

# What's New in SPECIATE 4.2?

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Presented by:

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# What is SPECIATE?

- Database of speciated emissions profiles by source category
- Species include metals, ions, elements, organic and inorganic compounds
- Consistent Units
- Contains three categories:
  - Particulate matter (PM)
  - Volatile organic compounds (VOC)
  - Other Gases (e.g. Hg, NO/NO<sub>2</sub>/HONO, semi-volatile organic compounds)
- PM profiles are size-segregated (e.g. PM<sub>10</sub>, PM<sub>2.5</sub>)
- Housed in Microsoft Access database



# Development of SPECIATE

- **Collaboration involving:**
  - EPA's Office of Research and Development (ORD)
  - Office of Air Quality Planning and Standards (OAQPS)
  - Office of Transportation and Air Quality (OTAQ)
  - Environment Canada
  - SPECIATE Workgroup



# Why Do We Need SPECIATE?

- Create speciated emissions inventories for photochemical modeling
- Estimate toxic air pollutant emissions from various emission sources
- Provide input to source-receptor models (CMB)
- Verify profiles derived from ambient measurements using multivariate receptor models (e.g., factor analysis and positive matrix factorization)
- Provide a repository of compounds searchable by source category and pollutant



# Brief History of SPECIATE Database

- Paper and computerized versions available in 1988 for EPA applications
- First electronic version (CD) distributed to the user community in 1993
- SPECIATE 3.2 posted to EPA's CHIEF website in Nov 2002
- SPECIATE 4.0 posted to EPA's CHIEF website Jan 2007
- SPECIATE 4.1 completed October 2007 for Environment Canada; final results included in SPECIATE 4.2
- SPECIATE 4.2 – Final Report Expected in April 2009, Web Browser posted March 2009



## Brief History (continued)

- SPECIATE 3.2 (2002)
  - Has a front-end via desk top application
  - 1503 PM profiles
  - 565 gas profiles
  - 890 unique species
- SPECIATE 4.0 (2007)
  - Housed in MS Access®
  - 2,865 PM profiles
  - 1,215 gas profiles
  - 1,902 unique species



# SPECIATE 4.2

- 3,326 PM profiles;
- 1,624 organic gas profiles;
- 237 Other Gases profiles;
- A total of 2,207 unique species
- Composite profiles for 58 (47 PM and 11 VOC) source categories;
- Every profile has been assigned to a SCC
- An updated SCC-to-SPECIATE profile cross-reference table accounting for over 80% of national VOC and PM emissions in the 2002 National Emissions Inventory (NEI)



# SPECIATE 4.2 (continued)

- Final Report is In-Press
- VOC-to-TOG conversion factors for applicable gas profiles;
- A protocol for expansion of the database;
- A mapping of the new VOC compounds into model species categories;
- Review and prioritization of 49 studies entailing 614 PM and 822 VOC profiles for potential inclusion in the future SPECIATE database.
- Web application developed to provide access through a simple web interface - allows complex searches and downloads



# Example of SPECIATE Data

Category	Subcategory	Profile Type	Bar Chart
Motor Vehicle (1,653 profiles)	Gasoline Exhaust Gasoline Diurnal Evaporative Gasoline Hot Soak Liquid Gasoline Diesel Exhaust Diesel Headspace Evaporative Tire Wear Brake Wear	TOG; PM; SVOC; Hg; NO/NO <sub>2</sub> / HONO	Figure 1
Agricultural Burning (78 profiles)	Rice Straw Wheat Straw	VOC; PM	Figures 2 & 3
Forest Fire (99 profiles)	Ponderosa Pine Loblolly Pine Western Hemlock Aceraceae/ Fagaceae Palmae/ Pinaceae Poaceae/Pinaceae	VOC; PM	Figure 4
Fireplace/ Wood Stove (144 profiles)	Pine Oak Eucalyptus	VOC; PM	Figure 4

