SPECIATE and using the Speciation Tool to prepare VOC and PM chemical speciation profiles for air quality modeling

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International Emissions Inventory Conference, Baltimore, MD, August 15, 2017
TRAINERS

- Mike Kosusko, EPA ORD
- Madeleine Strum, EPA OAQPS
- Tejas Shah, Ramboll Environ

LOGISTICS
COURSE OUTLINE

8:00 SPECIATE, SPECIATE 101
8:45 Speciation Concepts
9:30 Break
10:00 SPECIATE Data Gaps and Future Plan
10:30 The Speciation Tool
11:30 End of Class
CLASS OBJECTIVES

• To introduce you to SPECIATE, its content and use
• To introduce you to the SPECIATE Web Browser and its use
• To provide an opportunity to ask questions about SPECIATE
• To present the Speciation Tool and how to use it
SPECIATE 101

• What is Speciation?
• What is SPECIATE?
• The SPECIATE Data Browser
WHAT IS SPECIATION?

Speciation disaggregates inventory species (e.g. VOC, PM\textsubscript{2.5}) into more detailed species

VOC:
- propane
- ethylene
- formaldehyde
- acetaldehyde
- ethanol
- etc.

PM\textsubscript{2.5}:
- elemental carbon
- organic carbon
- nitrate
- sulfate
- aluminum
- silicon
- iron
- etc.
SPECIATION IN GENERAL (STEPS)

1. Emissions source for inventory pollutant, e.g. VOC, PM$_{2.5}$
2. Assign Speciation Profile to source
3. Multiply inventory emissions by profile fraction to get emissions of specific chemical compounds

- 100 tons of VOC
- Solvent Utilization; Surface Coating; Architectural Coatings; Total: All Solvent Types in Autauga County, AL (SCC = 2401001000)

- Profile Code: 8744
- Composite Profile - Architectural Coatings: Solvent Borne and Waterborne

- 50 tons mineral spirits
- 9 tons texanol
- 9 tons propylene glycol
- 5 tons ethylene glycol
- etc.
**SPECIATION IN GENERAL (SPECIATE)**

Assign Speciation Profile to source based on process (SCC)

- **SPECIATE** is EPA’s repository of speciation profiles.
- **SPECIATE 4.5** is the current version.
- Several hundred literature citations to SPECIATE have been found.
WHAT IS SPECIATE?

DATA SOURCES → SPECIATE → DATA USERS

- Peer-reviewed literature
- Source testing of speciated emissions
- Other

Input to Air Quality Models
-- NEI Modeling Platform
Source Apportionment/Source Receptor Models
Black Carbon Report to Congress
Air Toxics Inventories

Feedback on Data Gaps

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WHAT IS SPECIATE? (continued)

• A repository for speciated emissions profiles
• A searchable Microsoft Access database
• Profiles for three air pollution emission types:
  – Particulate Matter (PM)
  – Total Organic Gases (TOG)
  – Other Gases [Hg, NO/NO₂/HONO, semivolatile organic compounds (SVOC)]
• Available on EPA Website:
  https://www.epa.gov/air-emissions-modeling/speciate-version-45-through-40
WHAT IS SPECIATE? (continued)

- Species include metals, ions, elements, organic and inorganic compounds
- PM profiles are size-segregated ($PM_{10}$, $PM_{2.5}$)
- Lots of metadata (references, test methods, notes, geographic region…)
- Profiles are rated for quality – judgement (J), vintage (V), number of data points (D)
# KEY TABLES IN SPECIATE

- **PM_PROFILE**
  - List of profiles

- **GAS_PROFILE**

- **PM_SPECIES**
  - Weight percents by profile and species ID

- **GAS_SPECIES**

- **SPECIES_PROPERTIES**
  - Species ID, name, molecular weight, other IDs, formula, whether it is a HAP, non-VOC

- **REFERENCE**
  - Citation or source of data
KEY SPECIATE QUERIES

**VIEW_GAS_PROFILES**
- Date Created: 7/7/2005 8:42:...
- Date Modified: 5/5/2017 9:14:...

**VIEW_PM_PROFILES**
- Date Created: 7/7/2005 8:40:...
- Date Modified: 5/11/2017 11:...
EXAMPLES – USING MS ACCESS

1. How do I find a VOC profile that has “Oil and Gas” in the title? (106 of them, example: “95420 Oil and Gas Production - Composite Profile - Glycol Dehydrator, Uinta Basin”)
   A. How do I find the latest profiles?
   B. How would I know if a profile is for a specific geographic region? (Look at Region field for where test was conducted)
   C. How do I get out the weight percentages for any one profile? (View gas profiles or view PM profiles, filter on profile ID)

2. How do I find a PM profile that has "Combustion" in the title? (There are 248 of them, example: 91105, Residential Wood Combustion -- Composite)
KEY METADATA COLUMNS

- NOTES
- REGION
- T_METHOD (Test method)
- DOCUMENT (Reference)
- TEST_YEAR
- P_DATE (Profile date)
- QUALITY
- CONTROLS
- ORIG_COMPO (original or composite)
QUESTIONS?

Are there any questions on what we've covered so far?
THE SPECIATE DATA BROWSER

- Provides database access for the non-MS Access user
  - URL - https://cfpub.epa.gov/speciate/
- On-Line demo
  - Key strength of the browser is the ability to search for profiles,
  - View them, and
  - Download them to MS Excel for further manipulation
SPECIATE DATA BROWSER QUERY

• How do I find a VOC profile that has “Oil and Gas” in its title? [Use Keyword Search]

• How would I know if a profile is for a specific geographic region? [View profile information. See 4th row.]

• How do I download profiles to MS Excel? [Add to “Shopping Cart” (but note it’s free) from Search page. Download cart.]

