Work Order No. 582-20-10973-010
Contract No. 582-19-90500
Tracking No. 2020-02
Task 6.2

Prepared for:

Texas Commission on Environmental Quality
12100 Park 35 Circle MC 164
Austin, TX 78753

Prepared by:

Ramboll US Corporation
7250 Redwood Blvd., Suite 105
Novato, California 94945

June 29, 2020

# Processing Global Anthropogenic Emissions from CEDS – Final

PREPARED UNDER A CONTRACT FROM THE
TEXAS COMMISSION ON ENVIRONMENTAL QUALITY

*The preparation of this document was financed through a contract from the State of Texas through the Texas Commission on Environmental Quality.*
*The content, findings, opinions and conclusions are the work of the author(s) and do not necessarily represent findings, opinions or conclusions of the TCEQ.*

# Processing Global Anthropogenic Emissions from CEDS – Final

Ramboll
7250 Redwood Boulevard
Suite 105
Novato, CA 94945
USA

T +1 415 899 0700
https://ramboll.com

# Contents



## Appendix



## Table of Figures



## Table of Tables

# List of Acronyms and Abbreviations

| | |
|---|---|
| AIR_CDS | Aircraft Climbing & Descent |
| AIR_CRS | Aircraft Cruise |
| AIR_LTO | Aircraft Landing and Take Off |
| CAMx | Comprehensive Air Quality Model with Extensions |
| CH4 | Methane |
| CEDS | Community Emissions Data System |
| CMAS | Community Modeling and Analysis System |
| CSV | Comma-separated Values |
| ETHA | Ethane |
| EPA | Environmental Protection Agency |
| HTAP | Hemispheric Transport of Air Pollutants |
| NMVOC | Non-Methane VOC (VOC – methane) |
| NOx | Nitrogen Oxides |
| PEC | Particulate Elemental Carbon |
| PM10 | Particulate Matter with diameter smaller than 10 µm |
| PM2.5 | Particulate Matter with diameter smaller than 2.5 µm |
| POC | Particulate Organic Carbon |
| SMOKE | Sparse Matrix Operator Kernel for Emissions |
| TCEQ | Texas Commission on Environmental Quality |
| TOG | Total Organic Gasses |
| VOC | Volatile Organic Compounds |

# EXECUTIVE SUMMARY

International transport of pollution has increased in importance as the US National Ambient Air Quality Standards for ozone and particulate matter (PM) have become more stringent in recent years. International anthropogenic emissions contribute to ozone and PM transport into the continental United States. PM is a cause of regional haze and visibility degradation in protected areas such as National Parks located in Texas. Assessing international transport is important for several reasons, including improving the accuracy of modeling inputs (and hence model accuracy), improving attribution of ozone and visibility degradation to the correct sources, and accounting for effects of foreign emissions in air quality management plans. The purpose of this project is to develop a processing platform that uses publicly available emissions that cover the globe. The new Community Emissions Data System (CEDS) provides the most current global emissions. This project develops a CEDS processing platform to develop Comprehensive Air Quality Model with Extensions (CAMx) photochemical model inputs for areas lacking anthropogenic emissions in the expanded ozone transport and Hemispheric CAMx domains. Ramboll provided training via webinar and self-paced tutorial on using the SMOKE processing platform for CEDS and developed a User's Guide with detailed instructions.

# 1.0 BACKGROUND

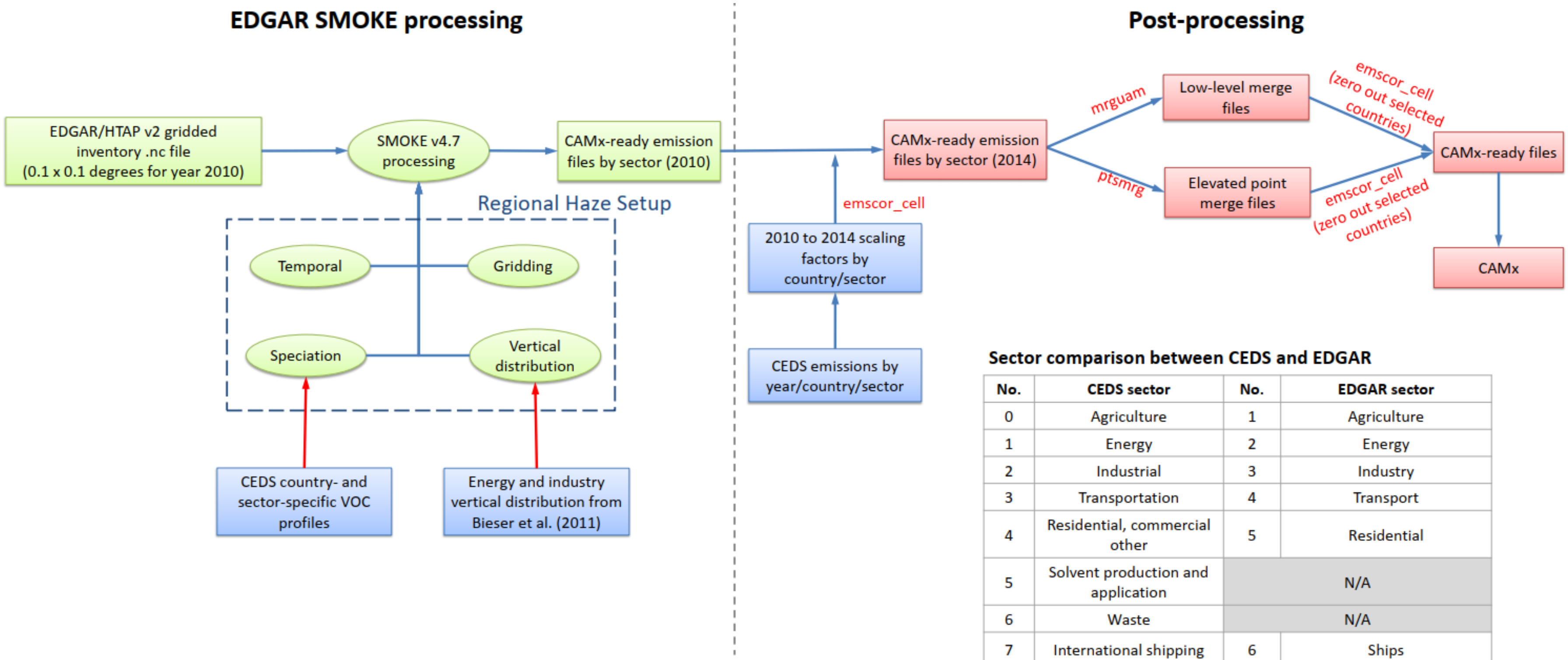
International transport of pollution has increased in importance as the US National Ambient Air Quality Standards for ozone and particulate matter (PM) have become more stringent in recent years. International anthropogenic emissions contribute to ozone and PM transport into the continental United States. PM is a cause of regional haze and visibility degradation in protected areas such as National Parks located in Texas. Assessing international transport is important for several reasons, including improving the accuracy of modeling inputs (and hence model accuracy), improving attribution of ozone and visibility degradation to the correct sources, and accounting for effects of foreign emissions in air quality management plans.

