

Organic Gas Speciation Profiles for Prescribed Burning and Agricultural Burning Emissions

OG1479–OG1485

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Introduction

Agricultural burning and prescribed burning are important biomass burning sources of reactive organic gases (ROG) and particulate matter. These emissions can contribute to ozone formation, secondary organic aerosol production, visibility impacts, and exposure to toxic air pollutants. Because these emissions are used in inventories and chemical transport models for regulatory and planning applications, accurate chemical speciation profiles are needed to represent their total organic gas (TOG) composition.

The existing California Air Resources Board's (CARB) agricultural and prescribed-burning profiles were developed from older datasets summarized in Yang (2018) [1]. Although those profiles improved on earlier simplified assignments, they were based on more limited chemical measurements than are available today. As a result, a substantial fraction of TOG remained unresolved, and many oxygenated volatile organic compounds (OVOCs) and other reactive compounds were either underrepresented or not explicitly included.

More recent Fire Influence on Regional to Global Environments and Air Quality (FIREX-AQ) campaign measurements provide improved chemical detail for crop-residue and prescribed fires. Travis et al. (2023) [2] reported aircraft-based measurements from 53 crop-residue fires and 22 prescribed fires, including rice, corn, soybean, winter wheat, piles, slash, grassland, shrubland, and the Blackwater River State Forest (BRSF) prescribed understory fire. These measurements include many oxygenated, hydrocarbon, nitrile, and other organic species that were not explicitly represented in the older profiles.

The objective of this report is to update CARB's TOG speciation profiles for agricultural and prescribed burning using recently available measurement data and supporting literature. The updated profiles are intended to better represent these sources in the CARB's speciation database by expanding chemical coverage, improving representation of reactive and toxic compounds, and replacing the current agricultural and prescribed burning assignments. The profiles discussed in this document are:

- OG1479: Rice crop residue burning
- OG1480: Crop residue burning
- OG1481: Pile burning
- OG1482: Slash burning
- OG1483: Prescribed grassland burning
- OG1484: Prescribed shrubland burning
- OG1485: Prescribed forest/woodland burning

Data Sources and Methods

Reference datasets and measurement basis

Agricultural and prescribed burning TOG speciation profiles were developed from FIREX-AQ measurements reported by Travis et al. (2023). The Travis dataset includes aircraft observations of crop-residue burning and prescribed fires across multiple fuel types. Agricultural fuels include residues from corn, rice, soybean, and winter wheat, while prescribed burning measurements include fuels such as slash, woody piles, shrubland vegetation, and grassland fuels.

Travis et al. (2023) derived emission factors from aircraft plume measurements and focused on primary emissions representative of fresh combustion plumes. In their analysis, plume segments influenced by photochemical processing were screened using the maleic anhydride-to-furan ratio (MA/F) measured by proton-transfer-reaction time-of-flight mass spectrometry (PTR-ToF-MS), with low MA/F values indicating relatively fresh plumes with limited atmospheric processing. Reported emission factors were also limited to compounds that showed strong correlations with carbon monoxide, helping ensure that the reported species were directly associated with combustion emissions. Importantly, the aircraft sampled fresh, minimally aged plumes after initial plume rise, cooling, and dilution, but before substantial photochemical processing. Residual smoldering or other emissions that remain near the ground may therefore be less completely represented.

The FIREX-AQ measurement suite combined PTR-ToF-MS with the University of California, Irvine Whole Air Sampler (UCI WAS), the National Oceanic and Atmospheric Administration integrated Whole Air Sampler (NOAA iWAS), and the National Center for Atmospheric Research Trace Organic Gas Analyzer with Time-of-Flight mass spectrometry (NCAR TOGA-TOF), together with instruments for major combustion gases. These complementary measurements provide broad gas-phase organic coverage and help resolve some isomeric compounds that cannot be uniquely identified by PTR-ToF-MS alone. Instrument coverage differs by species and fire, so profile completeness and compound-specific uncertainty remain dependent on the underlying measurements.

For context, the Travis prescribed-fire measurements were reviewed together with relevant biomass-burning measurements reported by Gkatzelis et al. (2024) [3] and Akagi et al. (2013) [4]. Akagi et al. (2013) provided an additional comparison for the forest/woodland prescribed-fire profile, including emission factors for several species measured in common. Andreae (2019) [5] and Shahid et al. (2024) [6] were reviewed as broader biomass-burning context. These external datasets were used to evaluate source representativeness and uncertainty and were not used to fill unmeasured species or construct the new profiles.

Fuel Selection and Development of TOG Speciation Profiles from Emission Factors

Measured emission factors (EFs) were used to construct the TOG speciation profiles. Reported species were mapped to CARB compound names and SAROAD codes. Carbon monoxide and carbon dioxide were excluded from the TOG, while methane was retained.

For each profile, the mass fraction of species i was calculated as:

$$f_i = \frac{EF_i}{\sum_j EF_j}$$

where EF_i is the mass-based emission factor for species i, and $\sum_j EF_j$ is the sum of the processed organic-gas emission factors included in the source dataset. For profile development, this summed value is treated as the TOG represented by the combined measurements. The normalization therefore assumes that the analytical methods used in the source study capture the organic-gas mass sufficiently well to provide a representative TOG composition. No molar conversion is applied because both the emission factors and resulting profile fractions are expressed on a mass basis.

The resulting fractions describe the organic-gas composition represented by the available measurements. They do not imply that every emitted organic compound was measured. Intermediate-volatility, semi-volatile, and other compounds that are not fully captured by the analytical methods may therefore remain underrepresented, which is a source of uncertainty in the TOG profiles.

Profile development follows the measured fuel and vegetation or land-cover information reported in the source studies. When these profiles are assigned in the emissions inventory, the most specific available fuel or vegetation information should be used. Table 1 summarizes the basis for each profile, and Appendix Table A1 provides the EIC/SCC crosswalk used for inventory assignment without creating new vegetation-specific sub-EICs.

Agricultural and Prescribed Burning

OG1479–OG1482 are agricultural-burning profiles derived from the aircraft measurements reported by Travis et al. (2023) [2]. The source measurements include crop-residue fires and woody agricultural burning sampled across several regions of the United States.

OG1479 represents rice-residue burning and is based on 12 rice-residue fires sampled in Mississippi, Kansas, Illinois, and Arkansas, comprising 29 plume measurements. OG1480 represents the broader crop-residue category and combines measurements from corn, rice, soybean, and winter-wheat residue burning. This profile is based on 53 fires and 142 plume measurements and represents the

average chemical composition of the crop-residue fires included in the FIREX-AQ dataset.

OG1481 represents stacked woody piles and is based on nine fires and 16 plume measurements from the south-central and southeastern United States. OG1482 represents woody slash and is based on seven fires and 34 plume measurements from the same general regions. These two profiles are retained separately because they represent different forms of woody material and burning activity.

OG1480 is not weighted to California crop activity. Instead, it represents the average composition of the crop-residue fires measured by Travis et al. (2023). Rice residue remains separately represented by OG1479 because rice-residue burning is maintained as a distinct category in the emissions inventory. The measured crop-residue fires showed generally similar TOG chemical patterns across the included crop types. Developing additional crop-specific profiles from the smaller number of measurements available for individual crops could increase sampling uncertainty without providing a clear improvement in chemical representativeness. For this reason, OG1480 is retained as the general crop-residue profile and can be revisited as additional crop-specific measurements become available.

Prescribed burning profiles

OG1483–OG1485 are organized by broad vegetation and land-cover type using the prescribed-fire measurements reported by Travis et al. (2023).

