobile emissions, biomass combustion emissions, agricultural emissions, methane emissions from reservoirs, SPECIATE | 2.1, 2.2, 2.3, 2.5, 2.6 |
| 4 | **Public Health and Environmental Exposures and Responses to Emerging Air Pollutants and Sources** | • Characterize airborne PFAS and EtO ambient concentration and emissions from sources<br>• Develop measurement methods and techniques for PFAS and EtO in air<br>• Gain better understanding of control technologies and potential for best use/practices<br>• Characterize dispersion, environmental fate, and impacts<br>• Identification of remaining critical knowledge gaps | 4.1, 4.3 |