The new Community Emissions Data System (CEDS) provides the most current global emissions. This project develops a CEDS processing platform based on the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system, which is distributed by the Community Modeling and Analysis System (CMAS) center. SMOKE supports global gridded inventories and can regrid them onto a desired modeling grid. It also supports chemical speciation and temporal profiles for each country and sector, accounts for time zones, and supports plume rise for elevated emission sectors.

# 2.0 INTRODUCTION

The purpose of this project is to use the latest CEDS global-scale emission inventories to develop Comprehensive Air Quality Model with Extensions (CAMx) photochemical model inputs for areas lacking anthropogenic emissions in the expanded ozone transport and Hemispheric CAMx domains. SMOKE can process global gridded emission data from the Hemispheric Transport of Air Pollutants Version 2 (HTAPv2) emission inventory with 0.1-degree resolution. Here, we develop additional ancillary data needed by SMOKE to process the latest CEDS global emissions data. The TCEQ will use SMOKE with CEDS data to develop input data for the Comprehensive Air quality Model with extensions (CAMx) applied to the expanded ozone transport and Hemispheric domains. Data from CEDS are needed outside of the US, Canada and Mexico. CEDS includes more recent years than HTAP but with coarser spatial resolution of 0.5 degree. Therefore, our methodology uses 2010 data from HTAPv2 with 0.1-degree resolution and applies CEDS-derived adjustment factors at a country and emissions sector level to build emissions for TCEQ's 2016 modeling platform. The processing steps are illustrated schematically in Figure 1.

Broadly speaking there are two key parts of this SMOKE processing system: (1) running SMOKE for individual HTAPv2 sectors; (2) applying projection factors derived from CEDS on a country/sector basis, merging inventory sectors, and zeroing-out areas with better anthropogenic emissions in the modeling domain. Chapter 2 describes how projection factors are derived from CEDS data. Chapter 3 provides details on the steps and settings needed to run SMOKE. Chapter 4 describes various post-processing steps needed to prepare CAMx-ready emissions.




**Sector comparison between CEDS and EDGAR**

| No. | CEDS sector | No. | EDGAR sector |
|---|---|---|---|
| 0 | Agriculture | 1 | Agriculture |
| 1 | Energy | 2 | Energy |
| 2 | Industrial | 3 | Industry |
| 3 | Transportation | 4 | Transport |
| 4 | Residential, commercial other | 5 | Residential |
| 5 | Solvent production and application | N/A | |
| 6 | Waste | N/A | |
| 7 | International shipping | 6 | Ships |
| 8 | Aircraft | 7/8/9 | air_crs/air_lto/air_cds |

**Figure 1. Flow diagram of processing global gridded inventories.**

# 3.0 COMMUNITY EMISSION DATA SYSTEM (CEDS)

CEDS is a recently produced global data set of anthropogenic emissions of gasses and carbon-containing aerosol (Hoesly et al., 2018). CEDS incorporates several regional emission inventories and elsewhere developed emission estimates from demographic and energy consumption data. The CEDS emissions are provided on an annual basis for years 1750 to 2014 by country and emissions sector. The gridded inventory files (0.5 degree spatial resolution with monthly variation) are available at https://esgf-node.llnl.gov/search/input4mips/. Appendix A provides instructions for downloading the gridded files. The CEDS gridded emission data are not directly used because of coarser spatial resolution but used to project emissions to recent year. Sector-specific annual emission total emissions are also available for each country and pollutant in a comma-separated values (CSV) format as part of the supplemental data of Hoesly et al. (2018).

## 3.1 Projecting EDGAR Emission Sectors from 2010 to 2014 using CEDS

The most recent HTAPv2 inventory year is 2010, which is six years prior to the TCEQ's modeling year of 2016. The most recent CEDS inventory year is 2014. Therefore, we use CEDS emissions totals for 2010 and 2014 to project forward the HTAPv2 gridded inventory to 2014 and so obtain a reasonable approximation of 2016.

CEDS provides 53 sub-level source sectors whereas the gridded HTAPv2 input files for SMOKE contain only 9 sectors. To develop projection factors, the CEDS sectors were mapped to HTAP sectors as shown in Table 1. The projection factors were calculated using CEDS emissions totals for 2010 and 2014. The country-specific projection factors are applied to gridded HTAP emissions by assigning each grid cell to a single country with a cell-mask file. The cell-mask file is developed through the intersection of shapefiles of the country boundaries with modeling grid.

