New Upgrades to EPA's SPECIATE Database

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ABSTRACT

The purpose of this project being conducted by E.H. Pechan & Associates, Inc. (Pechan) for EPA is to update the SPECIATE database. Speciation profiles in the latest SPECIATE 3.2 system have not been updated since 1999. Many of the profiles in SPECIATE 3.2 have become outdated, since some are the result of testing and/or studies that were conducted in the 1980s and, in some cases, the 1970s. There are a great deal of new particulate matter (PM), volatile organic compounds (VOC), and total organic gases (TOG) speciation data available from research studies and air quality management agency surveys. The primary purpose of this project was to update the SPECIATE database to capture recent and scientifically-meritorious VOC, TOG and PM speciation profile data available from EPA, state agencies, peer-reviewed literature and other relevant data sources. Another objective of this project was to revise the structure of the SPECIATE database to allow for storage of important information underlying each profile (meta data such as sampling and analysis methods, profile quality ratings, etc.).

Pechan is incorporating speciation data from 1,263 PM and 406 VOC and TOG data sources into the new SPECIATE database. Under this project, Pechan has reviewed speciation data and profiles from EPA, the California Air Resources Board (CARB), Desert Research Institute (DRI), the Texas Commission on Environmental Quality (TCEQ), and numerous peer-reviewed journals for inclusion in the new SPECIATE database. In addition, many other speciated datasets were collected. These data are being evaluated and included in the next phase of this project based on their usefulness to SPECIATE users.

Other than improving the SPECIATE database, two other important tasks are underway: revising the Source Classification Code (SCC) – Speciation Profile Cross Reference table and the TOG-to-VOC Conversion Factors table. Another enhancement related to the SPECIATE database considered by the project's technical workgroup was the development of an air quality "model species" profiles file. Photochemical modelers need the model species profiles to model ozone and particulate matter formation. Since most of the current emissions models (e.g. SMOKE, EMS, CONCEPT) have at least some capabilities for producing model species profiles from the SPECIATE profiles, incorporating a model species profile capability within SPECIATE was not included in the upcoming work.

This paper also provides examples of the impacts of these improved speciation data to modeling inventories or the development of speciated emission estimates of toxic air pollutants (TAPs) or climate change pollutants (e.g., methane, aerosol species). An example of these improved profiles is described with side by side comparison of "raw" speciation profiles and "model species" profiles.

INTRODUCTION

SPECIATE is the Environmental Protection Agency's (EPA) repository of total organic compounds (TOC) and particulate matter (PM) speciation profiles of air pollution sources. These source profiles are used to: 1) create speciated emissions inventories for regional haze, particulate matter less than 2.5 microns ($PM_{2.5}$), and ozone (O_3) air quality modeling; 2) estimate hazardous/toxic air pollutant and climate change pollutant emissions from total PM and TOC primary emissions; 3) provide input to chemical mass balance (CMB) receptor models; and, 4) verify profiles derived from ambient measurements using multivariate receptor models (e.g. factor analysis and positive matrix factorization).

Speciation profiles in the current version of SPECIATE, version 3.2, have not been updated since 1999. The SPECIATE 3.2 database contains profiles for important source categories that are outdated and are the result of testing and/or studies that were conducted in the 1980s, and, in some cases, the 1970s. However, there are numerous speciation profiles for particulate matter (PM), volatile organic compounds (VOC), and total organic gases (TOG, which include non-VOCs) available from recent research studies and air quality management agency surveys.

The SPECIATE user community has a wide range of interests and needs. Receptor modelers use SPECIATE as a source of data for emission source chemical profiles. Photochemical modelers make use of speciation data to properly characterize the photochemical reactivity of VOC emissions and the chemical composition of PM emissions. Emission inventory preparers will sometimes turn to SPECIATE to fill data gaps in inventories of TAPs (which include hazardous air pollutants) and climate change pollutants (e.g. methane, black carbon, other aerosol species). Also, control strategy analysts have an interest in the chemical make-up of VOC and PM emissions, so that control programs can better target the appropriate sources.

The steering committee for this project is organized as a working group of EPA and E.H. Pechan & Associates (Pechan) staff, University researchers, emission inventory developers, receptor/photochemical/dispersion modelers, and state agency staff. Members of the Workgroup contributed data and provided recommendations as to which speciation profiles to develop under this project.