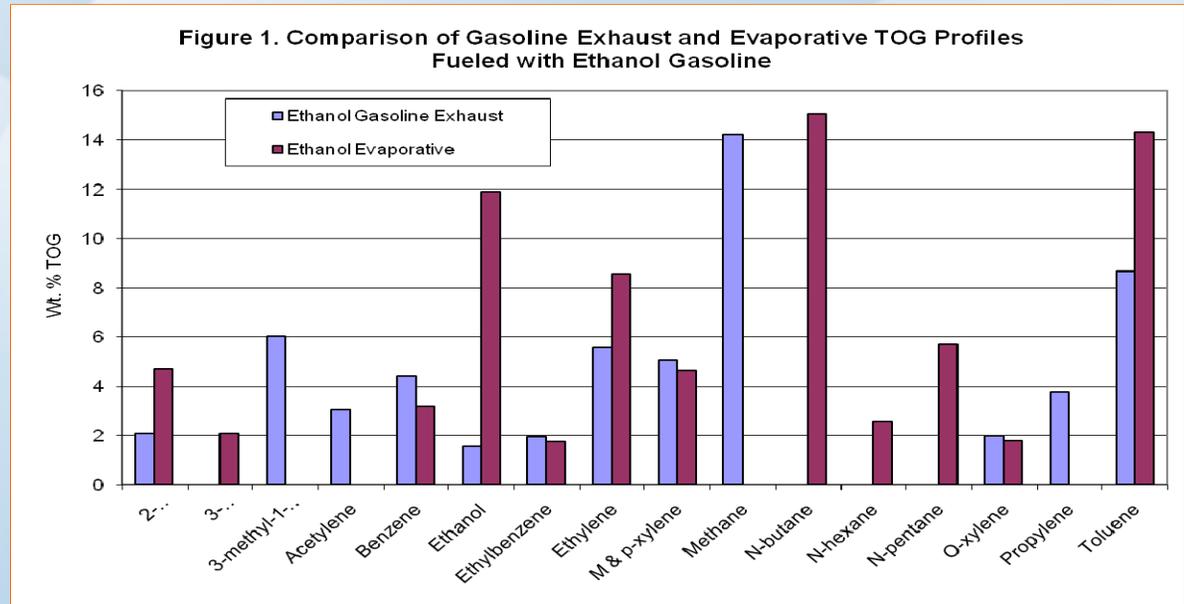


# Example Profiles

- Motor Vehicle (1,653 profiles)

- TOG; PM; SVOC; Hg;  
NO/NO2/HONO

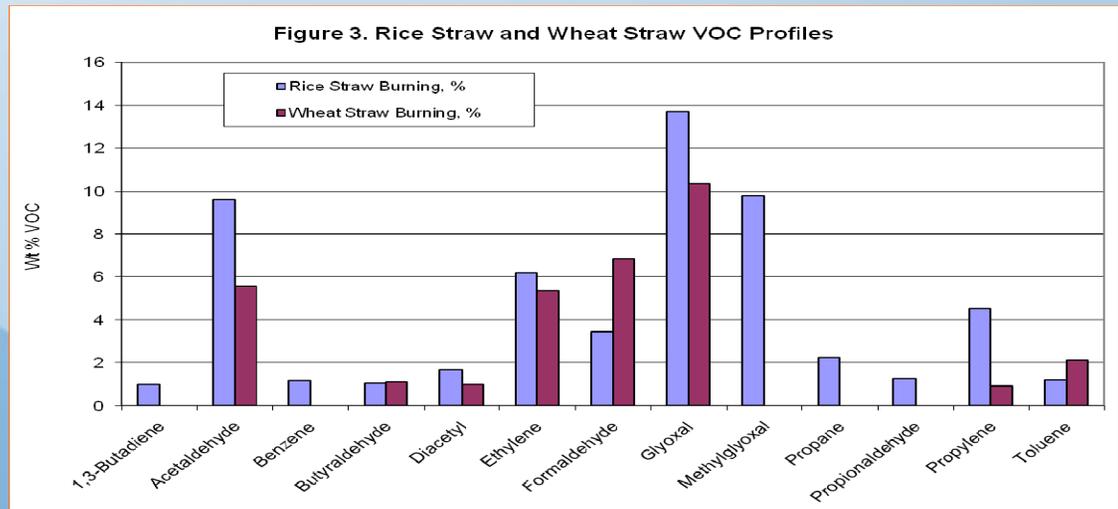
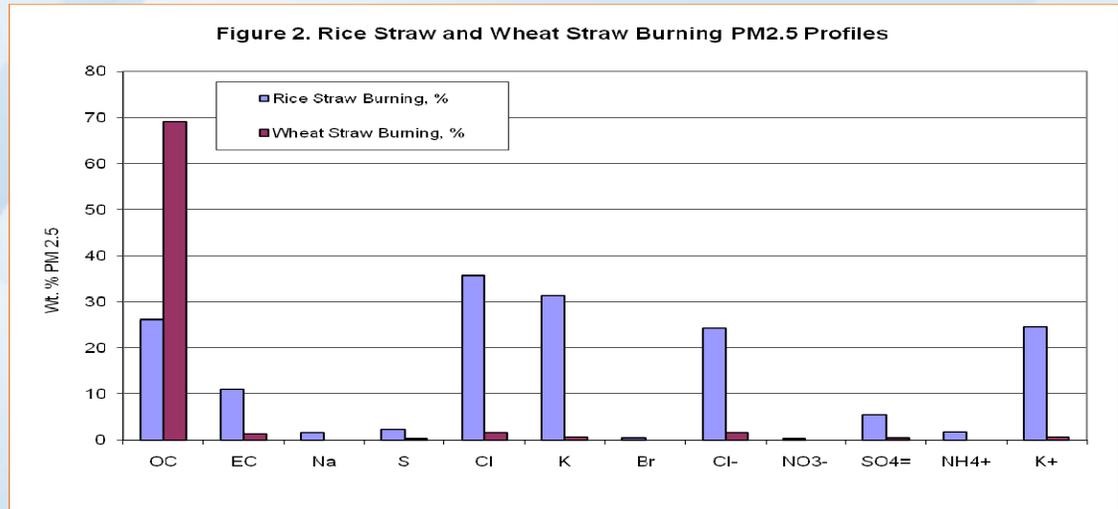
- Gasoline Exhaust
- Gasoline Hot Soak
- Liquid Gasoline
- Diesel Exhaust
- Tire Wear
- Brake Wear
- Diesel Headspace Evaporative
- Gasoline Diurnal Evaporative