**Table 1. Aggregating CEDS sub-level sector to HTAP sector.**

| CEDS sub-level sector | HTAP sector |
|---|---|
| 1A1a_Electricity-autoproducer | Energy |
| 1A1a_Electricity-public | Energy |
| 1A1a_Heat-production | Energy |
| 1A1bc_Other-transformation | Energy |
| 1A2a_Ind-Comb-Iron-steel | Industry |
| 1A2b_Ind-Comb-Non-ferrous-metals | Industry |
| 1A2c_Ind-Comb-Chemicals | Industry |
| 1A2d_Ind-Comb-Pulp-paper | Industry |
| 1A2e_Ind-Comb-Food-tobacco | Industry |
| 1A2f_Ind-Comb-Non-metalic-minerals | Industry |
| 1A2g_Ind-Comb-Construction | Industry |
| 1A2g_Ind-Comb-machinery | Industry |
| 1A2g_Ind-Comb-mining-quarying | Industry |
| 1A2g_Ind-Comb-other | Industry |
| 1A2g_Ind-Comb-textile-leather | Industry |

| CEDS sub-level sector | HTAP sector |
|---|---|
| 1A2g_Ind-Comb-transpequip | Industry |
| 1A2g_Ind-Comb-wood-products | Industry |
| 1A3b_Road | Transportation |
| 1A3c_Rail | Transportation |
| 1A3di_Oil_tanker_loading | Shipping |
| 1A3dii_Domestic-navigation | Transportation |
| 1A3eii_Other-transp | Transportation |
| 1A4a_Commercial-institutional | Residential |
| 1A4b_Residential | Residential |
| 1A4c_Agriculture-forestry-fishing | Residential |
| 1A5_Other-unspecified | Residential |
| 1B1_Fugitive-solid-fuels | Energy |
| 1B2_Fugitive-petr-and-gas | Energy |
| 1B2d_Fugitive-other-energy | Energy |
| 2A1_Cement-production | Industry |
| 2A2_Lime-production | Industry |
| 2Ax_Other-minerals | Industry |
| 2B_Chemical-industry | Industry |
| 2C_Metal-production | Industry |
| 2D_Chemical-products-manufacture-processing | Industry |
| 2D_Degreasing-Cleaning | Industry |
| 2D_Other-product-use | Industry |
| 2D_Paint-application | Industry |
| 2H_Pulp-and-paper-food-beverage-wood | Industry |
| 3B_Manure-management | Agriculture |
| 3D_Rice-Cultivation | Agriculture |
| 3D_Soil-emissions | Agriculture |
| 3E_Enteric-fermentation | Agriculture |
| 3I_Agriculture-other | Agriculture |
| 5A_Solid-waste-disposal | Residential |
| 5C_Waste-combustion | Residential |
| 5D_Wastewater-handling | Residential |
| 5E_Other-waste-handling | Residential |
| 6A_Other-in-total | N/A |
| 6B_Other-not-in-total | N/A |
| 1A3ai_International-aviation | Air |
| 1A3aii_Domestic-aviation | Air |
| 1A3di_International-shipping | Shipping |

### 3.2 VOC Speciation Profiles for CEDS

The CEDS data set provides VOC speciation data for 25 named VOC species by country and emissions sector[1]. Figure 2 provides a snapshot of CEDS VOC speciation data. TCEQ uses

[1] Source: https://github.com/JGCRI/CEDS (VOC_ratio_AllSectors.csv)

the Carbon Bond version 6 (CB6) chemical mechanism in CAMx. In order to create CB6 chemical mechanism profiles, the CEDS VOC species were mapped to species in the SPECIATE database[2] based on description and molecular weights, e.g., CEDS “acids” is mapped to acetic acid rather than acids unknown because the molecular weight matches acetic acid. CEDS “other alkanals” (VOC22) were equally split into “Isobutyraldehyde” and “Acetaldehyde”, and “ketones” (VOC23) were equally split into “Ketones-general” and “Acetone”. Table 2 provides the complete mapping of CEDS VOC species to SPECIATE species. This cross-reference allowed us to use the Speciation Tool[3] with the latest mechanism mappings to produce SMOKE profiles for CB6r4 chemical mechanism used in TCEQ’s modeling.

| sector | VOC01 | VOC02 | VOC03 | VOC04 | VOC05 | VOC06 | VOC07 | VOC08 | VOC09 | VOC12 | VOC13 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ELEC | 0.00802 | 0 | 0.08832 | 0.2017 | 0.35014 | 0.04551 | 0.0006 | 0 | 0 | 0.00066 | 0.09965 |
| ELEC | 0.11252 | 0 | 0.00881 | 0.06248 | 0.0404 | 0.07694 | 0.00983 | 0 | 0 | 0.00923 | 0.00995 |
| ELEC | 0.09256 | 0 | 0.00724 | 0.05138 | 0.03324 | 0.0633 | 0 | 0 | 0 | 0.00759 | 0.00817 |
| ELEC | 0.06919 | 0.00424 | 0.02429 | 0.08207 | 0.0868 | 0.09628 | 0.00821 | 0.00227 | 0.00245 | 0.02841 | 0.02741 |
| ELEC | 0.00068 | 0 | 0.09231 | 0.20791 | 0.36561 | 0.04257 | 0 | 0 | 0 | 5.59E-05 | 0.10416 |
| ELEC | 0.00821 | 0.00028 | 0.09017 | 0.20602 | 0.35663 | 0.04918 | 0.00026 | 0.00015 | 0.00016 | 0.0022 | 0.10174 |
| ELEC | 0 | 0 | 0.09622 | 0.21645 | 0.38107 | 0.04392 | 0 | 0 | 0 | 0 | 0.10858 |
| ELEC | 0.11251 | 0 | 0.00882 | 0.06246 | 0.0404 | 0.07695 | 0.00983 | 0 | 0 | 0.00924 | 0.00995 |
| ELEC | 0.06431 | 0 | 0.00651 | 0.03902 | 0.02894 | 0.04466 | 0 | 0 | 0 | 0.00528 | 0.00735 |
| ELEC | 0.00059 | 0.01366 | 0.03937 | 0.09272 | 0.11496 | 0.14806 | 0.00562 | 0.0073 | 0.00786 | 0.07311 | 0.04442 |
| ELEC | 0.01408 | 0.00442 | 0.07117 | 0.16669 | 0.26922 | 0.08367 | 0.00188 | 0.00237 | 0.00255 | 0.02485 | 0.0803 |
| ELEC | 0.09929 | 0 | 0.0458 | 0.14065 | 0.18622 | 0.08526 | 0 | 0 | 0 | 0.00815 | 0.05168 |
| ELEC | 0.05558 | 0.00658 | 0.01108 | 0.04788 | 0.02681 | 0.10364 | 0.00908 | 0.00353 | 0.0038 | 0.0398 | 0.0125 |
| ELEC | 0.01244 | 0.00549 | 0.06636 | 0.15556 | 0.24689 | 0.09054 | 0.00262 | 0.00294 | 0.00317 | 0.03042 | 0.07488 |
| ELEC | 0.02302 | 0 | 0.00177 | 0.01287 | 0.00843 | 0.01579 | 0 | 0 | 0 | 0.00186 | 0.002 |
| ELEC | 0.05558 | 0.00658 | 0.01108 | 0.04788 | 0.0268 | 0.10364 | 0.00906 | 0.00353 | 0.0038 | 0.03981 | 0.01251 |
| ELEC | 0.00495 | 0 | 0.09078 | 0.20609 | 0.35977 | 0.04464 | 0.00368 | 0 | 0 | 0.00041 | 0.10244 |
| ELEC | 0.0058 | 0.01266 | 0.04227 | 0.10092 | 0.1296 | 0.14343 | 0.00292 | 0.00678 | 0.0073 | 0.06829 | 0.0477 |
| ELEC | 0 | 0 | 0.09622 | 0.21645 | 0.38107 | 0.04392 | 0 | 0 | 0 | 0 | 0.10858 |
| ELEC | 0.06431 | 0 | 0.00653 | 0.03903 | 0.02894 | 0.04462 | 0 | 0 | 0 | 0.00525 | 0.00736 |