OG1483 represents grass-dominated prescribed burning and is based on four fires and 15 plume measurements from Nebraska, Kansas, and Oklahoma. OG1484 represents shrub-dominated prescribed burning and is based on one prescribed fire and one plume measurement in Missouri. OG1485 represents forest/woodland prescribed burning using the Blackwater River State Forest understory fire in Florida, which was sampled in 20 plume measurements from one independent fire event.

The prescribed-burning profiles therefore differ substantially in the number of independent fires available for profile development. The grassland profile is supported by measurements from multiple fires, while the shrubland and forest/woodland profiles are based on single fire events. For this reason, the profiles are retained at the broader vegetation-group level rather than further subdivided by individual fuel species or finer land-cover classes. This approach reflects the level of detail supported by the available measurements while limiting additional uncertainty from very small sample sizes.

Treatment of unresolved mass and compound allocations

Several organic-gas measurements in the FIREX-AQ dataset represent individual compounds, while others represent grouped compounds or formula-level signals that cannot be uniquely resolved by the primary measurement. Compound identities

and instrument-based assignments reported directly by Travis et al. (2023) were retained during profile development. For example, Travis et al. reported the C2H6O3 signal as ethene hydroxyperoxide based on CIT-CIMS measurements. No additional allocation was applied to this signal.

For some PTR-ToF-MS signals, Travis et al. (2023) reported more than one possible contributing compound and used complementary measurements or previously published FIREX laboratory results to interpret the measured signal. For example, the C4H6O2 signal was reported as a combination dominated by 2,3-butanedione, with a smaller unresolved contribution from other C4H6O2 compounds. Based on the interpretation reported by Travis et al. (2023), 87% of the parent signal was assigned to 2,3-butanedione and the remaining 13% was treated as unresolved C4H6O2 mass.

The unresolved C4H6O2 mass was treated conservatively when a compound-specific assignment was not adequately supported. For OG1479–OG1484, the residual was retained as unidentified organic-gas mass. For the forest/woodland profile OG1485, the residual was represented by 2-oxobutanal because independent wood-combustion measurements reported by Schauer et al. (2001) [7], and represented in CARB profile OG5491, provide source-relevant support for this compound assignment. This assignment is used as a representative treatment of the unresolved residual and does not imply that the entire residual was directly measured as 2-oxobutanal.

Where an additional compound-level allocation was needed for the CARB profiles, literature-based isomer distributions or compound identifications were applied when a defensible basis was available. These included residual butenenitrile distributions from Hatch et al. (2015) [8]; benzenediol and creosol assignments based on Schauer et al. (2001) [7]; propene- and butene-hydroxynitrate distributions from Teng et al. (2015) [9]; a representative C3H8O3 assignment supported by Liang et al. (2021) [10]; a nitrocresol assignment supported by Sakakibara et al. (2022) [11]; and nitrocatechol and methylnitrocatechol assignments from Xie et al. (2020) [12]. The combined beta-pinene/myrcene signal was divided equally because the source measurement did not provide a quantitative compound-specific ratio.

All multi-compound allocations preserve the mass of the original parent signal. Single representative assignments change the compound identity used for modeling but do not change the parent-signal mass. Where a defensible compound-level assignment could not be made, the mass was retained as unidentified organic gas rather than redistributed among identified species.

Appendix Table A4 documents only the additional literature-based and project-specific allocations applied during development of the final CARB profiles. Compound identities and assignments already provided in the FIREX-AQ source data are not repeated in Table A4. Appendix Table A5 summarizes the amount of profile mass affected by these additional allocations.

Results and Discussion

Table 1. Fuel- and vegetation-based description of OG1479–OG1485. All profiles were developed from Travis et al. (2023) [2].

Profile ID	Profile name	Fuel / vegetation basis	Profile development basis
OG1479	Rice crop residue burning	Rice crop residue	Direct rice-residue profile from Travis et al. (2023).
OG1480	Crop residue burning	Corn, rice, soybean, and winter wheat residues	Average of measured crop-residue fires reported by Travis et al. (2023); not a California activity-weighted crop mixture.
OG1481	Pile burning	Stacked woody biomass	Profile derived from measured woody-pile burning reported by Travis et al. (2023).
OG1482	Slash burning	Woody slash and pruning residues	Profile derived from measured woody-slash burning reported by Travis et al. (2023).

Profile ID	Profile name	Fuel / vegetation basis	Profile development basis
OG1483	Prescribed grassland burning	Grass-dominated vegetation	Average profile from grassland prescribed fires reported by Travis et al. (2023).
OG1484	Prescribed shrubland burning	Shrub-dominated vegetation	Profile from shrubland prescribed-fire measurements reported by Travis et al. (2023).
OG1485	Prescribed forest/woodland burning	Shrubs, grasses, and litter beneath pine, oak, and magnolia forest	Profile from the Blackwater River State Forest prescribed understory fire reported by Travis et al. (2023); one independent fire event sampled repeatedly.

Differences in Chemical Composition of Agricultural burning profiles

The updated agricultural burning profiles (OG1479–OG1482) show substantially expanded chemical detail relative to the previous crop residue burning profile (OG1474). Across the four updated agricultural profiles, the average ROG fraction was 79.10 ± 6.31% of TOG, with average CH4, NMHC, and OVOC fractions of 14.6 ±

6.7%, 16.8 ± 2.3%, and 62.0 ± 6.5%, respectively. By comparison, the previous crop residue burning profile had a ROG fraction of 87.45% of TOG, with CH4, NMHC, and OVOC fractions of 10.17%, 8.68%, and 35.20%, respectively.

The updated profiles also represent substantially more individual species. OG1479–OG1482 contain 148 to 153 ROG species, 72 to 75 NMHC species, 46 OVOC species, and 66 to 72 toxic species. OG1474 contains 32 ROG species, 18 NMHC species, 11 OVOC species, and 19 toxic species. These counts describe the chemical representation in the final profiles and include compound-level assignments from supported isomer splits. The broader representation primarily reflects the greater chemical coverage of the FIREX-AQ measurements, particularly for oxygenated and other reactive organic compounds.

Differences in Chemical Composition of Prescribed burning profiles

The updated prescribed burning profiles (OG1483-OG1485) also show substantially expanded chemical detail relative to the previous prescribed burning profiles used for comparison (OG1475, OG1473, and OG1472). Across the three updated prescribed burning profiles, the average ROG fraction was 80.2 ± 5.8% of TOG, with average CH4, NMHC, and OVOC fractions of 13.8 ± 5.2%, 17.7 ± 5.6%, and 62.8 ± 8.2%, respectively. The previous prescribed burning profiles had an average ROG fraction of 83.7 ± 4.7% of TOG, with average CH4, NMHC, and OVOC fractions of 13.4 ± 4.2%, 11.0 ± 4.9%, and 29.9 ± 7.2%, respectively.

The updated prescribed-burning profiles contain 114 to 150 ROG species, 53 to 73 NMHC species, 39 to 48 OVOC species, and 54 to 71 toxic species. By comparison, the previous prescribed-burning profiles contain substantially fewer represented species. As with the agricultural profiles, the larger number of represented compounds reflects the broader chemical coverage of the newer measurements, particularly for oxygenated and other reactive organic compounds that were only partly represented in the older profiles.

