# SPECIATE

Instructors: Madeleine Strum, strum.madeleine@epa.gov , and MarcMenetrez, menetrez.marc@epa.gov

## Questions and Answers

Q: What about toluene or other Non-NBAFMs? Are they used in speciation?

**A: Inventory pollutants that are HAPs and that aren’t “NBAFM” (naphthalene, benzene, acetaldehyde, formaldehyde and methanol) aren’t used in speciation, except for onroad and nonroad emissions generated by MOVES. This is the current choice we make in our modeling platform, and it is because non-NBAFM HAPs are not explicit in the chemical mechanism and we can model them using NEI emissions without using them for speciation.**

**For example, toluene is not explicit in the CB6 chemical mechanism. When we conduct emissions modeling for an air toxics photochemical model simulation, we use toluene for the toluene model species in the photochemical model (e.g., “TOLU” is the model species for toluene) but we don’t use it for chemical mechanism species “TOL” which is a lumped model species that contains toluene as well as other specific VOC compounds.**

Q: Is ALD2 on your slide twice on purpose?

A: **ALD2 is a CB6 species that consists only of acetaldehyde. It should not have been listed twice; that’s a typo and it has been corrected.**

Q: How do you figure out which species are used in modeling? If you don’t have PNCOM, it can’t be used in modeling, is that right?

A: **The species that are used in modeling are dependent on your chemical mechanism. The best way to find them in one of EPA’s modeling platforms is to read the speciation section of the Technical Support Document (TSD) for that modeling platform which will provide tables listing the species. Modeling platform TSDs are posted at https://www.epa.gov/air-emissions-modeling/emissions-modeling-platforms.**

**If you are not using a mechanism that uses particulate non-carbon organic matter (PNCOM) then you do not need it.**

**Knowing the species that are used in modeling doesn’t tell you which inventory pollutants are used. You can look at the TSD which will provide a list of inventory pollutants that are integrated. If you are developing a modeling platform and want to use more HAPS in from your inventory for speciation you can do that by running the Speciation Tool and specifying which HAPs you want to integrate. You also** need to provide SMOKE that information in the INVTABLE which is an ancillary file that SMOKE uses.

Q: When you do NATA modeling, do you have to use PNCOM, and is it related to integrating?

**A: Integration of HAPs for speciation is used only for VOC speciation and PNCOM is a species of PM speciation so PNCOM is not related to integration. However, for NATA modeling we use a version of CMAQ that uses the AE6 aerosol mechanism that requires PNCOM as a PM2.5 model species, so yes, NATA modeling does require us to use speciation profiles that include PNCOM.**

Q: Do we have a way to determine difference between toxic and carcinogenicity?

## **A: This data isn’t in speciate or NEI; it’s in a separate database on EPA’s “Fate, Exposure, and Risk Analysis (FERA)” website (**[**https://www.epa.gov/fera**](https://www.epa.gov/fera)**). In particular, the link** [**https://www.epa.gov/fera/dose-response-assessment-assessing-health-risks-associated-exposure-hazardous-air-pollutants**](https://www.epa.gov/fera/dose-response-assessment-assessing-health-risks-associated-exposure-hazardous-air-pollutants) **provides dose-response assessments that the Office of Air Quality Planning and Standards (OAQPS) uses for risk assessments of hazardous air pollutants. These data include acute, chronic, cancer and noncancer inhalation risks. Sources of data include but are not limited to EPA’s Integrated Risk Information System (IRIS) program.**

Q: What is the impact on the new finding that household products are low in the inventory (paper by Brian McDonald, et. al., “Volatile chemical products emerging as largest petrochemical source of urban organic emissions” Science 16 Feb 2018: Vol. 359, Issue 6377, pp. 760-764 DOI: 10.1126/science.aaq0524.

**A: Volatile products were found to contribute more in urban areas so it’s becoming more important now than mobile. We are aware of this work and have improved the speciation profiles we are currently using by updating the profiles to use CARB’s more recent consumer products survey. We’re planning to add about 100 new profiles for the next version of SPECIATE.**

**With the new data, will that pie piece (from Casey Bray’s VOC pie charts -slide 59) increase? No, that VOC won’t change but it will be speciated better. A change to the quantity of VOC emitted from these types of products would need to be made in the emission inventory, not the inventory speciation.**

Q: Each speciation profile has a separate voc to tog ratio, correct?

**A: Yes, that ratio depends on the species that are present in the profile and whether or not each is a VOC.**