| sector | VOC14 | VOC15 | VOC16 | VOC17 | VOC18 | VOC19 | VOC20 | VOC21 | VOC22 | VOC23 | VOC24 | VOC25 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ELEC | 0.05613 | 0.0007 | 0.00104 | 0 | 0 | 0 | 0 | 0.09037 | 0.00169 | 0.00256 | 0.00922 | 0.04371 |
| ELEC | 0.0246 | 0.00976 | 0.01456 | 0 | 0 | 0 | 0 | 0.06465 | 0.02365 | 0.03593 | 0.12933 | 0.36736 |
| ELEC | 0.02023 | 0.00802 | 0.01197 | 0 | 0 | 0 | 0 | 0.05319 | 0.01945 | 0.02955 | 0.1064 | 0.48771 |
| ELEC | 0.04351 | 0.06848 | 0.00895 | 0.02626 | 0 | 0 | 0 | 0.05609 | 0.01455 | 0.0221 | 0.09226 | 0.23618 |
| ELEC | 0.05736 | 5.91E-05 | 8.81E-05 | 0 | 0 | 0 | 0 | 0.09062 | 0.00014 | 0.00022 | 0.00078 | 0.03743 |
| ELEC | 0.05843 | 0.0049 | 0.00106 | 0.00176 | 0 | 0 | 0 | 0.09213 | 0.00173 | 0.00262 | 0.01029 | 0.01206 |
| ELEC | 0.05967 | 0 | 0 | 0 | 0 | 0 | 0 | 0.09411 | 0 | 0 | 0 | 0 |
| ELEC | 0.0246 | 0.00976 | 0.01454 | 0 | 0 | 0 | 0 | 0.06466 | 0.02366 | 0.03594 | 0.12932 | 0.36737 |
| ELEC | 0.01497 | 0.00558 | 0.00832 | 0 | 0 | 0 | 0 | 0.0384 | 0.01352 | 0.02054 | 0.07392 | 0.62867 |
| ELEC | 0.07814 | 0.20089 | 9.91E-05 | 0.08444 | 0 | 0 | 0 | 0.03198 | 0.00013 | 0.0002 | 0.0416 | 0.01486 |
| ELEC | 0.06392 | 0.06636 | 0.00182 | 0.02737 | 0 | 0 | 0 | 0.0744 | 0.00296 | 0.0045 | 0.02946 | 0.008 |
| ELEC | 0.04528 | 0.00862 | 0.01284 | 0 | 0 | 0 | 0 | 0.09425 | 0.02088 | 0.03172 | 0.11413 | 0.05526 |
| ELEC | 0.04219 | 0.1017 | 0.00719 | 0.04071 | 0 | 0 | 0 | 0.03523 | 0.01169 | 0.01775 | 0.08362 | 0.33965 |
| ELEC | 0.06484 | 0.08189 | 0.00161 | 0.03396 | 0 | 0 | 0 | 0.06835 | 0.00262 | 0.00397 | 0.03077 | 0.02069 |
| ELEC | 0.00512 | 0.00197 | 0.00309 | 0 | 0 | 0 | 0 | 0.01323 | 0.00476 | 0.00723 | 0.02646 | 0.87239 |
| ELEC | 0.04219 | 0.1017 | 0.00719 | 0.04071 | 0 | 0 | 0 | 0.03523 | 0.01168 | 0.01775 | 0.08362 | 0.33965 |
| ELEC | 0.05714 | 0.00043 | 0.00064 | 0 | 0 | 0 | 0 | 0.09125 | 0.00104 | 0.00158 | 0.00569 | 0.02947 |
| ELEC | 0.07697 | 0.18689 | 0.00075 | 0.07833 | 0 | 0 | 0 | 0.0379 | 0.00122 | 0.00185 | 0.04465 | 0.00375 |
| ELEC | 0.05967 | 0 | 0 | 0 | 0 | 0 | 0 | 0.09411 | 0 | 0 | 0 | 0 |
| ELEC | 0.01498 | 0.00555 | 0.0083 | 0 | 0 | 0 | 0 | 0.03841 | 0.01352 | 0.02055 | 0.07392 | 0.62872 |