• How do I find a PM profile that has “Combustion” in its title? [Use Keyword Search]
SPECIATE 4.5 HIGHLIGHTS

• New Profiles (September 2016)
  – 182 new PM profiles for a total of 3,782
  – 291 new TOG profiles for a total of 2,170
  – No new Other Gases profiles for a total of 249
  – 2,602 unique species
  – Composite profiles for 85 source categories

• New Profiles cover the following source types:
  – Oil and Natural Gas (RARE with EPA Region 8)
  – Motor Vehicle Exhaust
  – Biomass Combustion
  – Waste Incineration
  – Brake Wear Emission
QUESTIONS?

Are there any questions on what we've covered so far?
**SPECIATE AS PART OF EMISSIONS MODELING**

**SMOKE** software system performs **temporal allocation, speciation, and spatial allocation** to create...

- Total VOC and PM$_{2.5}$ need to be speciated into chemical components for photochemical modeling.
- Each speciation profile is cross-referenced to an inventory source by SCC, pollutant, and potentially by region.
- SCC-to-profile mapping is specific to the EPA modeling platform and is separate from the SPECIATE database itself.
- Thousands of SCCs in the NEI are mapped to a few hundred profiles.
- Onroad mobile source emissions species come directly from the EPA MOVES model.

**Final product:** gridded, hourly, speciated emissions in a format for an air quality model.
**SPECIATION FOR AQ-MODELING**

- Develop chemical–mechanism specific profiles from profiles in SPECIATE
- Assign sources to profiles

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**Diagram:**

1. **Emission Inventories**
   - Criteria Air Pollutants, Hazardous Air Pollutants

2. **Speciation Tool**
   - Speciation profiles, MW, VOCtoTOG

3. **SMOKE - Emissions Model**
   - GSPRO: mechanism-specific profiles, GSCNV

4. **Model Species Emissions**
   - GSREF: SCC/FIPs-to-profile mapping

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SPECIATION CONCEPTS

1. TOG (VOC) “Gas” Profiles” Terminology
2. PM Profiles and AE6
3. Assigning Inventory Sources to Profiles
4. VOC Integration
5. Composite Profiles
6. “Gap-Filling” Profiles
7. On-Road Speciation
8. Nonroad Speciation
9. Combination Profiles
VOC/TOG TERMINOLOGY

- Gas Profiles in SPECIATE can be based on VOC or TOG (see MASTER_POL field)
- Inventories have VOC (regulatory definition)
- TOG is “Total Organic Gases.”
- TOG includes low reactivity and low volatility (low vapor pressure)
- TOG profiles have a factor that allow you to convert VOC to TOG.

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- TOG profiles have a factor that allow you to convert VOC to TOG.

Googled and got this from CARB fact sheet

Total Organic Gases (TOG) means "compounds of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate."
The Electronic Code of Federal Register where the VOC information is available under Title 40 → Chapter I → Subchapter C → Part 51 → Subpart F → § 51.100:

http://www.ecfr.gov/cgi-bin/text-idx?SID=b77fd17464a534c225c8557b5ed4a469&node=40:2.0.1.1.2.3.8.1&rgn=div8

EPA’s Regulatory Definition of VOC
List of Compounds exempt from the Definition

(1) Includes any such organic compound other than the following, which have been determined to have negligible photochemical reactivity: Methane, ethane, methane chloride (chloromethane), 1,1,1-trichloro-1,2,2-trifluoroethane (CFC-113), 1,1-dichloro-1,2,2-trifluoroethane (CFC-115), 1,1,1-trichloro-1,2,2-trifluoroethane (CFC-123), 1,1-dichloro-1-trifluoroethane (CFC-141b), 1-chloro-1,1-difluoroethane (HCFC-142b), 1,1-chloro-1,2,2-trifluoroethane (HFC-123), 1,1,1,2-tetrafluoroethane (HFC-134a), 1,1-dichloro-1-fluoroethane (HFC-141a), 1-chloro-1,1-difluoroethane (HCFC-142a), 1,1-dichloro-1,2-fluoroethane (HFC-134b), 1,1-difluoroethane (HFC-152a), 1,1-dichloro-1,1-fluoroethane (HFC-152a), perfluorotributylamine (PCTFE), cyclo-, branched, or linear, completely methylated silicones, acrylonitrile, polyvinyl chloride (e.g., tetrafluoroethylene), 3,3-dichloro-1,1,2-perfluoropropane (HCFC-225ca), 1,3-dichloro-1,1,2,2-perfluoropropane (HCFC-225cb), 1,1,1,2,2,3,3,3-hexafluoropropane (HFC-236fa), 1,1,1,2,2,3,3,4,4,4-hexafluorobutane (HFC-227ea), ethylene (EPA-161), 1,1,1,2,2-pentafluoropropane (HFC-245fa), 1,1,1,2,3,3-pentafluoropropane (HFC-245fa), 1,1,1,2,3,3,3-hexafluoropropane (HFC-245eb), 1,1,1,2,3,3,4,4,4-heptafluorobutane (HFC-236fa), 1,1,1,2,2,3,3,3-hexafluoropropane (HFC-236fa), 1-chloro-1,1-difluoroethane (HFC-152a), 1,1,1,2,2,3,3,3-heptafluorobutane (HFC-236fa), 1,1,1,2,2,2,2,3,3,3-decafluoro-6-methylhexane (CF3CHCF2CF2CF3OCH2CH2CF3), 1,1,1,2,2,3,3,4,4,4-heptadecafluorobutane (HFC-236fa).
CURRENT STATUS OF VOC EXEMPTION

A VOC is exempt based on $O_3$ formation

List of Exempt VOC:

1. [http://www.ecfr.gov/cgi-bin/text-idx?SID=b77fd17146a534c225c8557b5ed4a469&node=40:2.0.1.1.2.3.8.1&rgn=div8](http://www.ecfr.gov/cgi-bin/text-idx?SID=b77fd17146a534c225c8557b5ed4a469&node=40:2.0.1.1.2.3.8.1&rgn=div8)