# Example Profiles (continued)

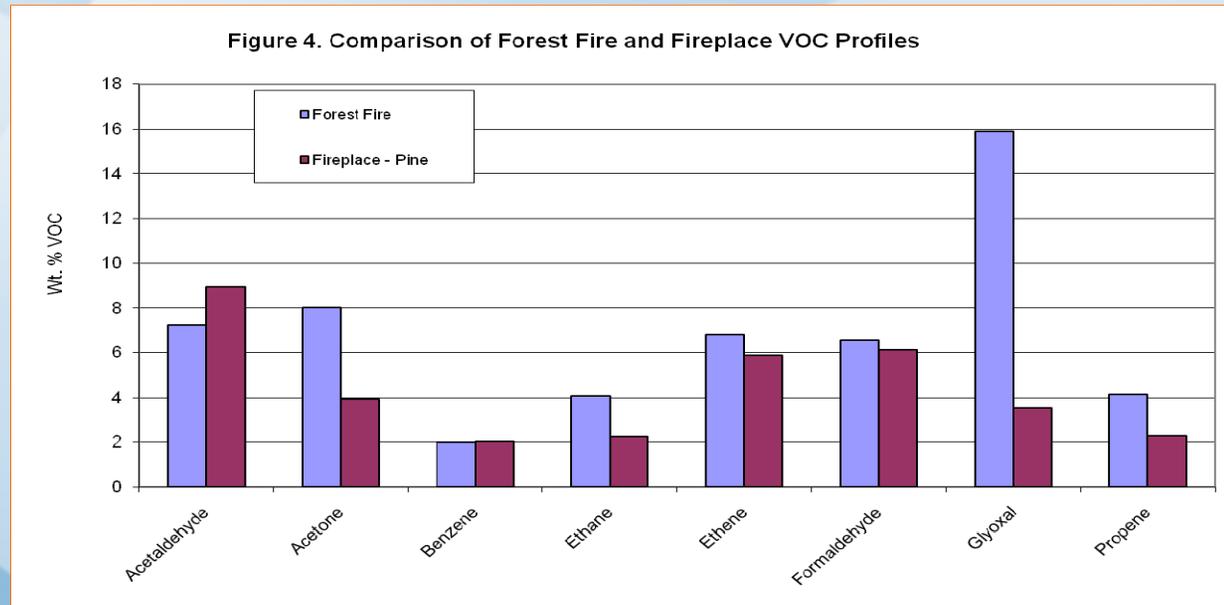
- Agricultural Burning (78 profiles)
- Rice Straw, Wheat Straw
- VOC; PM





