Recommended Best Practice for Quantifying Speciated Organic Gas Emissions from Aircraft Equipped with Turbofan, Turbojet, and Turboprop Engines

Version 1.0

United States
Environmental Protection
Agency

Recommended Best Practice for Quantifying Speciated Organic Gas Emissions from Aircraft Equipped with Turbofan, Turbojet, and Turboprop Engines

Version 1.0

Assessment and Standards Division
Office of Transportation and Air Quality
U.S. Environmental Protection Agency

and

AEE-300 - Emissions Division
Office of Environment and Energy
Federal Aviation Administration

EPA-420-R-09-901
May 2009

ACKNOWLEDGEMENTS

The Federal Aviation Administration (FAA) Office of Environment and Energy (AEE) and the U.S. Environmental Protection Agency (EPA) Office of Transportation Air Quality (OTAQ) would like to acknowledge the following agencies and individuals for their contribution to this document:

- FAA – Ralph Iovinelli, Mohan Gupta, Carl Ma, and Ed McQueen
- EPA – Bryan Manning, Rich Cook, Kent Helmer, Ken Petche, John Kinsey, Rich Wilcox, Kathryn Sergeant, Marion Hoyer, Laurel Driver, and Suzanne King
- California Air Resources Board – Steve Francis, Paul Allen, Wenli Yang, and Steve Church
- Aerodyne Research, Inc. – Rick Miake-Lye and Scott Herndon
- Montana State University – Berk Knighton
- KB Environmental Sciences, Inc. – Carrol Bryant, Mike Ratte, Paul Sanford, and Mike Kenney

This document was prepared for the Federal Aviation Administration, Office of Environment and Energy by KB Environmental Sciences Inc. with assistance from CSSI Inc. in support of CSSI's Contract DTFAWA-05-C-00044, Technical Directive Memorandum B-002-011.

EXECUTIVE SUMMARY

This document presents an approach to, and technical support for, the quantification of organic gas (OG) emissions including hazardous air pollutants (HAPs) from aircraft equipped with turbofan, turbojet and turboprop engines.[1,2,3] This Recommended Best Practice (RBP) was produced through an inter-agency partnership and collaborative effort between the Federal Aviation Administration (FAA) Office of Environment and Energy (AEE) and the U. S. Environmental Protection Agency (EPA) Office of Transportation Air Quality (OTAQ).[4] At the onset of the endeavor, the agencies agreed that the method used to quantify speciated OG emissions from aircraft engines should be:

- Nationally consistent,
- Supported by scientific data,
- Representative of today's flying fleet (to the extent possible), and
- A "living" process to reflect the state-of-the-science as new data becomes available.

Central to this RBP is the preparation of a revised speciation profile to identify most of the individual OG species that comprise the OG emissions from aircraft equipped with turbofan, turbojet, and turboprop engines (it should be noted that approximately 29 percent of the total amount of OG emissions from the tested engines remain characterized as unidentified). This new profile is based on recent field measurement campaigns and is considered representative of today's modern aircraft engines. The new profile (SPECIATE profile #5565), to be incorporated in to the next revision of EPA's SPECIATE (Version 4.0) database, is recommended as a replacement for all prior speciation profiles identified for aircraft and is the preferred profile that should be used to characterize gas-phase speciated OG emissions from aircraft equipped with turbofan, turbojet and turboprop engines.

The new speciation profile identifies 77 individual compounds, including 15 that are recognized by section 112 of the Clean Air Act as being hazardous air pollutants (HAPs). Two additional compounds also have potential toxic characteristics according to EPA's Integrated Risk Information System (IRIS) database. While future research will further define the unidentified component, in the interim, the unidentified mass has been generically characterized as longer carbon chain species (see Section 2.1 of this report) for air quality modeling practitioners that use chemical mechanisms such as the Statewide Air Pollution Research Center 1999 (SAPRC99), Carbon Bond 4, Carbon Bond 5, and the RADM-2 models.

It is important to acknowledge that the measurement of air emissions associated with aircraft engines is an evolving process that is still under development. This is especially relevant to the speciation of aircraft-related OG for which there is appreciably less experience, data, and

[1] This document does not address and/or provide speciation profiles for polynuclear aromatic hydrocarbons (PAH)/volatile organic compounds (VOC) or PAH/particulate matter.

[2] Although direct emission measurements from turboprop engines are not available at this time, it is recognized that turboprop engines operate with the same kerosene based fuels and have similar combustor temperature and pressures as the tested engines.

[3] This effort/document focuses on kerosene fueled turbofan, turbojet, and turboprop engines. Other engine types, including piston engines and those in auxiliary power units and ground service equipment, are not included in the analysis.

[4] EPA's Office of Research Development (ORD)/National Risk Management Research Laboratory (NRMRL) also participated in the development and review of this material.

information, when compared to other criteria pollutants or air pollutant emissions from other mobile sources (e.g., motor vehicles).

The FAA and EPA have agreed to continue further development of speciated OG from aircraft engines as new scientific information becomes available. Because this effort is a "living" methodology, air quality practitioners should verify that they have the most recent version of this document (by date and version number on the cover) and associated speciated profile before preparing an aircraft HAPs emissions inventory. New information and speciation profile will be posted on both FAA's and EPA's websites.[5] In addition, EPA's next revision to the SPECIATE database will incorporate this information.[6]

It is also important to acknowledge that there are currently no Federal regulatory guidelines specific to HAPs emissions from aircraft engines and, while the methodology discussed in this document is useful for disclosure, reporting, and comparative purposes, it does not provide results that are directly comparable to any regulatory or enforceable air quality standards.

[5] See www.FAA.gov/regulations_policies/policy_guidance/envir_policy/ and www.EPA.gov/otaq/aviation.htm
[6] USEPA. SPECIATE Version 4.0 (www.epa.gov/ttn/chief/software/speciate/index.html), December 2006.

