What Organic Compounds Evolve during Thermal Analysis of Carbonaceous Aerosols?

Identification of Specific Compounds in Different Temperature fractions of Thermal Evolution Methods

Joellen Lewtas, Ph.D
Human Exposure & Atmospheric Sciences Div.
National Exposure Research Laboratory
Office of Research & Development

Why is this a Critical Scientific Issue ?

Scientific Basis for Understanding
- **Carbon Fractions**
- **Measurement Issues**

Relationship to Organic Source Tracers for Source Apportionment

Basis for Improving Thermal Methods and Standards

Obstacles to Addressing this Issue

EPA

- **Selection/Standardization of OCEC Protocol(s)**
  - **Thermal Conditions**
  - **Definition of Specific Fractions**
- **Organic Characterization/Quantification Methods and Standards**
- **Integration of Research between the two Scientifc Communities:**
  - **Thermal Carbon Analysis**
  - **Organic Chemical Characterization**

Approaches to Addressing this Issue

- **Research Initiatives & RFAs (in progress)**
- **Organic Working Group (in progress)**
- **Possible Future Efforts**
  - **OCEC Working Group**
  - **Joint investigations between**

    Organic Speciation & Thermal OCEC

PM Organic Speciation Working Group: Goal

- **Goal:**

  Improve the Characterization and Quantification of Organic Compounds Associated with PM2.5 (Aerosols)

- **Organization/Sponsors:**

  EPA United States Environmental Protection Agency

  NIST National Institute of Standards and Technology

- **Contact:** lewtas.joellen@epa.gov

PM Organic Working Group: Why?

- To Improve Source Apportionment using Organic Tracers in Receptor Modeling
- To Facilitate Quantitative Comparison of Organic Species across Different Airsheds (Supersites)
- To Improve Aerosol Modeling through accounting for Organic Species
- To Determine the Role of Organics Species in Health Outcomes

PM Organic Working Group: Approach

EPA

- **Develop Standard Reference Materials (SRM)**
  - **Complex Realistic PM 2.5 SRM**
  - **Quantification & Calibration Standards**
  - **Dueterated Standards**
- **Identify & Analyze Key Target Analytes**
- **Conduct Inter-Laboratory Trials to Develop Consensus & Certified Values**
- **Development of Quality Assurance Procedures using Standard Reference Materials**

PM Organic Working Group: Participants

- **EPA PM Supersites, Centers & Related Programs (Universities, Research Institutes)**
- **Academic Scientists**
- **National Labs & other Research Centers**
- **Regional and State Laboratories**
- **NIST Laboratories**
- **EPA Laboratories (ORD, Regions)**
- **International (Canada, Europe, Asia)**
- **ORNL/NARSTO (data base development)**

Status of Working Group Activities

Developed Initial Target Analyte List

Survey of Organic Sampling Methods

Interlab Trial I Results 2002

Interlab Trial II Results 2003 (April Draft Report)

In progress: Development of Calibration Standards & Reference Materials

Future: Trial III (2003-2004)

Initial Target Analytes

- **Source Markers**
  - **Alkanes, Alkenes, Hopanes, …**
  - **Aromatics (PAH, Nitro-PAH,…)**
  - **Oxygenates (Acids, Aldehydes, Ketones, Quinones, Phenols, Sterols…)**
- **Toxic Organic Species**
  - **Polycyclic Aromatic Compounds (PAH, …)**
  - **Nitro Substituted Compounds**
  - **Reactive Oxygenates (Quinones,…)**

Intercomparison Trials: Reference Materials

EPA

- **Trial I (Feb-July, 2001)**
  - **SRM 1649a sieved to <63 microns**
  - **Extract of sieved SRM 1649a**
  - **SRM 1649a Urban Wash DC Particle <125 microns**
- **Trial II (2002-2003)**
  - **Interim Reference Material Baltimore $PM_{2.5}$ (20g)**
- **Trial III (2003-2004)**
  - **Bulk Baltimore $PM_{2.5}$ for new SRM (goal to collect 200g)**

Target Analytes Reported in Trial I

36 PAH	**14 Labs**
7 Nitro PAH	**2 Labs**
12 Alkanes & Alkenes	**6 Labs**
13 Hopanes, Colestanes, & Sterols	**5 Labs**
18 Carbonyls & Acids Aldehydes, Ketones, Lactones, etc.	**5 Labs**
8 Phenols	**none**

Standards Sub-Groups

Quinones & Ketones: - Barbara Zielinska (Lead) email: barbz@dri.edu, Doug Lane, Tony Miguel, Jake McDonald

Sugars & Phenols: - Chris Simpson (Lead), email: **simpson1@u.washington.edu ,** Mike Hayes,Barbara Zielinska , Lynn Reinhart

Hopanes and stearanes: - Jake McDonald (Lead) email: jmcdonal@LRRI.ORG , Mike Hayes, Barbara Zielinska , Steve McDow, John Offenberg, Wolfgang Rogge

Acids: - Mike Hayes (Lead), email: Hays.Michael@epa.gov, Lynn Reinhart, Steve McDow, and Tad Kleindienst

PAH Derivatives: Janet Arey (lead), email: **Janet.Arey@ucr.edu** Doug Lane, Barbara Zielinska, Chung Chiu, Brian McCarry, Steve McDow, Chris Simpson, Toney Miguel, Jake McDonald, Shao Mei Wong

New Investigations

- **Barbara Zielinska (DRI)**
  - **Thermal Desorption/Chemical Characterization**
  - **Temperature Ramps mimicing TOR Fractions**
- **Lara Gundel, Kirchstetter, Dod, Pang (LBL)**
  - **Comparison of thermograms of**
    - **Specific organic compounds**
    - **Ambient source**
    - **Surrogate PM**