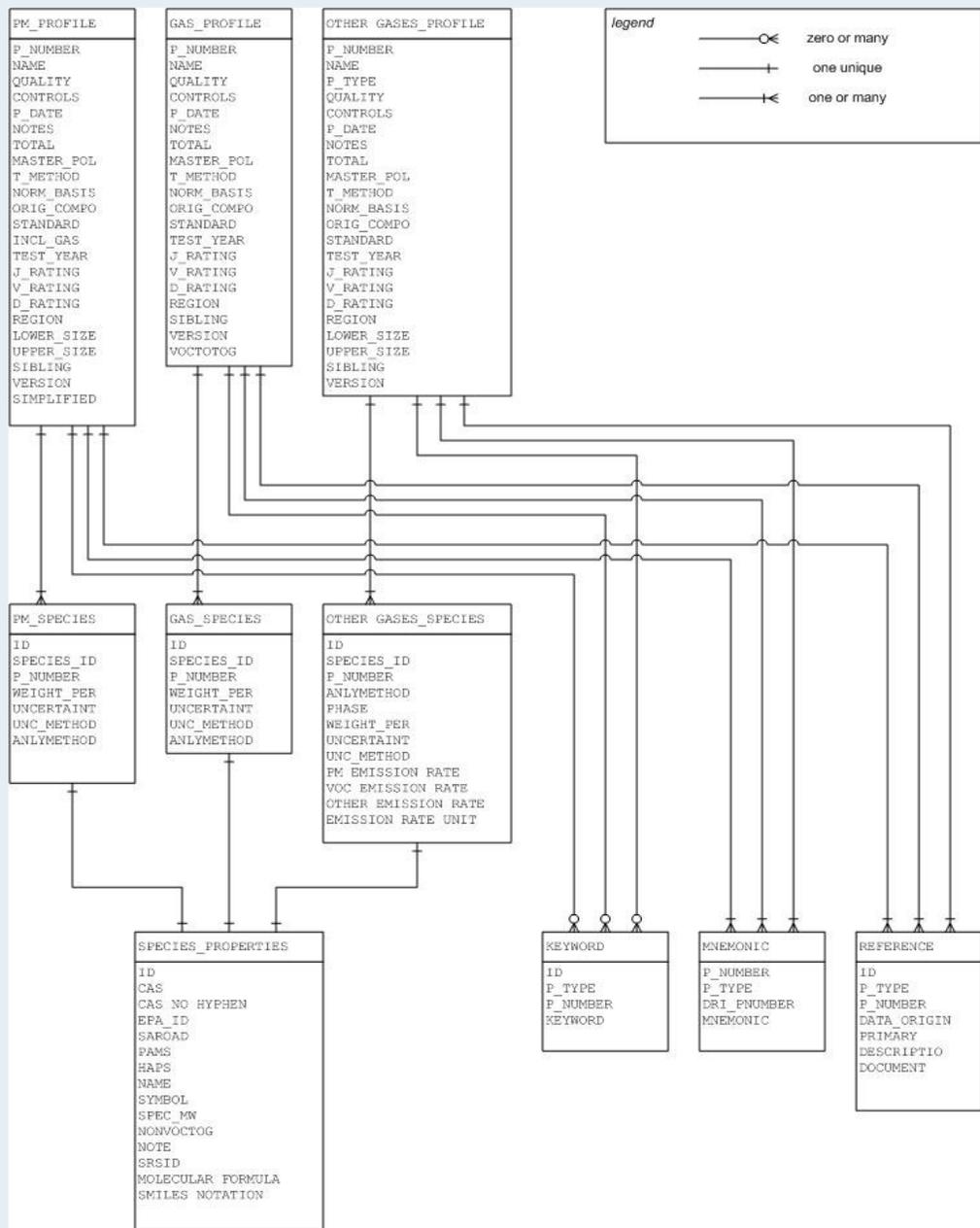
# Example Profiles (continued)

- Forest Fire (99 profiles) VOC, PM
  - Ponderosa Pine
  - Loblolly Pine
  - Western Hemlock
  - Aceraceae/ Fagaceae
  - Palmae/ Pinaceae
  - Poaceae/Pinaceae
- Fireplace/Wood Stove (144 profiles) VOC; PM
  - Pine
  - Oak
  - Eucalyptus





