MEMO

To **Alison Eyth, Madeleine Strum and Benjamin Murphy, EPA**

From **Ross Beardsley, Tejas Shah and Greg Yarwood**

Subject **Speciation Tool v5.0 Mechanism Mappings for CMAQ (AE7 and AE8) and CAMx (cf2)**

Attachments:

A. Memo: Mapping SPECIATE 5.0 compounds for photochemical models

B. Memo: Classification of SPECIATE 4.5 compounds as a function of estimated vapor pressure

C. Memo: Species Mappings for CB6 and CB05 for use with SPECIATE 4.5

Summary

Ramboll created new mechanism mappings[1] for the Speciation Tool v5.0 to accommodate recent changes in the gas speciation profiles of the EPA's SPECIATE 5.0 repository and specifically support the revised aerosol modules (AE7 and AE8) of the Community Multiscale Air Quality Model v5.3 (CMAQ). CMAQ mappings were created for the Carbon Bond 6 (CB6), SAPRC07TC, and the Common Representative Intermediates (CRI)[2] gas phase mechanisms. Minor revisions to mappings for the Comprehensive Air Quality Model with Extensions (CAMx)[3] mechanisms CB05, CB6 and SAPRC07 provide more consistent treatment of low volatility organic compounds (LVOC) across models. Detailed descriptions of the methods used to develop the mechanism mappings for each chemical mechanism were provided previously[4] and are included here as attachments for completeness.

The names of mechanism mappings are revised to more transparently indicate their purpose by including both the chemical mechanism name and the aerosol option in the mapping title. For example, the CB6 mappings for CMAQ AE7 and AE8 are titled CB6r3_AE7 and CB6r3_AE8, respectively, and the CB6 mapping for the CAMx two-mode coarse/fine aerosol option (CF2) is titled 'CB6r4_CF2'. CB6 mappings are named for the most recent CB6 revision present in the target model (r3 in CMAQ and r4 in CAMx).

A summary of the mechanism mappings in Speciation Tool v5.0 is provided in **Table 1.** The mechanism implementation details are available in respective model User's Guides. For example, CMAQ chemical mechanisms are described on CMAQ GitHub[5] and CAMx mechanism details are available in CAMx User's Guide[3]. **Table 2** lists chemical species names with their description common to all CB6 mechanisms. Similarly, **Table 3** and **Table 4** presents list of chemical species for SAPRC07 and CRI mechanisms respectively.

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[1] "Mechanism mapping" refers to the translating the detailed chemical constituents contained in the gas speciation profiles of air pollution sources in EPA's SPECIATE 5.0 repository to the "model species" used by condensed chemical mechanisms of photochemical air quality models. Mechanism mapping is implemented in software called the "Speciation Tool."

[2] http://mcm.leeds.ac.uk/CRI/

[3] http://www.camx.com/

[4] Ramboll technical memo to EPA titled "Mapping SPECIATE 5.0 compounds for photochemical models" dated October 11, 2018.

[5] https://github.com/USEPA/CMAQ/tree/master/CCTM/src/MECHS

Table 1. Summary of mechanism mappings in Speciation Tool v5.0

Mechanism Mapping Name	Purpose	Summary Description
CB6r4_cf2	Support for CAMx v6.5	Volatile organic species mapped for CAMx CB6r4 (also applicable for CB6r3 and CB6r2) Semi-volatile organic species mapped to model species NVOL ($c^* < 10^{2.5}$ µg m^{-3}) or IVOC ($c^* < 10^{6.5}$ µg m^{-3}) Inorganic species mapped for CAMx CF aerosol scheme, version 2 (cf2)
CB6r3_ae7	Support for CMAQv5.3	Volatile organic species mapped for CMAQ CB6r3 (with added model species NAPH and XYLMN) plus: - added explicit alpha-pinene (APIN) model species - acetic acid mapped to AACD - formic acid mapped to FACD Semi-volatile organic species mapped to IVOC and NVOL (as for CB6r4_cf2) Inorganic species mapped for CMAQ ae7 aerosol scheme
CB6r3_ae8	Support for AE8 in future CMAQ release	Volatile organic species mapped as CB6r3_ae7 except model species XYLMN renamed to XYL Semi-volatile organic species mapped to VBS model species (SVOCN1…IVOCP6, IVOCP5ARO, etc.) Inorganic species mapped for CMAQ ae8 scheme
SAPRC07_cf2	Support for CAMx v6.5	Volatile organic species mapped for CAMx SAPRC07 Semi-volatile organic species mapped to IVOC and NVOL (as for CB6r4_cf2) Inorganic species mapped for CAMx cf2 scheme
SAPRC07TC_ae7	Support for CMAQv5.3	Volatile organic species mapped for CMAQ SAPRC07TC with added explicit naphthalene (NAPH) Semi-volatile organic species mapped to IVOC and NVOL Inorganic species mapped for CMAQ ae7 scheme
SAPRC07TC_ae8	Prepare for ae8 in a future CMAQ release	Volatile organic species mapped as SAPRC07TC_ae7 Semi-volatile organic species mapped to VBS model species (SVOCN1…IVOCP6, IVOCP5ARO, etc.) Inorganic species mapped for CMAQ ae8 scheme
CRI_ae7	Support for CMAQv5.3 as-is	Volatile organic species mapped for CMAQ CRI with added explicit naphthalene (NAPH) Semi-volatile organic species mapped to IVOC and NVOL Inorganic species mapped for CMAQ ae7 scheme
CRI_ae8	Support for AE8 in future CMAQ release	Volatile organic species mapped as CRI_ae7 Semi-volatile organic species mapped to VBS model species (SVOCN1…IVOCP6, IVOCP5ARO, etc.) Inorganic species mapped for CMAQ ae8 scheme
CB05_cf2	Support for CAMx v6.5	Volatile organic species mapped for CAMx CB05 Semi-volatile organic species mapped to IVOC and NVOL (as for CB6r4_cf2) Inorganic species mapped for CAMx cf2 scheme

Table 2. Species names, descriptions and carbon numbers common to all CB6 Mechanisms

Species Name	Description	Carbon #
ACET	Acetone	3
ALD2	Acetaldehyde	2
ALDX	Propionaldehyde and higher aldehydes	2
BENZ	Benzene	6
CH4	Methane	1

Species Name	Description	Carbon #
ETH	Ethene	2
ETHA	Ethane	2
ETHY	Ethyne	2
ETOH	Ethanol	2
FORM	Formaldehyde	1
IOLE	Internal olefin carbon bond (R-C=C-R)	4
ISOP	Isoprene	5
KET	Ketone carbon bond (C=O)	1
MEOH	Methanol	1
OLE	Terminal olefin carbon bond (R-C=C)	2
PAR	Paraffin carbon bond (C-C)	1
PRPA	Propane	3
TERP	Monoterpenes	10
TOL	Toluene and other monoalkyl aromatics	7
XYL	Xylene and other polyalkyl aromatics	8

Table 3. Species names, descriptions and carbon numbers common to all SAPRC07 Mechanisms

Species Name	Description	Carbon #
ACET	Acetone	3
ACYE	Acetylene (ethyne)	2
ALK1	Alkanes and other non-aromatic compounds that react only with OH and have kOH (OH radical rate constant) between 2 and 5 x 10^2 ppm^{-1} min^{-1} (primarily ethane)	2
ALK2	Alkanes and other non-aromatic compounds that react only with OH and have kOH between 5 x 10^2 and 2.5 x 10^3 ppm^{-1} min^{-1} (primarily propane)	3
ALK3	Alkanes and other non-aromatic compounds that react only with OH and have kOH between 2.5 x 10^3 and 5 x 10^3 ppm^{-1} min^{-1}	4
ALK4	Alkanes and other non-aromatic compounds that react only with OH and have kOH between 5 x 10^3 and 1 x 10^4 ppm^{-1} min^{-1}	5
ALK5	Alkanes and other non-aromatic compounds that react only with OH and have kOH greater than 1 x 10^4 ppm-1 min-1	8
ARO1	Aromatics with kOH < 2x10^4 ppm^{-1} min^{-1}	7
ARO2	Aromatics with kOH > 2x10^4 ppm^{-1} min^{-1}	9
BACL	Biacetyl	4
BALD	Aromatic aldehydes	7
BENZ	Benzene	6
CCHO	Acetaldehyde	2
CH4	Methane	1
CRES	Phenols and Cresols	7
ETHE	Ethene	2
FACD	Formic Acid	1

Species Name	Description	Carbon #
GLY	Glyoxal	2
HCHO	Formaldehyde	1
IPRD	Lumped isoprene product species	5
ISOP	Isoprene	5
MACR	Methacrolein	4
MEK	Ketones and other non-aldehyde oxygenated products that react with OH radicals faster than 5 x 10^{-13} but slower than 5 x 10^{-12} cm^3 $molec^{-2}$ sec^{-1}	4
MEOH	Methanol	1
MGLY	Methyl Glyoxal	3
MVK	Methyl Vinyl Ketone	4
OLE1	Alkenes (other than ethene) with kOH < 7x10^4 ppm^{-1} min^{-1}	5
OLE2	Alkenes with kOH > 7x10^4 ppm^{-1} min^{-1}	5
PACD	Peroxyacetic and higher peroxycarboxylic acids	3
PRD2	Ketones and other non-aldehyde oxygenated products that react with OH radicals faster than 5 x 10^{-12} cm^3 $molec^{-2}$ sec^{-1}	6
RCHO	Propionaldehyde and larger aldehydes	3
TERP	Terpenes	10
RNO3	Lumped Organic Nitrates	6

Table 4. Species names, descriptions and carbon numbers common to all CRI Mechanisms

Species Name	Description	Carbon #
CH4	Methane	1
C2H6	Ethane	2
C3H8	Propane	3
NC4H10	Butane and larger alkanes	4
C2H4	Ethene	2
C3H6	Propene and larger terminal alkenes	3
TBUT2ENE	Trans-2-butene and other internal alkenes	4
APINENE	Alpha-pinene and similar terpenes	10
BPINENE	Beta-pinene and similar terpenes	10
C5H8	Isoprene	5
C2H2	Ethyne	2
BENZENE	Benzene	6
TOLUENE	Toluene and other monoalkyl aromatics	7
OXYL	Xylene and other polyalkyl aromatics	8
CH3OH	Methanol	1
C2H5OH	Ethanol	2
HCHO	Formaldehyde	1

Species Name	Description	Carbon #
CH3CHO	Acetaldehyde	2
C2H5CHO	Propionaldehyde and larger aldehydes	3
CH3COCH3	Acetone	3
MEK	Methyl Ethyl Ketone	5
UCARB10	Lumped oxygenated compounds	4
HCOOH	Formic acid	1
CH3CO2H	Acetic acid and larger carboxylic acids	2

Mapping of Semi-Volatile and Intermediate Volatility Organic Compounds

Some gas profiles of the SPECIATE 5.0 repository allocate mass to semi-volatile (SVOC) and intermediate volatility organic compounds (IVOC) that tend to form secondary organic aerosol (SOA) which tends to reduce their influence on oxidant chemistry. For this reason, species classified as SVOC or IVOC are mapped to model species that do not participate in gas-phase chemistry but are accounted for by SOA chemistry schemes. The classification of SPECIATE compounds by volatility is based on estimated saturation concentration (C*) as described previously.[6] As shown in **Table 5,** species with log (C*) less than or equal to 6.5 will not participate in oxidant chemistry.

SPECIATE SVOC and IVOC are mapped using two distinct methods that account for differences in the SOA schemes of CMAQ and CAMx. For CMAQ AE7 and CAMx CF2, SVOC and IVOC are mapped to model species NVOL and IVOC, respectively. For CMAQ AE8, the SPECIATE SVOC and IVOC are mapped to a larger number of CMAQ model species designed to work with the CMAQ VBS SOA scheme.[7] **Table 5** lists the CMAQ or CAMx model species used for SPECIATE SVOC and IVOC according to their binned volatility.

Table 5. Mapping of SPECIATE SVOC and IVOC to CMAQ and CAMx model species according to volatility bin

SVOC and IVOC Volatility Bin Upper Threshold in log(C*)	CMAQ AE8 VBS Species[1]	CMAQ AE7 and CAMx CFv2.2 Model Species
-0.5	SVOCN1	NVOL[2]
0.5	SVOCP0	
1.5	SVOCP1	
2.5	SVOCP2	
3.5	IVOCP3	IVOC
4.5	IVOCP4	
5.5	IVOCP5, IVOCP5ARO	
6.5	IVOCP6, IVOCP6ARO	

1 IVOCP5ARO and IVOCP6ARO specifically represent intermediate volatility aromatic compounds with C* of 10^5 and 10^6 µg/m^3, respectively
2 The upper threshold in log(C*) for NVOL was previously 3.5 in CAMx mappings, but was revised to 2.5 for consistency with the CMAQ VBS bins.

[6] Ramboll technical memo to EPA titled "Mapping SPECIATE 5.0 compounds for photochemical models" dated October 11, 2018.
[7] Robinson, A.L., Donahue, N.M., Shrivastava, M.K., Weitkamp, E.A., Sage, A.M., Grieshop, A.P., Lane, T.E., Pierce, J.R. and Pandis, S.N., 2007. Rethinking organic aerosols: Semivolatile emissions and photochemical aging. Science, 315(5816), pp.1259-1262.