ACRONYMS AND ABBREVIATIONS

AEE	FAA Office of Environment and Energy
APEX	Aircraft Particle Emissions Experiment
ASPM	Aviation System Performance Metrics (database)
CAA	Clean Air Act
CAEP	Committee on Aviation Environmental Protection
CARB	California Air Resources Board
CAS	Chemical Abstracts Service
DoD	U.S. Department of Defense
EDMS	Emissions and Dispersion Modeling System
EPA	U.S. Environmental Protection Agency
FAA	Federal Aviation Administration
FID	Flame Ionization Detector
HAPs	Hazardous air pollutants
HC	Hydrocarbon
ICAO	International Civil Aviation Organization
IRIS	Integrated Risk Information System
JETS	Jet Emission Testing for Speciation
kg	Kilogram
LTO	Landing-takeoff cycle
NASA	National Aeronautics and Space Administration
NEI	National Emission Inventory
NMOG	Non-methane organic gas
OG	Organic gas
OTAQ	Office of Transportation Air Quality
QAPP	Quality Assurance Plan
RBP	Recommended Best Practice
SAPRC99	Statewide Air Pollution Research Center 1999
SPECIATE	U.S. EPA data system of speciation profiles
TAC	Toxic air contaminant
TAF	Terminal Area Forecast
TAP	Toxic air pollutant
THC	Total hydrocarbons
TIM	Time in mode
TOG	Total organic gases
VOC	Volatile organic compounds

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

1.0 INTRODUCTION

> **Purpose of this Recommended Best Practice (RBP)**
> To provide a uniform approach to, and technical support for, the preparation of speciated gas-phase HC inventories (including HAPs) from aircraft equipped with turbofan, turbojet, and turboprop engines.

This document presents an approach for quantification of speciated organic gas (OG) emissions, including hazardous air pollutants (HAPs), from commercial aircraft equipped with turbofan, turbojet, and turboprop engines.[1,2,3,4] The preparation of an emissions inventory (an accounting of pollutant mass emissions from a source over a specific time interval) is the preferred approach for quantifying emissions from aircraft equipped with turbofan, turbojet, and turboprop engines. The aircraft-related speciation profile discussed in this document will also be used to update the speciated OG profile for aircraft equipment with turbofan, turbojet, and turboprop engines in the SPECIATE database[5], the U.S. Environmental Protection Agency's (EPA's) multi-sector repository for such data.

The focus of this document is only on aircraft equipped with turbofan, turbojet, and turboprop engines. The Federal Aviation Administration (FAA) intends to separately publish information that will address other airport-related sources (including other piston-powered aircraft engines). In these separate efforts, information will be provided for sources such as ground service equipment (includes vehicles such as aircraft tugs, baggage tugs, fuel trucks, maintenance vehicles, and other miscellaneous vehicles used to support aircraft operations), ground access vehicles (includes motor vehicles used by passengers, employees, freight operators, and other persons to enter and leave an airport such as shuttles, taxis, rental cars, and privately-owned vehicles), fuel storage and transfer facilities, stationary support services, and construction activities.

1.1 Background Information

The National Aeronautics and Space Administration (NASA), EPA, the Department of Defense (DoD), and FAA collaboratively sponsored three separate commercial aircraft engine exhaust measurement campaigns in 2004 and 2005, known as the Aircraft Particle Emission eXperiments (APEX1, APEX2, and APEX3). In addition, California Air Resources Board co-sponsored, as well as initiated, the JETS/APEX2 campaign (JETS (Jet Emission Testing for Speciation) is a California Air Resources Board (CARB) acronym).

---

[1] In this document, the term "hazardous air pollutants" and the accompanying acronym "HAPs" mean the same as "air toxics", "toxic air contaminants" or "TACs", and "toxic air pollutants" or "TAPs".

[2] This document does not address and/or provide speciation profiles for polycyclic aromatic hydrocarbons (PAH)/volatile organic compounds (VOC) or PAH/particulate matter.

[3] Although direct emission measurements from turboprop engines are not available at this time, it is recognized that turboprop engines operate on the same kerosene based fuels, and have similar combustor temperature and pressures as the tested engines.

[4] This effort/document focuses on kerosene fueled turbofan, turbojet, and turboprop engines. Other engine types, including piston engines, and those in auxiliary power units and ground service equipment, are not included in the analysis.

[5] USEPA. SPECIATE Version 4.0 (www.epa.gov/ttn/chief/software/speciate/index.html), December 2006.

The three campaigns were designed to evaluate the effects of engine thrust and fuel type on the levels of particulate matter and gaseous emissions from commercial aircraft engines, and specific measurements were made for speciated OG, including HAPs.

In the summer of 2007, the FAA and EPA formed a partnership and began a joint effort to use this newly acquired information and data to develop uniform protocols and methods to quantify the level of OG and HAPs from commercial aircraft. At the onset, the agencies agreed that the protocols and methods should be:

- Nationally consistent,
- Supported by scientific data,
- Representative of today's flying fleet to the extent possible, and
- A "living" process to reflect the state-of-the-science as new data becomes available.

The procedures that the FAA and EPA used to develop the uniform protocols and methods discussed in this document are outlined in the FAA/EPA *Quality Assurance Project Plan (QAPP) for the Development of a Commercial Aircraft Hazardous Air Pollutants Emission Inventory Methodology* [FAA/EPA, 2008]. In addition, the technical details and scientific information are available in a Technical Support Document [Knighton, Herndon, Miake-Lye, 2009]. Electronic copies of these documents are available on both FAA's and EPA's websites.[6]

1.2 Approach

It is important to acknowledge that the measurement of pollutant emissions in aircraft exhaust is an evolving science. In fact, new aircraft engine exhaust measurement campaigns and modeling studies are currently underway and more are planned in the future. This is especially relevant to aircraft-related speciated OG for which there is appreciably less experience, data, and information, when compared to criteria air pollutants (e.g., carbon monoxide and nitrogen oxides) and other mobile air pollutant sources (e.g., ground service equipment, motor vehicles).

Two guiding principles were followed during the course of this endeavor to develop uniform protocols and methods for quantifying aircraft-related gas-phase speciated OGs, while considering the current limitations and uncertainties associated with these specialized pollutants.

