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Speciation Methods in the U.S. EPA's Modeling Platforms

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The National Emissions Inventory

The National Emissions Inventory

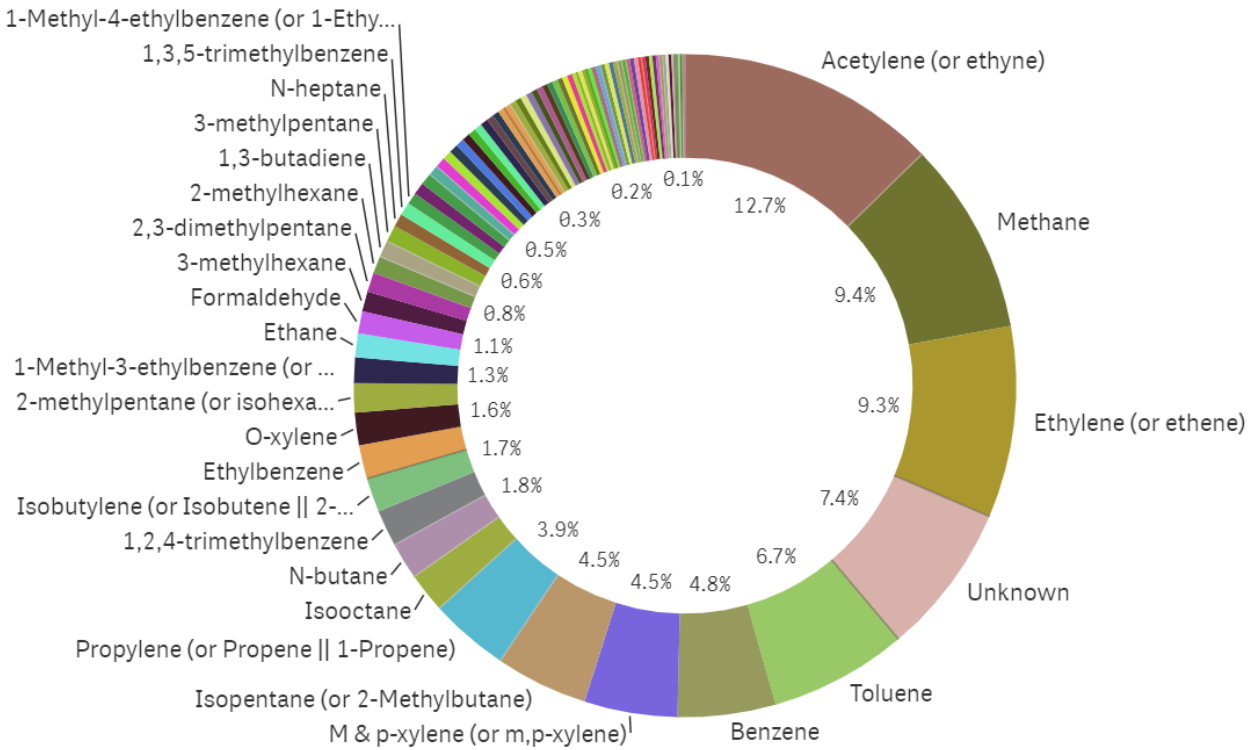
- The NEI is a national compilation of air emission estimates of criteria air pollutants (CAPs) and their precursors, and hazardous air pollutants (HAP).

CAPs in the NEI	CAP Precursors in the NEI	HAPs in the NEI
$PM_{2.5}$, PM_{10}, Carbon Monoxide, Lead, Sulfur Dioxide	Ammonia (precursor to PM), **Volatile Organic Compounds** (precursor to ozone and PM), Nitrogen Oxides (precursor to ozone and PM)	Benzene, Manganese, + 187 others

- **Particulate matter** and **volatile organic compounds** are not homogenous → composed of chemically distinct compounds.
  - Accurately speciating $PM_{2.5}$ and VOC is essential for source attribution research, evaluating photochemical models, and atmospheric chemistry/transport processes.
- Most HAPs are speciated $PM_{2.5}$ or VOC. For example, lead and benzene, respectively.