Some gas profiles in SPECIATE 5.0 contain CMAQ AE8 VBS species from **Table 5** directly in the profile creating a conceptual linkage of SPECIATE profiles to a specific aerosol scheme. AE8 VBS model species present in SPECIATE are treated by the Speciation Tool as one-to-one mappings for CB6r3_AE8 and mappings to either IVOC or NVOL for CB6r3_AE7 and CB6r4_CF2.

The mechanism mapping named CB6r4_CF2 can be used safely for other CB6 mechanisms in CAMx, namely CB6r3 and CB6r2h.

New Explicit CMAQ Model Species for CB6r3, CRI, and SAPRC07TC

New explicit model species are added to the mechanism mappings for CMAQ CB6r3, CRI, and SAPRC07TC chemical mechanisms with AE7 and AE8 aerosol options. The mappings intended for other models (e.g., CAMx) do not have these CMAQ-specific changes.

Naphthalene (SPECIATE ID: 611) is now mapped to the explicit species NAPH (naphthalene) in all CMAQ mappings to support CMAQv5.3. Naphthalene was previously mapped to XYL in the CMAQ CB6r3 mappings, and thus XYL is renamed as XYLMN (xylene minus naphthalene) in CB6r3_AE7 to match a naming convention of CMAQv5.3. Future CMAQ versions will simplify the name of XYLMN to XYL and accordingly CB6r3_AE8 uses the name XYL. In the CB6r4_CF2 mapping naphthalene is mapped to IVOC (rather than XYL) based on its estimated low volatility.

Alpha-pinene (SPECIATE ID: 1083) generally is mapped to the CB6 model species TERP (terpenes) but is now mapped to the explicit species APIN in the CMAQ CB6r3 mechanism mappings for AE7 and AE8.[8] We did not adopt a "terpene minus alpha-pinene" naming convention and so the TERP species remains in the CB6r3 mechanism mappings. Alpha-pinene is already a model species in CRI ('APINENE') and SAPRC07TC (see **Creation of the CMAQ SAPRC07TC mapping**).

Explicit (one-to-one) mappings were added for acetic acid (to AACD) and formic acid (to FACD) in the CMAQ CB6r3 mappings. Previously, acetic acid was mapped to PAR + UNR and formic acid to UNR. The recommended mappings of acetic and formic acid for CAMx were not changed because these species are predominantly secondary in the atmosphere and the CAMx developer assessed that changing the mappings would incur cost (larger emission files) for little benefit (little change in model concentration).

Creation of the CMAQ SAPRC07TC mapping

Previous versions of the Speciation Tool contained mechanism mappings for SAPRC07 but not SAPRC07TC, which includes many additional explicit model species to represent air toxics. The previous SAPRC07 mappings are revised to include the following explicit model species of SAPRC07TC: 1,3-butadiene (BDE13), acrolein (ACRO), a-pinene (APIN), 1,2,4-trimethyl benzene (B124), ethanol (ETOH), o-xylene (OXYL), m-xylene (MXYL), p-xylene (PXYL), propane (PRPE), sesquiterpenes (SESQ), and toluene (TOLU). Creating new mappings was straightforward for species that tend to be resolved in SPECIATE profiles, e.g., propane, 1,3-butadiene, toluene. Where SPECIATE profiles identified a compound mixture that clearly corresponds to a few explicit SAPRC07TC model species we made assumptions, e.g., that a previous mapping to XYL can be replaced by equal fractions of OXYL, MXYL and PXYL. The updated mappings are shown in **Table 6**. Where SPECIATE profiles identified complex mixtures that might contain an indeterminate amount of an explicit SAPRC07TC model species (e.g., "undefined petroleum distillates") we made no assumption and the previous mapping remains unchanged.

[8] See documentation here: https://github.com/USEPA/CMAQ/blob/master/DOCS/Release_Notes/biogenic_apinene.md

Table 6. Updated SAPRC07TC mappings of compound mixtures containing explicit model species

Species ID	Description	SAPRC07TC Mapping
326	C9 aromatics	0.2857*ARO1 + 0.6429*ARO2 + 0.0714*B124
507	Isomers of xylene	0.25*ARO1 + 0.25*MXYL + 0.25*OXYL + 0.25*PXYL
580	Misc. trimethylbenzenes	0.9*ARO2 + 0.1*B124
755	Trimethylbenzenes (mixed)	0.9*ARO2 + 0.1*B124
1962	C-3 Compounds	0.5*ALK2 + 0.5*PRPE

ATTACHMENT A

Mapping SPECIATE 5.0 compounds for photochemical models

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MEMO

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Summary

"Mechanism mapping" refers to translating the detailed chemical constituents identified in "speciation profiles" to the "model species" used by condensed chemical mechanisms of photochemical air quality models. Mechanism mapping is implemented in software called the "Speciation Tool." Ramboll reviewed version 5.0 of the Environmental Protection Agency's (EPA's) SPECIATE database of speciation profiles and created mechanism mappings for newly added and previously unmapped chemical species. We estimated the vapor pressure (p_i^o) of these compounds and those identified the low volatility organic compounds (LVOC) were not mapped to gas phase mechanisms. After removing LVOC, mechanism mappings for the remaining new or previously unmapped species were created for the Carbon Bond (CB), SAPRC07, and the Common Representative Intermediates (CRI) [1] gas phase mechanisms using methods developed previously.[2]

CLASSIFYING COMPOUNDS AS NVOL, IVOC, OR VOC

Some of the newly added or unmapped organic gas profiles within SPECIATE 5.0 repository allocate mass to LVOC that react in the atmosphere and rapidly move to the particulate phase limiting their influence on gas phase chemistry. For this reason, previous mechanism mappings for the Speciation Tool assigned some compounds to the non-volatile model species NVOL, removing them from the gas phase mechanism. However, the methodology for assigning compounds to NVOL was not well defined because the p_i^o of these compounds was not available within SPECIATE. A scheme was created previously to refine the identification of LVOCs within the SPECIATE 4.5 database and classify these compounds as NVOL or intermediate-volatility (IVOC) based on the definition of IVOC proposed by Robinson et al.[3] for the Volatility Basis Set SOA model. This task describes the

[1] http://mcm.leeds.ac.uk/CRI/

[2] Ramboll Environ technical memos to EPA titled "Species Mappings for CB6 and CB05 for use with SPECIATE 4.5" and "Classification of SPECIATE 4.5 compounds as a function of estimated vapor pressure" dated September 27, 2016 and September 29, 2017, respectively.

[3] Robinson, A.L, N. Donahue, M. Shrivastava, E.A. Weitkamp, A.M. Sage, A.P. Grieshop, T.E. Lane, J.R. Pierce, and S.N. Pandis. "Rethinking Organic Aerosols: Semivolatile Emissions and Photochemical Aging." Science 315, Issue 5816 (March 2, 2007): 1259-1262. doi:10.1126/science:1133061

application of this scheme to the newly added or previously unmapped species in SPECIATE 5.0.

Estimating Volatility

The MPBPWIN model (v1.43) within the EPA's Estimation Programs Interface (EPI) Suite (https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface) was utilized to estimate the p_i^o of compounds in SPECIATE 5.0 based on CAS# or simplified molecular-input line-entry system (SMILES) string provided in the SPECIATE species properties table. For compounds without a CAS# or SMILES string in SPECIATE, a SMILES string or estimate of p_i^o was obtained from an online repository (such as PubChem or ChemSpider) if readily available. In some cases the p_i^o of a surrogate compound was used, e.g. 1-undecene (ID: 1082) used for C11 Olefins (ID: 1930). Inorganic species, which were primarily mapped to NVOL previously, and other species lacking sufficient information to classify were assigned no mapping to ensure that they are not incorrectly treated as non-volatile organic species in the SOA modeling schemes of AQMs. Organic particulate matter species were assigned to NVOL (e.g. Organic Carbon II). The species assigned no mapping and the organic particulate matter species mapped to NVOL are listed in Table A1 and Table A2 of Appendix A, respectively.

In summary, the methodology used for estimating p_i^o of compounds in the SPECIATE database was as follows:

1. Use CAS# or SMILES string from the SPECIATE species property table.
2. If a CAS# or SMILES string is not available in SPECIATE, acquire SMILES string or p_i^o estimate from online repository such as PubChem (https://pubchem.ncbi.nlm.nih.gov/) or ChemSpider (http://www.chemspider.com/).
3. If a SMILES string cannot be readily obtained, assign the p_i^o of a surrogate.
4. If the properties of the species are unknown and a SMILES string or surrogate cannot be reasonably assigned, do not assign a mapping.

After estimating p_i^o, the saturation concentration of each species (C_i^*) was calculated at 298 K following Equation 1[4]:

$$C_i^* = \frac{10^6 MW_i p_i^o}{760RT} \quad (1)$$

where, MW_i is the molecular weight of each compound from the SPECIATE 5.0 database[5], R is the ideal gas constant (m^3 atm mol^{-1} K^{-1}), and T is the temperature (K).

Then, the species were classified as NVOL, IVOC or VOC using the volatility bins shown in Table 1, which are based on the volatility range propsed for IVOC in Robinson et al[3].

Table 1. Saturation concentration (C_i^*, µg m^{-3}) bins used in volatility classification

NVOL	$C_i^* < 3 \times 10^3$
IVOC	$3 \times 10^3 \leq C_i^* < 3 \times 10^6$
VOC	$3 \times 10^6 \leq C_i^*$

[4] Odum, J.R., T. Hoffmann, F. Bowman, D. Collins, R.C. Flagan, and J.H. Seinfeld. "Gas/Particle Partitioning and Secondary Organic Aerosol Yields." Environmental Science & Technology 30, no. 8 (July 1, 1996): 2580–85. doi:10.1021/es950943+.

[5] In cases in which the molecular weight was missing from the database or incorrect, a corrected or assigned molecular weight was used in these calculations.

Discussion of Volatility Estimates

The estimated C_i^* of SPECIATE 5.0 species are shown in Figure 1 as a function of molecular weight along with the defined volatility bins for VOC, IVOC, and NVOL. Using estimated vapor pressure to classify SPECIATE compounds allows for systematic identification, classification and removal of complex, low-volatility compounds.

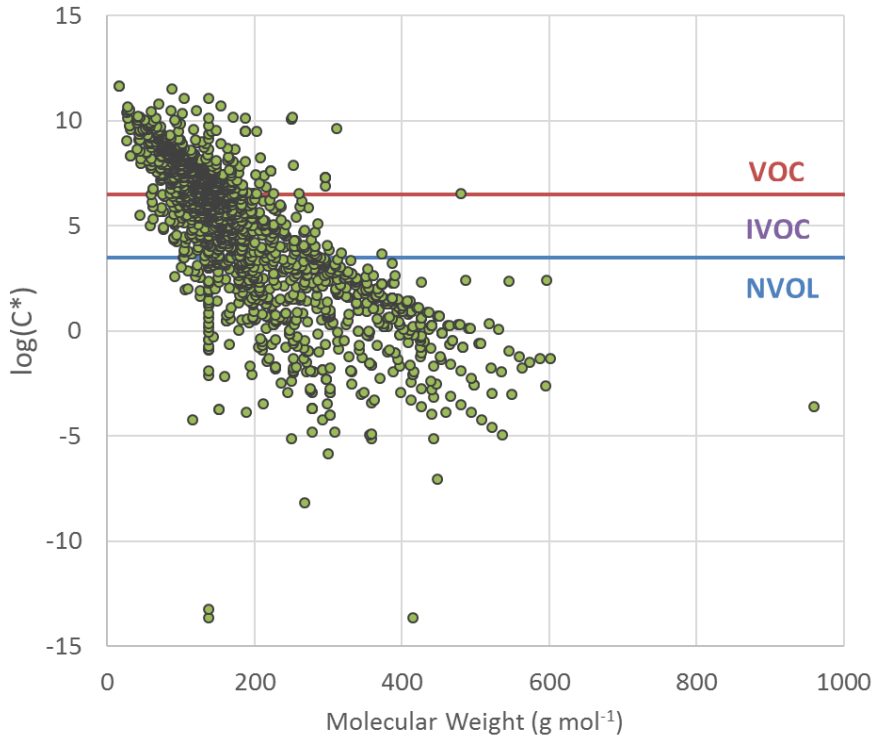

Figure 1. Estimated saturation concentrations (C_i^*) of species in SPECIATE 5.0 at 298 K as a function of molecular weight.

The number of species from SPECIATE 5.0 assigned to each bin is shown in Table 2, and approximately 50% are assigned to IVOC or NVOL based on their estimated p_i^o.

Table 2. Number of SPECIATE 4.5 compounds assigned to each volatility bin or not mapped.

Volatility Bin	Number of Compounds
VOC	1265
IVOC	619
NVOL	786
Not mapped*	124
Total	**2794**

* Inorganic species and other unknown species with insufficient information to characterize

MAPPING LVOC FOR ALL GAS-PHASE MECHANISMS

All gas-phase mechanism mappings for Speciation Tool version 5.0 use a new systematic methodology for mapping low volatility compounds. Compounds with very low vapor pressure are mapped to model species NVOL and intermediate volatility compounds are mapped to IVOC. By reviewing which compounds are mapped to IVOC and NVOL, representative molecular weights (MW) and numbers of carbon atoms (C#) were assigned to these species (Table 3). Consequently, the Speciation Tool version 5.0 produces speciation profiles that compute IVOC and NVOL in moles, which is consistent with all other model species in the gas-phase mechanisms. For consistency, air quality models that make use of IVOC and/or NVOL emissions from Speciation Tool version 5.0 should make use of the representative properties given in Table 3.