STATUS OF CURRENT SPECIATE UPDATES

This project is a work in progress, but represents the addition of 1,263 PM and 406 VOC and TOG profiles into the new SPECIATE database. EPA provided data for 155 gasoline and diesel liquid and headspace vapor profiles. Other EPA VOC, TOG and PM data incorporated into the database include the burning of foliar fuels, agricultural biomass burning, motor vehicles exhaust, pulp and paper boilers, small internal combustion engines, and iron and steel manufacturing facilities. CARB profiles are strong in area source TOG profiles (e.g. consumer products, aerosol coatings, architectural coatings, vehicle hot soak, and other motor vehicle sources powered by new reformulated gasoline). DRI provided many area and point source PM speciation profiles as the result of recent studies conducted in several states. Finally, the literature has provided valuable sources of speciation data.

Additional datasets were collected during Phase I of this study and we anticipate that these will be evaluated and incorporated in the next phase of the project based on their perceived priority - as recommended by the Workgroup. In order to facilitate the use of the new SPECIATE profiles by air quality modelers and emission inventory preparers, the Workgroup accepted Pechan's recommendation to update the following two tables during Phase II of this study.

SCC-Profile Cross-Reference Table

This table links individual SCCs to a SPECIATE profile. Users of SPECIATE rely on this table to identify appropriate speciation profiles to develop speciated emission inventories and to develop model species profiles for photochemical air quality modeling. The current version of this table is available on EPA's website: http://www.epa.gov/ttn/chief/emch/speciation/scc-profile_assignments_mar_4_2002.xls. During Phase II of this project, Pechan will update the cross-reference table.

New speciation profiles are available to cover sources contributing around 80% of the national VOC and PM emissions. Also, many assigned profiles are not in SPECIATE 3.2 (these were apparently dated profiles that were removed during the development of SPECIATE 3.2, but the cross reference table was not updated). Pechan's work in the current phase of the project will be to review SCCs for the top 80% of national VOC and PM emissions and assign appropriate speciation profiles. In some cases, profiles are different for regions and/or States (e.g., gasoline, road dust). The cross reference table needs to be expanded to include the applicable spatial assignment (FIPS county code), where needed. The SMOKE emissions model has the capability to assign different speciation profiles for different SCC-county combinations. For certain sources, Pechan will include the spatial assignment for different profiles (e.g., Federal reformulated gasoline, MTBE or ethanol oxygenated reformulated gasoline).

Another issue that won't be addressed in the current SPECIATE work is the temporal variation in speciation for certain sources. Again, using gasoline as an example, in many areas of the country, the composition differs between Summer and the rest of the year or Winter and the rest of the year. These differences are important to photochemical modelers and speciated emissions inventory developers.

Pechan has recommended that EPA develop a mechanism to allow for different speciation profiles to be assigned to the same SCC and county during different months of the year. This could be done through enhancements to SMOKE and other emissions modeling systems. The other alternative is to have the emission inventory developers break out the emission estimates into two separate SCCs (and provide appropriate temporal allocation profiles for each). Since this would result in new SCCs being created, additional problems would result (e.g., the new SCCs would not match the EPA Master List, which would make the associated emissions reporting to EPA non-compliant with the National Inventory Format).

TOG to VOC Conversion Factors by SCC

The current version of this table is available at EPA's website: http://www.epa.gov/ttn/chief/emch/speciation/voc-togconversions_apr_23_2003.xls. Conversion factors are contingent upon composition of the assigned profiles. This table is also part of the SMOKE model and needs to be updated at the same time as the SCC cross-reference table.

Profile Rating Criteria

As part of the meta data captured for each new speciation profile, quality ratings were developed based on the following criteria:

- *Final Score* = (V-rating) x (J-rating) x (D-rating);
- *V-rating (profile vintage)* is based on the vintage of the profile which reflects measurement technology and methodology. For profiles before Year 1980 – score = 1, 1980-1990 score = 2, 1991-1995 score = 3, 1996-2000 score = 4 and after Year 2000 score = 5;
- *J-rating (expert judgment)* is given a "1" (poor) to "5" (excellent) rating. This is an objective judgment based on the information underlying each profile [e.g. source representativeness (new formulations for consumer products or architectural coatings), measurement quality (e.g. if acrolein properly measured, etc.); and
- *D-rating (data quality)* is given a "2" (poor) to "5" (excellent) rating. This category is rated based on the number of samples: # of samples > 10 score = 5; 5-9 samples score = 4; 3-4 and composite samples score = 3; 1-2 or unknown # of samples score = 2.