2. Currently, we have about 68 exempt chemicals including methane and ethane.

3. More chemicals could be added to the list in future assessments.
Interim Guidance of 2005 (70 FR 54046-54051) is the guiding process to assess the viability of a VOC exemption based on:

1. $K_{OH}$: Reactivity with OH
2. MIR: Maximum Incremental Reactivity to form $O_3$
3. Toxicity and environmental fate
4. GWP: Global Warming Potential
5. ODP: Ozone Depletion Potential
6. Viability as a better substitute for the same end-uses of other chemicals
CONVERTING VOC TO TOG

• Ideally, when modeling you want TOG so you get all the species.
• TOG profiles have a factor that allow you to convert VOC to TOG.
• You can compute it
  \[
  \text{VOC-to-TOG} = \frac{100}{(\text{sum of VOC percent})}
  \]
• These factors are in the GSCNV SMOKE ancillary file.
### EXAMPLE TOG SPECIATION PROFILE
*(selected fields from the Query “View Gas Profiles”)*

<table>
<thead>
<tr>
<th>P_NUM</th>
<th>GAS_PROFILE</th>
<th>CONTROLS</th>
<th>P_DATE</th>
<th>TOTAL</th>
<th>VERSION</th>
<th>VOCtoTOG</th>
<th>SPECIES_ID</th>
<th>SPECIES_PROPERTIES.NAME</th>
<th>WEIGHT_PER</th>
<th>VOC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0051</td>
<td>Flares - Natural Gas</td>
<td>Uncontrolled</td>
<td>05-Jan-89</td>
<td>100</td>
<td>3.2</td>
<td>2</td>
<td>438</td>
<td>Ethane</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>0051</td>
<td>Flares - Natural Gas</td>
<td>Uncontrolled</td>
<td>05-Jan-89</td>
<td>100</td>
<td>3.2</td>
<td>2</td>
<td>465</td>
<td>Formaldehyde</td>
<td>20</td>
<td>YES</td>
</tr>
<tr>
<td>0051</td>
<td>Flares - Natural Gas</td>
<td>Uncontrolled</td>
<td>05-Jan-89</td>
<td>100</td>
<td>3.2</td>
<td>2</td>
<td>529</td>
<td>Methane</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>0051</td>
<td>Flares - Natural Gas</td>
<td>Uncontrolled</td>
<td>05-Jan-89</td>
<td>100</td>
<td>3.2</td>
<td>2</td>
<td>671</td>
<td>Propane</td>
<td>30</td>
<td></td>
</tr>
</tbody>
</table>

**Assume you have 100 lb VOC from Flare – How much propane?**

\[
\text{Mass of Propane} = 100 \text{ lb VOC} \times \left( \frac{30}{100} \right) \left[ \text{lb propane/lb TOG} \right] \times \left[ \frac{2 \text{ lb TOG}}{1 \text{ lb VOC}} \right] = 60 \text{ lb}
\]
QUESTIONS?

Are there any questions on what we've covered so far?
**PM$_{2.5}$ SPECIATION– MODELING PROFILE EXAMPLE**

Model species definitions

<table>
<thead>
<tr>
<th>species name</th>
<th>species description</th>
<th>AE5</th>
<th>AE6</th>
</tr>
</thead>
<tbody>
<tr>
<td>POC</td>
<td>organic carbon</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>PEC</td>
<td>elemental carbon</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>PSO4</td>
<td>sulfate</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>PNO3</td>
<td>nitrate</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>PMFINE</td>
<td>unspeciated PM$_{2.5}$</td>
<td>Y</td>
<td>N</td>
</tr>
<tr>
<td>PNH4</td>
<td>ammonium</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PNCOM</td>
<td>non–carbon organic matter</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PFE</td>
<td>iron</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PAL</td>
<td>aluminum</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PSI</td>
<td>silica</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PTI</td>
<td>titanium</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PCA</td>
<td>calcium</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PMG</td>
<td>magnesium</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PK</td>
<td>potassium</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PMN</td>
<td>manganese</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PNA</td>
<td>sodium</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PCL</td>
<td>chloride</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PH2O</td>
<td>water</td>
<td>N</td>
<td>Y</td>
</tr>
<tr>
<td>PMOTHR</td>
<td>unspeciated PM$_{2.5}$</td>
<td>N</td>
<td>Y</td>
</tr>
</tbody>
</table>

Example modeling speciation profile – AE6

Prescribed Burning – Composite (91109)

<table>
<thead>
<tr>
<th>pollutant</th>
<th>species</th>
<th>massfrac</th>
</tr>
</thead>
<tbody>
<tr>
<td>PM$_{2.5}$</td>
<td>POC</td>
<td>0.5019</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PEC</td>
<td>0.1093</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PSO4</td>
<td>0.0033</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PNO3</td>
<td>0.0107</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PNH4</td>
<td>0.0034</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PAL</td>
<td>0.0005</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PCA</td>
<td>0.0007</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PCL</td>
<td>0.0024</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PFE</td>
<td>0.0004</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PK</td>
<td>0.0014</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PMN</td>
<td>0.0001</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PMOTHR</td>
<td>0.0125</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PNA</td>
<td>0.0014</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PNCOM</td>
<td>0.3513</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PSI</td>
<td>0.0001</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>PTI</td>
<td>0.0007</td>
</tr>
</tbody>
</table>
HOW DO YOU KNOW THE PM$_{2.5}$ PROFILE HAS WHAT YOU NEED?

- Example 1 – 95126 Gas-fired process heater exhaust
  - This one does NOT have what you need for AE6.
- Example 2 – 95462 Composite - Brake Wear
  - This one does.
- Hints
  - But, we did add more recent profiles as well (search for PNCOM or PH20).
SIMPLIFIED PROFILES – PM$_{2.5}$ ONLY

• These are legacy profiles.
• They were used from AE5.
• Their function was superceded by the Speciation Tool.
ASSIGNING SOURCES TO PROFILES – GSREF

• Area & Mobile (county level)
  – You can assign profiles based on SCC and/or country/state/county.
  – Provides no sub-county variation - If you want this, you need your source to be inventoried as a point source.