Table 3. Representative molecular weights and numbers of carbon atoms for model species IVOC and NVOL

Model Species	Representative C#	Representative MW (g/mol)
IVOC	12	160
NVOC	18	260

MAPPING MIXTURES FOR ALL MECHANISMS

Several species in SPECIATE 5.0 are not a single species but represent a mixture of compounds, e.g. 1-methylcyclohexene; 4-methylheptane (ID:2677). For these compounds the average molecular weight of the compounds was used in estimating vapor pressure. Similarly, the mapping assignments of each compound in the mixture were averaged to get the mapping of the mixture.

MAPPING INORGANIC AND ORGANIC PARTICULATE MATTER SPECIES FOR ALL MECHANISMS

Inorganic species and species with unknown properties, which previously were primarily mapped to NVOL, were assigned no mapping to ensure that they are not incorrectly treated as non-volatile organic species by air quality models. These species are now implicitly mapped to UNK by the Speciation Tool along with all other species that are not mapped. Organic particulate matter species were mapped to NVOL. The species assigned no mapping and the organic particulate matter species mapped to NVOL are listed in Table A1 and Table A2 of Appendix A, respectively.

GAS-PHASE MECHANISM MAPPINGS

After the classification of the LVOCs contained in SPECIATE 5.0 database in Task 1, new gas phase mechanism mappings were created for the remaining VOCs based on the guidelines created for SPECIATE 4.5.[2]

Carbon Bond (CB) Mechanisms

Organic gases are mapped to the CB mechanism either as explicitly represented individual compounds (e.g. ALD2 for acetaldehyde), or as a combination of model species that represent common structural groups (e.g. ALDX for other aldehydes, PAR for alkyl groups). Table 4 lists the explicit and structural model species in the CB05 and CB6 mechanisms, each of which represents a defined number of carbon atoms. CB6 contains four more explicit model species than CB05 and an additional structural group to represent ketones.

Table 4. Model Species in the CB05 and CB6 chemical mechanisms

Model Species Name	Description	Number of Carbons	Included in CB05 (structural mapping)	Included in CB6
Explicit model species				
ACET	Acetone (propanone)	3	**No** (3 PAR)	Yes
ALD2	Acetaldehyde (ethanal)	2	Yes	Yes
BENZ	Benzene	6	**No** (1 PAR, 5 UNR)	Yes
CH4	Methane	1	Yes	Yes
ETH	Ethene (ethylene)	2	Yes	Yes
ETHA	Ethane	2	Yes	Yes
ETHY	Ethyne (acetylene)	2	**No** (1 PAR, 1 UNR)	Yes
ETOH	Ethanol	2	Yes	Yes
FORM	Formaldehyde (methanal)	1	Yes	Yes
ISOP	Isoprene (2-methyl-1,3-butadiene)	5	Yes	Yes
MEOH	Methanol	1	Yes	Yes
PRPA	Propane	3	**No** (1.5 PAR, 1.5 UNR)	Yes
Common Structural groups				
ALDX	Higher aldehyde group (-C-CHO)	2	Yes	Yes
IOLE	Internal olefin group (R_1R_2>C=C<R_3R_4)	4	Yes	Yes
KET	Ketone group (R_1R_2 >C=O)	1	**No** (1 PAR)	Yes
OLE	Terminal olefin group (R_1R_2>C=C)	2	Yes	Yes
PAR	Paraffinic group (R_1-C<R_2R_3)	1	Yes	Yes
TERP	Monoterpenes	10	Yes	Yes
TOL	Toluene and other monoalkyl aromatics	7	Yes	Yes
UNR	Unreactive carbon groups (e.g., halogenated carbons)	1	Yes	Yes
XYL	Xylene and other polyalkyl aromatics	8	Yes	Yes

CB6 and CB05 mappings of new VOCs (excluding species mapped to IVOC and NVOL) were created using the general guidelines for mapping provided in Table 5, and mapping guidelines for difficult to map compound classes and structural groups shown in Table 6.

Table 5. General guidelines for mapping using CB6 structural model species.

CB6 Species Name	Number of Carbons	Represents
ALDX	2	Aldehyde group. ALDX represents 2 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. propionaldehyde is ALDX + PAR
IOLE	4	Internal olefin group. IOLE represents 4 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. 2-pentene isomers are IOLE + PAR. *Exceptions:* • IOLE with 2 carbon branches on both sides of the double bond are downgraded to OLE
KET	1	Ketone group. KET represents 1 carbon and additional carbons are represented as alkyl groups (mostly PAR), e.g. butanone is 3 PAR + KET
OLE	2	Terminal olefin group. OLE represents 2 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. propene is OLE + PAR. Alkyne group, e.g. butyne isomers are OLE + 2 PAR.
PAR	1	Alkanes and alkyl groups. PAR represents 1 carbon, e.g. butane is 4 PAR. See UNR for exceptions.
TERP	10	All monoterpenes are represented as 1 TERP.
TOL	7	Toluene and other monoalkyl aromatics. TOL represents 7 carbons and any additional carbons are represented as alkyl groups (mostly PAR), e.g. ethylbenzene is TOL + PAR. Cresols are represented as TOL and PAR. Styrenes are represented using TOL, OLE and PAR.
UNR	1	Unreactive carbons are 1 UNR such as quaternary alkyl groups (e.g., neo-pentane is 4 PAR + UNR), carboxylic acid groups (e.g., acetic acid is PAR + UNR), ester groups (e.g., methyl acetate is 2 PAR + UNR), halogenated carbons (e.g., trichloroethane isomers are 2 UNR), carbons of nitrile groups (-C≡N)
XYL	8	Xylene isomers and other polyalkyl aromatics. XYL represents 8 carbons and any additional carbons are represented as alkyl groups (mostly PAR), e.g. trimethylbenzene isomers are XYL + PAR
IVOC	12	Intermediate volatility organic compounds with saturation concentrations (C_i^*) in the range: $3 \times 10^3 \mu g\ m^{-3} \leq C_i^* < 3 \times 10^6 \mu g\ m^{-3}$
NVOL	18	Low volatility organic compounds with saturation concentrations (C_i^*) in the range: $C_i^*\ \mu g\ m^{-3} < 3 \times 10^3$

Table 6. Mapping guidelines for some difficult to map compound classes and structural groups.

Compound Class/Structural group	CB model species representation
Chlorobenzenes and other halogenated benzenes	Guideline: • 3 or less halogens – 1 PAR, 5 UNR • 4 or more halogens – 6 UNR Examples: • 1,3,5-Chlorobenzene – 1 PAR, 5 UNR • Tetrachlorobenzenes – 6 UNR
Cyclodienes	Guideline: • 1 IOLE with additional carbons represented as alkyl groups (generally PAR) Examples: • Methylcyclopentadiene – 1 IOLE, 2 PAR • Methylcyclohexadiene – 1 IOLE, 3 PAR
Furans/Pyrroles	Guideline: • 2 OLE with additional carbons represented as alkyl groups (generally PAR) Examples: • 2-Butylfuran – 2 OLE, 4 PAR • 2-Pentylfuran – 2 OLE, 5 PAR • Pyrrole – 2 OLE • 1-Methylpyrrole – 2 OLE, 1 PAR
Heterocyclic aromatic compounds containing 2 non-carbon atoms	Guideline: • 1 OLE with remaining carbons represented as alkyl groups (generally PAR) Examples: • Ethylpyrazine – 1 OLE, 4 PAR • 1-methylpyrazole – 1 OLE, 2 PAR • 4,5-Dimethyloxazole – 1 OLE, 3 PAR
Triple bond(s)	Guideline: • Triple bonds are treated as PAR unless they are the only reactive functional group. If a compound contains more than one triple bond and no other reactive functional groups, then one of the triple bonds is treated as OLE with additional carbons treated as alkyl groups. Examples: • 1-Penten-3-yne – 1 OLE, 3 PAR • 1,5-Hexadien-3-yne – 2 OLE, 2 PAR • 1,6-Heptadiyne – 1 OLE, 5 PAR
Alkane isomers and cycloalkanes	Guideline: • UNR is calculated as the inverse of the carbon number (1/number of carbon) with the remaining treated as PAR. This includes alkane branches on rings and other compounds that do not have an explicitly defined structure • Cycloalkanes are assumed to be cyclohexane with additional carbons treated as described above unless explicitly defined Examples: • Branched C7 Alkanes – 6.86 PAR, 0.14 UNR • C10 Cycloalkanes – 9.75 PAR, 0.25 UNR

After applying the volatility classification summarized in Table 2, 50% of the existing CB mappings for SPECIATE 5.0 were assigned to IVOC or NVOL. Of the remaining 50%, 124 inorganic species were assigned no mapping (and consequently mapped to UNK by the Speciation Tool). The updated CB mappings were incorporated in the Speciation Tool.

SAPRC07 Mechanism

Mappings for the SAPRC07 mechanism were created for species added in SPECIATE 5.0 with the LVOC assigned to IVOC or NVOL as described previously for CB mechanisms. VOCs are represented in SAPRC by lumped model species classified by structure (e.g., alkane, alkene, etc.) and OH radical rate constant

(kOH). Existing species were used as examples to create mappings for the newly added and previously unmapped SPECIATE 5.0 compounds by analogy. For compounds where no analogous mappings existed, the AopWin v1.92 model in EPI Suite was used to estimate kOH and mappings were assigned based on structure and estimated kOH. The updated mappings were incorporated in the Speciation Tool.

CRI Mechanism

The CRI mechanism is a condensed mechanism developed from the Master Chemical Mechanism version 3.1[6]. There are several versions of the CRI mechanism with differing levels of condensation and the mappings described here are specific to version CRIv2r5. SPECIATE 5.0 VOCs were mapped by translating the updated SAPRC07 mappings (and CB06 mappings in some cases). All alkanes with 4 or more carbons were mapped to NC4H10 with the mapping factors equal to the ratio of the MW of the VOC to the MW of butane, which is consistent with the VOC mass weighting approach used in the development of the CRI mechanism[7,8]. Organic nitrates (RNO3 in SAPRC07) were treated as alkanes, and terpene mappings in SAPRC (TERP) were split evenly between APINENE and BPINENE except the compounds α-pinene and β-pinene. The CRI mechanism mappings for most terpenes could be improved.

The mapping guidelines are provided in Table 7. The updated mappings were incorporated in the Speciation Tool.

[6] http://mcm.leeds.ac.uk/CRI/

[7] Personal communication with CRI Developer Mike Jenkin

[8] Watson, L.A., D.E. Shallcross, S.R. Utembe, and M.E. Jenkin, A Common Representative Intermediates (CRI) mechanism for VOC degradation. Part 2: Gas phase mechanism reduction, Atmos. Environ., 42 7196-7204, 2008.

Table 7. Translation from SAPRC07 mappings to CRI mappings.

CRIv2r5 Species	SAPRC07 Translation
CH4	CH4
C2H6	ALK1
C3H8	ALK2
NC4H10	ALK3 + ALK4 + ALK5 (mapping weighted by the ratio of the MW of the compounds to the MW of butane)
C2H4	ETHE
C3H6	OLE1
TBUT2ENE	OLE2
APINENE	TERP/2
BPINENE	TERP/2
C5H8	ISOP
C2H2	ACYE
BENZENE	BENZ
TOLUENE	(ARO1 – BENZ*) + CRES + BALD
OXYL	ARO2
CH3OH	MEOH
C2H5OH	ETOH*
HCHO	HCHO
CH3CHO	CCHO
C2H5CHO	RCHO + GLY
CH3COCH3	ACET
MEK	MEK + PRD2
UCARB10	MACR + MVK + IPRD + BACL + MGLY
HCOOH	FACD
CH3CO2H	AACD
NROG	NROG
NVOL	NVOL

* CB06 model species

Appendix A

Inorganic species and species with unknown properties in SPECIATE 5.0 that were not assigned a mechanism mapping

Table A1. Inorganic species and species with unknown properties in SPECIATE 5.0 that were not assigned a mechanism mapping.