Profile quality is rated from A (excellent) to E (poor) as shown below:

Overall Profile Quality Ratings

Profile Quality	Final Score
A	75-125
B	50-74
C	30-49
D	16-29
E	2-15

CONSIDERATION OF AIR QUALITY MODEL SPECIES CAPABILITIES WITHIN SPECIATE

The workgroup gave consideration to whether SPECIATE should provide additional support for the development of air quality model species profiles. The term "model species" refers to the chemical species groups used by photochemical modelers to model ozone formation and other photochemical

processes. A list of model species is provided in Table 1 for three different air quality models. In order for a model to use speciation data, the data in the "raw" speciation profile (such as those in SPECIATE) must be converted into the appropriate model species. For example, acetaldehyde in a SPECIATE profile becomes part of the ALD2 (aldehydes) model species group. Similarly, hexane becomes part of the PAR (paraffins) model species group.

Table 1. List of model species used for air quality models.

CMAQ	PMCAMx	CAMx4	Species Description
ALD2	ALD2	ALD2	Aldehydes
ETH	ETH	ETH	Ethylene
FORM	FORM	FORM	Formaldehyde
ISOP	ISOP	ISOP	Isoprene
OLE	OLE	OLE	Olefins (anthropogenic only for PMCAMx and CAMx4)
	OLE2	OLE2	Olefins-biogenic (only for PMCAMx and CAMx4)
PAR	PAR	PAR	Paraffins
TOL	TOL	TOL	Toluene
XYL	XYL	XYL	Xylene
NH3	NH3	NH3	Ammonia
CO	CO	CO	Carbon monoxide
NO2	NO2	NO2	Nitrogen dioxide
NO	NO	NO	Nitrogen oxide
SULF	SULF	SULF	Sulfur
SO2	SO2	SO2	Sulfur dioxide
PMC			Primary PM-coarse "other" & crustal
PMFINE			Primary PM-fine "other" & crustal
PEC	PEC[1-10]	PEC	Primary PM-fine elemental carbon
PNO3	PNO3[1-10]	PNO3	Primary PM-fine nitrate
POA	POA[1-10]	POA	Primary PM-fine organic aerosol
PSO4	PSO4[1-10]	PSO4	Primary PM-fine sulfate
	CCRS[1-10]	CCRS	Primary PM-coarse crustal
	FCRS[1-10]	FCRS	Primary PM-fine crustal
	CPRM[1-10]	CPRM	Primary PM-coarse "other"
	FPRM[1-10]	FPRM	Primary PM-fine "other"

Currently, the SPECIATE system does not handle model species data. The current Carbon Bond-IV (CB-IV) version of these profiles, which is used by many modelers can be found on the EPA Emissions Modeling Clearinghouse (EMCH). The current table is based on profiles in SPECIATE 3.2: http://www.epa.gov/ttn/chief/emch/speciation/cbiv-profiles_mar_4_2002.xls).

Updating the model species table is thought to be an important item by members of the SPECIATE work group. If this table is not updated, air quality modelers may not take advantage of the new profiles in SPECIATE. The consequences are not limited to poor performance of air quality models but can also include inconsistencies between speciated emissions inventories and air quality modeling inventories, problematic State Implementation Plans (SIPs), and miss-directed control measures.

In addition to updating the model species profiles table with new profiles based on the new raw SPECIATE profiles, additional chemical compounds need to be mapped to the appropriate model species. The new SPECIATE profiles house tens to hundreds of individual compounds (e.g., xylene, benzene, etc.). As mentioned above, these comprehensive "raw" speciated profiles have to be converted into "model species" for air quality modeling. EPA has nearly completed an effort to develop code within SMOKE to convert raw (e.g., SPECIATE 3.2) profiles into model species profiles through work with the Carolina Environmental Program and Dr. Bill Carter. However, this mapping of new

compounds still needs to be done and may be incorporated into Phase II of the project (there are about 160 new VOC compounds that need to be mapped).