Table 2. A summary of chemical composition of the profiles in this study compared to previous profiles. Here composition is broadly summarized by Reactive Organic Gases (ROG), methane, Non-Methane Hydrocarbons (NMHC), and Oxygenated Volatile Organic Compounds (OVOC)

Parameter	Agricultural burning old (OG1474)	Agricultural burning new (OG1479–OG1482)	Prescribed burning old (OG1472, OG1473, OG1475)	Prescribed burning new (OG1483–OG1485)
ROG fraction (% of TOG)	87.45	79.1 ± 6.3	83.7 ± 4.7	83.3 ± 2.4

Parameter	Agricultural burning old (OG1474)	Agricultural burning new (OG1479–OG1482)	Prescribed burning old (OG1472, OG1473, OG1475)	Prescribed burning new (OG1483–OG1485)
CH4 fraction (% of TOG)	10.17	14.6 ± 6.7	13.4 ± 4.2	11.4 ± 1.3
NMHC fraction (% of TOG)	8.68	16.8 ± 2.3	11.0 ± 4.9	17.6 ± 5.5
OVOC fraction (% of TOG)	35.2	62.0 ± 6.5	29.9 ± 7.2	63.6 ± 6.9
Number of ROG compounds	32	148–153	14–45	114–150
Number of NMHC compounds	18	72–75	6–19	53–73
Number of OVOC compounds	11	46	7–21	39–48
Number of toxic species	19	66–72	9-28	54–71

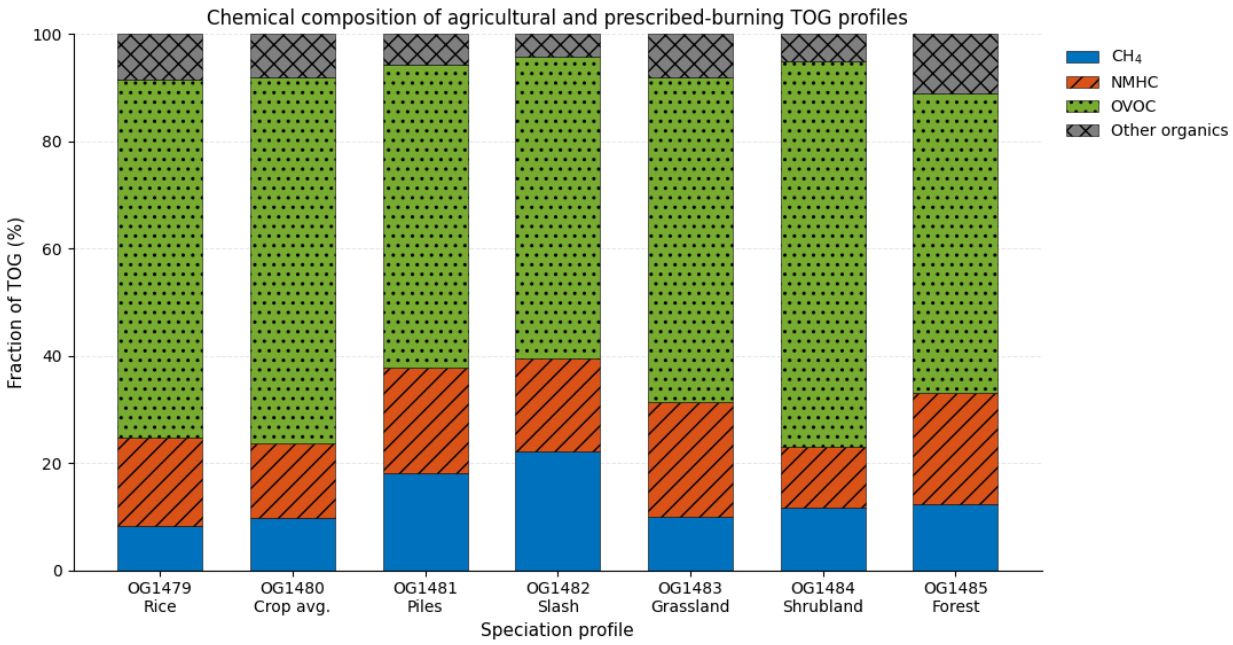


Figure 1. Comparison of chemical composition across newly developed agricultural and prescribed-burning TOG speciation profiles (OG1479–OG1485), illustrating differences in CH_4, NMHC, OVOC, and ROG fractions by fuel type.

Implications for Emission Inventory and Modeling

Representation of toxic air contaminants

The updated agricultural- and prescribed-burning profiles contain substantially more CEIDARS-designated toxic species than the previous profiles. The updated agricultural-burning profiles contain 66 to 72 toxic species per profile, compared with 19 in the previous crop-residue profile, OG1474. The updated prescribed-burning profiles contain 54 to 71 toxic species per profile, compared with 9 to 28 in the previous prescribed-burning comparison profiles.

For this comparison, toxic species were identified using CARB's CEIDARS toxic designation. For newly assigned species that are not yet included in the chemistry master table, the current CEIDARS pollutant table was used to determine toxic status. This approach provides a consistent basis for comparing the old and updated profiles.

The larger number of represented toxic species primarily reflects the broader chemical coverage of the FIREX-AQ measurements. In addition to compounds represented in the older profiles, such as formaldehyde, acetaldehyde, benzene, and toluene, the updated profiles include CEIDARS-designated toxic compounds such as acrolein, glyoxal, methacrylonitrile, carbon disulfide, nitromethane, furfural,

benzaldehyde, styrene, and naphthalene. Several toxic compounds that previously had no profile representation are therefore represented explicitly in the updated profiles.

The number of toxic species should be interpreted as a measure of chemical coverage rather than as an indication that every individual toxic emission factor is better constrained. These profiles were developed primarily for chemical speciation in emissions and air-quality modeling and therefore separate uncertainty was not quantified. Compound-specific uncertainty may also vary among species. Acrolein, for example, warrants particular caution because sampling and analytical uncertainty can affect its measured abundance.

Ozone formation potential

The updated profiles also increase the ozone formation potential (OFP) assigned to combustion emissions in the inventory. OFP was calculated by $OFP = \sum_1^i f_i \times MIR_i$. Where f_i is the fractional abundance of species i in TOG and MIR_i is its Maximum Incremental Reactivity (MIR) – a scale used to estimate reactivity to form ozone [13].

Across OG1479–OG1482, the updated agricultural-burning profiles have a mean MIR-weighted ozone formation potential of 4.10 ± 0.49 g O_3/g TOG, compared with 1.60 g O_3/g TOG for OG1474. The updated prescribed-burning profiles have a mean value of 4.37 ± 0.47 g O_3/g TOG, compared with 1.77 ± 0.06 g O_3/g TOG for the previous prescribed-burning profiles.

For an inventory-scale comparison, the profile-level MIR-weighted values were multiplied by the corresponding 2023 statewide TOG emissions (see **Table 3**). Using the 2023 inventory totals from CEPAM2019v1.04, the resulting MIR-based reactivity-equivalent metric increases from 18.7 to 48.0 tons O_3/day-equivalent for agricultural burning and from 56.8 to 140.3 tons O_3/day-equivalent for prescribed burning. Across both source groups, the metric increases from 75.5 to 188.3 tons O_3/day-equivalent.

These values provide a common basis for comparing the relative reactivity assigned by the old and updated profiles. They are not estimates of actual ozone produced in the atmosphere. Actual ozone formation depends on NOx concentrations, sunlight, dilution, background chemistry, plume processing, and other atmospheric conditions. The higher MIR-weighted values primarily reflect the broader representation of reactive organic compounds in the updated profiles, particularly oxygenated compounds and aldehydes with relatively high MIR values.

Table 3. MIR-weighted ozone formation potential and inventory-scale reactivity-equivalent metrics for the previous and new profiles.

Metric	Agricultural burning old	Agricultural burning new	Prescribed burning old	Prescribed burning new
TOG emissions (tons/day)	11.7	11.7	32.1	32.1
Mean OFP (g O_3/g TOG)	1.60	4.10 ± 0.49	1.77 ± 0.06	4.37 ± 0.47
Estimated ozone formation (tons/day)	18.6	48	56.8	140.3
Change (tons/day)	–	29.3	–	83.5
% change	–	157%	–	147%

Uncertainty and limitations

The updated profiles provide broader chemical resolution than the older CARB biomass-burning profiles, but several uncertainties remain. The FIREX-AQ aircraft measurements represent the fuels, burn conditions, and sampling conditions included in that campaign. The aircraft sampled fresh, minimally aged plumes after initial plume rise, cooling, and dilution but before substantial photochemical processing. Residual smoldering, low-temperature combustion, or emissions that remain close to the ground may therefore be less completely represented. Individual agricultural and prescribed burns may also differ because of crop type, residue composition, fuel moisture, fuel loading, combustion efficiency, and burn management practice.