# SPECIATE Data Diagram



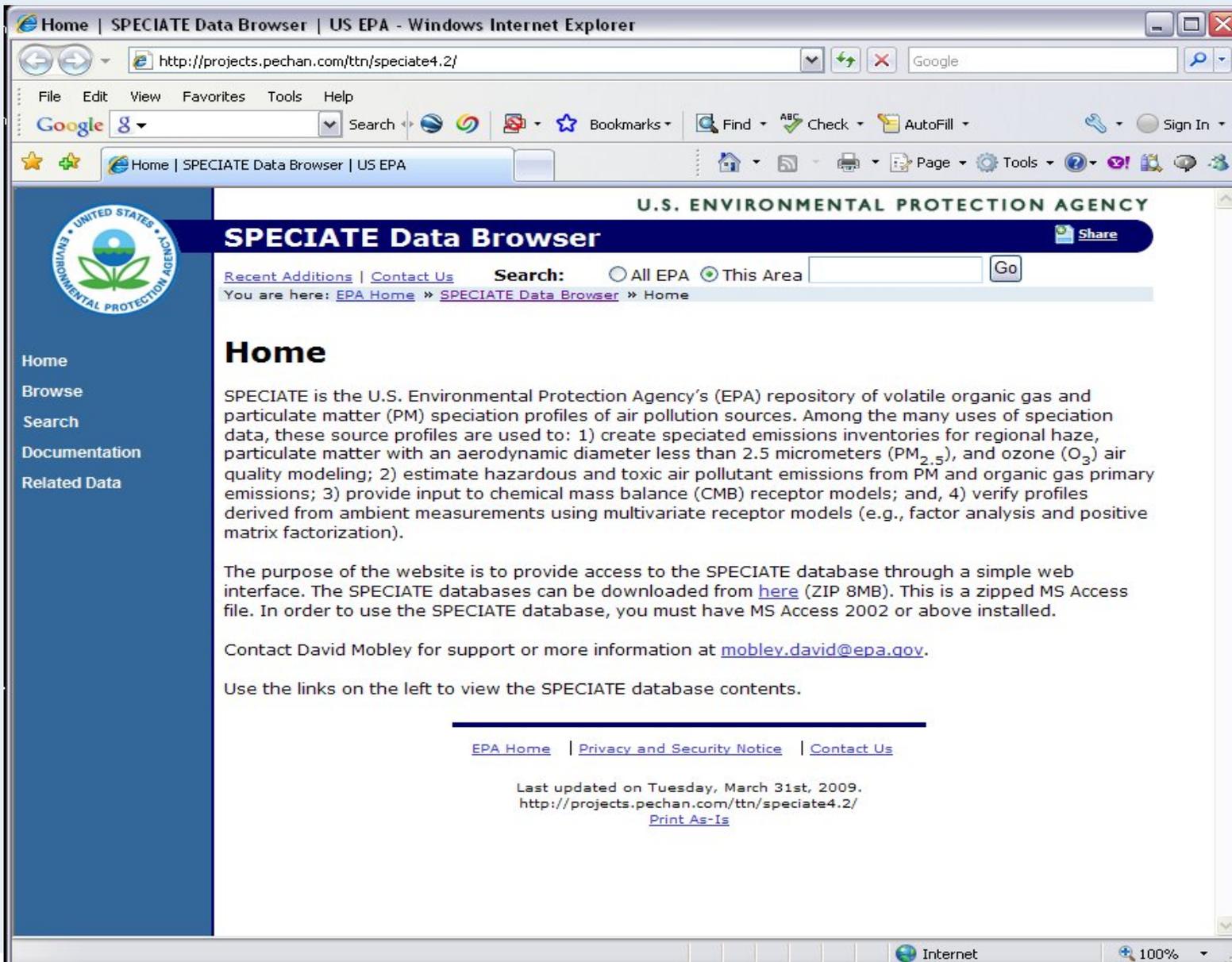


# The SPECIATE Data Browser

- Web-based application
  - ColdFusion® and Oracle®
- Accessed through internet browser
- Allows data searches by pollutant, key word, and category
- Allows data download
- No need to purchase or use Access

<http://projects.pechan.com/ttn/speciate4.2/>

# Home Index Screen



The screenshot shows a web browser window with the address bar displaying <http://projects.pechan.com/ttn/speciate4.2/>. The browser's title bar reads "Home | SPECIATE Data Browser | US EPA - Windows Internet Explorer". The page content includes the EPA logo, the title "SPECIATE Data Browser", a search bar with "All EPA" selected, and a navigation menu on the left with links for Home, Browse, Search, Documentation, and Related Data. The main text area contains a "Home" heading, a paragraph describing the SPECIATE database, a paragraph about the website's purpose, and contact information for David Mobley. At the bottom, there are links for "EPA Home", "Privacy and Security Notice", and "Contact Us", along with a "Last updated" date of Tuesday, March 31st, 2009, and a "Print As-Is" link.

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## Home

SPECIATE is the U.S. Environmental Protection Agency's (EPA) repository of volatile organic gas and particulate matter (PM) speciation profiles of air pollution sources. Among the many uses of speciation data, these source profiles are used to: 1) create speciated emissions inventories for regional haze, particulate matter with an aerodynamic diameter less than 2.5 micrometers (PM<sub>2.5</sub>), and ozone (O<sub>3</sub>) air quality modeling; 2) estimate hazardous and toxic air pollutant emissions from PM and organic gas 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).