First, the RBP should reflect the current state-of-the-science. The FAA and EPA recognize that even though the amount of aircraft engine emission test data is growing, the amount is still limited and there are research gaps that need to be addressed. However, by publishing this document, the FAA and EPA are establishing an initial and nationally-consistent approach for preparing speciated OG and HAPs emission inventories. While this is the case, air quality practitioners must recognize that the topic of speciating aircraft-related OG is

[6] See www.FAA.gov/regulations_policies/policy_guidance/envir_policy/ and www.EPA.gov/otaq/aviation.htm

relatively new and therefore in an evolutionary science. As a result, this RBP will be updated as scientific advancements are made.

Second, even though there is still some uncertainty related to gas-phase speciated OG emissions from commercial aircraft, there is an immediate and growing need for an accurate, up-to-date, and consistent method for estimating these emissions. Therefore, this document makes the best use of what is presently known about aircraft OGs with the expectation that this RBP may need to be updated as new information and data are available.

1.3 Regulatory Context

There are presently no Federal regulatory guidelines that address aircraft engine-related gas-phase OG species or HAPs emissions. By definition, aircraft are not subject to the regulations of Section 112 of the Federal Clean Air Act (CAA).[7] That said, there are 15 common HAPs detected in measurable concentrations in aircraft engine exhaust, and these HAPs are also listed in Section 112 of the CAA. These pollutants are 1,3 butadiene, acetaldehyde, acrolein, benzene, ethylbenzene, formaldehyde, isopropylbenzene, methanol, m-xylene and p-xylene, naphthalene, o-xylene, phenol, propionaldehyde, styrene, and toluene. EPA's Integrated Risk Information System (IRIS)[8] identifies two additional hazardous compounds measured in the exhaust from turbofan, turbojet, and turboprop engines: benzaldehyde and 2-methyl-naphthalene.

---

[7] Only major stationary sources are regulated by Section 112 of the CAA.

[8] EPA's IRIS (Integrated Risk Information System) is a compilation of electronic reports on specific substances found in the environment and their potential to cause human health effects. http://cfpub.epa.gov/ncea/iris/index.cfm

2.0 SPECIATED OG PROFILE

The initial speciation profile for use in the quantification of the level of OGs/HAPs emitted from aircraft equipped with turbofan, turbojet, and turboprop engines are provided in **Table 1** and in a companion spreadsheet to this document (posted mutually on FAA's and EPA's websites).[9] Because the intent of the FAA/EPA is to update the profile as additional data becomes available, air quality practitioners should verify that they have the most recent profile before beginning an evaluation.

The development of the recommended FAA/EPA speciation profile (provided in Table 1) is discussed in a Technical Support Document entitled *Aircraft Engine Speciated Organic Gases: Speciation of Unburned Organic Gases in Aircraft Exhaust* [Knighton, Herndon, Miake-Lye, 2009]. The most noteworthy findings of this effort are stated below:

- The current speciation profile chosen to represent organic gas emissions from aircraft engines is #1098[10] in the SPECIATE database, and was derived from a publication by Spicer et al. in 1994. This profile included data from a military variant of the CFM56 commercial engine.[11] Comparisons of data from Spicer's measurements for the CFM-56 and several of the CFM-56 engines measured in the APEX programs indicate that, with few exceptions, the Spicer and APEX data exhibit an overall agreement for species where the results of measurements are available. Notably, and again with few exceptions, all of the data are within one standard deviation of the measurements to the unit line (i.e., the unity line represents perfect agreement).

- The results of a comparison of Spicer's measurements for the CFM-56 and the APEX measurements for three models of the CFM-56 also provide strong support that speciated OG profile data are invariant across engine technologies for the commercial engines tested.

- Results of both studies (i.e., Spicer and APEX) indicate that at engine power conditions substantially higher than approximately 15 to 30 percent thrust, the engine combustion efficiency is close to 100 percent. Measurement of many OGs becomes difficult or impossible due to limitations of the instrument detection levels (the OG concentration is too small to measure). Therefore, the total amount of aircraft OG in an aircraft landing-takeoff cycle (LTO) is dominated by the OG emitted at low power settings (30 percent thrust or less).

---

[9] See www.FAA.gov/regulations_policies/policy_guidance/envir_policy/ and www.EPA.gov/otaq/aviation.htm.
[10] The results of this effort will be incorporated into the SPECIATE database as profile #5565.
[11] The CFM56 is a high bypass turbofan engine. Turbofan engines with a bypass ratio of 5 or greater are considered to be high bypass turbofan engines (Cumpsty, N., Jet Propulsion, Cambridge University Press, 2002, P. 46.). CFM56 and the CFM logo represent CFM International, a joint company of Snecma and General Electric. Snecma is a French manufacturer of engines for commercial and military aircraft, and space vehicles.

Table 1. Speciated Gas-Phase OG Profile for Aircraft Equipped with Turbofan, Turbojet, and Turboprop Engines.[c]