• Point
  – You can assign based on SCC and/or country/state/county and/or facility, unit, process, release point.

• You can assign a combination of multiple profiles to the same source (10% profile A, 35% profile B, 55% profile C).
Examples of Profile Assignments

SCC 39999999  
“Industrial Process, NEC”  
Assigned to profile 0000 - Overall Average (the King of Defaults)

SCC 2811015001  
Prescribed Forest Burning; Smoldering  
County=Autauga, AL  
Assigned to profile 95421 – Composite Profile - Prescribed fire southeast conifer forest

SCC 2811015001  
Prescribed Forest Burning; Smoldering  
County=Gila, AZ  
Assigned to profile 95422 – Composite Profile - Prescribed fire southwest conifer forest
COMPOSITE PROFILES

- Often, a single study may be too specific to apply to an inventory category or that study has multiple test scenarios or different operators.
- A composite profile combines these data into something usable.
- When using a composite of different profiles, one can take the mean or median of each species from the various profiles being composited.
- When compositing individual SPECIATE profiles, see NOTES for the P_NUMBERS used in the composite.
- Issue: Assigning metadata/ratings to composites
“GAP-FILLING” PROFILES

- This is DIFFERENT from “Compositing” – It is adding missing species to a profile.
- Why? – Some profiles may be missing species that are expected. (Be aware of this when assigning profiles.)
- We can create new profiles by filling in these species (gap-filling) from another profile.

We will need to figure out how to indicate which profiles are gap-filled and how (perhaps using the profile number and the NOTES field).

<table>
<thead>
<tr>
<th>profile</th>
<th>pollutant</th>
<th>missing</th>
</tr>
</thead>
<tbody>
<tr>
<td>95242</td>
<td>Poultry Farm - Hen and Animal Waste</td>
<td>Methane</td>
</tr>
<tr>
<td>95241</td>
<td>Swine Farm and Animal Waste</td>
<td>Ethane</td>
</tr>
<tr>
<td>95240</td>
<td>Beef Cattle Farm and Animal Waste</td>
<td></td>
</tr>
</tbody>
</table>

70% methane, 20% ethane
From profile 0203
(solid waste - animal waste decomposition)

Three new profiles for SPECIATE
QUESTIONS?

Are there any questions on what we've covered so far?
VOC INTEGRATION - CONCEPT

• Integration
  – Process of taking select VOC HAPs from the HAP inventory and speciating the remaining VOC because it is generally believed that the HAP inventory is a better source of HAP emissions than the speciated VOC
  – Want to avoid double counting of HAPs
  – Want to speciate the remaining VOC taking into account HAPs that were removed

• NBAFM chosen as “integration HAPs” in 2014 Modeling Platform
  – Naphthalene, Benzene, Acetaldehyde, Formaldehyde, Methanol
  – These are explicit VOC HAPs in the CB6-CMAQ chemical mechanism.

• NONHAPVOC
  – Remaining VOC after removing explicit VOC HAPs
  – NONHAPVOC = VOC - NBAFM
Integration Steps

VOC+ NBAFM

SMOKE

Compute NONHAPVOC

Convert to NONHAPTOG

SPECIATE NONHAPTOG and map NBAFM to model species

Model species (e.g., ACET, ALD2, ALDX, BENZ, CH4, ETH, ETHA, ETHY, ETOH, FORM, KET, IOLE, ISOP, OLE, PAR, PRPA, TOL, XYLNN, SOAALK, NAPH, BENZ, ALD2, FORM, MEOH, SESQ, TERP)
### Example of Integrated Profile

**No integrate/No use of HAP inventory**

<table>
<thead>
<tr>
<th>pollutant</th>
<th>species</th>
<th>massfrac</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOG</td>
<td>ACET</td>
<td>0.0393</td>
</tr>
<tr>
<td>TOG</td>
<td>ALD2</td>
<td>0.0895</td>
</tr>
<tr>
<td>TOG</td>
<td>ALDX</td>
<td>0.12</td>
</tr>
<tr>
<td>TOG</td>
<td>BENZ</td>
<td>0.0201</td>
</tr>
<tr>
<td>TOG</td>
<td>CH4</td>
<td>0.2163</td>
</tr>
<tr>
<td>TOG</td>
<td>ETH</td>
<td>0.0588</td>
</tr>
<tr>
<td>TOG</td>
<td>ETHA</td>
<td>0.0225</td>
</tr>
<tr>
<td>TOG</td>
<td>ETHY</td>
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</tr>
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<td>TOG</td>
<td>FORM</td>
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<tr>
<td>TOG</td>
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<td>0.014</td>
</tr>
<tr>
<td>TOG</td>
<td>ISOP</td>
<td>0.002153</td>
</tr>
<tr>
<td>TOG</td>
<td>KET</td>
<td>0.006088</td>
</tr>
<tr>
<td>TOG</td>
<td>NAPH</td>
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<tr>
<td>TOG</td>
<td>NVOL</td>
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</tr>
<tr>
<td>TOG</td>
<td>OLE</td>
<td>0.0331</td>
</tr>
<tr>
<td>TOG</td>
<td>PAR</td>
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</tr>
<tr>
<td>TOG</td>
<td>PRPA</td>
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</tr>
<tr>
<td>TOG</td>
<td>TOL</td>
<td>0.0798</td>
</tr>
<tr>
<td>TOG</td>
<td>UNR</td>
<td>0.0437</td>
</tr>
<tr>
<td>TOG</td>
<td>XYLMN</td>
<td>0.0203</td>
</tr>
</tbody>
</table>