The purpose of the website is to provide access to the SPECIATE database through a simple web interface. The SPECIATE databases can be downloaded from [here](#) (ZIP 8MB). This is a zipped MS Access file. In order to use the SPECIATE database, you must have MS Access 2002 or above installed.

Contact David Mobley for support or more information at [mobley.david@epa.gov](mailto:mobley.david@epa.gov).

Use the links on the left to view the SPECIATE database contents.

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<http://projects.pechan.com/ttn/speciate4.2/>  
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Internet 100%



# Keyword Search

Keyword Search | SPECIATE Data Browser | US EPA - Windows Internet Explorer

http://projects.pechan.com/ttn/speciate4.2/ehpa\_speciate\_search.cfm?txtKeywords=Road+Dust+and+TX&btnSearch=Search&optProfileType=P

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## Keyword Search

Road Dust and TX

**Profile Type**

- Volatile Organic Compound (VOC)
- Particulate Matter (PM)
  - PM Composite
  - PM Simplified
  - PM Detailed

[Search Help](#)

### Results

26 profiles

Details	Name	Controls	Notes	Version	
<a href="#">View [4349]</a>	Unpaved Road Dust	Uncontrolled	Composite of two unpaved road dust profiles from Guadalupe, TX, and Eagle Pass, TX (BVUNPV06 and BVUNPV09).	SPECIATE 4.0	<input type="button" value="Add to Cart"/>
<a href="#">View [4348]</a>	Unpaved Road Dust	Uncontrolled	Composite of two unpaved road dust profiles from Guadalupe, TX, and Eagle Pass, TX (BVUNPV06 and BVUNPV09).	SPECIATE 4.0	<input type="button" value="Add to Cart"/>
<a href="#">View [4347]</a>	Paved Road Dust	Uncontrolled	Composite of five paved road dust profiles from San Antonio, TX, and Laredo, TX (BVPVRD01, BVPVRD02, BVPVRD03, BVPVRD04, and BVPVRD05).	SPECIATE 4.0	<input type="button" value="Add to Cart"/>
<a href="#">View [4346]</a>	Paved Road Dust	Uncontrolled	Composite of five paved road dust profiles from San Antonio, TX, and Laredo, TX (BVPVRD01, BVPVRD02, BVPVRD03, BVPVRD04, and BVPVRD05).	SPECIATE 4.0	<input type="button" value="Add to Cart"/>
<a href="#">View [4221]</a>	Unpaved Road Dust	Uncontrolled	Unpaved road dust sample from Eagle Pass, TX, collected from aerosol sampling site dirt road (path) immediately next to sampler on 09/17/99.	SPECIATE 4.0	<input type="button" value="Add to Cart"/>
<a href="#">View [4220]</a>	Unpaved Road Dust	Uncontrolled	Unpaved road dust sample from Eagle Pass, TX, collected from aerosol sampling site dirt road (path) immediately next to sampler on 09/17/99.	SPECIATE 4.0	<input type="button" value="Add to Cart"/>
<a href="#">View [4219]</a>	Unpaved Road Dust	Uncontrolled	Unpaved road dust sample from Guadalupe, TX, collected from road next to sample shed on 11/01/99.	SPECIATE 4.0	<input type="button" value="Add to Cart"/>
<a href="#">View [4218]</a>	Unpaved Road Dust	Uncontrolled	Unpaved road dust sample from Guadalupe, TX, collected from road next to sample shed on 11/01/99.	SPECIATE 4.0	<input type="button" value="Add to Cart"/>



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## Browse Details

Profile Information	
<b>Number</b>	4349 <a href="#">Add to Cart</a>
<b>Name</b>	Unpaved Road Dust
<b>Master Pollutant</b>	PM
<b>Region</b>	Western Texas
<b>Controls</b>	Uncontrolled
<b>Notes</b>	Composite of two unpaved road dust profiles from Guadalupe, TX, and Eagle Pass, TX (BVUNPV06 and BVUNPV09).
<b>Test Year</b>	2002
<b>Entry Date</b>	Jun 30, 2004
<b>Version</b>	SPECIATE 4.0
<b>Particle Size Range</b>	0 µm to 2.5 µm