Compound	CAS Registry No.[a]	Mass Fraction		Compound	CAS Registry No.[a]	Mass Fraction
1,2,3-trimethylbenzene	526-73-8	0.00106		glyoxal	107-22-2	0.01816
1,2,4-trimethylbenzene	95-63-6	0.00350		isobutene/1-butene	106-98-9	0.01754
1,3,5-trimethylbenzene	108-67-8	0.00054		isopropylbenzene [d]	98-82-8	0.00003
1,3-butadiene[d]	106-99-0	0.01687		isovaleraldehyde	590-86-3	0.00032
1-decene	872-05-9	0.00185		methacrolein	78-85-3	0.00429
1-heptene	25339-56-4	0.00438		methanol [d]	67-56-1	0.01805
1-hexene	592-41-6	0.00736		methylglyoxal	78-98-8	0.01503
1-methyl naphthalene	90-12-0	0.00247		m-ethyltoluene	620-14-4	0.00154
1-nonene	124-11-8	0.00246		m-tolualdehyde	620-23-5	0.00278
1-octene	25377-83-7	0.00276		m-xylene and p-xylene [d]	108-38-3 / 106-42-3	0.00282
1-pentene	109-67-1	0.00776		naphthalene [d]	91-20-3	0.00541
2-methyl-1-butene	563-46-2	0.00140		n-decane	124-18-5	0.00320
2-methyl-1-pentene	763-29-1	0.00034		n-dodecane	112-40-3	0.00462
2-methyl-2-butene	513-35-9	0.00185		n-heptadecane	629-78-7	0.00009
2-methyl-naphthalene [e]	91-57-6	0.00206		n-heptane	142-82-5	0.00064
2-methylpentane	107-83-5	0.00408		n-hexadecane	544-76-3	0.00049
3-methyl-1-butene	563-45-1	0.00112		n-nonane	111-84-2	0.00062
4-methyl-1-pentene	691-37-2	0.00069		n-octane	111-65-9	0.00062
acetaldehyde [d]	75-07-0	0.04272		n-pentadecane	629-62-9	0.00173
acetone	67-64-1	0.00369		n-pentane	109-66-0	0.00198
acetylene	74-86-2	0.03939		n-propylbenzene	103-65-1	0.00053
acrolein [d]	107-02-8	0.02449		n-tetradecane	629-59-4	0.00416
benzaldehyde [e]	100-52-7	0.00470		n-tridecane	629-50-5	0.00535
benzene [d]	71-43-2	0.01681		n-undecane	1120-21-4	0.00444
butyraldehyde	123-72-8	0.00119		o-ethyltoluene	611-14-3	0.00065
c14-alkane	No CAS	0.00186		o-tolualdehyde	529-20-4	0.00230
c15-alkane	No CAS	0.00177		o-xylene [d]	95-47-6	0.00166
c16-alkane	No CAS	0.00146		p-ethyltoluene	622-96-8	0.00064
c18-alkane	No CAS	0.00002		p-tolualdehyde	104-87-0	0.00048
c4-benzene + c3-aroald	No CAS	0.00656		phenol [d]	108-95-2	0.00726
c5-benzene + c4-aroald	No CAS	0.00324		propane	74-98-6	0.00078
cis-2-butene	590-18-1	0.00210		propionaldehyde [d]	123-38-6	0.00727
cis-2-pentene	627-20-3	0.00276		propylene	115-07-1	0.04534
crotonaldehyde	4170-30-3	0.01033		styrene [d]	100-42-5	0.00309
dimethylnapthalenes	28804-88-8	0.00090		toluene [d]	108-88-3	0.00642
ethane	74-84-0	0.00521		trans-2-hexene	4050-45-7	0.00030
ethylbenzene [d]	100-41-4	0.00174		trans-2-pentene	646-04-8	0.00359
ethylene[f]	74-85-1	0.15461		valeraldehyde	110-62-3	0.00245
formaldehyde [d,f]	50-00-0	0.12310		*unidentified* [b]	*NA*	*0.29213*
Sum of all compounds						1.00000

[a] CAS = Chemical Abstracts Service

[b] See discussion of unidentified species in Section 2.1 of this report.

[c] For commercial, military, general aviation, and air taxi aircraft equipped with turbofan, turbojet, and turboprop engines.

[d] Identified as a HAP in Section 112 of the CAA (shaded above).

[e] Identified in IRIS as having toxic characteristics (shaded above).

[f] Values were adjusted from those shown in the Technical Support Document to account for rounding and to facilitate inclusion of the data in the SPECIATE database (where the required sum of the values is 1.00000).

Note: Values in this table may be revised in the future as additional engine data are available.

2.1 Representation of Unidentified Mass

Table 1 shows that approximately 29 percent of the OG mass associated with the exhaust from the tested commercial aircraft engines is presently unidentified. Future research by both the FAA and EPA may provide better quantification and definition of the currently unidentified mass. In the interim, the unidentified mass has been generically identified as longer carbon chain species not included in the measured OG species listed in Table 1. These longer carbon chain species, identified in **Table 2**, are based on scientific judgment from the APEX principal investigators, the EPA, and the FAA.

Table 2. Unidentified Mass Species Assignment

Species	CAS	Mass Fraction
C-10 paraffins	No CAS	0.14608
C-10 olefins	No CAS	0.05843
decanal	112-31-2	0.05843
dodecenal	1127 1786	0.02922
Total		0.29213

Both FAA and EPA recognize that the advanced atmospheric photochemical models used to simulate the transport, dispersion, and reactivity of aircraft engine emissions will benefit from the best available accounting of OGs. For the purpose of photochemical and other related modeling efforts, the EPA and FAA recommend the "best fit" speciation of the unidentified mass listed in Table 2 (recognizing that other assignments may be appropriate depending on the modeling effort provided assignments do not repeat or overlap with already identified species). This unidentified mass species assignment is recommended for use in existing chemical mechanisms such as the Statewide Air Pollution Research Center 1999 (SAPRC99), Carbon Bond 4, Carbon Bond 5, RADM-2 and other atmospheric chemistry models.

2.2 SPECIATE Database Rating

In the support documentation for the SPECIATE database, EPA explains the rating criteria developed for adding new profiles to the database. The aircraft engine speciation profile listed in Table 1 will also reside in EPA's SPECIATE database, as the FAA and EPA preferred profile for speciating OG emissions from aircraft equipped with turbofan, turbojet, and turboprop engines. The profile will replace and supersede all prior profiles.

The EPA rates all SPECIATE profiles using criteria to describe the confidence, data quality and robustness. These ratings assess the quality of the entire dataset used to generate a given profile, rather than each specific pollutant within the profile. These criteria are presented/discussed on the following page:

- *V-rating (profile vintage)* is based on the vintage of the profile which reflects measurement technology and methodology:
  - After year 2000 score = 5
  - 1996-2000 score = 4
  - 1991-1995 score = 3
  - 1980-1990 score = 2
  - For profiles before year 1980 – score = 1

The speciation profile presented in **Table 1** was assigned a V-rating of “5” because the profile is based on measurement techniques that were used and methodologies that have been accepted after the year 2000.