Table 2 provides an example of transforming a speciation profile in SPECIATE 3.2 into a model species profile format for use in air quality modeling. Table 2 is a TOG profile that is assigned to SCC 2501995120 (Storage and Transport: Petroleum and Petroleum Product Storage: All Storage Types: Working Loss: Gasoline). The petroleum marketing sector is often one of the top 10 area TOG emission sources.

The first step is to group individual compounds into appropriate categories. This mapping table is available at http://pah.cert.ucr.edu/~carter/emitdb/. Among the pollutants in Table 2, xylenes (m, o, p) are assigned to the XYL category as shown in Table 1 (Carter, 2004). Trimethylbenzene provides one mole of PAR and one mole of XYL. For profiles with methane, the methane is broken into 99% as NR (non-reactive) and 1% as PAR (paraffin). Acetone, n-butane, and n-hexane are grouped as PAR. This categorization step places all of the raw profile species into the appropriate model species group shown in the first column of Table 3.

After each raw species has been categorized, a few more steps are involved in calculating the mass fraction of each model species group. This series of procedures is described in the EPA document "Speciation Profiles and Assignment Files Located on EMCH" (http://www.epa.gov/ttn/chief/emch/speciation/emch_speciation_profile.pdf) and "Documentation of Speciation Preprocessor Programs for SMOKE" by Dr. Carter, presented in 2004 EPA Emission Inventory conference in Florida. Table 3 shows the converted model species profile based on the raw SPECIATE profile from Table 2.

Table 2. SPECIATE 3.2 profile # 1190 - gasoline marketing.

CAS No.	Pollutant	Percent
	M-XYLENE AND P-XYLENE	15.26
108-88-3	TOLUENE	15.22
95-47-6	O-XYLENE	6.41
25551-13-7	TRIMETHYLBENZENE	4.29
100-41-4	ETHYLBENZENE	4.07
110-54-3	N-HEXANE	3.91
	C8 PARAFFIN	3.84
25550-14-5	ETHYLTOLUENE	3.61
71-43-2	BENZENE	3.25
	ISOMERS OF BUTYLBENZENE	3.21
75-28-5	ISOBUTANE	2.65
79-29-8	2,3-DIMETHYLBUTANE	2.29
	C5 PARAFFIN	2.09
	C5 OLEFIN	1.91
142-82-5	N-HEPTANE	1.84
	METHYLPENTANE	1.76
	METHYLHEXANE	1.68
	C5-ALKYLBENZENES	1.43
	ETHYLDIMETHYLBENZENE	1.24
	C5 PARAFFIN/OLEFIN	1.08
25619-60-7	TETRAMETHYLBENZENE	1.03

Note: Due to file length, compounds less than 1% (by weight) are excluded from this table.

Table 3. Model species format for SPECIATE 3.2 profile # 1190 - gasoline marketing.

Species	Split Factor	Divisor	Mass Fraction
ALD2	0.000355	1	0.007679
FORM	2.5E-05	1	0.00035
ISOP	1.47E-06	1	0.0001
NR	0.002094	1	0.027333
OLE	0.000778	1	0.014494
PAR	0.026158	1	0.483296
TOL	0.002463	1	0.188683
XYL	0.003217	1	0.278265

IMPACT OF THE NEW SPECIATE DATA

The SPECIATE database update project has collected over 1,600 recent speciation profiles. Many of the new speciation profiles derived from these data will replace older counterparts in SPECIATE 3.2. For example, the SPECIATE 3.2 diesel exhaust profile was based on data collected over 20 years ago (see Table 4). The speciation profile is significantly different and much less detailed than the new profile (see Table 5). The previous profile has very limited use in the development of speciated emission estimates.

Following the steps described above, the model species profiles derived from the SPECIATE 3.2 profile and the new diesel exhaust profile are shown in Table 6. The model species profiles (mass fractions) are substantially different. Note that both FORM and ALD2 are much higher in the new profile, and that NR (nonreactive) species are much lower (aldehydes have a high ozone formation potential). Diesel exhaust is an important emission sector in most urban to regional scale inventories used for ozone modeling. The updates of speciation profiles and model species profiles are expected to greatly enhance the quality of modeling analyses of ozone, fine PM, and toxic air pollutants.