Name	Weight %	Uncertainty %	Analytical Method	Uncertainty Method
<a href="#">Aluminum</a> (Al)	3.3809	0.8635	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Ammonia</a> (NH3)	0	0	Automated Colorimetry	Standard deviation
<a href="#">Ammonium</a> (NH4+)	0.0525	0.0371	Automated Colorimetry	Standard deviation
<a href="#">Antimony</a> (Sb) [HAPS]	0.0011	0.0143	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Arsenic</a> (As) [HAPS]	0.001	0.0017	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Barium</a> (Ba)	0.3341	0.4062	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Bromine Atom</a> (Br)	0.0072	0.0063	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Cadmium</a> (Cd) [HAPS]	0	0.009	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Calcium</a> (Ca)	28.5589	4.0727	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Chloride ion</a> (Cl-)	0.0479	0.0301	Ion Chromatography (IC)	Standard deviation
<a href="#">Chlorine atom</a> (Cl)	0	0.1841	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Chromium</a> (Cr)	0.0049	0.0037	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Cobalt</a> (Co) [HAPS]	0	0.0248	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Copper</a> (Cu)	0.0026	0.0008	X-Ray Fluorescence (XRF)	Standard deviation
<a href="#">Elemental Carbon</a> (EC) [PAMS]	0.1549	1.0646	Thermal/Optical Reflectance	Standard deviation
<a href="#">Elemental carbon I</a> (EC1)	0.8244	0.4211	Thermal/Optical Reflectance	Standard deviation



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[ # [A](#) [B](#) [C](#) **D** [L](#) [M](#) [N](#) [O](#) [P](#) [S](#) ]

Name	Symbol	HAPS	PAMS
<a href="#">Di(2-ethylhexyl)phthalate</a>		Yes	No
<a href="#">Dibenzofuran , also noted as "DBZFUR"</a>	DBZF	Yes	No
<a href="#">Dibutyl phthalate</a>		Yes	No
<a href="#">Dimethyl phthalate</a>		Yes	No

[ # [A](#) [B](#) [C](#) **D** [L](#) [M](#) [N](#) [O](#) [P](#) [S](#) ]

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[http://projects.pechan.com/ttn/speciate/ehpa\\_speciate\\_browse\\_pollutant.cfm?pType=P&bHAPS=1&strBrowseFilter=D](http://projects.pechan.com/ttn/speciate/ehpa_speciate_browse_pollutant.cfm?pType=P&bHAPS=1&strBrowseFilter=D)  
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# Results for Dibenzofuran

<a href="#">View [4400]</a>	Oil Refinery	Unknown	Dilution tunnel sampling of a combined cycle generating unit employing a General Electric Frame 7FA gas turbine with steam augmentation at Site E. The unit is a single shaft design, with the single generator driven by a shaft common to both the gas and the steam turbine. Hot exhaust gases from the turbine pass through a heat recovery steam generator (HRSG) before venting into the atmosphere via the stack. The total nominal capacity of the cogeneration facility is 240 MW. The unit fired natural gas for these tests. #2 run (9/7/01).	<a href="#">Add to Cart</a>
<a href="#">View [4401]</a>	Oil Refinery	Unknown	Dilution tunnel sampling of a combined-cycle generating unit employing a General Electric Frame 7FA gas turbine with steam augmentation at Site E. The unit is a single shaft design, with the single generator driven by a shaft common to both the gas and the steam turbine. Hot exhaust gases from the turbine pass through a heat recovery steam generator (HRSG) before venting into the atmosphere via the stack. The total nominal capacity of the cogeneration facility is 240 MW. The unit fired natural gas for these tests. #3 run (9/8/01).	<a href="#">Add to Cart</a>
<a href="#">View [4403]</a>	Oil Refinery	Unknown	Average of CCGU_E1, CCGU_E2 and CCGU_E3.	<a href="#">Add to Cart</a>
<a href="#">View [4558]</a>	Vehicle exhaust - gasoline - Catalyst	Catalytic converter	Weight percentages are from the undened sampling train. Downstream of the organics denuder, OC = 31.8% of the fine particle mass.	<a href="#">Add to Cart</a>
<a href="#">View [4559]</a>	Vehicle exhaust - gasoline - Noncatalyst	None	Weight percentages are from the undened sampling train. Downstream of the organics denuder, OC = 58.3% of the fine particle mass.	<a href="#">Add to Cart</a>
<a href="#">View [4675]</a>	Medium duty trucks - diesel	Catalytic converter	Weight percentages are from the filter downstream of an organics denuder. On the undened filter, OC = 30.4% of the fine particle mass.	<a href="#">Add to Cart</a>