Species ID	Name/Description
292	Aluminum
294	Ammonia
296	Antimony
298	Arsenic
300	Barium
307	Bromine
328	Cadmium
329	Calcium
337	Chloride ion
339	Chlorine
347	Chromium
379	Cobalt
380	Copper
436	Total carbon
468	Gallium
477	Gold
487	Indium
488	Iron
519	Lanthanum
520	Lead
525	Magnesium
526	Manganese
528	Mercury
586	Molybdenum
612	Nickel
613	Nitrate
649	Palladium
665	Phosphate
666	Phosphorus
669	Potassium
689	Rubidium
693	Selenium
694	Silicon
695	Silver
696	Sodium
697	Strontium
699	Sulfate
700	Sulfur

Species ID	Name/Description
712	Thallium
714	Tin
715	Titanium
765	Uranium
767	Vanadium
777	Yttrium
778	Zinc
779	Zirconium
784	Ammonium
785	Sodium ion
788	Carbonate
794	Elemental carbon I
795	Chlorine atom
796	Elemental carbon III
797	Elemental Carbon
810	Bromine Atom
830	Sulfur dioxide
831	Hydrogen Sulfide
843	Sum of PM species
1027	Steroid-w , also noted as sterow
1166	Carbon dioxide
1190	Elemental carbon II
1423	Steroid-m , also noted as sterom
1680	Nitrite
1839	Beryllium
1847	Tellurium
1849	Dysprosium
1850	Lithium
1851	Neodymium
1852	Niobium
1853	Praseodymium
1854	Samarium
1855	Scandium
1856	Tantalum
1857	Terbium
1858	Thorium
1859	Tungsten
1860	Boron
1861	Cerium

Species ID	Name/Description
1862	Cesium
1863	Europium
1864	Gadolinium
1865	Germanium
1866	Hafnium
1867	Holmium
1868	Ytterbium
1869	Bismuth
1870	Iodine atom
1871	Fluoride ion
1872	hydrogen phosphate
1884	PM other
1919	Butyl
2032	Copper naphthenate
2302	Potassium ion
2303	Calcium ion
2586	Particulate Mercury
2587	Oxidized Mercury
2588	Elemental Mercury
2604	Reactive gas-phase Mercury
2605	Nitrogen Monoxide (Nitric Oxide)
2606	Nitrogen Dioxide
2607	Nitrous acid
2663	Protactinium
2664	Erbium
2665	Platinum
2668	Particulate Water
2670	Metal-bound Oxygen
2671	Other Unspeciated PM2.5
2672	Chromium(VI)
2686	Iridium
2687	Hydrated sulfate
2772	Magnesium ion
2839	Oxalate anion
2840	Acetate anion
2841	Formate anion (formic acid, ion)
2847	Calcium Oxide
2848	Aluminum Oxide (or Alumina)
2849	Iron Oxide

Species ID	Name/Description
2850	Potassium Carbonate
2851	Sodium Carbonate
2852	Magnesium Oxide
2853	Sulfur Trioxide
2854	Silica
2855	Titanium Oxide
2856	Lutetium
3041	Ruthenium
3042	Rhodium
3152	Corrosion Inhibitor

Table A2. Organic particulate matter species in SPECIATE 5.0 that were mapped to NVOL.

Species ID	Name/Description
626	Organic carbon
789	Organic carbon II
790	Organic carbon III
791	Organic carbon IV
792	Pyrolyzed organic carbon
1027	Steroid-w , also noted as sterow
1183	Organic carbon I
1423	Steroid-m , also noted as sterom
2298	Volatile Carbon
2669	Particulate Non-Carbon Organic Matter

ATTACHMENT B

Classification of SPECIATE 4.5 compounds as a function of estimated vapor pressure

September 29, 2017

MEMORANDUM

To: Alison Eyth and Madeleine Strum, OAQPS, EPA
From: Ross Beardsley, Tejas Shah and Greg Yarwood, Ramboll Environ
Subject: Classification of SPECIATE 4.5 compounds as a function of estimated vapor pressure

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Summary

Ramboll Environ (RE) implemented a scheme to identify and classify low volatility organic compounds (LVOC) contained within the gas speciation profiles of the Environmental Protection Agency's (EPA's) SPECIATE version 4.5 repository using estimated vapor pressure (p_i^o). These LVOC are not well represented by the model species of condensed gas phase mechanisms (e.g. CB6) and have little impact on atmospheric oxidants because their degradation products tend to be incorporate into aerosols. The purpose of this work is to remove these compounds from the gas phase mechanism and add LVOC emissions that can be utilized by secondary organic aerosol (SOA) schemes, such as the volatility basis set (VBS).

After classifying the LVOC species in the SPECIATE 4.5 repository, the Carbon Bond (CB) and SAPRC07 mechanism mappings of the remaining VOCs were reviewed and updated. Species added in SPECIATE 4.5 were mapped for CB6 and CB05 mechanisms previously[1], but existing mappings were not verified. Additionally, SAPRC07 mechanism mappings were created for the new species in SPECIATE 4.5 and some existing mappings were updated for consistency. Finally, VOC mappings were created for the model species of the Common Representative Intermediates (CRI) mechanism.[2] This memorandum is organized according to the specific project tasks listed in the Scope of Work (SOW).

Task 1: Implement a new scheme to classify compounds as NVOL, IVOC, or VOC

Some of the organic gas profiles within SPECIATE 4.5 repository allocate mass to LVOC that rapidly move to the particulate phase limiting their influence on gas phase chemistry. For this reason, current mechanism mappings for the Speciation Tool assign some compounds to the non-volatile model species NVOL, removing them from the gas phase mechanism. However, the methodology for assigning compounds to NVOL is not well defined because the p_i^o of these compounds are not available within SPECIATE. Additionally, refined classification of these compounds as NVOL or intermediate-volatility (IVOC) could improve support for SOA modeling schemes in air quality models (AQMs) such as CMAQ (http://www.cmascenter.org/cmaq/) and CAMx (http://www.camx.com).

[1] Ramboll Environ technical memo to EPA "Species Mappings for CB6 and CB05 for use with SPECIATE 4.5" dated September 27, 2016
[2] http://mcm.leeds.ac.uk/CRI/

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This task describes the implementation of a volatility based framework for classifying SPECIATE compounds by estimated p_i^o using the volatility groupings of the VBS SOA scheme in CAMx.

Methods

The MPBPWIN model (v1.43) within the EPA's Estimation Programs Interface (EPI) Suite (https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface) was utilized to estimate the p_i^o of compounds in SPECIATE 4.5 based on CAS# or simplified molecular-input line-entry system (SMILES) string provided in the SPECIATE species properties table. For compounds without a CAS# or SMILES string in SPECIATE, a SMILES string or EPI estimate of p_i^o was obtained from an online repository (such as PubChem or ChemSpider) if readily available. In some cases the p_i^o of a surrogate compound was used, e.g. 1-undecene (ID: 1082) used for C11 Olefins (ID: 1930). Some species in the database lack sufficient information to assign a SMILES string or surrogate (e.g. Species ID# 2285, Unknown 1), and these species were assumed to be volatile organic compounds (VOC). Inorganic species, which were primarily mapped to NVOL previously, were assigned no mapping to ensure that they are not incorrectly treated as non-volatile organic species in the SOA modeling schemes of AQMs.

In summary, the methodology used for estimating p_i^o of compounds in the SPECIATE database was as follows:

1. Use CAS# or SMILES string from the SPECIATE species property table.
2. If a CAS# or SMILES string is not available in SPECIATE, acquire SMILES string or EPI p_i^o estimate from online repository such as PubChem (https://pubchem.ncbi.nlm.nih.gov/) or ChemSpider (http://www.chemspider.com/).
3. If a SMILES string cannot be readily obtained, assign the p_i^o of a surrogate.
4. If the properties of the species are unknown and a SMILES string or surrogate cannot be reasonably assigned, classify the species as VOC. [3]

After estimating p_i^o, the saturation concentration of each species (C_i^*) was calculated at 298 K following Equation 1[4]:

$$C_i^* = \frac{10^6 MW_i p_i^o}{760RT} \qquad (1)$$

where, MW_i is the molecular weight of each compound from the SPECIATE 4.5 database, R is the ideal gas constant (m^3 atm mol^{-1} K^{-1}), and T is the temperature (K).

[3] The vapor pressures of 'Tetrabutyl orthotitanate' (ID: 2249) could not be estimated by the MPBPVP model of EPI Suite, but is low volatility and thus was assigned to NVOL instead of VOC.

[4] Odum, J.R., T. Hoffmann, F. Bowman, D. Collins, R.C. Flagan, and J.H. Seinfeld. "Gas/Particle Partitioning and Secondary Organic Aerosol Yields." Environmental Science & Technology 30, no. 8 (July 1, 1996): 2580–85. doi:10.1021/es950943+.

Then, the species were classified as NVOL, IVOC or VOC using the volatility bins shown in Table 1, which are based on the volatility range for IVOC from the VBS SOA scheme in CAMx.

Table 1. Saturation concentration (C_i^*, µg m^{-3}) bins used in volatility classification

NVOL	$C_i^* < 3 \times 10^3$
IVOC	$3 \times 10^3 \leq C_i^* < 3 \times 10^6$
VOC	$3 \times 10^6 \leq C_i^*$

Finally, after classifying compounds using the p_i^o estimated in EPI Suite, The Estimation of Vapour Pressure of Organics, Accounting for Temperature Intramolecular, and Non-addivity Effects (EVAPORATION) method of Compernolle et al.[5] was used to estimate the subcooled liquid vapor pressure ($p_{L,i}^o$) of a subset of compounds that were then compared to the EPI p_i^o estimates. The EVAPORATION method was more recently developed and was designed to specifically handle complex, polyfunctional molecules that are relevant to SOA formation. However, the scope of the model is somewhat limited by the functional groups it can handle (e.g. does not treat aromatics), and so this method could not be employed for all compounds. For this reason, the model was only applied to a subset of compounds that are within the scope of the model and whose EPI estimated C_i^* is within approximately one order of mangitude of the boundary of the NVOL/IVOC and IVOC/VOC bins.

Results and Discussion

The estimated C_i^* are shown in Figure 1A and 1B as a function of molecular weight for compounds previously treated as NVOL and as VOC, respectively, along with the newly defined volatility bins for VOC, IVOC, and NVOL. As can be seen, the lack of a defined methodology in previous mappings resulted in compounds with p_i^o corresponding to the VOC volatility bin being mapped to NVOL, and vice versa. Using estimated vapor pressure to classify SPECIATE compounds allows for systematic identification, classification and removal of complex, low-volatility compounds.

[5] Compernolle, S., K. Ceulemans, and J.-F. Müller, EVAPORATION: a new vapor pressure estimation method for organic molecules including non-additivity and intramolecular interactions, Atmos. Chem. Phys., 19431-9450, 2011. Accessed at: http://tropo.aeronomie.be/models/evaporation_run.htm

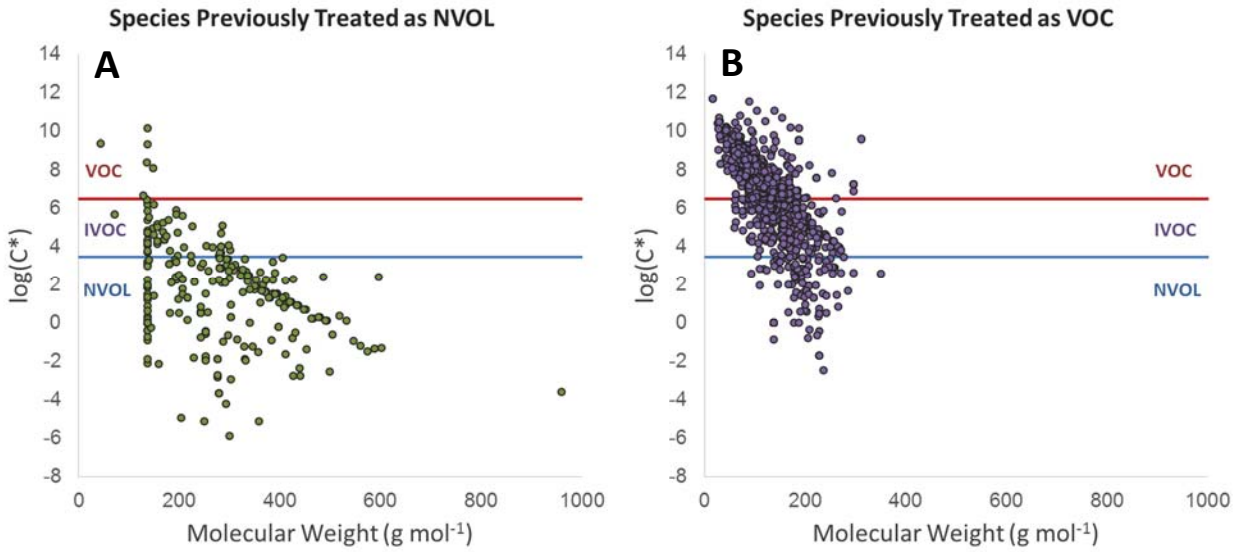

Figure 1. Estimated saturation concentrations (C_i^*) at 298 K as a function of molecular weight shown separately for species previously treated as NVOL (A) and as VOC (B).

The number of species from SPECIATE 4.5 assigned to each bin is shown in Table 2, and approximately 40% were assigned to IVOC or NVOL based on their estimated p_i^o. There are still a number of species that were not mapped for SPECIATE 4.4. The unmapped compounds are listed in Table A1 of Appendix A, and many of these compounds are inorganic or low volatility organic compounds (likely IVOC or NVOL).

Table 2. Number of SPECIATE 4.5 compounds assigned to each volatility bin or not mapped.