$PM_{2.5}$ and VOC Speciation

- The NEI includes primary $PM_{2.5}$ and select speciated $PM_{2.5}$ components. It also houses total VOC and VOC-HAPs.
- Photochemical models transport and deposit speciated $PM_{2.5}$. These models also require VOC emissions to be speciated.
- Compared to $PM_{2.5}$ speciation, VOC speciation for air quality modeling features greater chemical resolution.



Lawn Mowers – 4 Stroke (Profile 4738)
This is an explicit profile provided by SPECIATE

Inventory to Modeling Platform

- A modeling platform consists of all the emissions inventories and ancillary data files (e.g., profile-to-SCC cross reference files) used for emissions modeling, as well as the meteorological, initial condition, and boundary condition files needed to run the air quality model.

Example: **100 TPY VOC** → **50 TPY ETOH, 50 TPY ALD2**

HAP Treatment in Modeling Platforms

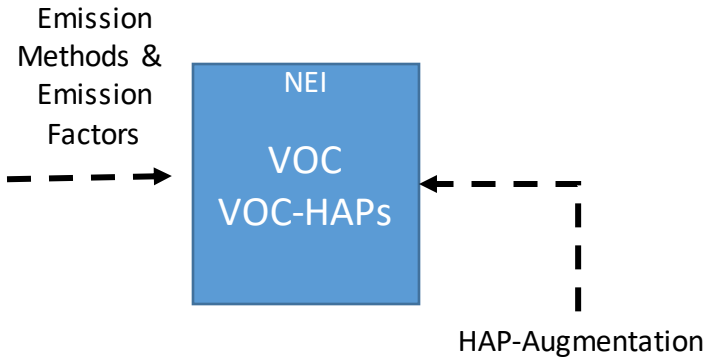
- Recall that HAPs are in the NEI and often components of VOC or $PM_{2.5}$. These emissions might better reflect what is emitted than what is in a speciation profile. As such, these speciated components are often incorporated into a modeling platform.
  - Integrate, HAP-use: HAPs from NEI are used, HAP mass is subtracted from VOC mass, residual VOC mass is speciated using a renormalized profile.
  - No-Integrate, HAP-use: HAPs from NEI are used, HAP mass is subtracted from VOC mass, residual VOC mass is speciated using a non-renormalized profile.
  - Criteria: HAPs are "generated" using a speciation profile.
- The method utilized when developing a modeling platform is sector specific.

Types of Modeling Platforms

- Currently, the EPA generates two types of modeling platforms, (1) HAP-CAP and (2) CAP-only. The speciation methods for these two platform types often overlap and vary by sector:

	Integrate, HAP-use	**No-Integrate, HAP-use**	**Criteria**
HAP-CAP	Onroad, Nonroad, Nonpoint	Point, Nonpoint (when HAP > VOC or no emissions of integrated species)	n/a
CAP-Only	Onroad, Nonroad, Nonpoint	n/a	Point, Nonpoint (when HAP > VOC or no emissions of integrated species)