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[http://projects.pecan.com/ttn/speciate/ehpa\\_speciate\\_browse.cfm?ptype=P&pollutant=873](http://projects.pecan.com/ttn/speciate/ehpa_speciate_browse.cfm?ptype=P&pollutant=873)

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# Results for profile 4400

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Profile Information	
<b>Number</b>	4400 <input type="button" value="Add to Cart"/>
<b>Name</b>	Oil Refinery
<b>Master Pollutant</b>	PM
<b>Region</b>	United States
<b>Controls</b>	Unknown
<b>Notes</b>	Dilution tunnel sampling of a combined-cycle generating unit employing a General Electric Frame 7FA gas turbine with steam augmentation at Site E. The unit is a single shaft design, with the single generator driven by a shaft common to both the gas and the steam turbine. Hot exhaust gases from the turbine pass through a heat recovery steam generator (HRSG) before venting into the atmosphere via the stack. The total nominal capacity of the cogeneration facility is 240 MW. The unit fired natural gas for these tests. #2 run (9/7/01).
<b>Test Year</b>	2001
<b>Entry Date</b>	Jun 30, 2004
<b>Version</b>	SPECIATE 4.0
<b>Particle Size Range</b>	0 µm to 2.5 µm

Name	Weight %	Uncertainty %	Analytical Method	Uncertainty Method
<a href="#">1&amp;2-ethylnaphthalene</a> (ENAP)	0.146150023	0.007767115	Filter/PUF/XAD/PUF Cartridges; GC/MS	Standard



139 Additional Compounds



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The contents of your shopping cart are listed below. If you would like to download all of the files in your cart, click the checkout button. If you would like to remove an item from your cart, click the associated delete button. Click [here to view the Export Data Dictionary](#).

Particulate Matter (PM) speciation profiles	
<a href="#">Paved Road Dust [4211]</a> Controls: Uncontrolled Paved road dust sample from the intersection of Cevallos & Pecos La Trinidad, San Antonio, TX, collected on 09/24/99.	<input type="button" value="Delete"/>
<a href="#">Unpaved Road Dust [4220]</a> Controls: Uncontrolled Unpaved road dust sample from Eagle Pass, TX, collected from aerosol sampling site dirt road (path) immediately next to sampler on 09/17/99.	<input type="button" value="Delete"/>
<a href="#">Paved Road Dust [4205]</a> Controls: Uncontrolled Paved road dust sample from the intersection of Rittiman & I-410, San Antonio, TX, collected on 09/25/99.	<input type="button" value="Delete"/>
<a href="#">Paved Road Dust [4209]</a> Controls: Uncontrolled Paved road dust sample from the intersection of Commerce & Pecos La Trinidad 1430, San Antonio, TX, collected on 09/24/99.	<input type="button" value="Delete"/>
<a href="#">Paved Road Dust [4210]</a> Controls: Uncontrolled Paved road dust sample from the intersection of Cevallos & Pecos La Trinidad, San Antonio, TX, collected on 09/24/99.	<input type="button" value="Delete"/>
<a href="#">Paved Road Dust [4346]</a> Controls: Uncontrolled Composite of five paved road dust profiles from San Antonio, TX, and Laredo, TX (BVPVRD01, BVPVRD02, BVPVRD03, BVPVRD04, and BVPVRD05).	<input type="button" value="Delete"/>
<a href="#">Paved Road Dust [4347]</a> Controls: Uncontrolled Composite of five paved road dust profiles from San Antonio, TX, and Laredo, TX (BVPVRD01, BVPVRD02, BVPVRD03, BVPVRD04, and BVPVRD05).	<input type="button" value="Delete"/>
<a href="#">Unpaved Road Dust [4349]</a> Controls: Uncontrolled Composite of two unpaved road dust profiles from Guadalupe, TX, and Eagle Pass, TX (BVUNPV06 and BVUNPV09).	<input type="button" value="Delete"/>

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# Conclusion

- SPECIATE 4.2 and its Data browser represent a significant enhancement of the data available to characterize emissions by species and source category.
- The SPECIATE Data Browser makes it easy for non Access users to view and use SPECIATE data
- New source profiles and application features will be added in future revisions
- You can help by supplying data
  - Electronic data preferred
- Questions/Comments/Suggestions
  - Frank Divita - [frank.divita@pechan.com](mailto:frank.divita@pechan.com)
  - Lee Beck - [beck.lee@epa.gov](mailto:beck.lee@epa.gov)
- <http://cfpub.epa.gov/si/speciate/>
- <http://projects.pechan.com/ttn/speciate4.2/>