**Integrate**

- Fireplace wood combustion - pine wood - 4642

<table>
<thead>
<tr>
<th>pollutant</th>
<th>species</th>
<th>massfrac</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOG</td>
<td>ACET</td>
<td>0.0481</td>
</tr>
<tr>
<td>TOG</td>
<td>ALD2</td>
<td>0.1468</td>
</tr>
<tr>
<td>TOG</td>
<td>CH4</td>
<td>0.2647</td>
</tr>
<tr>
<td>TOG</td>
<td>ETH</td>
<td>0.0719</td>
</tr>
<tr>
<td>TOG</td>
<td>ETHA</td>
<td>0.0275</td>
</tr>
<tr>
<td>TOG</td>
<td>ETHY</td>
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</tr>
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<td>TOG</td>
<td>IOLE</td>
<td>0.0172</td>
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</tr>
<tr>
<td>TOG</td>
<td>XYLMN</td>
<td>0.0248</td>
</tr>
</tbody>
</table>
WHY NOT INTEGRATE A SOURCE

• Point sources –
  – The State reports HAPs at a different process level than where they reported VOCs. So HAP is at the facility but there is no VOC at that process level to do the subtraction.
  – There is misalignment of VOC and HAP even though both are reported.

• Nonpoint sources –
  – There are no inventory NBAFM emissions at the source.
    • If there really shouldn’t be, then remove NBAFM from the profile.
  – NBAFM mass > VOC
TWO APPROACHES TO NO-INTEGRATE

1) Don’t use any HAPs from the HAP inventory.
   – Use the profile to generate all model species - HAPs and nonHAPs.

2) Assume HAP inventory is better than speciation:
   – Use the HAP inventory (NBAFM) for model species
   – Create TOG profiles that drop the mass of NBAFM.
   – TOG profiles will have less than 100% of mass if the profile has NBAFM.
<table>
<thead>
<tr>
<th>Platform Sector *</th>
<th>Approach for Integrating</th>
</tr>
</thead>
<tbody>
<tr>
<td>ptegu</td>
<td>No integration</td>
</tr>
<tr>
<td>ptnonipm</td>
<td>No integration</td>
</tr>
<tr>
<td>ptfire</td>
<td>No integration</td>
</tr>
<tr>
<td>othafdust</td>
<td>No integration</td>
</tr>
<tr>
<td>othar</td>
<td>No integration</td>
</tr>
<tr>
<td>othon</td>
<td>No integration</td>
</tr>
<tr>
<td>ag</td>
<td>N/A – sector contains no VOC</td>
</tr>
<tr>
<td>afdust</td>
<td>N/A – sector contains no VOC</td>
</tr>
<tr>
<td>biog</td>
<td>N/A – contains specific VOC model species</td>
</tr>
<tr>
<td>nonpt</td>
<td>Partial integration (NBAFM)</td>
</tr>
<tr>
<td>np_oilgas</td>
<td>Partial integration (NBAFM)</td>
</tr>
<tr>
<td>pt_oilgas</td>
<td>No integration</td>
</tr>
<tr>
<td>rwc</td>
<td>Partial integration (NBAFM)</td>
</tr>
<tr>
<td>nonroad</td>
<td>Full integration (calculated in MOVES)</td>
</tr>
<tr>
<td>c1c2rail</td>
<td>Partial integration (NBAFM)</td>
</tr>
<tr>
<td>othpt</td>
<td>Partial integration (NBAFM)</td>
</tr>
<tr>
<td>c3marine</td>
<td>Partial integration (NBAFM)</td>
</tr>
<tr>
<td>onroad</td>
<td>Full integration (calculated in the MOVES model)*</td>
</tr>
</tbody>
</table>

*See Modeling Platform technical support document for sector descriptions *(https://www.epa.gov/air-emissions-modeling).*
ONROAD SPECIATION

• MOVES2014 does speciation within MOVES for onroad sources
  – Uses inputs from the Speciation Tool
  – Different profiles for different vehicle model years, regulatory classes, fuel types, and emission processes
  – Previously used COMBO files or weighted profiles to approximate, but was a coarse approach

• PM$_{2.5}$
  – AE6 species come directly from MOVES (in mass).

• VOC
  – 16 pollutants are explicit, i.e. integrated.
  – Model species (moles) and inventory pollutants (mass) come directly from MOVES.
  – Need to specify chemical mechanism in the MOVES run
ONROAD SPECIATION IN MOVES

- **TOG**
  - Acetaldehyde
  - Formaldehyde
  - Benzene
  - Other individual toxics to be integrated

- **TOG** – integrated toxics (NONHAPTOG)

- **MOVES**
  - Speciation of NONHAPTOG with renormalized profile
  - Mapping of each integrated toxic
  - Summed CMAQ model species

- **Speciate Tool**
  - New CMAQ model species profiles renormalized without integrated toxics
  - Chemical mechanism for lumping measured species into CMAQ model species

- **OTAQ**
  - Speciation profiles with all measured species (e.g., based on EPAct data)

- **OAQPS**

- **SMOKE**

- **CMAQ**
NONROAD SPECIATION

• MOVES2014a provides nonroad emissions that are semi-speciated.
• Also provides individual HAPs - benzene, toluene, etc.
• And provides the remainder along with the profile code
  – e.g. NONHAPTOG_4452
    • NONHAPTOG is the difference between TOG and the sum of the HAPs.
    • 4452 is the profile code to use for NONHAPTOG.
  – Unlike onroad, the speciation is done in SMOKE.
  – Approach allows application of new chemical mechanisms in SMOKE without re-running MOVES.
COMBINATION PROFILES

• SMOKE now has a method of combining two or more speciation profiles for a specific SCC/FIPS.

• Examples:
  – Combine E0 and E10 fuel profiles
  – Combine flare profile with oil & gas process profile
COMBINATION PROFILES (cont.)