The other important note is that the new profiles contain speciated data for up to hundreds of compounds due to recent advances in technology. Since these tests are more comprehensive than those used to derive the older profiles in SPECIATE 3.2, there are approximately 160 new VOC compounds in the SPECIATE database. Preliminary review of profiles indicates that these new compounds (e.g., nonanal, decanal, undecanal) are in many of the new motor vehicle and combustion source TOG profiles.

New speciation data are available to cover the top 20 emission source sectors commonly-inventoried in the U.S. These are summarized in Table 7 below. The following examples are foreseeable major changes to future speciated and air quality modeling inventories using the new SPECIATE profiles:

1) Fireplaces (top # 6 VOC emissions, SCC 2104008001) and wood stoves (top # 11 VOC emission, SCC 2104008010) were assigned to a profile (Profile # 1167) which includes PAHs and aldehydes only – TAP emission estimates based on these profiles are overestimated. For an ongoing project that Pechan has, both sectors were assigned to Schauer's profile which has 22% methane and many other TOG species. Similar situations exist for forest fires (SCC 2810001000) and prescribed burning (SCC 2801500170, 2810015000);

2) By EPA default, VOC Profile Number 1190 (circa 1984) was assigned to the petroleum storage emission sector. This profile has no oxygenates like MTBE and ethanol, indicating that this profile does not properly characterize the source compositions (see Table 2). Based on recent source testing data, this sector is dominated by pentanes, MTBE, butanes, and other

species (xylenes) as shown in the recent profiles that Pechan incorporated into the database. VOC Profile 1190 contains xylenes (the largest constituent) at 22% by weight, compared to more recent data showing xylenes at less than 2%;

3) SCC 2460500000 (Solvent Utilization: Miscellaneous Non-Industrial: Consumer and Commercial: All Coatings and Related Products: Total: All Solvent Types) was assigned to an EPA VOC Profile 289 which has only one species – n-butyl alcohol. Consumer and commercial products are another important VOC source sector. Pechan recommended a profile from CARB, which is a composite profile including solvent and coating related products profiles. This CARB profile contains over 100 species and is now in the new SPECIATE database;

4) The onroad gasoline exhaust PM profile (35501) has 21% of crustal constituents and metals which are too high for a gasoline combustion source. Pechan recommends replacing this profile with those by DRI and Schauer et al. which have mostly elemental carbon and organic carbon. There are many gasoline exhaust PM profiles collected from many states in the new SPECIATE database;

5) Over 90% of onroad exhaust and evaporative VOC emissions were assigned to a single EPA Profile 1101. This profile was based on 45 cars fueled by leaded gasoline, circa 1987. There are many new non-leaded gasoline profiles by source sector (e.g. starts, hot soak, exhaust, etc.) incorporated into the new SPECIATE database. As can be imagined, emissions from gasoline combustion and evaporation are totally different processes. They should be characterized differently. On the other hand, there is also a need within SPECIATE for new composite profiles that can be applied directly to the source categories commonly developed in the United States. As an example, for the onroad sector, a composite profile is needed for VOC emissions from light-duty gasoline vehicles (which are often reported as a composite of exhaust and evaporative emissions); and

6) Diesel exhaust VOC is assigned to Profile 1201 in SPECIATE 3.2 which includes "C2 compounds 20%, C3 compounds", etc (see Table 4). Few individual species are provided. New profiles based on studies sponsored by CARB and the Coordinating Research Council are more appropriate for this important sector.