**Figure 2. Snapshot of CEDS VOC speciation data by country and sector.**

**Table 2. Mapping of CEDS VOC species to CB6 species.**

| No. | VOC species | Molecular weight | SPECIATE Species ID | SPECIATE Description |
|---|---|---|---|---|
| VOC01 | alcohols | 46.2 | 442 | Ethyl alcohol |
| VOC02 | ethane | 30.0 | 438 | Ethane |
| VOC03 | propane | 44.0 | 671 | Propane |
| VOC04 | butanes | 57.8 | 309 | Butane, branched & linear |
| VOC05 | pentanes | 72.0 | 2132 | Isomers of pentane |
| VOC06 | hexanes_plus_higher_alkanes | 106.8 | 2126 | Isomers of heptane |
| VOC07 | ethene | 28.0 | 452 | Ethylene (or ethene) |
| VOC08 | propene | 42.0 | 678 | Propylene (or Propene; 1-Propene) |
| VOC09 | ethyne | 26.0 | 282 | Acetylene (or ethyne) |
| VOC12 | other_alkenes_and_alkynes | 67.0 | 2133 | Isomers of pentene |
| VOC13 | benzene | 78.0 | 302 | Benzene |
| VOC14 | toluene | 92.0 | 717 | Toluene |
| VOC15 | xylene | 106.0 | 507 | Isomers of xylene |

[2] https://www.epa.gov/air-emissions-modeling/speciate

[3] https://github.com/CMASCenter/Speciation-Tool

| No. | VOC species | Molecular weight | SPECIATE Species ID | SPECIATE Description |
|---|---|---|---|---|
| VOC16 | trimethylbenzenes | 120.0 | 755 | Trimethylbenzenes (mixed) |
| VOC17 | other_aromatics | 126.8 | 3206 | C10 trialkylbenzenes |
| VOC18 | esters | 104.7 | 568 | Misc. esters |
| VOC19 | ethers | 81.5 | 445 | Ethyl ether |
| VOC20 | chlorinated_hydrocarbons | 138.8 | 7 | 1,1,2-trichloroethane |
| VOC21 | methanal | 30.0 | 465 | Formaldehyde |
| VOC22 | other_alkanals | 68.8 | 2585 | Isobutyraldehyde; Butyraldehyde |
| | | 68.8 | 279 | Acetaldehyde |
| VOC23 | ketones | 75.3 | 2137 | Ketones - general |
| | | 75.3 | 281 | Acetone |
| VOC24 | acids | 59.1 | 280 | Acetic acid |
| VOC25 | other_voc | 68.9 | 640 | Other, misc. VOC |

The CEDS speciation data were formatted for input to the Speciation Tool and over thousand CB6 profiles were produced in SMOKE format (GSPRO) which are being used in SMOKE processing. Upon further review of SMOKE profiles, we found that transportation sector profiles for some countries were missing ethene (ETH) which is inconsistent with the known VOC composition of gasoline vehicle exhaust, and important because ethene is photochemically reactive. We corrected this issue by adding ethene (assuming ethene = twice the sum of 1-alkenes, i.e., ETH = 2 x OLE) and renormalizing the profile.

### 3.3 Emission Height Profiles

The HTAP inventories do not provide stack parameters or other information that can be used to estimate plume rise for point sources. Consequently, vertical allocation profiles are used by SMOKE to characterize point source plume rise on a sector-wide basis. Among the HTAP sectors, only the aircraft, energy, ships, and industry sectors have a vertical profile applied. For agriculture, residential, and transport, all emissions remain in Layer 1 (height ~34 m).

Figure 3 compares the vertical profiles available from EPA's hemispheric modeling platform (Vukovich et al., 2019) and a peer-reviewed paper published in the *Environmental Pollution* (Bieser et al., 2011). As shown in Figure 3, the HTAP Energy and Industry sectors receive identical vertical profile in EPA's platform with 50% of emission injected above 400 m. Bieser et al. (2011) has different vertical profiles for combustion in energy and transformation industries (no emissions below 200 m) and combustion in manufacturing industry (almost all emissions below 200 m). Based on engineering judgement, the vertical profiles from Bieser et al. (2011) seem more reasonable and thus are used for vertical allocation of emissions as described in Section 3.2. The vertical profile "combustion in energy and transformation industries" is used for HTAP Energy sector and profile "combustion in manufacturing industry" is used for HTAP Industry sector. The HTAP aircraft sector vertical profiles are based on EPA's hemispheric modeling platform. The shipping sector uses vertical profile with 25% of emissions under 40 m and 75% between 40 – 81 m.

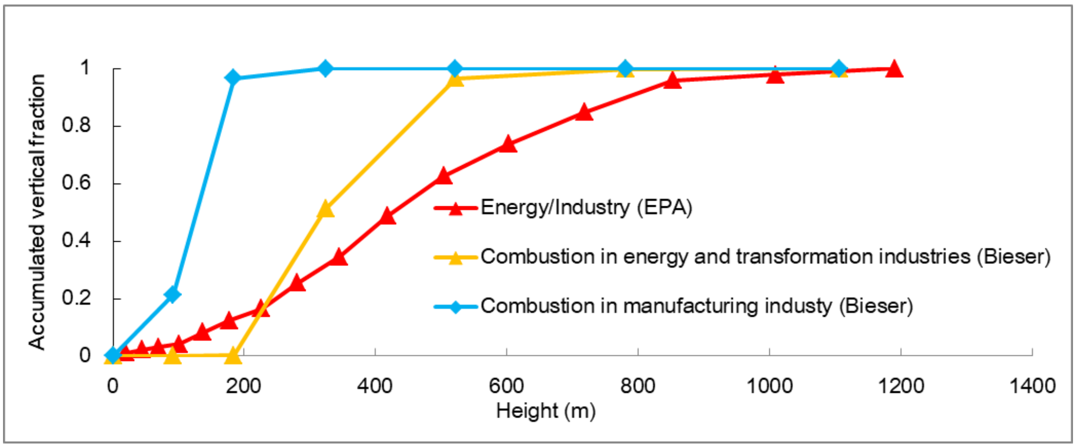



**Figure 3. Emission height profiles for HTAP sectors.**

# 4.0 SMOKE PROCESSING OF HTAP EMISSIONS

The system uses the latest version of Sparse Matrix Operator Kernel for Emissions (SMOKE) modeling system, version 4.7, which is distributed by the Community Modeling and Analysis System (CMAS) center[4]. It supports global gridded inventories and can re-grid them onto a desired modeling grid. It also supports chemical speciation and temporal profiles for each country and sector, accounts for time zones, and supports plume rise for elevated emission sectors.