Volatility Bin	Number of Compounds
VOC	1180
IVOC	459
NVOL	302
Not mapped*	30
Total	**1971**

* Inorganic species

Saturation concentrations estimated by EPI Suite and the EVAPORATION method are compared in Figure 2 for a subset of compounds. In general, the estimated p_i^o from EPI suite are higher than the corresponding EVAPORATION method estimates, especially for low volatility compounds, as is reflected in the slope of the intercept-free linear regression line. This results in a shift to higher volatility bins for some the classification of some compounds. More specifically, the use of saturation concentrations from EVAPORATION would result in 15% of the VOC compounds in the subset examined to be assigned to IVOC, and 12% of the IVOC species in the subset to be assigned to NVOL. However, there is relatively good overall agreement between the estimates of the two models for these purposes (R^2 = 0.81), and the broad applicability of the EPI Suite and the simplicity of estimating the p_i^o of a large number of compounds (using batch mode) makes it an effective tool for implementing the volatility classification. However, future application of a more recent and accurate method may be valuable.

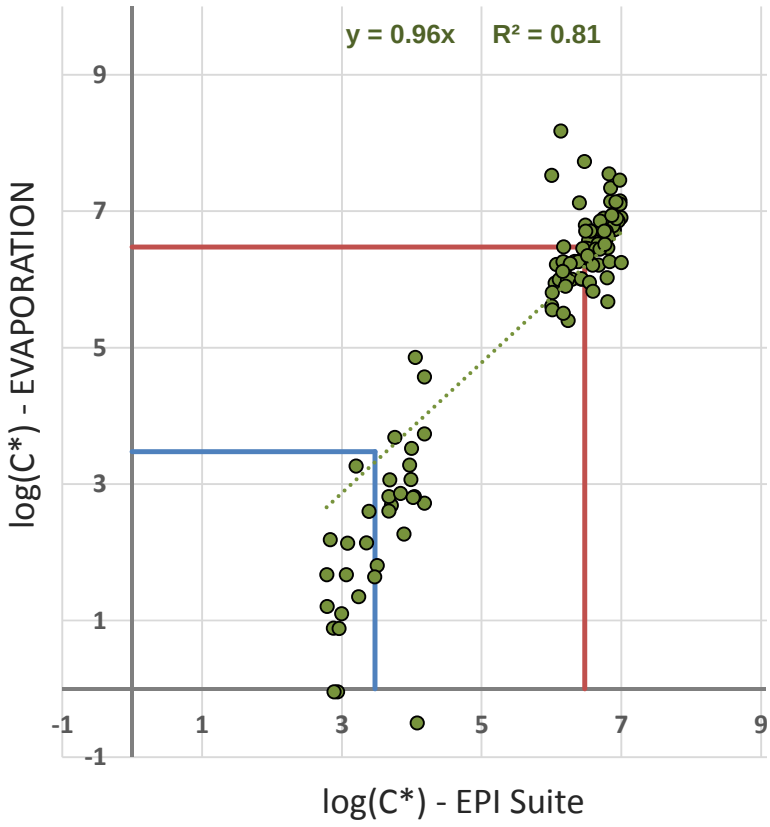

Figure 2. Comparison of the estimated Saturation Concentrations (C_i^*) at 298 K from the EPI Suite (x-axis) and the EVAPORATION method (y-axis).

Recommendation

The MPBPVP model of the EPI Suite was found to be an effective tool for implementing the volatility classification scheme described in this memo due to the simplicity of the approach and ability to handle a wide range of compounds. It is recommended that the EPI p_i^o classification is used for future additions to the SPECIATE database unless a more accurate, easily applied method capable of handling a wide range of compounds is made available. Now that a systematic method has been implemented for mapping low volatility compounds, mappings could be created for a number of compounds that were not mapped for SPECIATEv4.4 (listed in Table A1).

Task 2: Review all Carbon Bond VOC mappings for consistency with current mapping guidelines

After the classification of the LVOCs in SPECIATE 4.5 in Task 1, a systematic review of the existing CB6 and CB05 mechanism mappings was performed for the remaining VOCs based on the guidelines created for SPECIATE 4.5[1]. In addition, updated guidelines for mapping IVOC, NVOL, and inorganic species were established and applied.

Methods

CB Model Species

Organic gases are mapped to the CB mechanism either as explicitly represented individual compounds (e.g. ALD2 for acetaldehyde), or as a combination of model species that represent common structural groups (e.g. ALDX for other aldehydes, PAR for alkyl groups). Table 3 lists all of the explicit and structural model species in the CB05 and CB6 mechanisms, each of which represents a defined number of carbon atoms. CB6 contains four more explicit model species than CB05 and an additional structural group to represent ketones.

Table 3. Model Species in the CB05 and CB6 chemical mechanisms

Model Species Name	Description	Number of Carbons	Included in CB05 (structural mapping)	Included in CB6
Explicit model species				
ACET	Acetone (propanone)	3	**No** (3 PAR)	Yes
ALD2	Acetaldehyde (ethanal)	2	Yes	Yes
BENZ	Benzene	6	**No** (1 PAR, 5 UNR)	Yes
CH4	Methane	1	Yes	Yes
ETH	Ethene (ethylene)	2	Yes	Yes
ETHA	Ethane	2	Yes	Yes
ETHY	Ethyne (acetylene)	2	**No** (1 PAR, 1 UNR)	Yes
ETOH	Ethanol	2	Yes	Yes
FORM	Formaldehyde (methanal)	1	Yes	Yes
ISOP	Isoprene (2-methyl-1,3-butadiene)	5	Yes	Yes
MEOH	Methanol	1	Yes	Yes
PRPA	Propane	3	**No** (1.5 PAR, 1.5 UNR)	Yes
Common Structural groups				
ALDX	Higher aldehyde group (-C-CHO)	2	Yes	Yes
IOLE	Internal olefin group (R_1R_2>C=C<R_3R_4)	4	Yes	Yes
KET	Ketone group (R_1R_2 >C=O)	1	**No** (1 PAR)	Yes
OLE	Terminal olefin group (R_1R_2>C=C)	2	Yes	Yes
PAR	Paraffinic group (R_1-C<R_2R_3)	1	Yes	Yes
TERP	Monoterpenes	10	Yes	Yes
TOL	Toluene and other monoalkyl aromatics	7	Yes	Yes

Model Species Name	Description	Number of Carbons	Included in CB05 (structural mapping)	Included in CB6
UNR	Unreactive carbon groups (e.g., halogenated carbons)	1	Yes	Yes
XYL	Xylene and other polyalkyl aromatics	8	Yes	Yes

Updated mapping guidelines for non-explicit species

CB and all other gas-phase mechanism mappings for Speciation Tool version 4.5 use a new systematic methodology for mapping low volatility compounds (see Task 1). Compounds with very low vapor pressure are mapped to model species NVOL and intermediate volatility compounds are mapped to IVOC. By reviewing which compounds are mapped to IVOC and NVOL, representative molecular weights (MW) and numbers of carbon atoms (C#) were assigned to these species (Table 4). Consequently, the Speciation Tool version 4.5 produces speciation profiles that compute IVOC and NVOL in moles, which is consistent with all other model species in the gas-phase mechanisms. This is a change from previous versions of the Speciation Tool that generate profiles which compute NVOL emissions in grams. Air quality models that make use of IVOC and/or NVOL emissions from Speciation Tool version 4.5 can make use of the representative properties given in Table 4.

Table 4. Representative molecular weights and numbers of carbon atoms for model species IVOC and NVOL

Model Species	Representative C#	Representative MW (g/mol)
IVOC	12	160
NVOC	18	260

In addition, the mappings of inorganic species, which were primarily mapped to NVOL previously, were removed in order to ensure that they are not incorrectly treated as non-volatile organic species in the SOA modeling schemes of AQMs. These species are now implicitly mapped to UNK by the Speciation Tool along with all other species that are not mapped.

After the volatility classification of Task 1 was implemented, the CB6 and CB05 mappings of VOCs (excluding species mapped to IVOC and NVOL) were systematically reviewed using the general guidelines for mapping provided in Table 5, and mapping guidelines for difficult to map compound classes and structural groups shown in Table 6.

Table 5. General guidelines for mapping using CB6 structural model species.

CB6 Species Name	Number of Carbons	Represents
ALDX	2	Aldehyde group. ALDX represents 2 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. propionaldehyde is ALDX + PAR
IOLE	4	Internal olefin group. IOLE represents 4 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. 2-pentene isomers are IOLE + PAR. *Exceptions:* • IOLE with 2 carbon branches on both sides of the double bond are downgraded to OLE
KET	1	Ketone group. KET represents 1 carbon and additional carbons are represented as alkyl groups (mostly PAR), e.g. butanone is 3 PAR + KET
OLE	2	Terminal olefin group. OLE represents 2 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. propene is OLE + PAR. Alkyne group, e.g. butyne isomers are OLE + 2 PAR.
PAR	1	Alkanes and alkyl groups. PAR represents 1 carbon, e.g. butane is 4 PAR. See UNR for exceptions.
TERP	10	All monoterpenes are represented as 1 TERP.
TOL	7	Toluene and other monoalkyl aromatics. TOL represents 7 carbons and any additional carbons are represented as alkyl groups (mostly PAR), e.g. ethylbenzene is TOL + PAR. Cresols are represented as TOL and PAR. Styrenes are represented using TOL, OLE and PAR.
UNR	1	Unreactive carbons are 1 UNR such as quaternary alkyl groups (e.g., neo-pentane is 4 PAR + UNR), carboxylic acid groups (e.g., acetic acid is PAR + UNR), ester groups (e.g., methyl acetate is 2 PAR + UNR), halogenated carbons (e.g., trichloroethane isomers are 2 UNR), carbons of nitrile groups (-C≡N)
XYL	8	Xylene isomers and other polyalkyl aromatics. XYL represents 8 carbons and any additional carbons are represented as alkyl groups (mostly PAR), e.g. trimethylbenzene isomers are XYL + PAR
IVOC	12	Intermediate volatility organic compounds with saturation concentrations (C_i^*) in the range: $3 \times 10^3 \mu g\ m^{-3} \leq C_i^* < 3 \times 10^6 \mu g\ m^{-3}$
NVOL	18	Low volatility organic compounds with saturation concentrations (C_i^*) in the range: $C_i^*\ \mu g\ m^{-3} < 3 \times 10^3$

Table 6. Mapping guidelines for some difficult to map compound classes and structural groups

Compound Class/Structural group	CB model species representation
Chlorobenzenes and other halogenated benzenes	Guideline: • 3 or less halogens – 1 PAR, 5 UNR • 4 or more halogens – 6 UNR Examples: • 1,3,5-Chlorobenzene – 1 PAR, 5 UNR • Tetrachlorobenzenes – 6 UNR
Cyclodienes	Guideline: • 1 IOLE with additional carbons represented as alkyl groups (generally PAR) Examples:

	• Methylcyclopentadiene – 1 IOLE, 2 PAR • Methylcyclohexadiene – 1 IOLE, 3 PAR
Furans/Pyrroles	Guideline: • 2 OLE with additional carbons represented as alkyl groups (generally PAR) Examples: • 2-Butylfuran – 2 OLE, 4 PAR • 2-Pentylfuran – 2 OLE, 5 PAR • Pyrrole – 2 OLE • 1-Methylpyrrole – 2 OLE, 1 PAR
Heterocyclic aromatic compounds containing 2 non-carbon atoms	Guideline: • 1 OLE with remaining carbons represented as alkyl groups (generally PAR) Examples: • Ethylpyrazine – 1 OLE, 4 PAR • 1-methylpyrazole – 1 OLE, 2 PAR • 4,5-Dimethyloxazole – 1 OLE, 3 PAR
Triple bond(s)	Guideline: • Triple bonds are treated as PAR unless they are the only reactive functional group. If a compound contains more than one triple bond and no other reactive functional groups, then one of the triple bonds is treated as OLE with additional carbons treated as alkyl groups. Examples: • 1-Penten-3-yne – 1 OLE, 3 PAR • 1,5-Hexadien-3-yne – 2 OLE, 2 PAR • 1,6-Heptadiyne – 1 OLE, 5 PAR

Results

Following the volatility classification in Task 1, 40% of the existing CB mappings for SPECIATE 4.5 were assigned to IVOC or NVOL (Table 2). Of the remaining 60%, 30 inorganic species were assigned no mapping (and consequently mapped to UNK by the Speciation Tool) and 16 mappings were updated for consistency with the current guidelines. Molecular weights were added for 15 compounds. The updated mappings were incorporated in the Speciation Tool.

Task 3: Update SAPRC07 mappings

Mappings for the SAPRC07 mechanism were created for species added in SPECIATE 4.5 and low volatility species were assigned to IVOC or NVOL. VOCs are represented in SAPRC by lumped model species classified by structure and OH radical rate constant (kOH). Existing species were used as examples to create mappings for the added SPECIATE 4.5 compounds by analogy. For compounds where no analogous mappings existed, the AopWin v1.92 model in EPI Suite was used to estimate kOH. Excluding the species assigned to NVOL or IVOC, 140 new mappings were created and 15 were updated for consistency. The updated mappings were incorporated in the Speciation Tool.

Task 4: Create mappings for the CR1v2r5 mechanism

Methods and Results

The CRI mechanism is a condensed mechanism developed from the Master Chemical Mechanism version 3.1[6]. SPECIATE 4.5 VOCs were mapped by translating the updated SAPRC07 mappings (and CB06 mappings in some cases). All alkanes with 4 or more carbons were mapped to NC4H10 with the mapping factors equal to the ratio of the MW of the VOC to the MW of butane, which is consistent with the VOC mass weighting approach used in the development of the CRI mechanism[7,8]. Organic nitrates (RNO3 in SAPRC07) were treated as alkanes, and terpene mappings in SAPRC (TERP) were split evenly between APINENE and BPINENE except the compounds α-pinene and β-pinene. The mapping guidelines are provided in Table 7. The updated mappings were incorporated in the Speciation Tool.