- *D-rating (number of samples)* is given a “4” (excellent) to “1” (poor) rating. This category is rated based on the number of samples:
  - Number of samples greater than 10 score = 4
  - 5-9 samples score = 3
  - 3-4 and composite samples score = 2
  - 1-2 or unknown number of samples score = 1

The speciation profile presented in Table 1 has been assigned a D-rating of “4” because the profile is based on more than 10 samples (the multiple Spicer and APEX testing for CFM-56 engines).

- *Final Score* = (V-rating) x (D-rating). Profile quality is then rated from A (excellent) to E (poor) as shown in **Table 3**.

Table 3. Overall Profile Quality Ratings

Final Score Ranges	Profile Quality
17-20	A
13-16	B
9-12	C
5-8	D
<5	E

The final profile quality rating for the speciation profile in Table 1 is 20, or “A”.

- *J-rating (expert judgment)* is given a “5” (excellent) to “1” (poor) rating. This value is based on the information underlying each profile including, but not limited to:
  - Profile composition;
  - Relative ratios of species within the profile;
  - Sum of the speciated mass fractions;
  - Confidence in investigator/group collecting the data; and
  - Supporting documentation.

EPA does not provide objective rules on how to assign the J-rating. This inherently qualitative value has been assigned by the principal investigators of the profile (Aerodyne Research, Inc. and EPA's Office of Research Development-National Risk Management Research Laboratory) with input from the participants on this project.

The speciation profile in Table 1 has been assigned a J-rating of "5" (excellent).

3.0 CONVERSION FACTORS

OG emissions are defined a variety of ways depending on the reason for the analysis (e.g., preparation of an emissions inventory or photochemical analysis), the modeling need, and/or the regulatory context. The definitions include total organic gases (TOG)[18], non-methane OGs (NMOG), total HC (THC), and volatile organic compounds (VOC). The individual and groups of OGs included in each defined set/subset of gases are described in the following and illustrated on **Figure 1**:

- TOG –TOG is defined by CARB as compounds of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate. TOG includes all organic gas compounds emitted to the atmosphere, including the low reactivity compounds (e.g., methane, ethane, various chlorinated fluorocarbons, acetone, perchloroethylene, volatile methyl siloxanes, and oxygenated OG).

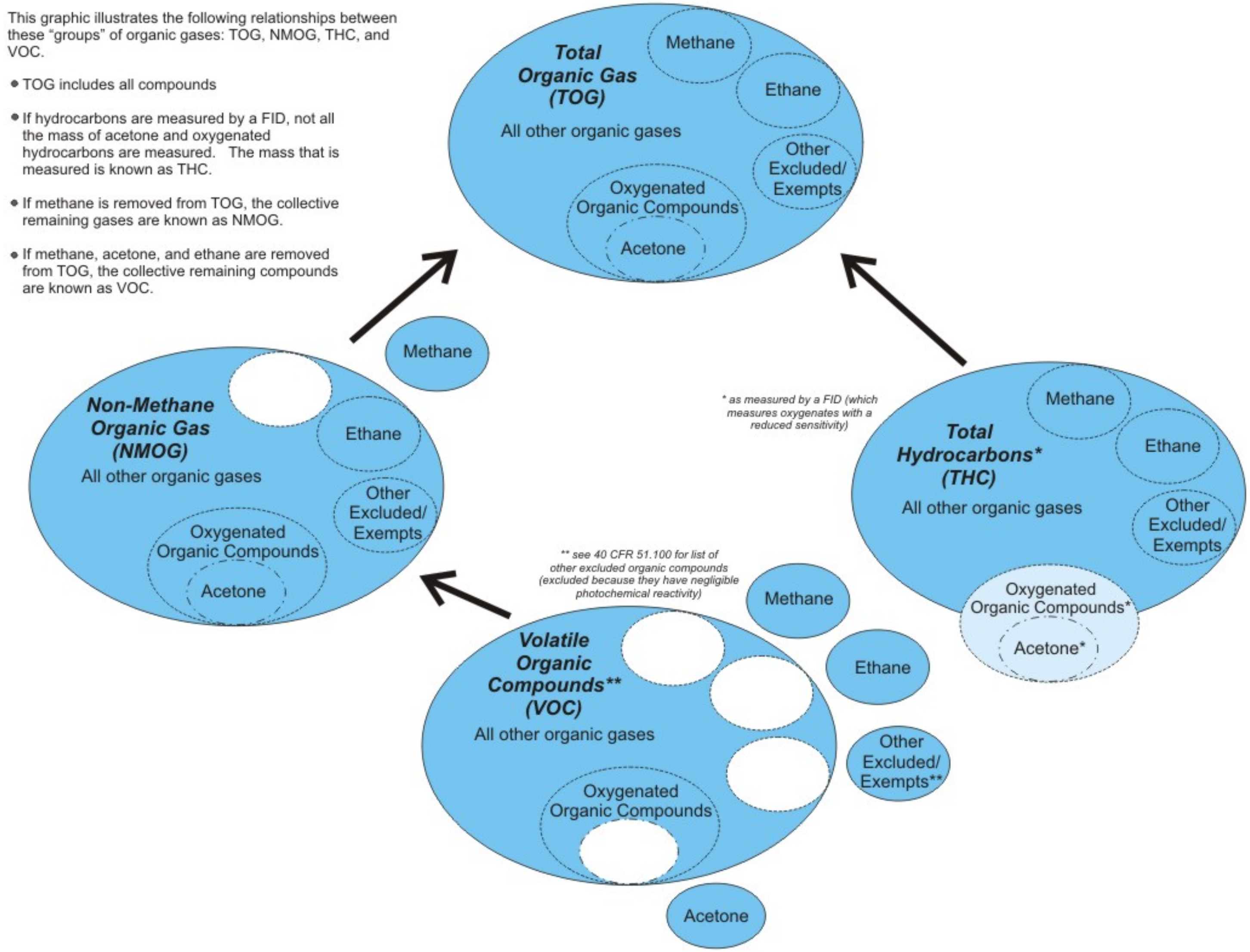
- NMOG - As implied, NMOGs include all organic compounds except methane which is the most common OG and a greenhouse gas that is sometimes excluded from the analysis of organic compounds.