- Combine flare profile with oil & gas process profile
  - Based on output from the Oil and Gas Tool (software & data that is used to develop EPA Oil and Gas estimates for the NEI)

<table>
<thead>
<tr>
<th>SCC</th>
<th>PROFILE CODE</th>
<th>POLLUTANT</th>
<th>FIPS</th>
<th>FACTOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>2310021010</td>
<td>SWFLA_R</td>
<td>NONHAPVOC</td>
<td>56045</td>
<td>0.0456</td>
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<tr>
<td>(Oil &amp; Gas:On-Shore Gas Prod;Cond. Storage Tank)</td>
<td>(Oil and Gas -SW Wyoming Basin Flash Gas Composition for Condensate Tanks)</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>2310021010</td>
<td>FLR99</td>
<td>NONHAPVOC</td>
<td>56045</td>
<td>0.9544</td>
</tr>
<tr>
<td>(Natural Gas Flare Profile with DRE &gt;98%)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
QUESTIONS?

Are there any questions on what we've covered so far?
SPECIATE DATA GAPS AND FUTURE PLANS
DATA GAP ANALYSIS – AN ONGOING PROCESS

• Goal: Every inventory source is assigned to a good profile that best fits its source category.
  – Are assignments appropriate?
  – How good are the available profiles?
  – What research is needed to meet the goal?
• Past Efforts: Analyses leading toward 2011 NEI Modeling Platform improvements
• Current Efforts: Gaps and needs analysis
PAST EFFORT: 2008 NEI (2013 VOLUNTEER)

- Found low-hanging fruit in the 2008 NEI Platform
- Reviewed VOC emission profiles applied to SCCs that are the largest sources of VOCs
- Identified opportunities for Pulp & Paper
  - Over 200 source operations linked to generic profiles
  - Profile 1185: Coal Fired Boiler – Industrial linked to eight largest operations (43 of 144 kTpy)
- The 2008 NEI had > 500 kTpy of TOG speciated with the default profile (0000).
IMPACT OF MISMATCHED PROFILES

Chemical Composition: Coal-Fired Boiler - Industrial vs. Pulp & Paper Mills - Kraft Mill Bleach Plants (wt.%)
PAST EFFORTS: 2011 NEI MODELING PLATFORM IMPROVEMENTS

- EPA developed and applied appropriate composite source profiles for the Pulp & Paper and Chemical Manufacturing sectors from SPECIATE emissions profiles.
- Pulp and Paper: 97 of 121 kTpy (80%) reassigned from profiles 0000 and 1185
- Chemical Manufacturing: 20 of 90 kTpy (22%) reassigned from profile 0000
- Composite profiles were added to SPECIATE 4.5.
Assessment of Important SPECIATE Profiles in EPA’s Emissions Modeling Platform and Current Data Gaps

• Casey Bray, NC State & EPA/ORD Intern
• Goals
  – Elucidate profiles/categories of most importance for air quality modeling purposes
  – Evaluate current profiles
  – Identify and articulate research needs

Come to Casey’s talk FRIDAY @ 8 am
Major PM$_{2.5}$ Profiles (% of mass assigned in 2014 EPA modeling platform)* - from Bray’s work

*excludes emissions from the onroad mobile sector

International Emissions Inventory Conference, Baltimore, MD, August 15, 2017
VOC PROFILES – REGIONAL DIFFERENCES*
(From Bray)

Southwest: UT, CO, AZ, NM
Northeast: ME, NH, VT, RI, CT, NY, NJ, DE, PA, MD

953,352 tons/year
- Crude Oil Storage Tanks 12%
- Oil and Gas Production - Glycol Dehydrator, Uinta Basin 3%
- Oil and Gas -Permian Basin Produced Gas Composition for Non-CBM Wells 4%
- Oil and Natural Gas Production - Condensate Tanks 5%
- Oil and Gas -Production - Oil Tank Vent Gas, Uinta Basin 6%
- Oil and Gas -South San Juan Basin Produced Gas Composition from Non-CBM Gas Wells 7%
- Prescribed fire southwest conifer forest 12%

823,885 tons/year
- Natural Gas Production 11%
- Other 51%
- Household Products 4%
- Graphic Arts - (Printing) 7%
- Solvents And Coating Related Products 5%
- Gasoline Headspace Vapor - 0% Ethanol (EO) 5%
- Architectural Coatings: Solvent Borne and water borne 7%
- Fireplace wood combustion - pine wood 10%

*excludes emissions from the onroad and nonroad mobile sectors
THE SPECIATE WORKGROUP AND FUTURE PLANS

- EPA’s SPECIATE Workgroup
- Modelers tell us what is important
- Ongoing literature searches
- Peer-reviewed journal articles preferred
- The “Master List” of references
- Needs Analysis Project - data gaps
- Please let us know if you’ve got data that could be added!
FUTURE SPECIATE PLANS

• Develop Standard Operating Procedure (SOP) for SPECIATE Profile Selection, Collection, and Entry
  – Allow In-House Processing of Profiles
  – Improve Documentation of Metrics and Processes
  – Identify Key Metrics for Quality Profiles
  – Formalize Prioritization Process

• ACCESS database structure improvements (including use of forms to add to profiles)

• Continue Oil and Natural Gas Emissions profiles started with Region 8 RARE

• Comparison of Emissions Inventory HAPs vs. those from speciated VOC to improve VOC/HAP integration
THE SPECIATION TOOL
ACKNOWLEDGEMENTS

- Greg Yarwood – Ramboll Environ
- Madeleine Strum EPA/OAQPS
- Zac Adelman – Institute for the Environment – UNC
- Michele Jimenez – Ramboll Environ
DEFINITIONS

- AQM – Air Quality Model
  - CMAQ, CAMx, etc.

- Model Species – Model species are used in the AQM
  - e.g., OLE, PAR, etc. in CB mechanisms

- Profile – list of mass fractions (or wt. %) of compounds

- Organic Compounds – Organic compounds included in SPECIATE profiles
  - e.g., 1-Methylcyclopentene, isomers of hexane, etc.

- SPECIATE – EPA’s SPECIATE database

- SPTOOL – The stand-alone Speciation Tool
Atmospheric chemistry consists of millions of reactions among many thousands of chemical compounds.