The crop-residue fires measured by Travis et al. (2023) showed generally similar normalized TOG chemical patterns across the included crop types, supporting use of OG1480 as the general crop-residue profile. Developing additional crop-specific profiles from the smaller number of measurements available for individual crops could increase sampling uncertainty without a clear gain in chemical

representativeness. For prescribed burning, OG1483 is supported by multiple grassland fires, whereas OG1484 and OG1485 are based on single shrubland and forest/woodland fire events, respectively. These categories should be refined as additional source-specific measurements become available.

The isomer assignments applied to selected grouped species preserve total TOG mass but do not represent burn-specific compound-resolved measurements in every case. Across OG1479–OG1485, parent mixture rows that were resolved or assigned using supporting literature account for 2.27% to 3.99% of TOG. These allocations improve compound-level specificity for modeling, but they remain an additional source of speciation uncertainty and should be revisited when direct source-specific isomer measurements become available.

The profiles emphasize measured gas-phase organic compounds. Intermediate-volatility organic compounds, semivolatile organic compounds, condensable organics, and low-volatility oxygenated compounds may be incompletely represented because of instrument- and inlet-specific transmission and detection limitations. This incomplete coverage is relevant to both the assumed TOG normalization basis and secondary organic aerosol precursors. The profile update primarily changes how a given TOG emission total is chemically allocated; it does not demonstrate an equivalent reduction in uncertainty in the underlying total TOG emission factor or activity estimate.

References

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Appendix A

Table A1. Mapping of EICs to the newly added profiles

EIC/SCC	Category	Subcategory 1	Subcategory 2	Subcategory 3	New OG Profile ID
67066002620000	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - PRUNINGS	AGRICULTURAL WASTE	SUB-CATEGORY UNSPECIFIED	OG1481
67066002629842	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - PRUNINGS	AGRICULTURAL WASTE	ATTRITION	OG1482
67066002629856	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - PRUNINGS	AGRICULTURAL WASTE	GRAPE VINES/STUMPS	OG1481
67066002629862	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - PRUNINGS	AGRICULTURAL WASTE	ORCHARD REMOVAL	OG1481
67066002629884	MANAGED BURNING	AGRICULTURAL BURNING - PRUNINGS	AGRICULTURAL WASTE	TREE PRUNINGS	OG1482

EIC/SCC	Category	Subcategory 1	Subcategory 2	Subcategory 3	New OG Profile ID
	AND DISPOSAL				
67066002629888	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - PRUNINGS	AGRICULTURAL WASTE	UNTREATED GRAPE STAKES	OG1481
67066002629892	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - PRUNINGS	AGRICULTURAL WASTE	VINEYARD REMOVAL	OG1481
67066202620000	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - FIELD CROPS	AGRICULTURAL WASTE	SUB-CATEGORY UNSPECIFIED	OG1480
67066202629878	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - FIELD CROPS	AGRICULTURAL WASTE	RICE STUBBLE	OG1479
67066202629882	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - FIELD CROPS	AGRICULTURAL WASTE	STUBBLE	OG1480

EIC/SCC	Category	Subcategory 1	Subcategory 2	Subcategory 3	New OG Profile ID
67066402000000	MANAGED BURNING AND DISPOSAL	RANGE IMPROVEMENT	SOLID FUEL (UNSPECIFIED)	SUB-CATEGORY UNSPECIFIED	OG1483
67066602000000	MANAGED BURNING AND DISPOSAL	FOREST MANAGEMENT	SOLID FUEL (UNSPECIFIED)	SUB-CATEGORY UNSPECIFIED	OG1485
67066802000000	MANAGED BURNING AND DISPOSAL	WEED ABATEMENT	SOLID FUEL (UNSPECIFIED)	SUB-CATEGORY UNSPECIFIED	OG1484
67066802009858	MANAGED BURNING AND DISPOSAL	WEED ABATEMENT	SOLID FUEL (UNSPECIFIED)	NOXIOUS WEEDS	OG1484
67066802009872	MANAGED BURNING AND DISPOSAL	WEED ABATEMENT	SOLID FUEL (UNSPECIFIED)	PONDING/LEVEE BANKS/DITCHBANK/CANAL	OG1483

EIC/SCC	Category	Subcategory 1	Subcategory 2	Subcategory 3	New OG Profile ID
67066802009886	MANAGED BURNING AND DISPOSAL	WEED ABATEMENT	SOLID FUEL (UNSPECIFIED)	TUMBLEWEEDS	OG1484
67066802009894	MANAGED BURNING AND DISPOSAL	WEED ABATEMENT	SOLID FUEL (UNSPECIFIED)	WEED ABATEMENT - OTHER	OG1484
67099502409852	MANAGED BURNING AND DISPOSAL	OTHER	SOLID WASTE (UNSPECIFIED)	DISEASED FIELD CROPS	OG1480
50100202	SOLID WASTE DISPOSAL	GOVERNMENT	OPEN BURNING DUMP	VEGETATION ONLY	OG1481
50200201	SOLID WASTE DISPOSAL	COMMERCIAL/INSTITUTIONAL	OPEN BURNING	WOOD	OG1481
50200204	SOLID WASTE DISPOSAL	COMMERCIAL/INSTITUTIONAL	OPEN BURNING	VINE CROPS	OG1481

EIC/SCC	Category	Subcategory 1	Subcategory 2	Subcategory 3	New OG Profile ID
50200206	SOLID WASTE DISPOSAL	COMMERCIAL/INSTITUTIONAL	OPEN BURNING	ORCHARD CROPS	OG1481
50300201	SOLID WASTE DISPOSAL	INDUSTRIAL	OPEN BURNING	WOOD/VEG/LEAVES	OG1481

Table A2. New species to be added to CEIDAR database

SAROAD	Species	Type	CAS	Formula	Mol Wt.
51071	1,2-ethanediol, 1-nitrate	Isomer	16051-48-2	C2H5NO4	107.06
50842	2(3h)-furanone	Isomer	20825-71-2	C4H4O2	84.07
51541	2,6-dimethoxyphenol	Isomer	91-10-1	C8H10O3	154.16
51391	2-nitrophenol	Isomer	88-75-5	C6H5NO3	139.11
50961	3-furaldehyde	Isomer	498-60-2	C5H4O2	96.08
51082	anisole	Isomer	100-66-3	C7H8O	108.14
51031	benzonitrile	Isomer	100-47-0	C7H5N	103.12
50741	ethyl formate	Isomer	109-94-4	C3H6O2	74.08
51240	hydroxyquinone	Isomer	2474-72-8	C6H4O3	124.09
51021	phenylacetylene	Isomer	536-74-3	C8H6	102.14
51360	tricyclene	Isomer	508-32-7	C10H16	136.24