- THC – Organic compounds in exhaust, as measured by a flame ionization detector (FID) per the International Civil Aviation Organization's (ICAO's) Annex 16.[19] Notably, a FID does not accurately measure all of the mass of oxygenated OG, which influences the abundances of specific chemical compounds relative to the total in the measured exhaust. This is important because these abundances dictate the amounts of each speciated compound in the exhaust plume

- VOC – VOC is defined by EPA as any compound of carbon that participates in atmospheric photochemical reactions. For aircraft, this is further defined as exhaust TOG corrected to exclude the mass of methane, ethane, and acetone and to fully account for the mass of formaldehyde and acetaldehyde [U.S. EPA 2007].[20] Notably, additional compounds are excluded/exempt from this group of OG when sources other than aircraft engines are being considered. VOC also excludes carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate.

[18] Also referred to as total organic compounds (TOC) when discussed in an air quality context.
[19] ICAO's Annex 16 addresses protection of the environment from the effect of aircraft noise and aircraft engine emissions.
[20] Per the EPA definition of VOC at http://www.epa.gov/ttn/naaqs/ozone/ozonetech/def_voc.htm

Figure 1
Groups of OGs



Unlike emissions from other transportation sources, international certification standards require that OG emissions from newly certified aircraft engines be reported in units of methane equivalency.[21] As part of the effort to develop an approach to quantifying individual OG and HAPs species, the OG, in methane equivalency, is converted to TOG according to the average molecular weight of the entire specific profile (discussed in more detail in the Technical Support Document) listed in **Table 1**. The derivations of conversion factors for various types of defined OGs are discussed in a companion spreadsheet to this document that is entitled *Aircraft Engine Speciated Hydrocarbons: Speciation Profile Spreadsheet* [Miake-Lye, 2008]. The factors for converting THC to TOG, VOC to TOG and factors to/from the other groups of organic compounds are provided in **Table 4**.

Table 4. Conversion Factors[a]

THC to TOG	VOC to TOG	THC to NMOG	THC to VOC	NMOG to TOG	TOG to VOC	TOG to NMOG
1.16	1.01	1.16	1.15	1.00	0.99	1.00

[a] For the purpose of reporting, application, and comparison, the units for the compounds in this table are referenced as follows: THC measured as methane equivalent (following procedures established by ICAO's Committee on Aviation Environmental Protection (CAEP)) , TOG as TOG, VOC as VOC, and NMOG as NMOG (see Technical Support Document for additional information).
Source: Aircraft Engine Speciated Hydrocarbons: Speciation Profile Spreadsheet, Miake-Lye, 2008.

It should be noted that the conversion factors in Table 4 supersede all factors previously published by the EPA for aircraft. These conversion factors are needed because the EPA National Emissions Inventory (NEI) reports emissions as VOC, rather than THC, which is the mass of hydrocarbons measured by a Flame Ionization Detector (FID). The FID does not accurately measure the mass of some compounds, such as formaldehyde and acetaldehyde (oxygenated OGs). VOC as defined above excludes methane. The turbine engine aircraft emissions profile presented in this RBP does not include methane. When a detailed quantification of methane is made in the future, the measured levels will be used to better identify all of the emissions that occur at low power. It is worth noting, however, that consumption of methane at high powers more than compensates for production of this compound at low powers, so the net budget of methane will indicate consumption and it will not be an important aircraft engine emission. Regardless, quantifying the amount of methane in aircraft engine exhaust will provide a more complete speciation of idle emissions.

Previously there were slightly different profiles for commercial, military, air taxi and general aviation turbine engine aircraft, due to different time in mode (TIM) estimates. Currently, it is recommended that one profile be used for all aircraft equipped with turbofan, turbojet, and turboprop engines, regardless of aircraft classification. A key difference between the old and new profiles is that while methane was previously assumed to be about 9 percent of hydrocarbon exhaust, methane is no longer considered to be an emission from aircraft gas turbine engines burning Jet A at higher power settings and is, in fact, consumed in net at these higher powers. This is an area of continuing scientific research—the results of which

[21] Procedures in the Emissions Certification of Aircraft Engines, Annex 16, Volume II, International Civil Aviation Organization. www.icao.int

will clarify if methane emissions are significant at lower power settings and should thereby be considered in fully speciating the low power emissions profile. FAA and EPA agree to re-visit the development of an organic profile that reflects these developments as the data becomes available. [Knighton, Herndon, Miake-Lye, 2008].

4.0 EMISSION INVENTORIES

This section describes the recommended steps to prepare an emission inventory of speciated OGs, including HAPs, for commercial, military, general aviation, and air taxi aircraft that are equipped with turbofan, turbojet, and turboprop engines. The emission inventories discussed in this document provide an estimation of the speciated OG and HAPs associated with aircraft activity. The results of the aircraft engine-related emission inventories are typically expressed in units of pounds per day or tons per year for each pollutant.[22]

4.1 Aircraft Operational Data

The aircraft operational characteristics that are of primary significance for preparation of an emissions inventory of ground-based pollutants and pollutants below the atmospheric mixing height are:

- The number of aircraft operations (i.e., landings and takeoffs) by aircraft type,
- The type and number of aircraft engines, and
- Times-in-mode for each of the aircraft operational modes (i.e., approach, taxi-in, taxi-out, idle (delay), takeoff, and climbout) within the atmospheric mixing zone.[23,24]

Some of this data are available from airport planning and design documents. Certain data (i.e., times-in-mode for the landing/take off cycle) may also be acquired from aircraft performance manuals, airport-specific data, and the FAA's Aviation System Performance Metrics (ASPM) database, Terminal Area Forecast (TAF) and/or Emissions and Dispersion Modeling System (EDMS) model.