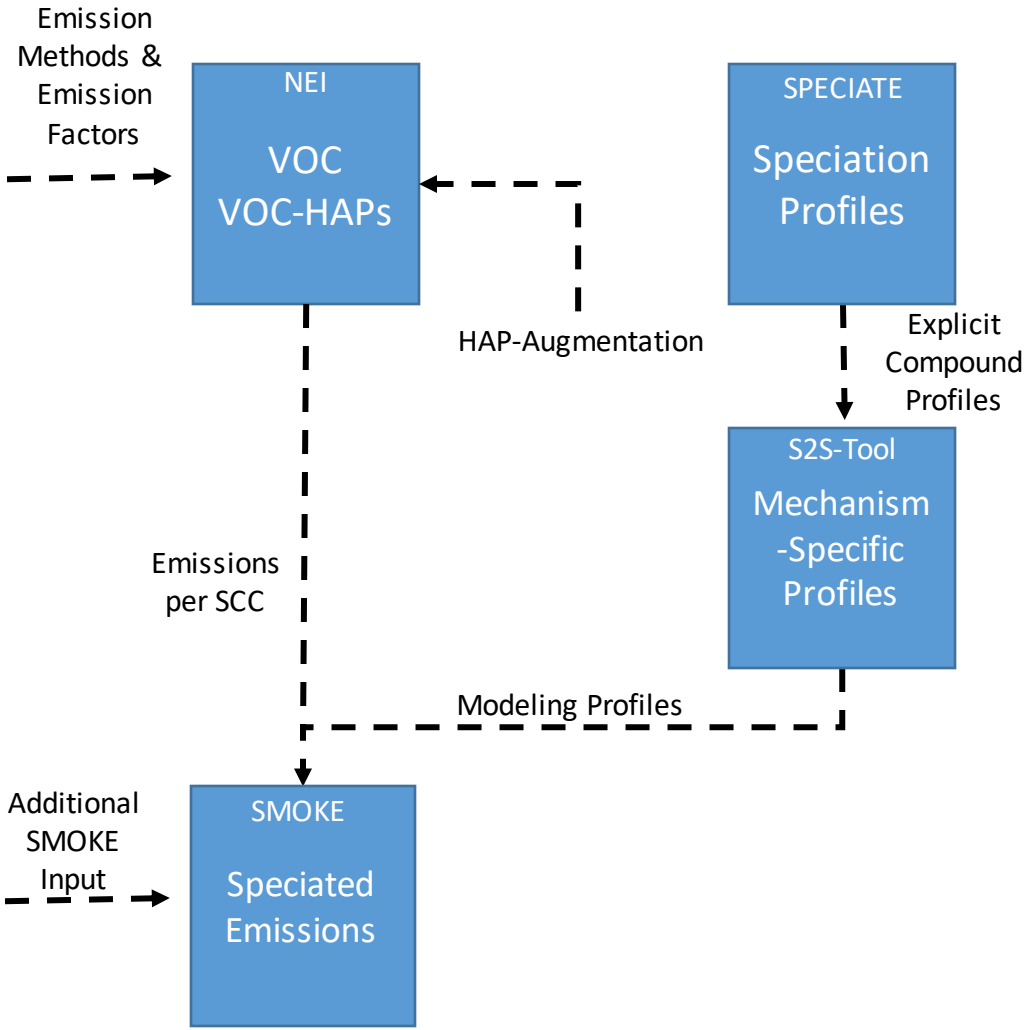
VOC Speciation Tools at the EPA: Overview



The National Emissions Inventory

- EIAG incrementally updates methods to better characterize emissions in the NEI.
- Both the VOC and VOC-HAPs are housed in the NEI and used in modeling platforms.
- NEI VOC-HAP emissions are largely generated using "HAP-augmentation" in EIS (nonpoint, point), provided by MOVES (mobile), or submitted/added from the Toxics Release Inventory (point).