The SMOKE processing system input data consist of emissions inventories and ancillary data files for specifying the timing and chemical nature of emissions. SMOKE ancillary data files used in the processing system are largely based on EPA hemispheric modeling SMOKE setup but speciation and vertical profiles are updated based on more recent information available from CEDS and Bieser et al. as described in Chapter 2.

## 4.1 HTAPv2 Inventories

The system is setup to process 2010 HTAPv2 gridded inventories. The HTAPv2 inventory includes 9 sectors: agriculture (g_ag), air (g_air_cds, g_air_crs, g_air_lto), energy (g_energy), industry (g_industry), residential (g_residential), transport (g_transport) and shipping (g_ships). Even though agriculture burning sector inventory is available from HTAPv2, it is not used in this system to avoid potential double counting with the separately processed "FINN" fire inventory. For all the sectors except air and shipping, monthly inventories are available from HTAPv2. Gridded 2010 HTAP emissions can be downloaded from EPA's hemispheric modeling platform ftp site ftp://newftp.epa.gov/Air/emismod/2011/hemispheric/.

## 4.2 SMOKE Ancillary Files

SMOKE needs ancillary data files for temporal allocation, chemical speciation, and vertical distribution of elevated emissions sector as described below.

### 4.2.1 Temporal Allocation

Each HTAP sector has a single set of temporal profiles (weekly and diurnal, and also monthly for sectors without monthly inventories) that is applied to the entire sector. These temporal profiles were obtained from EPA's hemispheric modeling which were estimated using North American source-specific examples and engineering judgement. A temporal cross-reference file (ATREF) and three temporal profile files (ATPRO_MONTH/ATPRO_WEEKLY/ATPRO_HOURLY) are needed to convert annual/monthly emissions to hourly emissions.

4 SMOKE (http://www.smoke-model.org/)

#### 4.2.2 Spatial Allocation

The HTAP dataset includes gridded annual and monthly datasets on a global 0.1° latitude by 0.1° longitude grid. Spatial allocation of these inventories in SMOKE consists of two steps. First, in the SMOKE program Smkinven, each 0.1° by 0.1° point on the global grid is mapped to a country code (GEOCODE) and a time zone using a file called the GRIDMASK. Then, the SMOKE program Grdmat spatially reallocates emissions from the global input grid to the TCEQ's "na_12km" domain.

#### 4.2.3 Chemical Speciation

HTAP inventories include the following pollutants: "non methane VOC" (NMVOC); black carbon (BC, mapped to model species PEC); organic carbon (OC, mapped to model species POC); total PM2.5; and other standard CAPs (CO, NH3, NOx, PM10, SO2). Similar to temporal allocation, speciation cross-reference (GSREF) and profile (GSPRO) files are needed for processing and applying a sector-average speciation profile to individual HTAP sector.

The VOC speciation profiles are developed based on CEDS speciation data and processed to develop CB6 profiles as described in Section 2.2. The GSREF file is also developed with country code embedded so country-specific VOC profiles can be applied. For regions or countries that are not covered by the CEDS VOC speciation data, the EPA hemispheric modeling profiles are used. Since the HTAP inventories specify "NMVOC" instead of "VOC", the profiles do not include methane (CH4), but do include other species which may be considered part of TOG but not VOC, such as ethane (ETHA). There is no VOC-to-TOG conversion prior to speciation like there is in traditional emissions modeling, since these profiles are computed on the basis of (NM)VOC.

For PM2.5 speciation, the HTAP inventories include emissions for black carbon, organic carbon, and total PM2.5. In SMOKE modeling, we map black carbon to the model species PEC, and organic carbon to the model species POC. Since PEC and POC are also part of total PM2.5, we must subtract PEC and POC from total PM2.5 in order to prevent a double count. Prior to SMOKE modeling, an additional set of gridded inventory files is generated for PM2_5_OTH (other PM2.5), which is equal to total PM2.5 minus PEC minus POC. Then, PM2_5_OTH is speciated using speciation profiles based on EPA's hemispheric modeling, which map to the remaining PM species needed for modeling. The PM profiles from EPA are in terms of AE6 aerosol-phase mechanism and AE6 model species are converted to CAMx PM species using species mapping in the post processing.

For all HTAP sectors, NOx is speciated to NO and NO2 using a 90/10 split. The SULF species is calculated as a percentage of SO2 in the HTAP energy (2.2%), industry (0.9%), and residential (1.48%) sectors.

#### 4.2.4 Vertical Allocation

Among HTAP sectors, only the aircraft, energy, ships, and industry sectors have a vertical profile applied. For agriculture, residential, and transport, all emissions remain in Layer 1.

As described in Section 2.3, vertical profiles for Energy and Industry sectors were updated based on Bieser et al. (2011). The HTAP aircraft sector vertical profiles are based on EPA's hemispheric modeling platform. The ships sector uses vertical profile with 25% of emissions under 40 m and 75% between 40 – 81 m.

## 4.3 SMOKE Assign File and Run Scripts

The first part of setting up SMOKE system for a case is to create an Assigns file and script files. For sectors that have monthly variations (e.g. transport, industry), SMOKE needs to be run for 12 months, and sectors that do not have monthly variation (e.g. ships, air) SMOKE needs to be run only for one month. To run SMOKE, just execute the run script. One SMOKE run script should be executed at a time, so you don't overwrite intermediate files created by SMOKE. For air, ships and agriculture sectors, one representative day of emissions for each month is processed; for all other sectors, seven representative days of emissions for each month is processed. The Assigns file defines SMOKE home directory, case name, running dates, etc. SMOKE run scripts are created for each sector.

