# OG Speciation Profile for Aircraft—Jet Fuel (OG5861)

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## 1 Introduction

The current CARB organic gas (OG) speciation profile for aircraft—jet fuel combustion is OG586, which is a composite profile of three EPA aircraft landing/takeoff profiles: 1097 (military), 1098 (commercial) and 1099 (general aviation) [1]. These three profiles were made based on a series of studies performed by Spicer et al [2] in the 1980s. A wide range of organic gases emitted from aircraft engines were quantified in the studies.

In 2003, NASA initiated a series of aircraft engine emission measurement programs called Aircraft Particle Emission eXperiment (APEX), with FAA, CARB, EPA and other sponsors. The APEX studies focused on commercial aircraft particulate matter emissions, and also included organic gaseous emissions analysis. Because more advanced sampling and analytical techniques were used in the APEX studies, more gaseous organic species were identified relative to the previous Spicer's chemical list. Based on the test results, a new OG speciation profile was created by US EPA and FAA in 2009 [3], and the profile was added to the SPECIATE 4.3 database as No. 5565 in 2011. The data of this profile are used in this work to create a new jet aircraft OG profile for CARB to replace the current OG586. The new CARB aircraft-jet fuel profile is OG5861.

## 2 Methodology

Because some of the chemical species in the new profile do not have corresponding CARB SAROAD codes in the existing CEIDARS POLLUTANT table and chem3.d table, new CARB SAROAD codes are created in this work for them (Table 1).

**Table 1. New CARB SAROAD codes to be added to the CEIDARS POLLUTANT table**

| *CARB SAROAD* | *CAS* | *Chemical Name* | *Formula* | *Molecular Weight* |
|---|---|---|---|---|
| 45504 | 529204 | o-tolualdehyde | C8H8O | 120.15 |
| 45505 | | C11 aromatics | C11H16 | 147.70 |
| 45506 | 82107899 | dodecenal | C12H22O | 182.30 |
| 43125 | | C10 Olefins | C10H20 | 140.27 |
| 43126 | | C14 alkanes | C14H30 | 198.39 |
| 43127 | | C15 alkanes | C15H32 | 212.41 |
| 43124 | | C16 alkanes | C16H34 | 226.44 |
| 43119 | | C18 alkanes | C18H38 | 254.49 |

## 3 Results and Discussion

Most of the species contributions in the new profile are comparable to the current profile OG586. For example, ethylene and formaldehyde are two of the most abundant species in both profiles. However, the role of methane is very different: OG586 shows that 11.4% of the exhaust TOG is methane [1], but no methane is in the new profile. Because the APEX studies found methane in the aircraft exhaust was below the ambient level, it is not considered to be a significant emission from aircraft engine burning jet fuel and then is not included in the new profile created based APEX data (Table 2).

This profile can be used to convert emissions based on FID-THC (Flame Ionization Detector-Total Hydrocarbon) measurements to TOG. Assuming that mass THC is based on the molecular weight of methane (16.04) per carbon measured, the actual weight of each compound can be calculated and the carbonyl emissions added to the THC emissions. Based on the above profile, the TOG/THC fraction is 1.366 which converts THC emission mass (expressed as methane) to actual weight TOG. The ROG (=TOG – methane –ethane -acetone) fraction of TOG is 0.9911.

**Table 2. OG speciation profile for aircraft—jet fuel**

| *Species Name* | *SAROAD* | *Weight Percentage (%)* |
|---|---|---|
| 1,2,3-trimethylbenzene | 45225 | 0.106 |
| 1,2,4-trimethylbenzene | 45208 | 0.350 |
| 1,3,5-trimethylbenzene | 45207 | 0.054 |
| 1,3-butadiene | 43218 | 1.687 |
| 1-butene | 43213 | 1.754 |
| 1-decene | 43268 | 0.185 |
| 1-heptene | 98005 | 0.438 |
| 1-hexene | 43245 | 0.736 |
| 1-methyl-2-ethylbenzene | 99915 | 0.065 |
| 1-methyl-3-ethylbenzene | 99912 | 0.154 |
| 1-methyl-4-ethylbenzene | 99914 | 0.064 |
| 1-methylnaphthalene | 91124 | 0.247 |
| 1-nonene | 43267 | 0.246 |
| 1-octene | 43265 | 0.276 |
| 1-pentene | 43224 | 0.776 |
| 2-methyl-1-butene | 43225 | 0.140 |
| 2-methyl-1-pentene | 98040 | 0.034 |
| 2-methyl-2-butene | 43228 | 0.185 |
| 2-methyl-2-propenal | 43506 | 0.429 |
| 2-methylnaphthalene | 91123 | 0.206 |
| 2-methylpentane | 43229 | 0.408 |
| 3-methyl-1-butene | 43223 | 0.112 |
| 4-methyl-1-pentene | 98135 | 0.069 |
| acetaldehyde | 43503 | 4.272 |
| acetone | 43551 | 0.369 |
| acetylene | 43206 | 3.939 |
| acrolein | 43505 | 2.449 |
| benzaldehyde | 45501 | 0.470 |
| benzene | 45201 | 1.681 |
| butyraldehyde | 43510 | 0.119 |
| C10-aromatics | 98050 | 0.656 |
| C10-olefins | 43125 | 5.843 |
| C10-paraffins | 99323 | 14.606 |