Table 7. Translation from SAPRC07 mappings to CRI mappings

CRIv2r5 Species	SAPRC07 Translation
CH4	CH4
C2H6	ALK1
C3H8	ALK2
NC4H10	ALK3 + ALK4 + ALK5 (mapping weighted by the ratio of the MW of the compounds to the MW of butane)
C2H4	ETHE
C3H6	OLE1
TBUT2ENE	OLE2
APINENE	TERP/2
BPINENE	TERP/2
C5H8	ISOP
C2H2	ACYE
BENZENE	BENZ
TOLUENE	(ARO1 – BENZ*) + CRES + BALD
OXYL	ARO2
CH3OH	MEOH
C2H5OH	ETOH*
HCHO	HCHO
CH3CHO	CCHO
C2H5CHO	RCHO + GLY
CH3COCH3	ACET
MEK	MEK + PRD2
UCARB10	MACR + MVK + IPRD + BACL + MGLY
HCOOH	FACD

[6] http://mcm.leeds.ac.uk/CRI/

[7] Personal communication with CRI Developer Mike Jenkin

[8] Watson, L.A., D.E. Shallcross, S.R. Utembe, and M.E. Jenkin, A Common Representative Intermediates (CRI) mechanism for VOC degradation. Part 2: Gas phase mechanism reduction, Atmos. Environ., 42 7196-7204, 2008.

CRIv2r5 Species	SAPRC07 Translation
CH3CO2H	AACD
NROG	NROG
NVOL	NVOL

* CB06 model species

Recommendation

- Refine the current approach of mapping most terpenes evenly between APINENE and BPINENE.

Appendix A

Unmapped Species from SPECIATEv4.4 that Remain Unmapped for v4.5

Table A1. Unmapped species from SPECIATEv4.4 that remain unmapped for v4.5

Species ID, Name	Species ID, Name	Species ID, Name
2838: 3-Methylcholanthrene	2495: 2,4-Dimethylbenzoic acid	1016: G-decanolactone
2839: Oxalate anion	2496: 2,5-Dimethylbenzoic acid	1017: C27-20R5a(H),14(H),17(H)-cholestane , also noted as c27rch
2840: Acetate anion	2497: Myristoleic acid	1019: C27-20R5a(H),14a(H),17a(H)-cholestane , also noted as c27rac
2841: Formate anion (formic acid, ion)	2498: Trans-2-decenoic acid	1021: 1-Hexadecene
2847: Calcium Oxide	2499: o-Toluic acid	1022: C28-20R5a(H),14(H),17(H)-ergostane
2848: Aluminum Oxide (or Alumina)	2500: Maleic acid	1024: C28-20R5a(H),14a(H),17a(H)-ergostane
2849: Iron Oxide	2501: p-Toluic acid	1025: C29-20S5a(H),14a(H),17a(H)-stigmastane
2850: Potassium Carbonate	2502: m-Toluic acid	1026: C29-20R5a(H),14(H),17(H)-stigmastane
2851: Sodium Carbonate	2503: Salicylic acid	1027: Steroid-w , also noted as sterow
2852: Magnesium Oxide	2504: Ergosterol	1044: 4-formyl-guaiacol-TMS , also noted as f4gucl
2853: Sulfur Trioxide	2505: Tetradecanedioic acid	1056: Me-succinic acid-TMS
2854: Silica	2506: 1-Nitrobenzoepyrene	1066: Sitostane
2855: Titanium Oxide	2507: 20S 24RS-Ethylcholestane	1120: G-nonanoic lactone
2856: Lutetium	2508: 20R 24R-Ethylcholestane	1123: Trans-2-heptenal
2857: Oleic Acid (or cis-9-Octadecenoic Acid)	2509: 2-nitroanthracene	1127: 7-Hexadecene
2858: trans-Oleic acid (trans-9-Octadecenoic acid)	2510: 3-Nitrobenzoepyrene	1166: Carbon dioxide
2859: 2-Octadecenoic acid	2511: C19-tricyclic terpane	1174: Benzofluoranthenes
2860: 2-pentacosenoic acid	2512: C20-tricyclic terpane	1183: Organic carbon I
2861: Eicosanedioic acid	2513: C21-tricyclic terpane	1190: Elemental carbon II
2862: n-Octadecanol	2514: C22-tricyclic terpane	1194: Undecanoic-g-lactone
2863: 1-Nonadecanol	2515: C21--sterane	1254: A-Methylbiphenyl
2864: n-Eicosanol	2516: C21--sterane	1257: A-MePyMeFl
2865: Henicosanal	2517: C22--sterane	1267: B-Methylbiphenyl
2866: Docosanal	2518: C23--dimethyl-a-butylpodocarpane	1269: B-methylphenanthrene
2867: Tricosanal	2519: C24--dimethyl-a-methylbutylpodocarpane	1270: B-Methylpyrene
2868: Tetracosanal	2520: C25-tricyclic terpane	1275: Benzo(b+j+k)fluoranthene
2869: Pentacosanal	2521: C26-tricyclic terpane	1280: B-MePyMeFl
2870: 14-Methylhexadecanoic acid	2522: C26-tricyclic triterpane-22R	1281: Benzonaphthothiophene
2871: 16-Methyloctadecanoic acid	2523: C26-tricyclic triterpane-22S	1289: C-Methylbiphenyl
2872: n-Docasanoic acid	2524: C27-20S--cholestane	1290: C-methylfluorene
2873: Heptacosanedioic acid	2525: C27--Trisnorhopane	1293: 1-MeFl+C-MePyFl
2874: Methyl hexadecanoate	2526: C27--Trisnorneohopane	1296: C-MePyMeFl
2875: Methyl 14-methylhexadecanoate	2527: C27-tetracyclicterpane-22R	1312: D-MePyMeFl
2876: Methyl nonadecanoate	2528: C27-tetracyclicterpane-22S	1313: D-Trimethylnaphthalene
2877: Methyl heneicosanoate	2529: C28-20R--methylcholestane	1315: E-Methylpyrene

Species ID, Name	Species ID, Name	Species ID, Name
2878: Methyl heptacosanoate	2530: C28-20S--methylcholestane	1317: 2-ethyl-1-methylnaphthalene
2879: Ethyl docosanoate	2531: C28-20S--methylcholestane	1321: F-Methylpyrene
2880: Ethyl tetracosanoate	2532: C28-20R-Ba-diasterane	1326: G-Methylpyrene
2881: 9,12-Octadecenoic acid, methyl ester	2533: C28-20S-Ba-diasterane	1328: H-Trimethylnaphthalene
2882: Methyl eicosenoate	2534: C29-20S-Ba-diasterane	1352: 1,2,8-trimethylnaphthalene
2883: Methyl 2-docosenoate	2535: C28-aaB-Bisnorhopane	1357: Nitro-benzo(a)anthracene
2884: Behenic acid, methyl ester (or Methyl behenate; Methyl docosanoate; n-Docosanoic acid methyl ester)	2536: C28-tetracyclicterpane-22R	1387: 18a(H),21(H)-22,29,30-Trisnorhopane
2885: Methylparaben	2537: C28-tetracyclicterpane-22S	1390: 17a(H),18a(H),21(H)-28,30-Bisnorhopane
2886: 2-Phenylpropanoic acid	2538: C29-aB-Norneohopane	1391: 17a(H),21(H)-30-Norhopane , also noted as ab30nh
2887: Matairesinol	2539: C30-Tricyclicterpane-22R	1392: 17(H),21a(H)-30-Norhopane , also noted as ba30nh
2888: Cinnamaldehyde	2540: C30-Tricyclicterpane-22S	1393: 18a(H),21(H)-30-Norneohopane
2889: Hydroxyquinol (or 1,2,4-Benzenetriol; 1,2,4-Trihydroxybenzene)	2541: C32-22R--bishomohopane	1396: 17(H),21a(H)-hopane , also noted as bahop
2890: Phloroglucinol	2542: C32-22S--bishomohopane	1397: 22S-17a(H),21(H)-30-Homohopane , also noted as sabhhp
2891: Pyrogallol (or 1,2,3-Trihydroxybenzene; Pyrogallic acid)	2543: C33-22R--trishomohopane	1398: 22R-17a(H),21(H)-30-Homohopane , also noted as rabhhp
2892: 1,4-Naphthalenedione	2544: C33-22S--trishomohopane	1402: 22S-17a(H),21(H)-30,31,32-Trisomohopane
2893: Methoxynaphthol (or 2-Methoxy-1-naphthol)	2545: C34-22R--tetrakishomohopane	1407: C27-20S-13a(H),17(H)-diasterane
2894: 1,43,6-Dianhydro-D-mannitol	2546: C34-22S--tetrakishomohopane	1408: C27-20R-13a(H),17(H)-diasterane
2674: Trans-3-hexene; 3-methylcyclopentene	2547: C35-22R--pentakishomohopane	1409: C28-20S-13(H),17a(H)-diasterane
2675: 2-methyl-2-hexene; cis-3-heptene	2548: C35-22S--pentakishomohopane	1410: C29-20R-13a(H),17(H)-diasterane
2676: 3-methyl-trans-3-hexene; Trans-2-heptene	2549: Trisnorhopane	1411: C27-20S5a(H),14a(H)-cholestane
2677: 1-methylcyclohexene; 4-methylheptane	2550: c29 20R--ethylcholestane	1413: C27-20S5a(H),14(H),17(H)-cholestane , also noted as c27sbc
2678: 1-pentene; 2-butyne	2551: c28 20R--methylcholestane	1415: Ster45+40(cholestane)u
2679: Cyclohexene; 3-methylhexane	2552: c29 20r--ethylcholestane	1416: C28-20S5a(H),14a(H),17a(H)-ergostane
2680: 2,4,4-trimethyl-1-pentene; 2,3-dimethyl-2-pentene	2553: 22R-17a(H),21(H)-30-homohopane	1418: Ergostane , also noted as ergos
2681: 4-methyl-cis-2-pentene; 2-methylpentane (isohexane)	2554: 22S-17a(H),21(H)-30-homohopane	1423: Steroid-m , also noted as sterom
2682: 2,3-dimethylheptane; 2-methyloctane	2555: 4-Nitropyrene	1437: 4-ethyl-syringol-TMS , also noted as e4syrg
2683: Trans-1,3-dimethylcyclohexane; Cis-1,4-dimethylcyclohexane	2556: 2-Nitrofluorene	1438: 4-ethyl-guaiacol-TMS , also noted as e4gucl

Species ID, Name	Species ID, Name	Species ID, Name
2685: 4-nonene	2557: C27-20R5a(H),14a(H),17a(H)-cholestane	1460: Propylgyaiacol
2686: Iridium	2558: 20R--cholestane	2345: 1,3-Dimethylnaphthalene
2687: Hydrated sulfate	2561: 1-methoxy-2-Propanone	2347: anteiso-Hentriacontane
2648: 1-methylfluoranthene; 3-methylfluoranthene	2565: 2,2-Dimethylpropanal	2348: anteiso-Heptacosane
2649: Picene	2569: 1,3-dimethyldibenzothiophene	797: Elemental Carbon
2650: Dibenzoa,hpyrene	2586: Particulate Mercury	2349: anteiso-Hexacosane
2651: Heptatriacontane	2587: Oxidized Mercury	2350: anteiso-Nonacosane
2652: Octatriacontane	2588: Elemental Mercury	2351: anteiso-Octacosane
2653: Nonatriacontane	2298: Volatile Carbon	2352: anteiso-Pentacosane
2654: 2,3-dimethoxybenzoic acid	2302: Potassium ion	2353: anteiso-Tetracosane
2655: 2,5-dimethoxybenzoic acid	2303: Calcium ion	2354: iso-Dotriacontane
2656: 3,5-dimethoxybenzoic acid	2340: abieta-6,8,11,13-tetraen-18-oic acid	2356: iso-Heptacosane
2657: 2,4-dimethoxybenzoic acid	2342: Iso-tritriacontane	2357: iso-Hexacosane
2658: Palustric acid	2343: Ethylphenols	2358: iso-Octacosane
2660: Benzoafluoranthene	2344: Myosmine	2359: iso-Pentacosane
2661: Malonic acid (or 1,3-Propanedioic acid)	2035: Cyclopenta-anthracenes	2360: iso-Tetracosane
2662: Syringic acid	2060: Dimethylcyclobutanone	2361: Linoleic acid, 9,12-Octadecadienoic acid (9Z,12Z)-
2663: Protactinium	2147: Methyl C12 ester	2362: Monopalmitin, Hexadecanoic acid, monoester with 1,2,3-propanetriol
2664: Erbium	2222: Pentenyne	2363: Monostearin, Glyceryl monostearate
2665: Platinum	2296: 6,7-Dimethoxy-coumarin	2364: Hexatriacontane
2668: Particulate Water	292: Aluminum	2365: Pinonic acid
2669: Particulate Non-Carbon Organic Matter	294: Ammonia	2366: Stigmasterol
2670: Metal-bound Oxygen	296: Antimony	2369: N-Methylolacrylamide
2671: Other Unspeciated PM2.5	298: Arsenic	2370: Pentachloroethane
2672: Chromium(VI)	300: Barium	2371: Phosgene
2374: 1-Nonadecene	307: Bromine	2714: Trans-2-octene; Trans-1,2-dimethylcyclohexane
2375: 1-Eicosene	328: Cadmium	2739: Bromochloromethane
2376: 1-Heneicosene	329: Calcium	2742: 3,5-Dimethoxyphenol
2377: 1-Docosene	337: Chloride ion	2743: Syringealdehyde
2378: 1-Tricosene	347: Chromium	2744: 1,2-Benzenedicarboxylic acid, 4-methyl-
2379: 1-Tetracosene	379: Cobalt	2745: 1,2,3-Benzenetricarboxylic Acid
2380: 1-Pentacosene	380: Copper	2746: 1,2,4-Benzenetricarboxylic Acid
2381: 1-Hexacosene	436: Total carbon	2747: 1,3,5-Benzenetricarboxylic Acid