ADDITIONAL RECOMMENDATIONS FOR SPECIATE

The following is a short list of additional recommendations for future work that Pechan feels is needed for the SPECIATE database:

1. Develop a set of composite profiles for important source sectors. Most inventories prepared in the U.S. are developed at a level of aggregation higher than that embodied in the SPECIATE profiles. For example, motor vehicle VOC emissions are often composites of exhaust and evaporative source components. Similarly, PM emissions are composites of exhaust and brake/tire wear;

2. Incorporate additional motor vehicle speciation data. A large amount of speciation data are available from CARB, EPA's Office of Transportation and Air Quality, and the Coordinating Research Council. The current coverage of these important sources by SPECIATE is less than optimum;

3. Revise profiles containing large amounts of unresolved mixtures. The best example of these are VOC profiles assigned to solvents or coatings categories containing large amounts of mineral spirits or other petroleum distillates. In some cases, the profile may contain unresolved mixtures

of 30% by mass. Speciation data are available for these unresolved mixtures, and they should be put to use to reflect complete profiles. This issue has large implications for both air quality modeling and speciated inventory development; and

4. Revise the SPECIATE front-end software. Until, the SPECIATE front-end software is updated, the new profile data structure (including all of the meta data) can not be populated into the system.

Table 4. SPECIATE 3.2 Diesel Exhaust VOC profile #1201.

Profile Name Light-Duty Diesel Vehicles

Controls Uncontrolled

Original Quality C

Date Profile Added 1/5/89

CAS No.	Pollutant	Percent
75070	ACETALDEHYDE	2.91
100527	BENZALDEHYDE	0.55
	C-1 COMPOUNDS	5.8
	C-10 COMPOUNDS	3.52
	C-11 COMPOUNDS	3.58
	C-12 COMPOUNDS	2.2
	C-13 COMPOUNDS	3.43
	C-14 COMPOUNDS	4.45
	C-15 COMPOUNDS	4.35
	C-16 COMPOUNDS	3.49
	C-17 COMPOUNDS	3.06
	C-18 COMPOUNDS	2.04
	C-19 COMPOUNDS	1.56
	C-2 COMPOUNDS	19.96
	C-20 COMPOUNDS	0.91
	C-21 COMPOUNDS	0.75
	C-22 COMPOUNDS	0.59
	C-23 COMPOUNDS	0.48
	C-24 COMPOUNDS	0.48
	C-25 COMPOUNDS	0.54
	C-26 COMPOUNDS	0.44
	C-27 COMPOUNDS	0.22
	C-28 COMPOUNDS	0.32
	C-29 COMPOUNDS	0.14
	C-3 COMPOUNDS	5.21
	C-30 COMPOUNDS	0.32
	C-31 COMPOUNDS	0.29
	C-32 COMPOUNDS	0.27
	C-33 COMPOUNDS	0.22
	C-34 COMPOUNDS	0.24
	C-35 COMPOUNDS	0.16
	C-36 COMPOUNDS	0.2
	C-37 COMPOUNDS	0.08
	C-38 COMPOUNDS	0.05
	C-39 COMPOUNDS	0.11
	C-4 COMPOUNDS	4.08
	C-40 COMPOUNDS	0.02
	C-41 COMPOUNDS	0.05
	C-42 COMPOUNDS	0.02
	C-43 COMPOUNDS	0.01
	C-5 COMPOUNDS	2.36
	C-6 COMPOUNDS	4.3
	C-7 COMPOUNDS	2.89
	C-8 COMPOUNDS	1.13
	C-9 COMPOUNDS	0.75
123739	CROTONALDEHYDE	1.01
50000	FORMALDEHYDE	8.61
66251	HEXANAL	0.08
123386	PROPIONALDEHYDE	1.77