4.2 Calculating THC, VOC, or NMOG Emissions

For each unique aircraft/engine combination, air quality practitioners will first prepare an emissions inventory for THC, VOC, or NMOG emissions. The inventories can be prepared using either the FAA's EDMS model or by manual calculation using the EDMS database or ICAO's Engine Exhaust Emissions Databank.[25]

For commercial aircraft, the easiest way to obtain an estimate of these emissions is to use FAA's EDMS model. For demonstrative purposes, the following example shows how to obtain an estimate of THC emissions using ICAO data. Estimates of THC are calculated

[22] The emission inventory results can also be expressed in metric system equivalents (e.g., kilograms per day).
[23] The time spent in the approach and climbout modes of the landing/take-off cycle is directly related to the height of the "mixing zone." The mixing zone is the layer of the earth's atmosphere where air is completely mixed and pollutants emitted anywhere within the layer will be carried down to the ground level. The height of the mixing zone for a given location typically varies by season and time of day.
[24] Aircraft also emit OG during "start-up". These emissions are will be addressed through future research and included in updates to this document (including updates to the speciation profile at the time such an update is appropriate.
[25] The ICAO Engine Exhaust Emissions Databank is available at http://www.caa.co.uk/default.aspx?catid=702&pagetype=90 .

based on the amount of fuel consumed by an aircraft in each of the aircraft operational modes and engine-specific THC emission indices (specific to each aircraft operational mode).

4.2.1 Example THC Calculation

An air quality practitioner is charged with speciating aircraft-related THC emissions for an Airbus A320-100 equipped with two CFM56-5A1 turbofan engines. Over the period of interest, the A320-100 performs 1,000 operations (500 landing-takeoff cycles). Based on the configuration of the airport and field surveys, each aircraft has an average combined taxi/idle (delay) time of 26 minutes per landing-takeoff cycle (a taxi in time of 7 minutes and a taxi-out time, including delay, of 19 minutes). This aircraft and operational data are summarized in **Table 5**.

Table 5. Example Aircraft Operational Data

Aircraft	Engine	Number of Engines	Number of Operations[a]	Taxi Time (Minutes) In	Taxi Time (Minutes) Out
Airbus A320-100	CFM56-5A1	2	1,000	7	19
[a] 1,000 operations equals 500 landing-takeoff cycles or 500 arrivals and 500 departures.					

The fuel flow rates and THC emission indices for the CFM56-5A1 are provided in Table 6.

Table 6: Example Fuel Flow Rates/Emission Indices

Data	Aircraft Operational Mode			
	Takeoff	Climbout	Approach	Idle
Fuel Flow Rate (kilograms/second)	1.05100	0.86200	0.29100	0.10110
THC Emission Indices (grams/kilogram of fuel)	0.2300	0.2300	0.4000	1.4000

Assuming a scenario specific atmospheric mixing height[26] and using the aircraft operational data (i.e., number of arrivals, number of departures, times-in-mode) and the base data (i.e., fuel flow rates and THC emission indices), the THC emissions, by aircraft operational mode is calculated, are calculated, and then summed for each mode, as detailed in **Equations No. 1 and 2**.[27]

[26] The national default atmospheric mixing height is 3,000 feet. Site-specific data should be used when such data is readily available.
[27] Notably, HAPs emissions are greatest during the taxi and idle aircraft operational modes and emissions attributable to the approach and climbout modes will vary depending on the scenario specific atmospheric mixing height.

Equation No. 1:

Fuel Consumption By Aircraft Operational Mode

Fuel Flow Rate for Operational Mode (kg/sec) x Time-in-Mode (secs) = Total Fuel Consumption/Engine for Operational Mode (kg)

Equation No. 2:

THC Emissions By Aircraft Operational Mode

Total Fuel Consumption for Operational Mode (kg) x THC Emission Indices (g/1000 kg of fuel) x Number of Engines x Number of Operations x kg/1000 g = THC Emissions by Mode (kg)

For the A320 aircraft example, the fuel flow rate and THC emission indices are provided in **Table 7**. The estimated level of THC from each of the aircraft operational modes and the THC for all of the A320 activity (all 1,000 operations or 500 landing-takeoff cycles) is also provided. As shown, the level of THC varies substantially depending on the aircraft operational mode with emissions being the highest during the taxi in and taxi out modes and the lowest during approach, takeoff, and climbout.

Table 7. Example THC Estimate

Fuel Flow Rate (Per Engine)[a]		Time in Mode (mins)[a]	Fuel Consumption (Per Engine Per Operation – kg)	THC Emission Indices (g/kg Fuel Consumed)[a]	Number of		THC (kg)
Mode[b]	Rate (kg/sec)				Engines	Operations	
Approach	0.29100	4.12	71.935	0.40	2	500	28.77
Taxi In	0.10110	7.00	42.562	1.40	2	500	59.45
Taxi Out	0.10110	19.00	115.254	1.40	2	500	161.36
Takeoff	1.05100	1.51	95.221	0.23	2	500	21.90
Climbout	0.86200	0.53	27.412	0.23	2	500	6.30
Total	--	--	--	--	--	--	277.78

[a] Obtained from FAA's EDMS databases.
[b] This example does not include data and/or assumptions for auxiliary power units.

As shown in **Table 7**, 277.78 kg of THC emissions are estimated to result from the operations performed by the Airbus A320-100.

4.3 Converting to TOG

As previously stated, the profile data in Table 1 should be applied to inventories of TOG to obtain estimates of individual (speciated) OGs. Before applying the profile data to an estimate of THC emissions (or NMOG or VOC), the THC must first be converted to TOG. This application is detailed in **Equation No. 3**.

Equation No. 3:

Conversion to TOG

THC Emissions (kg) x TOG Conversion Factor = TOG (kg)

As shown in Table 4, the THC to TOG conversion factor is 1.16. Therefore, the amount of TOG emitted by the A320 aircraft in this example is an estimated 322.22 kg.

4.4 Applying Speciation Profile Data

To speciate TOG emissions, an air quality practitioner should obtain the latest OG speciation profile (from Table 1 or from the FAA/EPA websites). To derive the emission rates for an individual OG, the mass fractions in the profiles are multiplied by the total amount of TOG. The calculation for obtaining the estimated emission rate for an individual OG and/or HAP is provided in **Equation No. 4**.