Table A3. Weight Percentages of organic gases in TOG in newly added profiles

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
45208	1,2,4-trimethylbenzene	C9H12	0.0318	0.0245	0.0401	0.0317	0.0177	0.0396	0.0169
43221	1,2-butadiene	C4H6	0.0114	0.0122	0.0050	0.0106	0.0265	0.0119	0.0169
51071	1,2-ethanediol, 1-nitrate	C2H5NO4	0.0023	0.0031	0.0006	0.0026	0.0044		0.0225
43208	1,2-propadiene	C3H4	0.0386	0.0398	0.0351	0.0343	0.1391	0.0356	0.0902
45207	1,3,5-trimethylbenzene	C9H12	0.0046	0.0061	0.0075	0.0132		0.0158	
43218	1,3-butadiene	C4H6	0.3568	0.3550	0.3381	0.3325	0.7131	0.1583	0.4282
43222	1,3-butadiyne	C4H2	0.0023			0.0026	0.0110		0.0113
43213	1-butene	C4H8	0.3204	0.2693	0.2579	0.2850	0.2826	0.2611	0.2141
98131	1-butyne	C4H6	0.0159	0.0184	0.0150	0.0132	0.0353	0.0158	0.0225
43268	1-decene	C10H20	0.0545	0.0367	0.0351	0.0211	0.0419	0.0277	0.0225
98005	1-heptene	C7H14	0.0591	0.0551	0.0451	0.0317	0.0751	0.0237	0.0563

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
43245	1-hexene	C6H12	0.1205	0.1071	0.0701	0.0607	0.1788	0.0514	0.1296
47048	1-hydroxy-2-propanone	C3H6O2	3.3052	3.2169	2.0914	1.7606	2.3524	3.6843	1.3767
99915	1-methyl-2-ethylbenzene	C9H12	0.0159	0.0122	0.0100	0.0132	0.0133	0.0277	0.0113
99912	1-methyl-3-ethylbenzene	C9H12	0.0273	0.0214	0.0601	0.0290	0.0221	0.0356	0.0169
99914	1-methyl-4-ethylbenzene	C9H12	0.0205	0.0184	0.0150	0.0158	0.0133	0.0317	0.0113
51350	1-nitrooxy-2-butanol	C4H9NO4	0.0031	0.0025	0.0040	0.0029	0.0018		
51210	1-nitrooxy-2-propanol	C3H7NO4	0.0014	0.0019	0.0015	0.0016	0.0014		
43267	1-nonene	C9H18	0.0364	0.0306	0.0276	0.0238	0.0530	0.0158	0.0225
43265	1-octene	C8H16	0.0500	0.0428	0.0326	0.0343	0.0508	0.0198	0.0338
43224	1-pentene	C5H10	0.1000	0.0796	0.0551	0.0660	0.0795	0.0831	0.0676
43209	1-propyne	C3H4	0.1295	0.1377	0.1302	0.1293	0.4106	0.1504	0.3043

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
50842	2(3H)-furanone	C4H4O2	2.3408	2.3686	1.5150	1.3801	2.2959	2.7300	2.2539
43276	2,2,4-trimethylpentane	C8H18	0.0091	0.0153	0.0200	0.0053	0.0088	0.0119	0.0044
47033	2,3-butanedione	C4H6O2	3.3414	3.3014	2.0936	1.7631	2.1511	2.8295	1.2648
43274	2,3-dimethylpentane	C7H16		0.0428	0.0050	0.0053	0.0088		0.0056
43271	2,4-dimethylpentane	C7H16	0.0318	0.0367	0.0551	0.0739	0.0133	0.0594	0.0113
43330	2,5-dimethylfuran	C6H8O	0.7850	0.6867	0.5630	0.6200	0.3866	0.3604	0.3124
51541	2,6-dimethoxyphenol	C8H10O3	0.2750	0.4070	0.3631	0.4961	0.1325	0.0712	0.0958
43552	2-butanone	C4H8O	0.7340	0.6886	0.5434	0.5700	0.3289	0.7003	0.2986
98156	2-butenal	C4H6O	1.0181	1.0038	0.7412	0.5251	1.4372	0.7320	0.5522
50671	2-butenenitrile	C4H5N	0.0816	0.0558	0.0238	0.0170	0.0602	0.0151	0.0198
98133	2-butyne	C4H6	0.0068	0.0061		0.0079	0.0110		0.0056
43329	2-ethylfuran	C6H8O	0.1784	0.1561	0.1280	0.1409	0.0879	0.0819	0.0710

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
50780	2-hydroxyethyl hydroperoxide	C2H6O3	0.0500	0.0551	0.0351	0.0422	0.0773	0.1504	0.0620
43225	2-methyl-1-butene	C5H10	0.0773	0.0643	0.0601	0.0739	0.0442	0.0594	0.0338
43228	2-methyl-2-butene	C5H10	0.0432	0.0306	0.0626	0.0369	0.0199		0.0113
43506	2-methyl-2-propenal	C4H6O	0.6386	0.4774	0.3456	0.4512	0.3908	0.4154	0.7269
51530	2-methyl-6-nitrophenol / 2-nitro-o-cresol	C7H7NO3	0.0250	0.0214	0.0150	0.0158	0.0199	0.0594	0.0225
43327	2-methylfuran	C5H6O	0.1818	0.2601	0.3280	0.6914	0.0905		0.0282
43275	2-methylhexane	C7H16	0.0295	0.0275	0.0326	0.0079	0.0155		0.0169
43229	2-methylpentane	C6H14	0.0159	0.0275	0.0276	0.0211	0.0353	0.0119	0.0338
98036	2-methylpropanal	C4H8O	0.2091	0.1622	0.1052	0.1267	0.1104	0.1860	0.1183
51351	2-nitrooxy-1-butanol	C4H9NO4	0.0083	0.0067	0.0109	0.0077	0.0048		
51211	2-nitrooxy-1-propanol	C3H7NO4	0.0032	0.0042	0.0035	0.0037	0.0030		

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
51391	2-nitrophenol	C6H5NO3	0.0159	0.0153		0.0106	0.0133		0.0338
43577	2-oxobutanal	C4H6O2							0.1890
50670	3-butenenitrile	C4H5N	0.1129	0.1008	0.0430	0.0307	0.0822	0.0274	0.0432
43223	3-methyl-1-butene	C5H10	0.0500	0.0428	0.0401	0.0475	0.0508	0.0475	0.0394
51691	3-methyl-6-nitrocatechol	C7H7NO4	0.0091	0.0107	0.0063	0.0066	0.0078	0.0159	0.0113
43328	3-methylfuran	C5H6O	0.0568	0.0673	0.1077	0.0976	0.0265		0.0225
43295	3-methylhexane	C7H16	0.0114	0.0153	0.0426	0.0106	0.0287		0.0113
43230	3-methylpentane	C6H14	0.0091	0.0122	0.0175	0.0106	0.0177		0.0451
51690	4-methyl-5-nitrocatechol	C7H7NO4	0.0091	0.0107	0.0063	0.0066	0.0078	0.0159	0.0113
43575	4-methylguaiacol	C8H10O2	0.5477	0.5876	0.7412	1.3432	0.3797	0.2809	0.4113
51550	4-nitrocatechol	C6H5NO4	0.0432	0.0459	0.0301	0.0238	0.0265	0.0554	0.0225
43363	5-methylfurfural	C6H6O2	1.9999	1.9280	1.6652	2.2034	1.4901	1.1335	1.6088
98025	a-pinene	C10H16	0.0932	0.0490	0.4457	0.4987	0.0464		0.4282