Table 5. New Diesel Exhaust VOC Profile

Pollutant	CAS No.	Percent	Molecular Weight
Acetaldehyde	75-07-0	22.6161	44.05
Formaldehyde	50-00-0	12.0656	30.03
Propionaldehyde	123-38-6	7.5748	58.08
Crotonaldehyde	4170-30-3	7.2502	70.09
Ethylene	74-85-1	4.6314	28.05
Methyl ethyl ketone (2-butanone)	78-93-3	4.0579	72.1
Acetophenone	98-86-2	2.7594	120.15
Acetylene	74-86-2	2.4889	26.04
2-methyl-2-propenal	78-85-3	2.1642	70.09
Toluene	108-88-3	2.1534	92.13
N-butane	106-97-8	2.0722	58.12
Benzaldehyde	100-52-7	2.0560	106.13
Acrolein (2-propenal)	107-02-8	1.8396	56.07
Heptanal	111-71-7	1.7314	114.19
Octanal	124-13-0	1.6773	128.21
Isopentane	78-78-4	1.4825	72.15
Benzene	71-43-2	1.4825	78.11
M & p-xylene	1330-20-7	1.2607	106.168
Hexaldehyde	66-25-1	1.1903	100.16
Glyoxal	107-22-2	1.1362	58.04
N-pentane	109-66-0	1.0064	72.15
Methylglyoxal	78-98-8	0.9198	72.0634
Butyraldehyde	123-72-8	0.7034	72.12
2,2,4-trimethylpentane	540-84-1	0.6709	114.22
Isobutylene	115-11-7	0.6168	56.1
2-methylpentane	107-83-5	0.5032	86.17
diacetyl	431-03-8	0.4870	86.0902
1,2,4-trimethylbenzene (1,3,4-trimethylbenzene)	95-63-6	0.4761	120.19
O-xylene	95-47-6	0.4491	106.16
Propylene	115-07-1	0.4220	42.08
2,3-dimethylpentane	565-59-3	0.3896	100.2
Hexadecane	544-76-3	0.3847	226.44
3-methylpentane	96-14-0	0.3625	86.17
Tetradecane	629-59-4	0.3403	198.39
Methylcyclopentane	96-37-7	0.3355	84.16
Naphthalene	91-20-3	0.3338	128.17
Heptadecane	629-78-7	0.3322	240.47
2-methylnaphthalene	91-57-6	0.3306	142.2
Octadecane	593-45-3	0.3252	254.49
2,3-dimethylbutane	79-29-8	0.3084	86.17
2-methylhexane	591-76-4	0.3084	100.2
Methylcyclohexane	108-87-2	0.2813	98.21
1-Methyl-4-ethylbenzene	622-96-8	0.2813	120.2
Trans-2-butene	624-64-6	0.2813	56.11
N-dodecane	112-40-3	0.2722	170.33
N-tridecane	629-50-5	0.2581	184.36
Ethylbenzene	100-41-4	0.2543	106.16
N-heptane	142-82-5	0.2543	100.2

Pollutant	CAS No.	Percent	Molecular Weight
Nonadecane	629-92-5	0.2224	268.52
2,4-dimethylpentane	108-08-7	0.2218	100.2
Cyclopentane	287-92-3	0.2218	70.14
Pentadecane	629-62-9	0.2153	212.41
1-Methylnaphthalene	90-12-0	0.2045	142.2
1,3-butadiene	106-99-0	0.1677	54.09
2,2-dimethylbutane	75-83-2	0.1677	86.17
2,3,4-trimethylpentane	565-75-3	0.1677	114.22
3-methylhexane	589-34-4	0.1677	100.2
1,3,5-trimethylbenzene	108-67-8	0.1407	120.19
2-methyl-1-butene	563-46-2	0.1407	70.13
Cis-2-butene	590-18-1	0.1407	56.11
N-octane	111-65-9	0.1407	114.23
Nonanoic acid	112-05-0	0.1299	158.24
2-methyl-2-pentene	625-27-4	0.1136	84.16
3-ethylhexane	619-99-8	0.1136	114.23
Cyclohexane	110-82-7	0.1136	84.16
Cyclopentene	142-29-0	0.1136	68.11
1-Methyl-3-ethylbenzene	620-14-4	0.1136	120.19
Eicosane	112-95-8	0.1115	282.55
Undecanoic acid	112-37-8	0.1115	186.29
2,3-dimethylhexane	584-94-1	0.0866	114.22
3-methyl-1-butene	563-45-1	0.0866	70.13
N-nonane	111-84-2	0.0866	128.26
Trans-2-hexene	4050-45-7	0.0866	84.16
Octanoic acid	124-07-2	0.0676	144.21
2-methylheptane	592-27-8	0.0541	114.23
Cis-2-hexene	7688-21-3	0.0541	84.16
N-propylbenzene	103-65-1	0.0541	120.19
Phenanthrene	85-01-8	0.0504	178.23
Pentylcyclohexane	4292-92-6	0.0454	154.2948
Decanoic acid-TMS	334-48-5	0.0394	172.26
2-methylcholanthrene	129-00-0	0.0389	202.25
Acenaphthylene	208-96-8	0.0379	152.19
n-Heneicosane	629-94-7	0.0356	296.57
Fluorene	86-73-7	0.0353	166.22
Lauric acid-TMS	143-07-7	0.0317	200.32
Fluoranthene	206-44-0	0.0287	202.25
2,4-dimethylhexane	589-43-5	0.0271	114.22
2,5-dimethylhexane	592-13-2	0.0271	114.22
Trans-2-pentene	646-04-8	0.0271	70.13
Decylcyclohexane	1795-16-0	0.0207	224.4288
Fluorene	86-73-7	0.0187	166.22
3-methyl-phenanthrene	832-71-3	0.0164	192.2598
Dibenzofuran , also noted as "DBZFUR"	132-64-9	0.0155	168.19
Octylcyclohexane	1795-15-9	0.0142	196.3752
N-Nonylcyclohexane	2883-02-5	0.0134	210.4
9-methylphenanthrene	883-20-5	0.0124	192.2598
Heptylcyclohexane	5617-41-4	0.0108	182.3484
Acenaphthene	83-32-9	0.0104	154.21

