Analysis of VOC Emissions using EPA's SPECIATE Database

Heather Simon[+], Lee Beck*, Prakash Bhave[+], Frank Divita[#], Ying Hsu[#], Deborah Luecken[+], David Mobley[+], George Pouliot[+], Adam Reff[&], Golam Sarwar[+], and Madeleine Strum[&]

[+]National Exposure Research Laboratory, EPA, Research Triangle Park, NC 27711
*** National Risk Management Research Laboratory, EPA, Research Triangle Park, NC 27711**
[#]E.H. Pechan and Associates, 3622 Lyckan Parkway, Durham, NC 27707
[&] Office of Air Quality Planning and Standards, EPA, Research Triangle Park, NC 27711

EPA's SPECIATE DATABASE

- Product of the U.S. Environmental Protection Agency (EPA) that serves as the repository for source category-specific emission speciation profiles
- Profiles contain weight fractions of chemical species of both volatile organic compounds (VOC) and particulate matter (PM)
- Data come from a variety of sources including peer-reviewed journal articles and emissions testing conducted primarily by the EPA.
- Original source profile is documented in the SPECIATE database.
- Includes a quality indicator field which ranks the quality of specific profiles.
- SPECIATE 4.2 Features
  - Composite profiles for 58 (47 PM and 11 VOC) source categories
  - Every profile has been assigned to a SSC
  - An updated SCC-to-SPECIATE profile cross-reference table accounting for national VOC and PM emissions in the 2002 National Emissions Inventory (NEI)
  - VOC-to-TOG conversion factors for applicable gas profiles
  - A protocol for expansion of the database
  - A mapping of the new VOC compounds into model species categories
  - Web browser application developed to provide access through a simple web interface – allows complex searches and downloads
  - Review and prioritization of 49 studies entailing 614 PM and 822 VOC profiles for potential inclusion in the future SPECIATE database
- SPECIATE 4.3 will be released in 2011

"Views" of the 2005NEI using SPECIATE 4.2 profiles by source category: typical July day

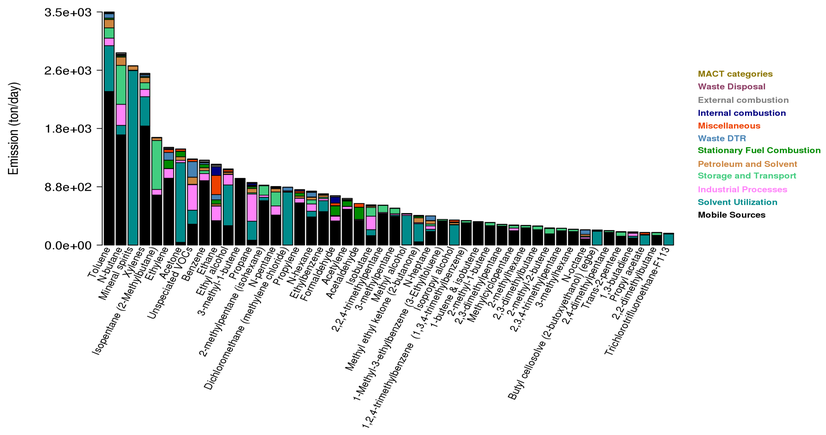
- Apply SCC to Profile Cross Reference to all VOCs in 2005 NEI
- Incorporate SPECIATE database directly into the Emission Processor to get VOC compound-SCC profile
- $E_{i,j}=E_{TOG,j}X_{i,j}$
  - $E_{i,j}$ = mass emissions of compound i from source type j
  - $E_{TOG,j}$ = Emissions of total organic gas from source, j
  - $X_{i,j}$ = weight fraction of compound i with respect to total organic gas emissions
- Weight the Emission Factors based on Mass, Ozone Reactivity, or Relative Toxicity
  - Reactivity weighting calculated by multiplying $E_{i,j}$ by the Maximum Incremental Reactivity (Carter, 1994) for compound i
  - Non-cancer toxicity weighting calculated by dividing $E_{i,j}$ by the reference concentration (RfC), below which no effects are noted. Lower RfCs indicate pollutants with higher relative toxicity.
- Compare 96 HAP VOCs from 2005 Criteria with the 2005 Toxic Inventory

References

- Database: **http://www.epa.gov/ttn/chief/software/speciate/index.html**
- Browser: **http://cfpub.epa.gov/si/speciate/**
- Report: SPECIATE4.2 – Speciation Database Development Documentation (EPA/600-R-09/038, June 2009)
- Mobley, D., L. Beck, Y. Hsu, F. Divita. What's New in Speciate 4.2? http://www.cmascenter.org/conference/2009/
- Mobley, J. D., L. L. Beck, G. Sarwar, A. Reff and M. Houyoux (2008). SPECIATE – EPA's Database of Speciated Emission Profiles. Air Pollution Modeling and Its Application XIX. C. Borrego and A. I. Miranda, Springer Netherlands: 665-666.
- Simon, H., Beck, L., Bhave, P., Divita, F., Hsu, Y., Luecken, D., Mobley, D., Pouliot, G., Reff, A., Sarwar, G., Strum, M. The Development and Uses of EPA's SPECIATE Database. Atmospheric Pollution Research, In press.
- Carter, W. P. L., Development of ozone reactivity scales for volatile organic compounds. Journal of the Air & Waste Management Association 1994, 44, 881-899.