Species ID, Name	Species ID, Name	Species ID, Name
2382: 1-Heptacosene	468: Gallium	2748: 1,2,3,4-Benzenetetracaroboxylic Acid
2383: 1-Octacosene	477: Gold	2749: Galactosan
2384: 14-Methyl-hexadecanoic acid	487: Indium	2750: 1,6-anhydro-beta-D-mannopyranose (Mannosan)
2385: n-Hentriacontanoic acid	488: Iron	2751: Glycerol monooleate (9-Octadecenoic acid (9Z)-, 2,3-dihydroxypropyl ester)
2386: n-Dotriacontanoic acid	519: Lanthanum	2752: 1-Monostearin (Octadecanoic acid, 2,3-dihydroxypropyl ester)
2387: n-Tritriacontanoic acid	520: Lead	2753: Cholestanol (Cholestan-3-ol, Dihydrocholesterol)
2388: n-Tetratriacontanoic acid	525: Magnesium	2765: 1-Nitro-2-methylnaphthalene
2389: n-Pentatriacontanoic acid	526: Manganese	2766: 22S-17a(H),21b(H)-29-Homohopane
2390: n-Hexatriacontanoic acid	528: Mercury	2767: 22R-17a(H),21b(H)-29-Homohopane
2391: 10-Undecenoic acid	586: Molybdenum	2768: 22S-17a(H),21b(H)-29,30-Bishomohopane
2392: Tetradecenoic acid	612: Nickel	2769: 22R-17a(H),21b(H)-29,30-Bishomohopane
2393: Hexadecenoic acid	613: Nitrate	2770: 22R-17a(H),21b(H)-29,30,31-Trishomohopane
2394: Nonadecenoic acid	626: Organic carbon	2772: Magnesium ion
2395: Eicosenoic acid	649: Palladium	2773: Heptachlor
2396: Heneicosenoic acid	665: Phosphate	2774: Aldrin
2397: Docosenoic acid	666: Phosphorus	2775: Heptachlor epoxide
2398: Tricosenoic acid	669: Potassium	2776: Endosulfan
2399: Tetracosenoic acid	689: Rubidium	2777: 2,2,5-Trichlorobiphenyl
2400: Hexacosenoic acid	693: Selenium	2778: 2,4,5-Trichlorobiphenyl
2401: Undecanedioic acid	694: Silicon	2779: 2,4,4-Trichlorobiphenyl
2402: Hexadecanedioic acid	695: Silver	2780: 2,2,5,5-Tetrachlorobiphenyl
2403: Docosanedioic acid	696: Sodium	2781: 2,2,3,5-Tetrachlorobiphenyl
2404: Tetracosanedioic acid	697: Strontium	2782: 2,2,4,5,5-Pentachlorobiphenyl
2405: Pentacosanedioic acid	699: Sulfate	2783: 2,2,3,4,5,6-Hexachlorobiphenyl
2406: Hexacosanedioic acid	700: Sulfur	2784: 2,2,4,4,5,5-Hexachlorobiphenyl
2407: Methyl heptadecanoate	712: Thallium	2785: 2,2,3,4,4,5,5-Heptachlorobiphenyl
2408: Methyl eicosanoate	714: Tin	2786: Decachlorobiphenyl
2409: Heneicosanoic acid	715: Titanium	2895: Coumarin
2410: Methyl docosanoate	765: Uranium	2896: Methoxyhydroxycoumarin
2411: Methyl tricosanoate	767: Vanadium	2897: 5-Acetoxymethyl-2-furaldehyde
2412: Methyl tetracosanoate	777: Yttrium	2898: 16,17-Bisnordehydroabietic acid
2413: Methyl pentacosanoate	778: Zinc	2899: Secodehydroabietic acid
2414: Methyl hexacosanoate	779: Zirconium	2900: 19-Norabieta-8,11,13-triene

Species ID, Name	Species ID, Name	Species ID, Name
2415: Methyl octacosanoate	784: Ammonium	2901: Methyl deisopropyldehydroabietate
2416: Methyl nonacosanoate	785: Sodium ion	2902: Pimarinal
2417: Methyl triacontanoate	788: Carbonate	2903: Methyl 8,15-pimaradien-18-oate
2418: Methyl hentriacontanoate	789: Organic carbon II	2904: Methyl iso-pimarate
2419: Methyl dotriacontanoate	790: Organic carbon III	2905: Methyl 16,17-bisnordehydroabietate
2420: Methyl tetratriacontanoate	791: Organic carbon IV	2906: Dehydroabietal
2421: Methyl cis-9-octadecenoate	792: Pyrolyzed organic carbon	2907: Juvabione
2422: Methyl trans-9-octadecenoate	794: Elemental carbon I	2908: Todomatuic acid
2423: Methyl 9,12-octadecadienoate	795: Chlorine atom	2909: Friedelin
2424: Methyl tetracosenoate	796: Elemental carbon III	2910: trans-Methoxy-iso-eugenol
2425: Methyl hexacosenoate	810: Bromine Atom	2911: 7-Oxo-abieta-8,11,13,15-tetraen-18-oic acid
2426: 4-Vinylguaiacol	830: Sulfur dioxide	2912: Manoyl oxide
2427: Vanillic acid	831: Hydrogen Sulfide	2913: 18-Norisopimara-4(19),7,15-triene
2428: Methyl homovanillate	843: Sum of PM species	2914: Neoabietic acid
2429: Methoxyeugenol	853: Benz(a)anthracene-7,12-dione	2915: Pinostrobin chalcone
2430: cis-Methoxy-iso-eugenol	861: 9,10-dihydrobenzo(a)pyrene-7(8H)-one	2916: Umbelliferone
2431: Methoxybenzenediols	862: Benzanthrone; 7H-benzdeanthracen-7-one	2917: Monomethyl inositol
2432: Hydroxyacetophenone	865: 2,3-Benzofluorene	2918: Conidendrin
2433: 3,4,5-Trimethoxybenzoic acid	866: 5&6-methylchrysene	2919: Methyl-2-deoxomatairesinol
2434: Benzenepropanoic acid	869: 1,4-chrysenequinone	2920: Benzenetriols
2435: Diguaiacyl ethanes	870: 4H-cyclopenta(def)phenanthrene	2921: Ethyl hexacosanate
2436: Syringyl guaiacyl ethane	872: Dibenz(ah+ac)anthracene	2922: 20-Methyldocosanoic acid
2437: Disyringyl methane	875: 1,7-dimethylnaphthalene	2923: Octacosanal
2438: Disyringyl ethane	894: 7-methylbenzo(a)pyrene	2924: Hexacosanal
2439: 2-Deoxomatairesinol	897: C-Methylpyrene	2925: Eicosanal
2440: Phenylnaphthalene	910: 1,3-dinitronaphthalene	2926: 1-Hydroxyheptadecane
2441: 1-Naphthalenol	911: 1,3-dinitropyrene	2927: 1-triacontene
2442: 2-naphthalenol	912: 1,5-dinitronaphthalene	2928: Allobetul-2-ene
2443: Methylnaphthol	913: 1,6-dinitropyrene	2929: Allobetulone
2444: 1,43,6-Dianhydro--D-glucopyranose	914: 1,8-dinitronaphthalene	2930: Allobetulin (or (18)-19,28-Epoxyoleanan-3-ol)
2445: Tetramethoxyisoflavone	915: 1,8-dinitropyrene	2931: Betulin
2446: Dibenzofuranols	916: 1-nitronaphthalene	2932: Manool
2447: Benzonaphthofurans	917: 1-nitropyrene	2933: Dehydrojuvabione
2448: Deisopropyldehydroabietic acid	918: 2,7-dinitrofluorene	2934: 1-Heneicosanol
2449: 16-Nordehydroabietic acid	919: 2-nitrobiphenyl	2935: Syringaresinol dimethyl ether
2450: Secodehydroabietic acids	920: 2-nitronaphthalene	2958: 2,3,7,8-Tetrachlorodibenzo-p-dioxin (or 2,3,7,8-TCDD)

Species ID, Name	Species ID, Name	Species ID, Name
2451: Levopimaric acid	921: 3-nitrobiphenyl	2959: 1,2,3,7,8-Pentachlorodibenzo-p-dioxin (or 1,2,3,7,8-PeCDD)
2452: 18-Norabieta-8,11,13-triene	922: 3-nitrofluoranthene	2960: 1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin (or 1,2,3,6,7,8-HxCDD)
2453: 19-norabieta-4,8,11,13-tetraene	923: 3-nitrophenanthrene	2961: 1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin (or 1,2,3,7,8,9-HxCDD)
2454: 18-norabieta-4(19),8,11,13-tetraene	924: 4-nitrobiphenyl	2962: 1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin (or 1,2,3,4,6,7,8-HpCDD)
2455: Dehydroabietane	925: 4-nitrophenanthrene	2963: 1,2,3,4,6,7,8,9-Octachlorodibenzo-p-dioxin (or OCDD)
2456: Methyl 6,8,11,13-abietatetraen-18-oate	926: 6-nitrobenzapyrene	2964: 2,3,7,8-Tetrachlorodibenzofuran (or 2,3,7,8-TCDF)
2457: Methyl 8,11,13,15-abietatetraen-18-oate	927: 6-nitrochrysene	2965: 1,2,3,7,8-Pentachlorodibenzofuran (or 1,2,3,7,8-PeCDF)
2458: Methyl dehydroabietate	928: 7-nitrobenz(a)anthracene	2966: 2,3,4,7,8-Pentachlorodibenzofuran (or 2,3,4,7,8-PeCDF)
2459: Methyl abietate	929: 9,10-dinitroanthracene	2967: 1,2,3,4,7,8-Hexachlorodibenzofuran
2460: Methyl-7-oxodehydroabietate	930: 9-nitroanthracene	2968: 1,2,3,6,7,8-Hexachlorodibenzofuran (or 1,2,3,6,7,8-HxCDF)
2461: Stigmasta-3,5-dien-7-one	931: 9-nitrophenanthrene	2969: 1,2,3,7,8,9-Hexachlorodibenzofuran
2462: Stigmasta-4,6-dien-3-one	932: G-Trimethylnaphthalene	2970: 2,3,4,6,7,8-Hexachlorodibenzofuran
2602: Heptadecane; Pristane	933: Abietic acid-TMS	2971: 1,2,3,4,6,7,8,9-Octachlorodibenzofuran (or OCDF)
2603: C29-20S5a(H),14(H),17(H)-stigmastane	936: Azelaic acid-TMS (Nonanedioic acid)	2972: N-Nitroso-N-diphenylamine
2604: Reactive gas-phase Mercury	938: 1,2,4-butanetriol-TMS	2973: N-Nitrosodimethylamine
2605: Nitrogen Monoxide (Nitric Oxide)	939: Cholesterol-TMS , also noted as chlsrl	2974: N-Nitrosomorpholine
2606: Nitrogen Dioxide	940: Cis-pinonic acid-TMS	2975: 22R-17a(H),21(H)-30,31,32-Trisomohopane
2607: Nitrous acid	942: Dehydroabietic acid-TMS	2976: Tetracontane
2617: Propylcyclopentane; Ethylcyclohexane	943: Docosanoic acid-TMS	2977: 1-Methyl-5-nitronaphthalene
2463: Stigmastan-3-ol	944: Eicosanoic acid-TMS	2978: 2,7-Dinitro-9-fluorenone
2464: Stigmastan-3-one	945: Elaidic acid-TMS	2979: 2-Nitrophenanthrene
2465: Beta-amyrone	946: Glutaric acid-TMS	2980: 2-Nitropyrene
2466: Alpha-amyrone	948: Henicosanoic acid	2981: 1-Methyl-4-nitronaphthalene
2467: Methyl indanones	949: Heptanedioic acid-TMS	2982: 2-Methyl-4-nitronaphthalene
2468: Delta-tocopherol; 8-methyltocol	953: Isophthalic acid-TMS	2983: 5-Nitroacenaphthene