### 4.3.1 Steps to Run SMOKE

A detailed set of instructions to run SMOKE are available in the User's Guide (refer to the "Final_UserGuide_TCEQ_CEDS_11Jun2020.docx"). Briefly, prior to running the SMOKE processing system:

- Review/update SMOKE executable folder
- Review/update directories in the inventory list files (one for each sector)
- Edit Assigns file with correct SMOKE directory and check/modify MCIP path in this file
- Review/update SMOKE run scripts (set correct SMOKE directory, modify ancillary files if needed)

# 5.0 POST-PROCESSING STEPS

After running SMOKE for each sector, a series post processing steps need to be executed to develop CAMx input emissions. This is the second part of the flow chart process in Figure 1.

1. Convert SMOKE 3D files in CMAQ model format to CAMx format for energy, industry, air and ships sectors using the "cmaq2camx" converter[5].
   For energy, industry, air and ships sectors, SMOKE will generate 3D netCDF files, which are converted to CAMx gridded and elevated files. This step requires METCRO3D met files from MCIP to generate CAMx files. For each day, two CAMx files are generated: (1) CAMx gridded file and (2) CAMx point source (PTSOURCE) file.

2. Convert SMOKE 2D files in CMAQ model format to CAMx format for transport, residential and agriculture sectors using "smk2emis" conversion program available in SMOKE.

3. Scale 2010 emissions to 2014 emissions based on projection factors using "emscor" program.
   Projection factors were created for each emissions sector to scale emissions from 2010 to 2014 as described in Section 2.1. The projection factor file is a CSV file with scaling factors assigned to each gridcell. For US, Canada and Mexico, projection factors are set to zero, whereas all other countries in the TCEQ's "na_12km" domain are assigned country-specific projection factors based on CEDS data (see details in Section 2.1). Emissions are scaled using "emscor" program with projection factors as input.

4. Merge Emissions
   Merge all sectors to generate CAMx-ready emissions using "mrguam" and "mrgpts" programs and convert AE6 PM species to CAMx CF species using the CAMx "xspcmap" program[5].

5. SMOKE creates emission files in UTC time zone. Since the TCEQ runs CAMx in local time, the emission files need to be time shifted to CST time zone.

6. Window for subdomains
   The SMOKE processing system will create model-ready files for the "na_12km" grid because MCIP data are based on TCEQ's WRF modeling– same extent as the "na_36km" but at a finer 12km resolution. In this step, two sets of files are generated: (1) aggregate to produce "na_36km" gridded files; (2) window to generate "us_12km" files. Both steps can be done using the CAMx "window" program.

[5] http://www.camx.com/download/support-software.aspx

# 6.0 SUMMARY OF CEDS TRAINING

Ramboll provided training via webinar and self-paced tutorial on using the SMOKE processing platform for CEDS. We also developed a User's Guide with detailed instructions on using the global emissions processing platform. The training agenda, presentation materials, and electronic files for the practice run were provided to the TCEQ Project Manager before the training. Eight TCEQ staff attended the training. We organized the training to give presentations in the morning and hands-on practice session using the TCEQ's AMDA Linux system in the afternoon. For the hands-on training, we provided virtual assistance while participants practiced running the SMOKE processing platform on their own.

# 7.0 SUMMARY AND RECOMMENDATIONS

This project developed a processing system to use the latest CEDS global-scale emission inventories to develop CAMx model inputs for areas lacking anthropogenic emissions in the expanded ozone transport and Hemispheric CAMx domains. The processing system uses 2010 data from HTAPv2 with 0.1-degree resolution and applies CEDS-derived adjustment factors at a country and emissions sector level to build emissions for TCEQ's 2016 modeling platform. We developed additional ancillary data needed by SMOKE to process the latest CEDS global emissions data. Specifically, we developed emission sector specific CB6 profiles for each country based on CEDS VOC speciation data and emission height profiles based on Bieser et al. (2011) for vertical allocation of elevated emission sectors.

Ramboll delivered the processing platform including inventory files, scripts, ancillary data files, expected outputs, and User's Guide. We provided training via webinar and self-paced tutorial on using the SMOKE processing platform for CEDS to TCEQ staff. We recommend that TCEQ staff should use the processing system to develop emissions for areas lacking anthropogenic emissions in the expanded modeling domain.

# 8.0 REFERENCES

Bieser, J., Aulinger, A., Matthias, V., Quante, M., & Denier van der Gon, H.A.C. (2011). Vertical emission profiles for Europe based on plume rise calculations. *Environmental Pollution*, 159(10), p.2935-2946.

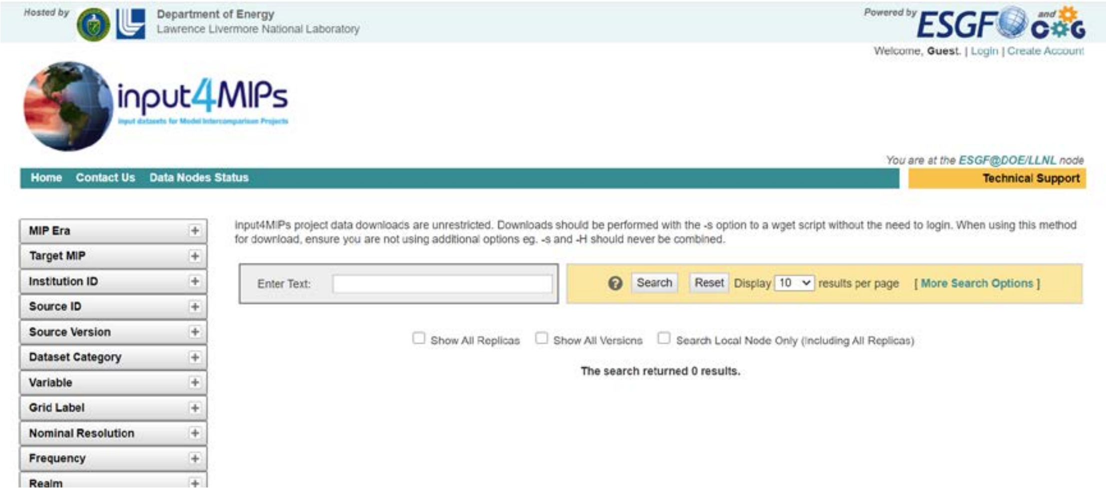
Hoesly, R. M., Smith, S. J., Feng, L., Klimont, Z., Janssens-Maenhout, G., Pitkanen, T., Seibert, J. J., Vu, L., Andres, R. J., Bolt, R. M., Bond, T. C., Dawidowski, L., Kholod, N., Kurokawa, J. I., Li, M., Liu, L., Lu, Z., Moura, M. C. P., O'Rourke, P. R., & Zhang, Q. (2018). Historical (1750-2014) anthropogenic emissions of reactive gases and aerosols from the Community Emissions Data System (CEDS). *Geoscientific Model Development*, *11*(1), 369-408. https://doi.org/10.5194/gmd-11-369-2018