VOC Emission Species by Mass

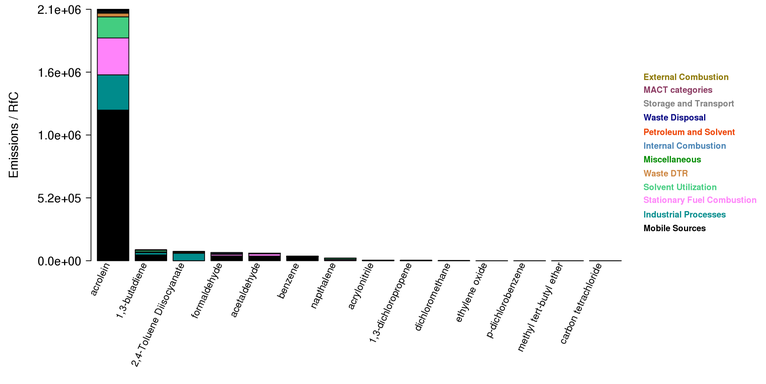
2005 National Emissions Inventory (typical July day)



- 50 species comprise 80% of total emitted VOC mass
- Mobile sources are the single largest source sector contributing to emitted mass for most VOC species
- Storage and transport, solvent utilization, and industrial processes also emit a great deal of VOC mass

VOC Emission Species weighted by Relative Toxicity (non-cancer risk)

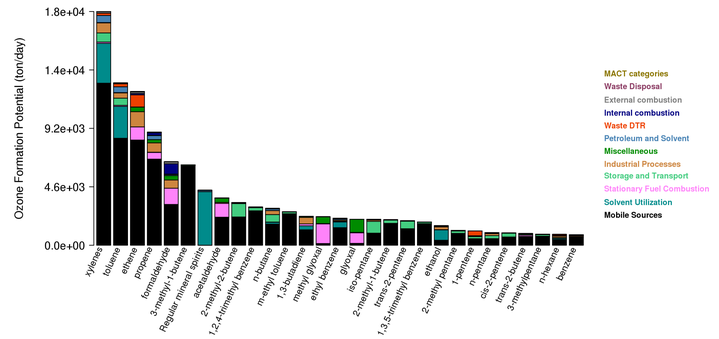
2005 National Emissions Inventory (Typical July day)



- Acrolein has a low RfC (Reference Concentration) and a moderate mass emission rate, making it an important contributor to toxicity-weighted emissions
- Toluene diisocyante has a similar RfC, but lower mass emissions, making it relatively less important as an emitted toxic organic compound

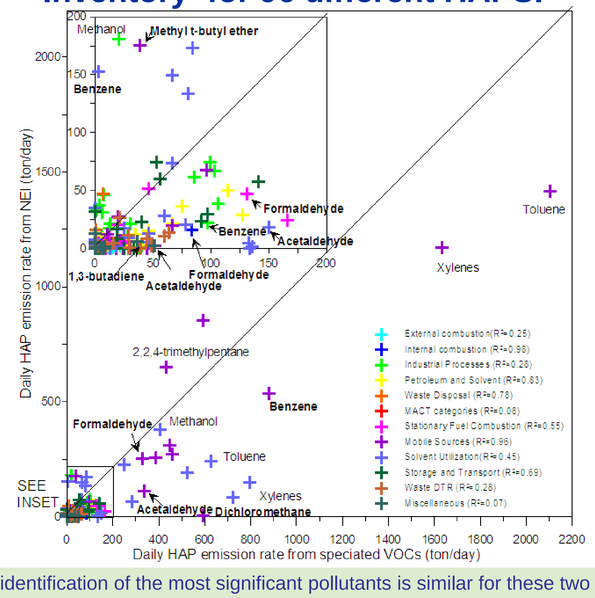
VOC Emission Species weighted by Ozone Potential

2005 National Emissions Inventory (typical July day)



- Xylene emissions are large both on a mass basis and on a reactivity-weighted basis
- Isopentane has a relatively larger importance in the reactivity weighted scheme than the mass emissions ranking
- Mobile sources and solvent utilizations potentially have a large impact on ozone production

Comparison of Speciated VOC from the 2005 NEI criteria inventory with the 2005 NEI HAP Inventory for 96 different HAPS.



- General identification of the most significant pollutants is similar for these two inventories.
- The predicted magnitude of emissions can be very different
- Emissions estimates from the mobile source category correlate strongly between the two inventories
- Emissions from internal combustion and MACT categories have almost no correlation between the two inventories
- Extensive work is needed to identify the causes of discrepancies between these inventories