Equation No. 4:

Computing Speciated Aircraft OG Emissions Using TOG

$$TOG\ (kg) \times Speciation\ Profile_i\ (mass\ fraction) = OG_i\ (kg)$$

Where: i = OG of interest

For illustrative purposes, **Table 8** provides the OG emission estimate for the A320 example for three individual OG/HAPs (the table does not include all of the speciated OGs in Table 1). The three OGs/HAPs are ethylene, formaldehyde, and toluene.

Table 8. Example Speciated OG Emission Levels

Aircraft Type	Engine Type / No. of Engines	TOG (kg)	OG	Speciation Profile (mass fraction)	OG Emission Inventory (kg)
A320-100	CFM-56 / 2	322.22	ethylene	0.15459	49.81
			formaldehyde	0.12308	39.66
			toluene	0.00642	2.09

As shown in Table 8, the estimated emission rates for ethylene, formaldehyde, and toluene emissions are approximately 50, 40, and 2 kg, respectively, for the A320 example.

4.5 Presentation of Results

The emissions inventory provides an estimate of the amount of aircraft-related HAPs emitted in the timeframe of the inventory. For consistency with emission inventories that are prepared for the EPA criteria air pollutants, the results should be expressed in units of tons or pounds per year or pounds per day or as equivalent metric system units. Because the output data can be overly complex and voluminous, the data are most conveniently presented in tabular form. **Table 9** provides a sample table format for presenting the aircraft-related OG/HAP emission estimates. The format of Table 1 (including CAS Registry numbers) may also be used.

Table 9. Example Format for Reporting Speciated OGs

Year	OG	Estimated Emissions (kg)
2008	ethylene	50
	formaldehyde	40
	toluene	2

Depending on the purpose and scope of the assessment, the results can be further segregated by analysis year, airport operational level or project alternative. For reviewing purposes, the emission estimation results should be accompanied by 1) a summary explanation of how the assessment was conducted (information and data sources, major assumptions, computational methods), 2) how the results are interpreted or compared (between alternatives or compared to any applicable significance criteria) and 3) any noteworthy limitations to the understanding and application of the outcome(s).

LIST OF REFERENCES

CAA, 1977, 42 U.S.C. 7401 to 771q, Clean Air Act.

CARB, 2000, *FACT SHEET #1: Development of Organic Emission Estimates For California's Emission Inventory and Air Quality Models*, August.

CARB, 2000, Statewide Air Pollution Research Center 1999 Mechanism (SAPRC99), May.

FAA, 2007, *Emissions and Dispersion Modeling System (EDMS) User's Manual*, FAA Office of Environment and Energy, prepared by CSSI, Inc., January.

FAA and U.S. EPA, 2008, *Quality Assurance Project Plan for the Development of a Commercial Aircraft Hazardous Air Pollutants Emission Inventory Methodology*, prepared by KB Environmental Sciences, Inc., March 31.

Gery et al, 1988, 1989. Carbon Bond IV Mechanism (CB4).

ICAO, Annex 16, Volume II - Aircraft Engine Emissions.

Knighton, W. B., Herndon, S.C., and Miake-Lye, R.C. (2009). *Aircraft Engine Speciated Organic Gases: Speciation of Unburned Organic Gases in Aircraft Exhaust*.

Lobo, P., et al., 2007. *The Development of Exhaust Speciation Profiles for Commercial Jet Engines*. Final Report, Contract No. 04-344, California Air Resources Board, Sacramento, CA, October 31.

Stockwell, Regional Atmospheric Chemistry Mechanism (RADM-2), 1997.

Systems Applications International, *An Updated Photochemical Mechanism for Modeling Urban and Regional Air Quality: Carbon Bond, Version 5 (CB-V),* December 4, 2002.

USAF, 1984, *Composition and Photochemical Reactivity of Turbine Engine Exhaust*, prepared by Battelle Laboratories, prepared for the Air Force Engineering and Services Center, September.

USAF, 1987a, *Aircraft Emissions Characterization: TF41-A2, TF30-P103, and TF30-P109 Engines,* December (Spicer et. al.)

USAF, 1987b, *Aircraft Emissions Characterization: TF33-P3, TF33-P7, and J79 (Smokeless) Engines*, August (Spicer et.al)

USAF, 1990, *Aircraft Emissions Characterization: F101 and F110 Engines,* March (Spicer et.al)

USAF, 1994, *Developing an Emission Factor for Hazardous Air Pollutants for an F-16 Using JP-8 Fuel*, U.S. Air Force, September 1994

USAF, 1999a, *Aircraft Engine and Auxiliary Power Unit Emissions Testing; Volume 1, Executive Summary.* U.S. Air Force, March 1999 (Gerstle, Virag, Wade, Kimm)

USAF, 1999b, *Aircraft Engine and Auxiliary Power Unit Emissions Testing; Volume 2, Detailed Sampling Approach and Results.* March 1999 (Gerstle, Virag, Wade, Kimm)

USAF, 1999c, *Aircraft Engine and Auxiliary Power Unit Emissions Testing; Volume 3, Particulate Matter Results*, U.S. Air Force, March 1999 (Gerstle, Virag, Wade, Kimm)

USAF, 2002, *Aircraft Engine and Auxiliary Power Unit Emissions Testing: Final Report. Addendum. F199-PW-100 Engine Emissions Testing Report*, June 2002 (Gerstle, Virag, Wade, Kimm)

U.S. EPA, 2000, *Compilation of Air Pollutant Emission Factors*, AP-42, November.

Wey, C. C. et al., 2006. Aircraft particle emissions experiment (APEX). NASA TM-2006-214382, September.

U.S. EPA, 2006, SPECIATE 4.0, Speciation Database Development Documentation, Final Report, November.

U.S. EPA, 2007, *Converting Aircraft Total Hydrocarbons (THC) to VOC*, Memorandum from Rich Cook to Bryan Manning, National Vehicle and Fuel Emissions Laboratory, Office of Transportation and Air Quality, June 27.

U.S. EPA. Integrated Risk Information System (IRIS). [Online] Available http://cfpub.epa.gov/ncea/iris/index.cfm, June 2, 2008.