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
43503	acetaldehyde	C2H4O	8.6585	7.7731	5.8596	5.1721	8.9849	8.1900	6.9872
43404	acetic acid	C2H4O2	3.9588	4.1623	3.2548	3.3062	3.4907	6.5211	4.9835
43551	acetone	C3H6O	2.7044	2.3839	1.9432	2.2588	1.5740	2.3700	1.8651
43702	acetonitrile	C2H3N	1.2022	0.9762	0.4983	0.4486	0.8455	0.5777	0.4902
43206	acetylene	C2H2	0.7227	0.6427	0.5284	0.4275	2.1436	0.7438	1.5327
43505	acrolein	C3H4O	2.8407	2.8552	2.4640	1.9817	3.0686	2.9278	2.7836
43704	acrylonitrile	C3H3N	0.1864	0.1867	0.1127	0.1135	0.3996	0.1978	0.2198
51082	anisole	C7H8O	0.8693	0.8049	0.6799	0.8325	0.5685	0.3680	0.4226
98026	b-pinene	C10H16	0.0261	0.0184	0.1277	0.0343	0.0166		0.0563
45501	benzaldehyde	C7H6O	0.3523	0.3275	0.3155	0.3272	0.4261		0.5409
45201	benzene	C6H6	1.2386	1.1139	1.3647	1.4804	2.8478		2.9808
50313	benzofuran	C8H6O	0.2273	0.2295	0.2254	0.2269	0.2627		0.2367
51031	benzonitrile	C7H5N	0.1727	0.1285	0.1077	0.1056	0.1612	0.1068	0.1183

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
43510	butyraldehyde	C4H8O	0.1568	0.1224	0.1027	0.1003	0.0662	0.1385	0.0733
43289	C6 olefins	C6H12	0.0159	0.0122		0.0106			0.0113
98049	C9 aromatics	C9H12	0.2659	0.1775	0.2629	0.2322	0.1391		0.2254
99332	camphene	C10H16	0.0091	0.0184	0.1077	0.0633	0.0243		0.0225
98030	carbon disulfide	CS2	0.0023		0.0011		0.0044		0.0033
98031	carbonyl sulfide	COS	0.1136	0.1132	0.1628	0.0449	0.1258	0.1227	0.0451
45801	chlorobenzene	C6H5Cl	0.0023		0.0025				0.0018
43217	cis-2-butene	C4H8	0.0750	0.0704	0.0801	0.0871	0.0397	0.0514	0.0282
43227	cis-2-pentene	C5H10	0.0227	0.0214	0.0225	0.0264	0.0199	0.0237	0.0113
43248	cyclohexane	C6H12	0.0295	0.0184	0.0250	0.0106	0.0375	0.0119	0.0169
43242	cyclopentane	C5H10	0.0068	0.0061	0.0050	0.0053	0.0110		0.0056
43292	cyclopentene	C5H8	0.0182	0.0184	0.0225	0.0264	0.0375		0.0113
43802	dichloromethane	CH2Cl2	0.0205	0.0153					

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
99278	dimethyl sulfide	C2H6S	0.0364	0.0490	0.0526	0.0079	0.0110	0.0317	0.0225
43202	ethane	C2H6	1.5522	1.6281	2.2011	2.5042	1.0243	2.3146	1.1890
43302	ethanol	C2H6O	0.6636	0.7865	1.7278	0.4249	0.6822		0.5353
43203	ethene	C2H4	3.4089	2.8644	2.6794	2.7180	6.4021	3.2602	5.0319
43812	ethyl chloride	C2H5Cl	0.0046	0.0061	0.0025		0.0022	0.0040	0.0010
50741	ethyl formate	C3H6O2	0.9640	0.9383	0.6100	0.5135	0.6861	1.0746	0.4015
47054	ethyl nitrate	C2H5NO3	0.0046					0.0039	0.0022
45203	ethylbenzene	C8H10	0.1250	0.1010	0.1277	0.1135	0.1391	0.0594	0.1578
43502	formaldehyde	CH2O	5.3178	5.3555	4.9080	4.7235	7.6383	8.5461	9.1285
43403	formic acid	CH2O2	1.6385	1.7841	1.6327	1.0925	1.9891	5.9348	3.1386
99902	furan	C4H4O	0.7840	0.9517	1.0142	2.6652	0.7506		0.3212
99312	furfural	C5H4O2	0.1000	1.1690	1.5676	0.1214	0.0375		0.0169
43380	glycerol	C3H8O3	0.0500	0.0673	0.0401	0.0211	0.0265	0.0910	0.0282

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
47045	glycolaldehyde	C2H4O2	1.9499	2.0501	1.6031	1.6284	1.7193	3.2119	2.4545
90121	glyoxal	C2H2O2	1.0545	1.2823	0.7287	0.6360	1.5829	0.7953	1.7919
43576	guaiacol	C7H8O2	1.9317	1.9371	1.7153	2.3353	0.9978	1.3848	0.9748
43332	hydrogen cyanide	CHN	1.0840	0.9487	0.9991	0.6043	1.7352	0.4985	1.3467
51240	hydroxyquinone	C6H4O3	0.4159	0.4193	0.3656	0.3879	0.3510	0.5262	0.5353
43214	isobutane	C4H10	0.0386	0.0398	0.0576	0.0739	0.0265	0.0594	0.1240
43215	isobutylene	C4H8	0.3500	0.3060	0.2730	0.3747	0.2649	0.3244	0.2085
99173	isocyanic acid	CHNO	1.5681	1.5210	1.6001	0.8497	2.3180		3.9895
98132	isopentane	C5H12	0.0750	0.0612	0.0726	0.0581	0.0530	0.0277	0.1014
43243	isoprene	C5H8	1.1113	0.8691	2.4841	0.6782	0.4570		0.4733
43304	isopropanol	C3H8O	0.0227	0.0275	0.0175	0.0211	0.0287	0.0040	0.0169
98043	isopropylbenzene	C9H12	0.0023	0.0061	0.0075	0.0106	0.0133		0.0113
99024	m & p-xylene	C8H10	0.2591	0.1591	0.1778	0.2718	0.1126	0.0752	0.1634

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
43568	m-benzenediol / resorcinol	C6H6O2	0.0169	0.0162	0.0140	0.0186	0.0126	0.0096	0.0129
99008	maleic anhydride	C4H2O3	0.1773	0.1959	0.2154	0.1610	0.2406	0.5777	0.5466
98120	methacrylonitrile	C4H5N	0.0705	0.0612		0.0369	0.1082		0.0282
43201	methane	CH4	8.3176	9.7010	18.1797	22.1923	9.9784	11.7509	12.3967
43301	methanol	CH4O	3.8861	4.8964	5.2586	5.9901	2.4504	5.9743	3.6570
43432	methyl acetate	C3H6O2	2.5478	2.4797	1.6121	1.3571	1.8133	2.8400	1.0612
43819	methyl bromide	CH3Br	0.0182	0.0122	0.0150		0.0110	0.0021	0.0028
43801	methyl chloride	CH3Cl	1.1295	1.4934	0.2354	0.0633	0.3576	2.3502	0.1240
99295	methyl formate	C2H4O2	0.1023	0.1255	0.0952	0.1267	0.0817	0.2849	0.0789
47051	methyl iodide	CH3I	0.0046	0.0031	0.0075	0.0026	0.0022	0.0018	0.0036
99280	methyl mercaptan	CH4S	0.1250	0.0857	0.0826	0.0238	0.0839		0.0113
47053	methyl nitrate	CH3NO3	0.0068	0.0092	0.0075	0.0026	0.0088	0.0079	0.0113
47047	methyl vinyl ketone	C4H6O	1.8408	1.6097	1.5400	1.3907	1.3378	1.3136	1.6454