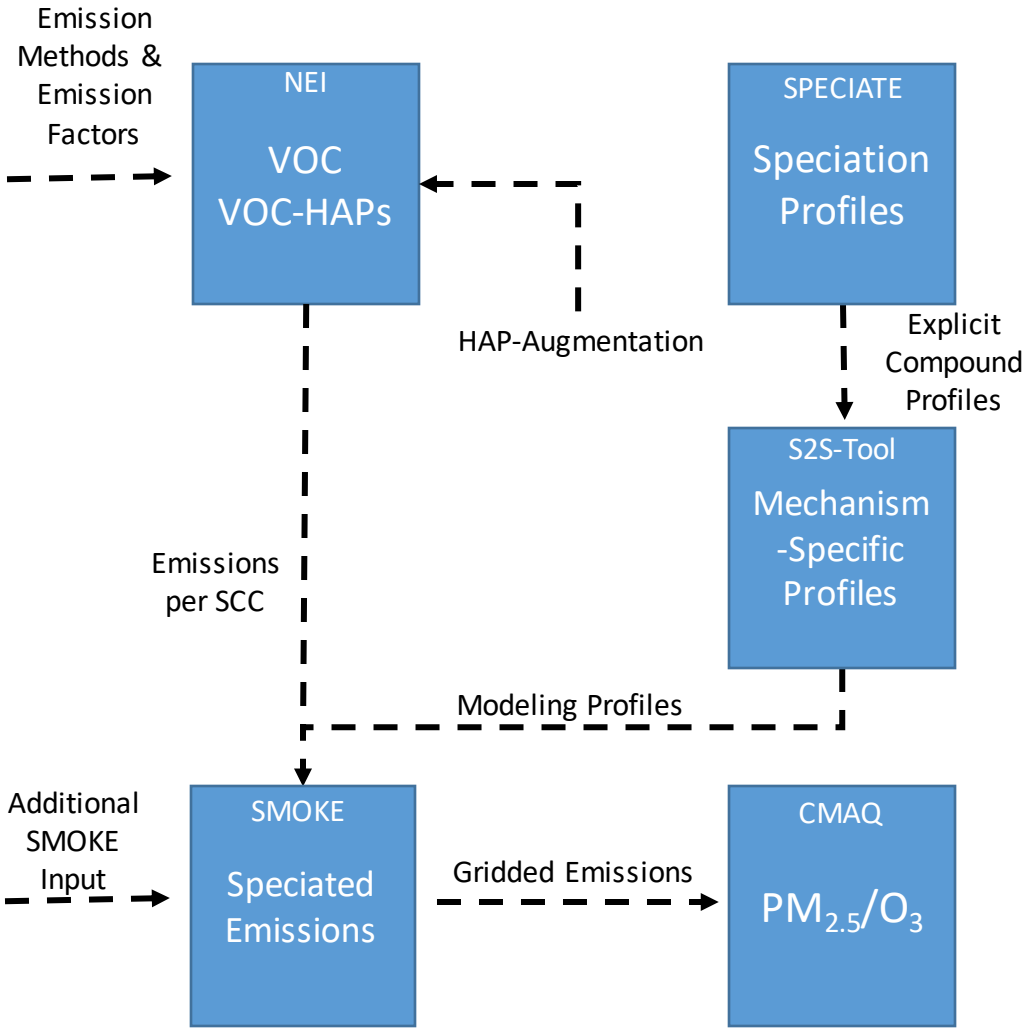
VOC Speciation Tools at the EPA: Overview



Modeling Platform VOC Speciation

- SPECIATE houses explicit VOC speciation profiles for various emissions sources.
- The S2S-Tool translates these explicit VOC profiles into chemical mechanism-specific profiles.
  - S2S: SPECIATE-to-SMOKE
  - Formerly done by the Speciation Tool.
  - e.g., translates octane to 8 PAR and ethanol to 1 ETOH for CB6R5; model species needed for CMAQ and CAMx.
- SMOKE combines data from the NEI, S2S-Tool, and other sources to generate gridded, speciated photochemical modeling files.