Pollutant	CAS No.	Percent	Molecular Weight
1-methylphenanthrene	832-69-9	0.0092	192.26
Hexylcyclohexane	4292-75-5	0.0081	168.3216
Tridecanoic acid-TMS	638-53-9	0.0071	214.34
Anthracene	120-12-7	0.0068	178.23
Anthracene, 2-methyl-	613-12-7	0.0056	192.26
Benzo[ghi]fluoranthene	203-12-3	0.0031	226.28
Myristic acid-TMS	544-63-8	0.0029	228.37
Chrysene	218-01-9	0.0018	228.29
Benz(a)anthracene	56-55-3	0.0016	228.29
Cyclopenta[cd]pyrene	27208-37-3	0.0011	228.29

Table 6. Comparison of diesel exhaust profiles in SPECIATE 3.2 and the new SPECIATE database.

		SPECIATE 3.2 Profile #1201		New SPECIATE Profile	
Model Species	Symbol	Split Factor	Mass Fraction	Split Factor	Mass Fraction
Paraffins	PAR	0.0224	0.4734	1.5944	0.2530
Olefins	OLE	0.0019	0.0381	0.1688	0.0607
Toluene	TOL	0.0017	0.0438	0.0494	0.0371
Xylene	XYL	0.0002	0.0050	0.0327	0.0278
Formaldehyde	FORM	0.0029	0.0861	0.4471	0.1347
Aldehydes	ALD2	0.0014	0.0472	0.9088	0.3597
Ethylene	ETH	0.0035	0.0665	0.1651	0.0463
Non-reactive	NR	0.0142	0.2397	0.4387	0.0807

Table 7. Examples of Important Source Sectors Covered by New Data in SPECIATE.

1999 NEI VOC Sectors			1999 NEI PM_{10} Sectors		
Rank	(ton/day)	Primary Source	Rank	(ton/day)	Primary Sources
1	9906	Gasoline Motor Vehicle/Nonroad	1	1235	Prescribed/Wildfires
2	3275	Surface Coatings	2	995	Agricultural Equipment
3	3118	Gasoline Refueling	3	910	Unpaved Roads
4	2355	Degreasing	4	520	Electric Generation
5	2201	Diesel Vehicles	5	505	Diesel On-Highway
6	1733	Automotive Aftermarket	6	490	Quarry, Mining
7	1581	Heavy-Duty Gasoline Vehicles	7	374	Electric Generation Coal
8	1491	Pesticides	8	344	Woodstoves
9	1343	Misc. Solvents and Adhesives	9	250	Wood Boiler
10	1087	Asphalt	10	216	Light Duty Gasoline
11	906	Non-Industrial Adhesives	11	176	Paved Road Dust
12	903	Oil and Gas Production	12	161	EGU Oil
13	720	Wood Furniture	13	147	Pulp and Paper Sulfate
14	685	Personal Care Products	14	137	Agricultural dust
15	679	Auto Refinishing	15	134	Nonroad Equipment
16	677	Fireplaces	16	101	Gray Iron Foundries
17	631	Dry Cleaning			
18	606	Graphic Arts			
19	540	Household Products			

KEYWORD
Speciation profile
SPECIATE
Speciated emissions inventories
Model species