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
43261	methylcyclohexane	C7H14	0.0046	0.0061	0.0376	0.0132	0.0221	0.0079	0.0169
43262	methylcyclopentane	C6H12	0.0182	0.0153	0.0250	0.0106	0.0155	0.0040	0.0113
43805	methylene bromide	CH2Br2	0.0046	0.0031	0.0025		0.0022	0.0023	0.0014
90122	methylglyoxal	C3H4O2	3.9543	4.1926	2.3564	2.4462	4.6580	2.3739	3.0259
43123	monoterpenes	C10H16	0.6431	0.2571	2.5041	1.5331	0.4018		0.9016
90051	myrcene	C10H16	0.0261	0.0184	0.1277	0.0343	0.0166		0.0563
43212	n-butane	C4H10	0.1954	0.1744	0.1528	0.1979	0.1369	0.1701	0.2648
43238	n-decane	C10H22	0.0227	0.0275	0.0250	0.0264	0.0287	0.0356	0.0169
43232	n-heptane	C7H16	0.0636	0.0490	0.0626	0.0501	0.0905	0.0317	0.0394
43231	n-hexane	C6H14	0.0477	0.0490	0.0501	0.0475	0.0618	0.0435	0.0902
43235	n-nonane	C9H20	0.0318	0.0275	0.0401	0.0264	0.0177	0.0317	0.0113
43233	n-octane	C8H18	0.0386	0.0306	0.0501	0.0264	0.0287	0.0198	0.0225
43220	n-pentane	C5H12	0.0932	0.0735	0.0851	0.0765	0.0927	0.0514	0.1296

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
47055	n-propyl nitrate	C3H7NO3						0.0009	0.0004
45209	n-propylbenzene	C9H12	0.0159	0.0122	0.0075	0.0106	0.0133	0.0237	0.0056
43241	n-undecane	C11H24	0.0136	0.0122	0.0326	0.0106	0.0618	0.0158	
98046	naphthalene	C10H8	0.3182	0.2112	0.2504	0.2217	0.5409		0.6649
99004	nitromethane	CH3NO2	0.1818	0.1897	0.1878	0.1399	0.3201		0.5071
43569	o-benzenediol / catechol	C6H6O2	1.9830	1.9118	1.6512	2.1848	1.4775	1.1239	1.5122
98021	o-cresol (2-methyl-benzenol)	C7H8O	0.2977	0.3152	0.2880	0.3536	0.2053	0.2295	0.2085
45204	o-xylene	C8H10	0.0886	0.0796	0.0876	0.1135	0.0618	0.0475	0.0789
43571	p-benzenediol / hydroquinone	C6H6O2							0.0837
45300	phenol	C6H6O	0.4545	0.4958	0.3356	0.3193	0.4106	0.4392	0.3719
51021	phenylacetylene	C8H6	0.0273	0.0306	0.0351	0.0158	0.1082	0.0158	0.0620
43504	propanal	C3H6O	0.8704	0.8018	0.7587	0.6043	0.9250	0.8704	0.6255

SAROAD	Species	Formula	OG1479 (%)	OG1480 (%)	OG1481 (%)	OG1482 (%)	OG1483 (%)	OG1484 (%)	OG1485 (%)
43204	propane	C3H8	0.4818	0.5019	0.6210	0.7785	0.1899	0.6726	0.4902
43205	propene	C3H6	1.5476	1.2945	1.3147	1.5437	1.4813	1.2107	1.1044
47049	propionitrile	C3H4N	0.1364	0.1255	0.0651	0.0475	0.1766	0.0752	0.0507
47050	pyrrole	C4H5N	0.2578	0.2076	0.0885	0.0632	0.1888	0.0564	0.0835
45220	styrene	C8H8	0.2523	0.2081	0.2629	0.1953	0.4040		0.4226
45202	toluene	C7H8	0.9977	0.8140	0.8514	1.0133	0.9427	0.5816	1.0312
90100	trans-1,3-pentadiene	C5H8	0.0864	0.0826	0.0776	0.0924	0.0949	0.0752	0.0563
43216	trans-2-butene	C4H8	0.0977	0.0918	0.1052	0.1108	0.0442	0.0594	0.0338
43226	trans-2-pentene	C5H10	0.0455	0.0459	0.0376	0.0449	0.0243	0.0237	0.0169
51360	tricyclene	C10H16	0.0068	0.0245	0.0551	0.0238	0.0110		0.0113
99999	unidentified	–	2.2566	2.0828	1.6241	1.7796	1.3418	1.2430	0.7779
98134	vinylacetylene	C4H4	0.0341	0.0398	0.0376	0.0317	0.1369	0.0317	0.0902
	Total		100.0000	100.0000	100.0000	100.0000	100.0000	100.0000	100.0000

Table A4. Literature-based and project-specific compound allocation rules used to resolve grouped or unresolved organic-gas signals in the updated profiles

Source signal / mixture	Formula	Split set / use	Assigned compound	SAROAD	Allocation (%)	Reference and allocation
Benzenediols	C6H6O2	OG1485 only	o-benzenediol / catechol	43569	94	OG1485 was allocated 94.0% catechol, 5.2% hydroquinone, and 0.8% resorcinol using the Schauer et al. (2001) pine-fireplace distribution represented in CARB profile OG5491. OG1479–OG1484 were not reallocated.
Benzenediols	C6H6O2	OG1485 only	p-benzenediol / hydroquinone	43571	5.2	Same OG1485-only Schauer/OG5491 allocation as above.
Benzenediols	C6H6O2	OG1485 only	m-benzenediol / resorcinol	43568	0.8	Same OG1485-only Schauer/OG5491 allocation as above.
beta-pinene + myrcene	C10H16	All profiles	beta-pinene	98026	50	Equal allocation applied because the grouped source measurement did not provide a quantitative compound-specific ratio.
beta-pinene + myrcene	C10H16	All profiles	myrcene	90051	50	Same allocation as above.
Butene hydroxynitrate isomers	C4H9NO4	All profiles	1-nitrooxy-2-butanol	51350	27	Teng et al. (2015), Table 5, 1-butene hydroxy-nitrate isomer distribution.

Source signal / mixture	Formula	Split set / use	Assigned compound	SAROAD	Allocation (%)	Reference and allocation
Butene hydroxynitrate isomers	C4H9NO4	All profiles	2-nitrooxy-1-butanol	51351	73	Same Teng et al. (2015) allocation as above.
Butenenitrile isomers	C4H5N	OG1479–OG1484	3-butenenitrile	50670	64.33	Hatch et al. (2015) vegetation/no-peat relative 3-/2-butenenitrile abundance, giving 64.33%/35.67% within the residual portion.
Butenenitrile isomers	C4H5N	OG1479–OG1484	2-butenenitrile	50671	35.67	Same Hatch et al. (2015) vegetation/no-peat allocation as above.
Butenenitrile isomers	C4H5N	OG1485	3-butenenitrile	50670	68.57	Hatch et al. (2015) black spruce + ponderosa pine relative abundance, giving 68.57%/31.43% within the residual portion.
Butenenitrile isomers	C4H5N	OG1485	2-butenenitrile	50671	31.43	Same Hatch et al. (2015) forest/conifer allocation as above.
C3H8O3 isomers	C3H8O3	All profiles	glycerol	43380	100	Glycerol used as a representative surrogate, with Liang et al. (2021) providing supporting biomass-burning evidence.
Creosols	C8H10O2	All profiles	4-methylguaiacol / 2-methoxy-4-methylphenol	43575	100	4-methylguaiacol selected based on Schauer et al. (2001) pine-combustion measurements represented in CARB profile OG5491.