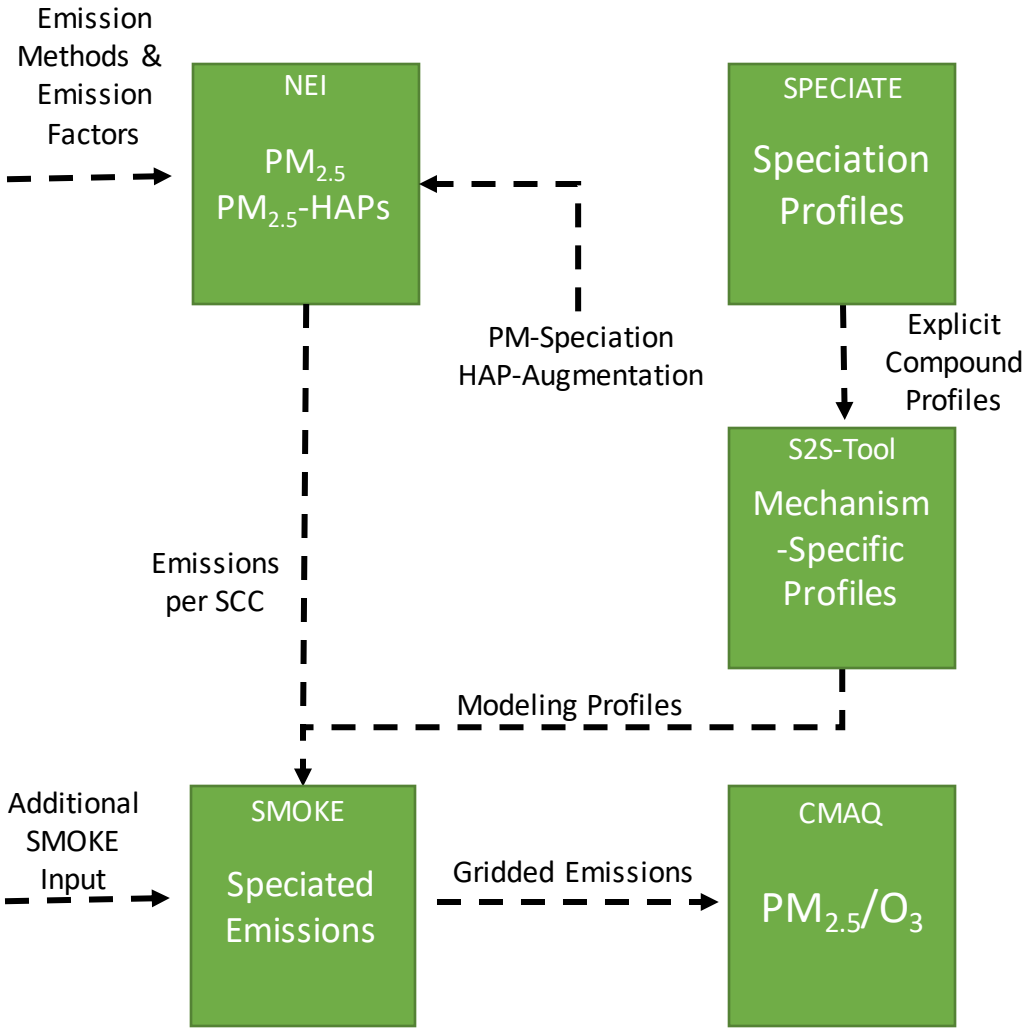
VOC Speciation Tools at the EPA: Overview



Photochemical Modeling

- Gridded emission files generated by SMOKE are used in photochemical models, such as CMAQ or CAMx, to simulate air quality.
  - Different chemical-mechanisms simulate the chemistry of the atmosphere.

$PM_{2.5}$ Speciation Tools at the EPA: Overview



- Methods are conceptually the same as VOC speciation.
- PM-Speciation is performed in EIS to generate a broad estimate of speciated $PM_{2.5}$ emissions (EC, OC, SO_4, NO_3, PMOTHR).

HAP-Augmentation

CAPs (e.g., VOC) are used to estimate HAP emissions within EIS. EPA uses a similar process is performed for PM-Speciation for the NEI.

Example HAP-Augmentation profile:

Augmentation Type	Profile Name	Input Pollutant Code	Input Pollutant Description	Output Pollutant Code	Output Pollutant Description	Multiplication Factor	SCC Assignment	SCC Description Level 1	SCC Description Level 2	SCC Description Level 3
HAP	2460100000_HAP-VOC	VOC	Volatile Organic Compounds	108883	Toluene	0.00157	2460100000	Solvent Utilization	Miscellaneous Non-industrial: Consumer and Commercial	All Personal Care Products
HAP	2460100000_HAP-VOC	VOC	Volatile Organic Compounds	111422	Diethanolamine	0.00113	2460100000	Solvent Utilization	Miscellaneous Non-industrial: Consumer and Commercial	All Personal Care Products
HAP	2460100000_HAP-VOC	VOC	Volatile Organic Compounds	122996	Phenyl Cellosolve	0.00103	2460100000	Solvent Utilization	Miscellaneous Non-industrial: Consumer and Commercial	All Personal Care Products
HAP	2460100000_HAP-VOC	VOC	Volatile Organic Compounds	171	Glycol Ethers	0.000659	2460100000	Solvent Utilization	Miscellaneous Non-industrial: Consumer and Commercial	All Personal Care Products
HAP	2460100000_HAP-VOC	VOC	Volatile Organic Compounds	110543	Hexane	0.00054	2460100000	Solvent Utilization	Miscellaneous Non-industrial: Consumer and Commercial	All Personal Care Products
HAP	2460100000_HAP-VOC	VOC	Volatile Organic Compounds	85449	Phthalic Anhydride	0.00027	2460100000	Solvent Utilization	Miscellaneous Non-industrial: Consumer and Commercial	All Personal Care Products

