

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

<i>CARB SAROAD</i>	<i>CAS</i>	<i>Chemical Name</i>	<i>Formula</i>	<i>Molecular Weight</i>
45504	529204	o-tolualdehyde	C ₈ H ₈ O	120.15
45505		C11 aromatics	C ₁₁ H ₁₆	147.70
45506	82107899	dodecenal	C ₁₂ H ₂₂ O	182.30
43125		C10 Olefins	C ₁₀ H ₂₀	140.27
43126		C14 alkanes	C ₁₄ H ₃₀	198.39
43127		C15 alkanes	C ₁₅ H ₃₂	212.41
43124		C16 alkanes	C ₁₆ H ₃₄	226.44
43119		C18 alkanes	C ₁₈ H ₃₈	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

<i>Species Name</i>	<i>SAROAD</i>	<i>Weight Percentage (%)</i>
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

<i>Species Name</i>	<i>SAROAD</i>	<i>Weight Percentage (%)</i>
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 naphthalene	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

<i>Species Name</i>	<i>SAROAD</i>	<i>Weight Percentage (%)</i>
<i>Total</i>		<i>100.000</i>

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

<i>SCC/EIC</i>	<i>Names</i>		
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
8108081400000	jet aircraft	military	jet fuel
8108081430000	jet aircraft	military	jet naphtha (JP-5)
8108101400000	jet aircraft	commercial	jet fuel
8108101450000	jet aircraft	commercial	Jet-A a fuel
8108121400000	jet aircraft	civil	jet fuel
8108121450000	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 O ₃ /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.