Source signal / mixture	Formula	Split set / use	Assigned compound	SAROAD	Allocation (%)	Reference and allocation
Methylnitrocatechols	C7H7NO4	All profiles	4-methyl-5-nitrocatechol	51690	50	Equal split between the two likely C7H7NO4 isomers identified by Xie et al. (2020); no quantitative isomer ratio was reported.
Methylnitrocatechols	C7H7NO4	All profiles	3-methyl-6-nitrocatechol	51691	50	Same Xie et al. (2020)-based allocation as above.
Nitrocatechols	C6H5NO4	All profiles	4-nitrocatechol	51550	100	Assigned to 4-nitrocatechol based on authentic-standard identification by Xie et al. (2020).
Nitrocresols	C7H7NO3	All profiles	2-methyl-6-nitrophenol / 2-nitro-o-cresol	51530	100	Represented by 2-methyl-6-nitrophenol based on gas-phase nitrophenol evidence from Sakakibara et al. (2022).
Propene hydroxynitrate isomers	C3H7NO4	All profiles	1-nitrooxy-2-propanol	51210	31	Teng et al. (2015), Table 5, propene hydroxy-nitrate isomer distribution.
Propene hydroxynitrate isomers	C3H7NO4	All profiles	2-nitrooxy-1-propanol	51211	69	Same Teng et al. (2015) allocation as above.
Residual C4H6O2 isomer mass	C4H6O2	OG1485 only	2-oxobutanal	43577	100% of residual (13% of parent)	For OG1485, the 13% unresolved C4H6O2 residual was represented by 2-oxobutanal using supporting wood-combustion measurements from Schauer et al. (2001) and CARB profile OG5491. OG1479–OG1484 retain this residual as unidentified mass.

Table A5. Mass contributions of compounds produced by the additional allocation and isomer-splitting rules used in the updated profiles

Profile ID	Profile name	Total mixture mass resolved/assigned (% TOG)	Multi-compound split (% TOG)	Single representative assignment (% TOG)
OG1479	Rice crop residue burning	0.9468	0.2809	0.6659
OG1480	Crop residue burning	0.9523	0.2301	0.7222
OG1481	Pile burning	1.1811	0.3547	0.8264
OG1482	Slash burning	1.5493	0.1454	1.4039
OG1483	Prescribed grassland burning	0.6548	0.2022	0.4526
OG1484	Prescribed shrubland burning	0.5610	0.0743	0.4867
OG1485	Prescribed forest/woodland burning	2.4806	1.8070	0.6736

Table A6. Leading species contributing to the mean MIR-weighted ozone formation potential of the updated agricultural- and prescribed-burning profiles

Source group	Rank	Compound	Mean mass fraction (% TOG)	MIR_2010	OFP contribution (g O3/g TOG)	Share of group OFP (%)
Agricultural burning (OG1479–OG1482)	1	methylglyoxal	3.2374	16.560	0.5361	13.08
Agricultural burning (OG1479–OG1482)	2	2,3-butanedione	2.6249	20.090	0.5273	12.86
Agricultural burning (OG1479–OG1482)	3	formaldehyde	5.0762	9.460	0.4802	11.72
Agricultural burning (OG1479–OG1482)	4	acetaldehyde	6.8658	6.540	0.4490	10.95
Agricultural burning (OG1479–OG1482)	5	ethene	2.9177	9.000	0.2626	6.41

Source group	Rank	Compound	Mean mass fraction (% TOG)	MIR_2010	OFP contribution (g O3/g TOG)	Share of group OFP (%)
Agricultural burning (OG1479–OG1482)	6	acrolein	2.5354	7.450	0.1889	4.61
Agricultural burning (OG1479–OG1482)	7	propene	1.4251	11.660	0.1662	4.05
Agricultural burning (OG1479–OG1482)	8	methyl vinyl ketone	1.5953	9.650	0.1539	3.76
Agricultural burning (OG1479–OG1482)	9	isoprene	1.2857	10.610	0.1364	3.33
Agricultural burning (OG1479–OG1482)	10	furan	1.3538	9.150	0.1239	3.02

Source group	Rank	Compound	Mean mass fraction (% TOG)	MIR_2010	OFP contribution (g O3/g TOG)	Share of group OFP (%)
Agricultural burning (OG1479–OG1482)	11	glyoxal	0.9254	12.500	0.1157	2.82
Agricultural burning (OG1479–OG1482)	12	glycolaldehyde	1.8079	5.100	0.0922	2.25
Agricultural burning (OG1479–OG1482)	13	1-hydroxy-2-propanone	2.5935	3.230	0.0838	2.04
Agricultural burning (OG1479–OG1482)	14	crotonaldehyde	0.8221	9.390	0.0772	1.88
Agricultural burning (OG1479–OG1482)	15	propanal	0.7588	7.080	0.0537	1.31

Source group	Rank	Compound	Mean mass fraction (% TOG)	MIR_2010	OFP contribution (g O3/g TOG)	Share of group OFP (%)
Agricultural burning (OG1479–OG1482)	16	2,5-dimethylfuran	0.6637	7.880	0.0523	1.28
Agricultural burning (OG1479–OG1482)	17	monoterpenes	1.2344	4.040	0.0499	1.22
Agricultural burning (OG1479–OG1482)	18	1,3-butadiene	0.3456	12.610	0.0436	1.06
Agricultural burning (OG1479–OG1482)	19	toluene	0.9191	4.000	0.0368	0.90
Agricultural burning (OG1479–OG1482)	20	methanol	5.0078	0.670	0.0336	0.82

Source group	Rank	Compound	Mean mass fraction (% TOG)	MIR_2010	OFP contribution (g O3/g TOG)	Share of group OFP (%)
Prescribed burning (OG1483–OG1485)	1	formaldehyde	8.4376	9.460	0.7982	18.26
Prescribed burning (OG1483–OG1485)	2	methylglyoxal	3.3526	16.560	0.5552	12.70
Prescribed burning (OG1483–OG1485)	3	acetaldehyde	8.0540	6.540	0.5267	12.05
Prescribed burning (OG1483–OG1485)	4	ethene	4.8981	9.000	0.4408	10.09
Prescribed burning (OG1483–OG1485)	5	2,3-butanedione	2.0818	20.090	0.4182	9.57

Source group	Rank	Compound	Mean mass fraction (% TOG)	MIR_2010	OFP contribution (g O3/g TOG)	Share of group OFP (%)
Prescribed burning (OG1483–OG1485)	6	acrolein	2.9267	7.450	0.2180	4.99
Prescribed burning (OG1483–OG1485)	7	glyoxal	1.3900	12.500	0.1738	3.98
Prescribed burning (OG1483–OG1485)	8	propene	1.2655	11.660	0.1476	3.38
Prescribed burning (OG1483–OG1485)	9	methyl vinyl ketone	1.4323	9.650	0.1382	3.16
Prescribed burning (OG1483–OG1485)	10	glycolaldehyde	2.4619	5.100	0.1256	2.87

Source group	Rank	Compound	Mean mass fraction (% TOG)	MIR_2010	OFP contribution (g O3/g TOG)	Share of group OFP (%)
Prescribed burning (OG1483–OG1485)	11	crotonaldehyde	0.9071	9.390	0.0852	1.95
Prescribed burning (OG1483–OG1485)	12	1-hydroxy-2-propanone	2.4711	3.230	0.0798	1.83
Prescribed burning (OG1483–OG1485)	13	propanal	0.8070	7.080	0.0571	1.31
Prescribed burning (OG1483–OG1485)	14	1,3-butadiene	0.4332	12.610	0.0546	1.25
Prescribed burning (OG1483–OG1485)	15	toluene	0.8518	4.000	0.0341	0.78

Source group	Rank	Compound	Mean mass fraction (% TOG)	MIR_2010	OFP contribution (g O3/g TOG)	Share of group OFP (%)
Prescribed burning (OG1483–OG1485)	16	acetic acid	4.9984	0.680	0.0340	0.78
Prescribed burning (OG1483–OG1485)	17	isoprene	0.3101	10.610	0.0329	0.75
Prescribed burning (OG1483–OG1485)	18	furan	0.3573	9.150	0.0327	0.75
Prescribed burning (OG1483–OG1485)	19	2-methyl-2-propenal	0.5110	6.010	0.0307	0.70
Prescribed burning (OG1483–OG1485)	20	2,5-dimethylfuran	0.3531	7.880	0.0278	0.64