AQM models use a condensed chemical mechanism with a manageable number of reactions and model species:
- CB05, CB6r2, CB6r4
- SAPRC99, SAPRC07, SAPRC11
- RACM2
- CRIv2r5
- etc.
ATMOSPHERIC CHEMISTRY IN AQM

- An integral part of any condensed chemical mechanism is the assignment from real organic compounds to model species of the condensed mechanism.

- Chemical mechanism provides a basis for computer modeling studies of ozone, particulate matter (PM), visibility, acid deposition and air toxics issues.
PREPARING EMISSIONS FOR MODELING

- Emissions processing converts from inventory pollutants to chemical mechanism model species, e.g., total VOC converted to CB OLE, PAR etc.
  - Emissions processing step referred to as ‘speciation’

- AQMs require emitted gaseous species in molar and PM species in mass units
SMOKE ancillary files GSPRO and GSCNV are used for speciation.

GSPRO contains factors to speciate inventory pollutants:
- Split Factor: numerator for mole-based speciation
- Divisor: denominator for the mole-based speciation
- Split Factor/Divisor = moles of model species per ton of TOG
- For PM, divisor = 1

GSCNV contains VOC-to-TOG conversion factors to convert inventory VOC (or ROG) to TOG to apply TOG-based speciation profiles.
SPECIATION STEPS IN MODELING TOOLS

- Speciation Tool: creates SMOKE ancillary files GSPRO and GSCNV
  - Uses SPECIATE profiles
  - Uses mechanism-specific chemical mapping, e.g., CB6 different from CB05

- SMOKE: assigns profiles to sources and uses ancillary files GSPRO and GSCNV to compute AQM emission files

- Emissions Modeling Framework: can be used as an interface for managing inventories and related data (profiles), and interface for running the Speciation Tool and SMOKE
SPECIATION FOR AQ MODELING

SPECIATE profiles → Speciation Tool → Mechanism-Specific Speciation Profiles (GSPRO and GSCNV)

Assign Chemical Mechanism-specific Speciation Profile(s) to source based on process (SCC), location (GSREF)

Multiply Inventory emissions by profile factor to get emissions of AQM species: moles for gases, mass for particulates

Emissions Source for Inventory Pollutant—e.g. VOC, PM2.5

Mechanism-Specific chemical mapping

ethane → ETHA
ethene → ETH
propene → OLE
butane → PAR
pentane → ....
## SMOKE GSPRO and GSCNV files

### GSPRO sample profile

<table>
<thead>
<tr>
<th>Speciation profile number</th>
<th>Pollutant ID (name)</th>
<th>Species ID (name)</th>
<th>Split factor</th>
<th>Divisor</th>
<th>Mass Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>0051</td>
<td>TOG</td>
<td>CH4</td>
<td>0.2</td>
<td>16.042</td>
<td>0.2</td>
</tr>
<tr>
<td>0051</td>
<td>TOG</td>
<td>ETHA</td>
<td>0.3</td>
<td>30.069</td>
<td>0.3</td>
</tr>
<tr>
<td>0051</td>
<td>TOG</td>
<td>FORM</td>
<td>0.2</td>
<td>30.026</td>
<td>0.2</td>
</tr>
<tr>
<td>0051</td>
<td>TOG</td>
<td>PRPA</td>
<td>0.3</td>
<td>44.096</td>
<td>0.3</td>
</tr>
</tbody>
</table>

### GSCNV sample profile

<table>
<thead>
<tr>
<th>Name of pollutant converting from</th>
<th>Name of pollutant converting to</th>
<th>Speciation profile code</th>
<th>Conversion factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>VOC</td>
<td>TOG</td>
<td>0051</td>
<td>2</td>
</tr>
</tbody>
</table>
SPTOOL is a stand-alone tool that was developed to generate the GSPRO and GSCNV ancillary data SMOKE uses for speciation.

SPTOOL implemented using open source PostgreSQL database and Perl interface.

SPTOOL SOFTWARE REQUIREMENTS

- PostgreSQL can be downloaded from [http://www.postgresql.org](http://www.postgresql.org)

- Perl and the database drivers can be downloaded from [http://www.perl.com](http://www.perl.com)

- User must have database create privileges in PostgreSQL to run the Speciation Tool
1. Create a Speciation Tool directory

2. Extract the Speciation Tool installation files
   a) Change to the Speciation Tool directory
   b) Copy the Speciation Tool package to this directory
   c) Extract the zipped file

3. Verify required software packages are available.
   a) Run ./spool_reqd_checks.sh

4. Set environment variables
   a) Edit Assigns.sptool; Set SPTOOL_HOME
   b) Source Assigns.sptool
5. Initialize the Speciation Tool database
   a) Execute ./init_sptooldb_v4.0.csh

6. Execute the provided test case
   a) Change to the run directory; cd /run
   b) Run ./test_all.job

7. Review results
   a) Change to output directory; cd ../output
SPTOOL INSTALLATION

- Create SPTOOL home directory with any valid directory name

- Copy the installation file to home directory and extract
  - `tar -xvzf tar_Speciation_Tool_v4.0_11jan2017.tgz`

- Run script to check for required software and verify user PostgreSQL authorizations
  - Run `sptool_reqd_checks.sh`
Speciation Tool must be initialized prior to making any runs. Initialization steps include:

- Update and source the assigns file `Assigns.sptool`
  - Set the home directory
- Run the initialization script
  - `./init_sptooldb_v4.0.csh`

What happens during the SPTOOL initialization?