| *Species Name* | *SAROAD* | *Weight Percentage (%)* |
|---|---|---|
| C11-aromatics | 45505 | 0.324 |
| C14-alkanes | 43126 | 0.186 |
| C15-alkanes | 43127 | 0.177 |
| C16-alkanes | 43124 | 0.146 |
| C18-alkanes | 43119 | 0.002 |
| cis-2-butene | 43217 | 0.210 |
| cis-2-pentene | 43227 | 0.276 |
| crotonaldehyde | 98156 | 1.033 |
| decanal | 47024 | 5.843 |
| dimethyl napthalene | 99365 | 0.090 |
| dodecenal | 45506 | 2.921 |
| ethane | 43202 | 0.521 |
| ethylbenzene | 45203 | 0.174 |
| ethylene | 43203 | 15.461 |
| formaldehyde | 43502 | 12.310 |
| glyoxal | 90121 | 1.816 |
| heptadecane | 43282 | 0.009 |
| hexadecane | 43281 | 0.049 |
| isopropylbenzene | 98043 | 0.003 |
| isovaleraldehyde | 98056 | 0.032 |
| m & p-xylene | 99024 | 0.282 |
| methyl alcohol | 43301 | 1.805 |
| methyl glyoxal | 90122 | 1.503 |
| m-tolualdehyde | 99455 | 0.278 |
| naphthalene | 98046 | 0.541 |
| n-decane | 43238 | 0.320 |
| n-dodecane | 43255 | 0.462 |
| n-heptane | 43232 | 0.064 |
| n-nonane | 43235 | 0.062 |
| n-octane | 43233 | 0.062 |
| n-pentane | 43220 | 0.198 |
| n-propylbenzene | 45209 | 0.053 |
| n-tridecane | 43258 | 0.535 |
| n-undecane | 43241 | 0.444 |
| o-tolualdehyde | 45504 | 0.230 |
| o-xylene | 45204 | 0.166 |
| pentadecane | 43260 | 0.173 |
| phenol | 45300 | 0.726 |
| propane | 43204 | 0.078 |
| propionaldehyde | 43504 | 0.727 |
| propylene | 43205 | 4.534 |
| p-tolualdehyde | 99397 | 0.048 |
| styrene | 45220 | 0.309 |
| tetradecane | 43259 | 0.416 |
| toluene | 45202 | 0.642 |
| trans-2-hexene | 98034 | 0.030 |
| trans-2-pentene | 43226 | 0.359 |
| valeraldehyde | 98200 | 0.245 |

| *Species Name* | *SAROAD* | *Weight Percentage (%)* |
|---|---|---|
| *Total* | | *100.000* |

## 4 Estimated Impacts of the Profile Update on the Emission Inventory

The newly-developed profile, OG5861, will replace the current profile OG586 for the inventory categories associated with jet aircraft combustion. The related SCCs/EICs are summarized in Table 3.