Species ID, Name	Species ID, Name	Species ID, Name
2469: Beta-tocopherol; 5,8-dimethyltocol	955: Levoglucosan-TMS	2984: 1-Methyl-6-nitronaphthalene
2470: Gama-tocopherol; 7,8-dimethyltocol	960: Oleic acid-TMS	2985: Benzobfluorene
2472: Benzobkjfluoranthene	963: Phthalic acid-TMS (1,2-Benzenedicarboxylic Acid)	2986: Dibenzoa,epyrene
2473: 1-methylfluoranthene, C-methylpyrenefluoranthene	964: Picolinic acid-TMS	2987: Dibenz(a,h)acridine or Dibenzo(a,h)acridine
2475: Hexadecane & Norpristane	965: Sitosterol-TMS	2988: Dibenzo(a,i)pyrene or Dibenz(a,i)pyrene
2476: 8-abietic acid	971: Tetracosanoic acid-TMS	2989: Dibenz(a,j)acridine or Dibenzo(a,j)acridine
2477: 2,3 & 3,5-dimethylbenzoic acid	972: Tricosanoic acid-TMS	2990: Dibenz(a,j)anthracene or Dibenzo(a,j)anthracene; 3,4,5,6-Dibenzanthracene
2478: C28-20S5a(H),14(H),17(H)-ergostane	973: 2-nitrofluoranthene	2991: Dibenzo(a,l)pyrene or Dibenzo(def,p)chrysene; 1,2,9,10-Dibenzopyrene
2479: C27-20R5a(H),14a(H),17a(H)-cholestane & C29-20S13(H),17a(H)-diasterane	979: Butylated Hydroxytoluene	2992: Dibenzo(b,k)fluoranthene or Naphth(2,3-e)acephenanthrylene
2480: C29-20R5a(H),14a(H),17a(H)-stigmastane	986: Nitrobap	2993: 7H-Dibenzo(c,g)carbazole
2481: C27-20R5a(H),14(H)-cholestane	988: Nitropyrene	2994: 7,12-Dimethylbenz(a)anthracene
2482: C27-20R-13(H),17a(H)-diasterane	989: C27-tetracyclic terpane	2995: 4H-Cyclopentadefphenanthrene
2483: 17a(H),21(H)-22,29,30-Trisnorhopane	990: C28-tetracyclic terpane	2996: 5-Methylchrysene5-Methylchrysene
2484: 17a(H),18a(H),21(H)-25,28,30-Trisnorhopane	993: 17a(H),18a(H),21(H)-25,28,30-Trisnorhopane ,	2997: 9-phenylanthracene
2485: 2,3,5 & I-trimethylnaphthalene	994: 17a(H),21(H)-22,29,30-Trisnorhopane	3041: Ruthenium
2486: C-methylpyrene & methylfluoranthene	999: 17a(H),21(H)-Hopane	3042: Rhodium
2487: Methylpyrenesfluoranthenes	1000: 17(H),21(H)-Hopane	
2488: 2-methylglutaric acid	1004: 22S-17(H),21(H)-Hopane	
2489: 3-Methyladipic acid	1005: 22S-17a(H),21(H)-30,31-Bishomohopane	
2490: 2,6-dimethoxybenzoic acid	1006: 22R-17a(H),21(H)-30,31-Bishomohopane	
2491: Dodecanedioic acid	1008: 22R-17a(H),21(H)-30,31,32-Trishomohopane	
2492: 2,6-Dimethylbenzoic acid	1010: C27-20S-13(H),17a(H)-diasterane	
2493: 3-Methylglutaric acid	1011: C27-20R-13(H),17(H)-diasterane	
2494: 3,4-Dimethylbenzoic acid	1015: Caprolactone	

ATTACHMENT C

Species Mappings for CB6 and CB05 for use with SPECIATE 4.5

September 27, 2016

MEMORANDUM

To: Alison Eyth and Madeleine Strum, OAQPS, EPA
From: Ross Beardsley and Greg Yarwood, Ramboll Environ
Subject: Species Mappings for CB6 and CB05 for use with SPECIATE 4.5

Summary

Ramboll Environ (RE) reviewed version 4.5 of the SPECIATE database, and created CB05 and CB6 mechanism species mappings for newly added compounds. In addition, the mapping guidelines for Carbon Bond (CB) mechanisms were expanded to promote consistency in current and future work.

Background

The Environmental Protection Agency's SPECIATE repository contains gas and particulate matter speciation profiles of air pollution sources, which are used in the generation of emissions data for air quality models (AQM) such as CMAQ (http://www.cmascenter.org/cmaq/) and CAMx (http://www.camx.com). However, the condensed chemical mechanisms used within these photochemical models utilize fewer species than SPECIATE to represent gas phase chemistry, and thus the SPECIATE compounds must be assigned to the AQM model species of the condensed mechanisms. A chemical mapping is used to show the representation of organic chemical species by the model compounds of the condensed mechanisms.

This memorandum describes how chemical mappings were developed from SPECIATE 4.5 compounds to model species of the CB mechanism, specifically CB05 (http://www.camx.com/publ/pdfs/CB05_Final_Report_120805.pdf) and CB6 (http://aqrp.ceer.utexas.edu/projectinfoFY12_13/12-012/12-012%20Final%20Report.pdf).

Methods

CB Model Species

Organic gases are mapped to the CB mechanism either as explicitly represented individual compounds (e.g. ALD2 for acetaldehyde), or as a combination of model species that represent common structural groups (e.g. ALDX for other aldehydes, PAR for alkyl groups). Table 1 lists all of the explicit and structural model species in CB05 and CB6 mechanisms, each of which represents a defined number of carbon atoms allowing for carbon to be conserved in all cases. CB6 contains four more explicit model species than CB05 and an additional structural group to represent ketones. The CB05 representation of the five additional CB6 species is provided in the '*Included in CB05*' column of Table 1.

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In addition to the explicit and structural species, there are two model species that are used to represent organic gases that are not treated by the CB mechanism:

NVOL – Very low volatility SPECIATE compounds that reside predominantly in the particle phase and should be excluded from the gas phase mechanism. These compounds are mapped by setting NVOL equal to the molecular weight (e.g. decabromodiphenyl oxide is mapped as 959.2 NVOL), which allows for the total mass of all NVOL to be determined.

UNK – Compounds that are unable to be mapped to CB using the available model species. This approach should be avoided unless absolutely necessary, and will lead to a warning message in the speciation tool.

Table 1. Model species in the CB05 and CB6 chemical mechanisms.

Model Species Name	Description	Number of Carbons	Included in CB05 (structural mapping)	Included in CB6
Explicit model species				
ACET	Acetone (propanone)	3	**No** (3 PAR)	Yes
ALD2	Acetaldehyde (ethanal)	2	Yes	Yes
BENZ	Benzene	6	**No** (1 PAR, 5 UNR)	Yes
CH4	Methane	1	Yes	Yes
ETH	Ethene (ethylene)	2	Yes	Yes
ETHA	Ethane	2	Yes	Yes
ETHY	Ethyne (acetylene)	2	**No** (1 PAR, 1 UNR)	Yes
ETOH	Ethanol	2	Yes	Yes
FORM	Formaldehyde (methanal)	1	Yes	Yes
ISOP	Isoprene (2-methyl-1,3-butadiene)	5	Yes	Yes
MEOH	Methanol	1	Yes	Yes
PRPA	Propane	3	**No** (1.5 PAR, 1.5 UNR)	Yes
Common Structural groups				
ALDX	Higher aldehyde group (-C-CHO)	2	Yes	Yes
IOLE	Internal olefin group (R_1R_2>C=C<R_3R_4)	4	Yes	Yes
KET	Ketone group (R_1R_2 >C=O)	1	**No** (1 PAR)	Yes
OLE	Terminal olefin group (R_1R_2>C=C)	2	Yes	Yes
PAR	Paraffinic group (R_1-C<R_2R_3)	1	Yes	Yes
TERP	Monoterpenes	10	Yes	Yes
TOL	Toluene and other monoalkyl aromatics	7	Yes	Yes
UNR	Unreactive carbon groups (e.g., halogenated carbons)	1	Yes	Yes
XYL	Xylene and other polyalkyl aromatics	8	Yes	Yes
Not mapped to CB model species				
NVOL	Very low volatility compounds	*	Yes	Yes
UNK	Unknown	*	Yes	Yes

* Each NVOL represents 1 g mol^{-1} and low volatility compounds are assigned to NVOL based on molecular weight. UNK is unmapped and thus does not represent any carbon.

Mapping guidelines for non-explicit organic gases using CB model species

SPECIATE compounds that are not treated explicitly are mapped to CB model species that represent common structural groups. Table 2 lists the carbon number and general mapping guidelines for each of the structure model species.

Table 2. General Guidelines for mapping using CB6 structural model species.

CB6 Species Name	Number of Carbons	Represents
ALDX	2	Aldehyde group. ALDX represents 2 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. propionaldehyde is ALDX + PAR
IOLE	4	Internal olefin group. IOLE represents 4 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. 2-pentene isomers are IOLE + PAR. *Exceptions:* • IOLE with 2 carbon branches on both sides of the double bond are downgraded to OLE
KET	1	Ketone group. KET represents 1 carbon and additional carbons are represented as alkyl groups (mostly PAR), e.g. butanone is 3 PAR + KET
OLE	2	Terminal olefin group. OLE represents 2 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. propene is OLE + PAR. Alkyne group, e.g. butyne isomers are OLE + 2 PAR.
PAR	1	Alkanes and alkyl groups. PAR represents 1 carbon, e.g. butane is 4 PAR. See UNR for exceptions.
TERP	10	All monoterpenes are represented as 1 TERP.
TOL	7	Toluene and other monoalkyl aromatics. TOL represents 7 carbons and any additional carbons are represented as alkyl groups (mostly PAR), e.g. ethylbenzene is TOL + PAR. Cresols are represented as TOL and PAR. Styrenes are represented using TOL, OLE and PAR.
UNR	1	Unreactive carbons are 1 UNR such as quaternary alkyl groups (e.g., neo-pentane is 4 PAR + UNR), carboxylic acid groups (e.g., acetic acid is PAR + UNR), ester groups (e.g., methyl acetate is 2 PAR + UNR), halogenated carbons (e.g., trichloroethane isomers are 2 UNR), carbons of nitrile groups (-C≡N).
XYL	8	Xylene isomers and other polyalkyl aromatics. XYL represents 8 carbons and any additional carbons are represented as alkyl groups (mostly PAR), e.g. trimethylbenzene isomers are XYL + PAR

Some compounds that are multifunctional and/or include hetero-atoms lack obvious CB mappings. We developed guidelines for some of these compound classes to promote consistent representation in this work and future revisions. Approaches for several compound classes are explained in Table 3. We developed guidelines as needed to address newly added species in SPECIATE 4.5 but did not systematically review existing mappings for “difficult to assign” compounds that could benefit from developing a guideline.

Table 3. Mapping guidelines for some difficult to map compound classes and structural groups

Compound Class/Structural group	CB model species representation
Chlorobenzenes and other halogenated benzenes	Guideline: • 3 or less halogens – 1 PAR, 5 UNR • 4 or more halogens – 6 UNR Examples: • 1,3,5-Chlorobenzene – 1 PAR, 5 UNR • Tetrachlorobenzenes – 6 UNR
Cyclodienes	Guideline: • 1 IOLE with additional carbons represented as alkyl groups (generally PAR) Examples: • Methylcyclopentadiene – 1 IOLE, 2 PAR • Methylcyclohexadiene – 1 IOLE, 3 PAR
Furans/Pyrroles	Guideline: • 2 OLE with additional carbons represented as alkyl groups (generally PAR) Examples: • 2-Butylfuran – 2 OLE, 4 PAR • 2-Pentylfuran – 2 OLE, 5 PAR • Pyrrole – 2 OLE • 1-Methylpyrrole – 2 OLE, 1 PAR
Heterocyclic aromatic compounds containing 2 non-carbon atoms	Guideline: • 1 OLE with remaining carbons represented as alkyl groups (generally PAR) Examples: • Ethylpyrazine – 1 OLE, 4 PAR • 1-methylpyrazole – 1 OLE, 2 PAR • 4,5-Dimethyloxazole – 1 OLE, 3 PAR
Triple bond(s)	Guideline: • Triple bonds are treated as PAR unless they are the only reactive functional group. If a compound contains more than one triple bond and no other reactive functional groups, then one of the triple bonds is treated as OLE with additional carbons treated as alkyl groups. Examples: • 1-Penten-3-yne – 1 OLE, 3 PAR • 1,5-Hexadien-3-yne – 2 OLE, 2 PAR • 1,6-Heptadiyne – 1 OLE, 5 PAR

These guidelines were used to map the new species from SPEICATE4.5, and also to revise some previously mapped compounds. Overall, a total of 175 new species from SPECIATEv4.5 were mapped and 7 previously mapped species were revised based on the new guidelines.

Recommendation

1. Complete a systematic review of the mapping of all species to ensure conformity with current mapping guidelines. The assignments of existing compounds that are similar to new species were reviewed and revised to promote consistency in mapping approaches, but the majority of existing species mappings were not reviewed as it was outside the scope of this work.
2. Develop a methodology for classifying and tracking larger organic compounds based on their volatility (semi, intermediate, or low volatility) to improve support for secondary organic aerosol (SOA) modeling using the volatility basis set (VBS) SOA model, which is available in both CMAQ and CAMx. A preliminary investigation of the possibility of doing so has been performed, and is discussed in a separate memorandum.