SPECIATE

- SPECIATE is an Access database that provides source-specific profiles of organic gases, $PM_{2.5}$, and mercury.
- The database can be downloaded or explored via a web-based tool.
- SPECIATE v5.3 soon to be published.
  - 50 new profiles were added to the database; total database is now 6,895 profiles.

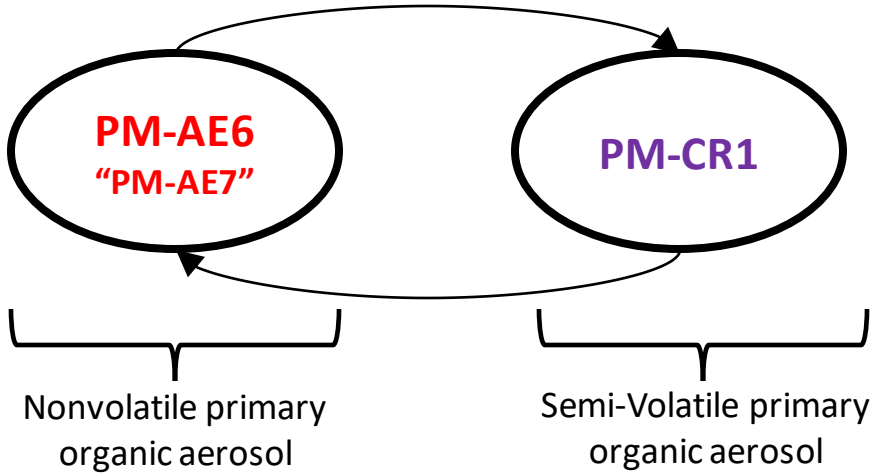
S2S-Tool

- U.S. EPA's S2S-Tool generates speciation input files (GSPRO, GSCNV) for SMOKE.
- Recently, v2.0 of the Tool was published.
  - Available via the USEPA's GitHub.
- Prior to the S2S-Tool's development, we used the "Speciation Tool." Advantages of the S2S-Tool include:
  - Developed/maintained in-house, Python-based, includes "mechanism mapping" scripts, generates semi-volatile primary organic aerosol profiles, generates files to allow speciation outside of MOVES.
- S2S-Tool meets the needs for:
  - Various modeling platform speciation setups, integrated HAP treatments, treatments of primary organic aerosol, mechanisms (9 gas, 2 PM), and models (2 AQMs) → yields 64 runtime configurations.
- A User's Guide is available detailing all input, modules, and methods of the Tool.

Semi-Volatile Organic Aerosol

- Organic $PM_{2.5}$ can partition between the aerosol and gas-phase. Older chemical mechanisms exclusively treated primary organic aerosol as non-volatile and do not allow partitioning.
- S2S-Tool enables all $PM_{2.5}$ profiles in SPECIATE to be cross compatible with different chemical mechanisms and treatments of primary organic aerosol.
  - The POA_VolatilityBins input file in S2S-Tool allows users to specify source-specific organic aerosol volatility profiles.

PM treatments in CMAQ:



Conclusions

- VOC and $PM_{2.5}$ speciation are important steps in the compilation of our emissions inventories and in air quality modeling.
- Various methods are employed at the EPA to incorporate HAPs from a base inventory into the modeling platforms.
- NEI VOC-HAP emissions are largely generated using "HAP-augmentation" in EIS (nonpoint, point), provided by MOVES (mobile), or submitted (point).
- Speciating emissions from a base inventory for a modeling platform requires many databases and tools:
  - SPECIATE, HAP-Augmentation, S2S-Tool, SMOKE
- We are continually looking to make updates and improvements to our tools and datasets. Please reach out with any questions, comments, or concerns regarding speciation!

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Thank you – any questions?

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