**Table 3. SCCs/EICs associated with jet aircraft**

| *SCC/EIC* | *Names* | | |
|---|---|---|---|
| 125 | commercial | jet aircraft | taxi |
| 126 | commercial | jet aircraft | take-off |
| 127 | commercial | jet aircraft | climb-out |
| 128 | commercial | jet aircraft | cruise |
| 129 | commercial | jet aircraft | descent |
| 131 | commercial | jet aircraft | approach |
| 47555 | other aircraft | jet aircraft | commercial jet |
| 47571 | government aircraft | military | jet aircraft |
| 47589 | other aircraft | jet aircraft | civil jet aircraft |
| 20100501 | electric generation | jet fuel | turbine |
| 20100901 | electric generation | keronaptha jet fuel | turbine |
| 20100902 | electric generation | keronaptha jet fuel | reciprocating |
| 20200901 | industrial | keronaptha jet fuel | turbine |
| 20200902 | industrial | keronaptha jet fuel | reciprocating |
| 20300901 | commercial | keronaptha jet fuel | turbine: jp-4 |
| 20400101 | engine testing | aircraft | turbojet |
| 20400102 | engine testing | aircraft | turbo shaft |
| 20400112 | engine testing | aircraft | JP-4 fuel |
| 27501014 | fixed wing aircraft | military | JP-4 fuel |
| 27501015 | fixed wing aircraft | military | JP-5 fuel |
| 27502011 | fixed wing aircraft | commercial | Jet-A fuel |
| 27505011 | fixed wing aircraft | civil | Jet-A fuel |
| 27601014 | rotary wing aircraft | military | JP-4 fuel |
| 27601015 | rotary wing aircraft | military | JP-5 fuel |
| 27602011 | rotary wing aircraft | commercial | Jet-A fuel |
| 27605011 | rotary wing aircraft | civil | Jet-A fuel |
| 81080814000000 | jet aircraft | military | jet fuel |
| 81080814300000 | jet aircraft | military | jet naphtha (JP-5) |
| 81081014000000 | jet aircraft | commercial | jet fuel |
| 81081014500000 | jet aircraft | commercial | Jet-A a fuel |
| 81081214000000 | jet aircraft | civil | jet fuel |
| 81081214500000 | jet aircraft | civil | Jet-A fuel |

The statewide annual average TOG emissions of jet aircraft exhausts are 30.50 tons/day, , 0.44% of the statewide total TOG emissions, based on the 2009 Almanac data for year

2010 [4]. Using the new profile OG5861, the ROG will be 30.23 tons/day, which is 11.1% higher than the ROG estimated based on the current profile OG586. The ozone forming potential (OFP) calculated based on SAPRC07 mechanism is 6.47 for the new profile; while the one for the current profile is 6.75. The emissions of the five toxic species listed in Table 4 are all reduced if the new profile is applied to the related categories (Table 3).

**Table 4. Changes on emissions of $PM_{2.5}$ species for jet aircraft categories (2010)**

| *Statewide Annual Ave. Emissions* | | *Current OG586 (tons/day)* | *New OG5861 (tons/day)* | *Change* | |
|---|---|---|---|---|---|
| | | | | *Emissions(tons/day)* | *Percentage* |
| ROG | | 27.21 | 30.23 | 3.02 | 11.1% |
| Ozone formation potential (MIR), (g O3/g ORG) | | 6.75 | 6.47 | -0.28 | -4.1% |
| Toxics | Benzene | 0.67 | 0.51 | -0.16 | -23.2% |
| | Formaldehyde | 5.18 | 3.75 | -1.42 | -27.5% |
| | 1,3-butadiene | 0.61 | 0.51 | -0.10 | -15.7% |
| | Acrolein | 0.78 | 0.75 | -0.03 | -4.3% |
| | Acetaldehyde | 1.60 | 1.30 | -0.30 | -18.6% |
| | PAHs | 0.36 | 0.33 | -0.03 | -8.9% |

## 5 Version Control

This section will be completed after management approval and after the CEIDARS FRACTION table and PMPROFILE table are updated. Version information from CEIDARS FRACTION table will be copied here.

**References:**


1. California Air Resources Board Main Speciation Profiles. In Jan 1, 2012 ed.; California Air Resources Board: 2012.
2. Spicer, C. W.; Holdren, M. W.; Lyon, T. F.; Riggin, R. M. *Composition and Photochemical Reactivity of Turbine Engine Exhaust*; ESL-TR-84-28 Air Force Engineering and Services Center (RDVS): Tyndall AFB, FL, 1984.
3. Knighton, W. B.; Herndon, S. C.; Miake-Lye, R. C. *Aircraft Engine Speciated Organic Gases: Speciation of Unburned Organic Gases in Aircraft Exhaust*; EPA-420-R-09-902; U.S. Environmental Protection Agency and Federal Aviation Administration: May 2009.
4. CEPAM. In California Air Resources Board: 2011.