Vukovich, J., & Eyth, A. (2019). Technical Support Document (TSD) Preparation of Emissions Inventories for the Version 7.1 2016 Hemispheric Emissions Modeling Platform.

# Appendix A

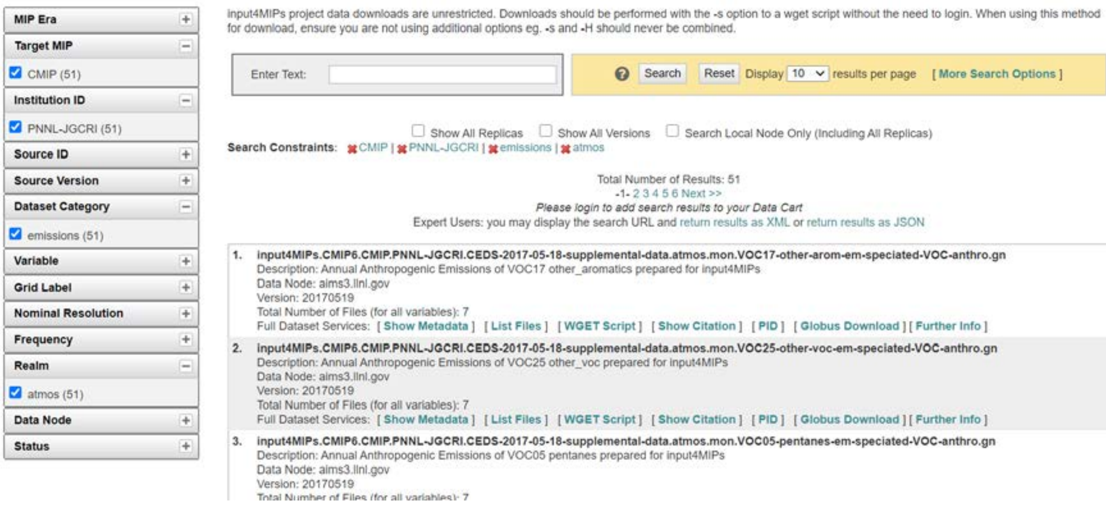
## Instructions on Downloading CEDS Data

The CEDS gridded data can be downloaded via this link: [https://esgf-node.llnl.gov/search/input4mips/](https://esgf-node.llnl.gov/search/input4mips/)




The CEDS anthropogenic emissions data is published within the ESGF system under the following metadata. On the left panel, select the following options, then click "Search".

:Target MIP = "CMIP";
:Institution ID = "PNNL-JGCRI";
:Dataset Category = "emissions";
:Realm = "atmos";




Click "List Files", download options are provided on the right.

Total Number of Results: 51
-1- 2 3 4 5 6 Next >>
*Please login to add search results to your Data Cart*
Expert Users: you may display the search URL and return results as XML or return results as JSON

1. **input4MIPs.CMIP6.CMIP.PNNL-JGCRI.CEDS-2017-05-18-supplemental-data.atmos.mon.VOC17-other-arom-em-speciated-VOC-anthro.gn**
Description: Annual Anthropogenic Emissions of VOC17 other_aromatics prepared for input4MIPs
Data Node: aims3.llnl.gov
Version: 20170519
Total Number of Files (for all variables): 7
Full Dataset Services: [ **Show Metadata** ] [ **Hide Files** ] [ **WGET Script** ] [ **Show Citation** ] [ **PID** ] [ **Globus Download** ] [ **Further Info** ]

**Total Number of Files: 7**

| | | |
|---|---|---|
| 1 | **VOC17-other-arom-em-speciated-VOC-anthro_input4MIPs_emissions_CMIP_CEDS-2017-05-18-supplemental-data_gn_175001-179912.nc**<br>checksum: 8aef963fe27e516d1b65546843f71caa5c3c737231efd35cbffcad5c56df2af3<br>size: 211753460<br>tracking_id: hdl:21.14100/47d4f25b-636c-413e-8a2b-cc58b29f9e6d<br>[ More File Metadata ] | Single File Access:<br>HTTP Download<br>OpenDAP<br>Download<br>Globus Download |
| 2 | **VOC17-other-arom-em-speciated-VOC-anthro_input4MIPs_emissions_CMIP_CEDS-2017-05-18-supplemental-data_gn_180001-184912.nc**<br>checksum: f1b90867e7f7ff38bbb18d407853807c4b3b772e0d0a69a050960875bf671757<br>size: 254707814<br>tracking_id: hdl:21.14100/8b53bce4-32c3-4ac5-8d56-0391eb3f80d8<br>[ More File Metadata ] | Single File Access:<br>HTTP Download<br>OpenDAP<br>Download<br>Globus Download |
| 3 | **VOC17-other-arom-em-speciated-VOC-anthro_input4MIPs_emissions_CMIP_CEDS-2017-05-18-supplemental-data_gn_185001-185012.nc**<br>checksum: d9daf4151a92b2b94afdc2e4340f4a9f1fd4c79d08d9bb5f167770cb825794ae<br>size: 10232738 | Single File Access:<br>HTTP Download<br>OpenDAP |