- Create database, set permissions, create the *shared* schema and table definitions for the tool data, and import data to the *shared* schema.
Initialization creates the sptoolv4_0 PostgreSQL database with schema shared. Each run will create an additional named schema based on the user specs.
Assigns.sptool file can be found in the top level SPTOOL home directory
  - Update and source the Assigns.sptool file

Assigns file sets environment variables that are required for the database initialization
  - SPTOOL home directory
  - Database name
  - File names of input speciation data
SPTOOL INPUT FILES

- PROFILES_GAS – gas profile description and documentation

- WEIGHTS_GAS – organic gas mass fraction profiles (in weight percent)

- PROFILES_PM – PM profile description and historical information

- WEIGHTS_PM – PM mass fraction profiles (in weight percent)
SPTOOL INPUT FILES

- SPECIES_PROPERTIES – properties of individual organic compound, including molecular weight
- MECHANISM – mechanism mappings
  - moles model species / mole organic compound
- MECHANISMPM – PM2.5 mechanism mappings
  - mass model species / mass PM2.5
- CARBONS – number of carbon atoms in each model species
SPTOOL OUTPUT FILES

- SPLITS_OUT (GSPRO) – SMOKE speciation profiles
  - Split Factor: numerator for mole-based speciation
  - Divisor: denominator for the mole-based speciation
  - Split Factor/Divisor = moles of model species per ton of TOG
  - For PM, divisor = 1

- CNV_OUT (GSCNV) – SMOKE VOC-to-TOG conversion factor file
RUNNING SPTOOL

- First source the Assigns.sptool file to set the required environment variables SPTOOL_HOME and SPTOOL_DB

- SPTOOL must be initialized prior to making any runs

- Run script – The perl program run_sptool.pl creates output SMOKE profile files – GSPRO and GSCNV

- The run script requires the SPTOOL database name, a name to uniquely label the database schema, and a run control file name as input
  - perl $SPTOOL_SRC_HOME/run_sptool.pl $SPTOOL_DB cmaq_cb6_criteria RUNCTL
SPTOOL RUN CONTROL FILE

- The run control file indicates run parameters and run-specific data files required for the Speciation Tool run.

- The format of the run control file is `<keyword>, <option>`
  Examples,
  MECH_BASIS, CB05
  OUTPUT, VOC
  RUN_TYPE, CRITERIA
  AQM, CAMX
RUN PARAMETERS

- **MECH_BASIS** – select chemical mechanism to use

- **OUTPUT** – select which output profiles to generate. Options are “VOC” for gas species and “PM” for particulates

- **RUN_TYPE** – The RUN_TYPE options are: CRITERIA, INTEGRATE, NOINTEGRATE, HAPLIST, and VBS

- **AQM** – this parameter selects model–correct species names for output files

- **TOLERANCE** – specifies acceptable deviation from 100% for the sum of weight percentages (default is 5%)
What happens when an organic compound used by a profile lacks a defined molecular weight?

- Any detailed organic compound with an undefined molecular weight is dropped from the profile because a molecular weight is required to compute splits factors. Dropped mass fraction due to missing molecular weights may take the profile sum outside the selected tolerance, causing the profile to be dropped. This problem should be resolved by specifying missing molecular weights in the species properties.
What happens when an organic compound used by a profile lacks an assignment in the mechanism mapping?
- SPTOOL issues a warning and the compound is assigned to UNK

When does SPTOOL renormalize a profile?
- If the sum of mass fractions for a profile is not 100%, and nothing is done to correct the profile, subsequent SMOKE processing will not conserve mass. SPTOOL renormalizes all gas profiles whose sum is within the tolerance thereby preserving VOC mass. Profiles outside the tolerance are dropped and a warning is issued.
- For the AE6 PM profiles, when sum of AE6 PM species is less than 100%, the remaining mass gets assigned to PMOTH (=100% – sum of AE6). When the sum is greater than 100%, the profiles are dropped with a warning.
Carbon Bond (CB) mechanisms represent some organic compounds explicitly
- e.g., ethane (ETHA), ethene (ETH), ethyne (ETHY), etc.
- more explicit species in CB6 than CB05

CB mechanisms lump other organic compounds according to carbon bonding type
- alkanes (paraffins) to PAR
- alkenes (olefins) to OLE or IOLE
- aromatics to TOL or XYL

example: propene: \[ \text{PAR} + \text{OLE} \]
### Example profile (first two columns) of organic compounds

### CB6 mapping in third column

### Right column shows CB6 model species per mole of TOG emitted

<table>
<thead>
<tr>
<th>Organic Compound</th>
<th>Mole Fraction</th>
<th>CB6 Mapping (mol/mol)</th>
<th>CB6 Profile (mol/mol TOG)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ethane</td>
<td>0.2</td>
<td>1 ETHA</td>
<td>0.2 ETHA</td>
</tr>
<tr>
<td>butane</td>
<td>0.1</td>
<td>4 PAR</td>
<td>0.4 PAR</td>
</tr>
<tr>
<td>ethene</td>
<td>0.05</td>
<td>1 ETH</td>
<td>0.05 ETH</td>
</tr>
<tr>
<td>propene</td>
<td>0.1</td>
<td>1 PAR + 1 OLE</td>
<td>0.1 PAR + 0.1 OLE</td>
</tr>
<tr>
<td>formaldehyde</td>
<td>0.1</td>
<td>1 FORM</td>
<td>0.1 FORM</td>
</tr>
<tr>
<td>acetaldehyde</td>
<td>0.15</td>
<td>1 ALD2</td>
<td>0.15 ALD2</td>
</tr>
<tr>
<td>toluene</td>
<td>0.1</td>
<td>1 TOL</td>
<td>0.1 TOL</td>
</tr>
<tr>
<td>ethylbenzene</td>
<td>0.05</td>
<td>1 PAR + 1 TOL</td>
<td>0.05 PAR + 0.05 TOL</td>
</tr>
<tr>
<td>xylene</td>
<td>0.15</td>
<td>1 XYL</td>
<td>0.15 XYL</td>
</tr>
<tr>
<td>TOG</td>
<td>1.0</td>
<td></td>
<td>0.2 ETHA + 0.55 PAR + 0.05 ETH + 0.1 OLE + 0.1 FORM + 0.15 ALD2 + 0.15 TOL + 0.05 XYL</td>
</tr>
</tbody>
</table>