Supporting Information

For manuscript entitled:

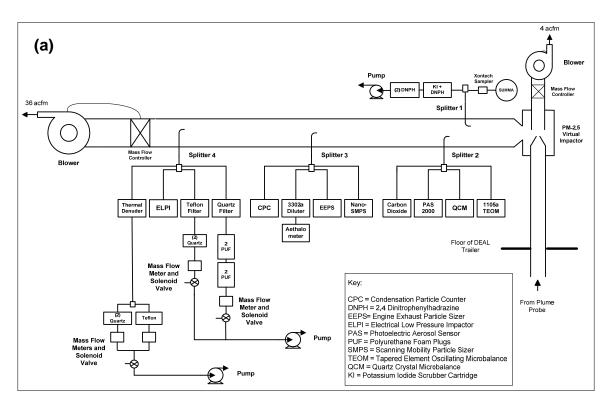
"Chemical Characterization of the Fine Particle Emissions from Commercial Aircraft Engines during the Aircraft Particle Emissions eXperiment (APEX) 1 to 3"

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Instrumentation

As discussed in the main paper, a variety of instruments were used during the three Aircraft Particle Emissions eXperiment (APEX) sampling campaigns. Figure S1 shows the typical Diesel Emissions Aerosol Laboratory (DEAL) instrumentation configuration used during the APEX campaigns for collection and speciation of both the engine exhaust and the ambient background air. Table S1 presents the specific instrumentation installed in the DEAL along with the sampling location, measured parameters, and description of each instrument.

During the three APEX campaigns, the instrument configuration varied slightly from that shown in Figure S1 depending on whether a particular test was speciated or non-speciated, whether the plume or background was being monitored, etc. Recall that "speciated" refers to a test where the chemical composition of the emissions was determined by time-integrated sampling. In APEX-1, three of the nine tests were speciated. During APEX-2, all sampling equipment configurations in the DEAL were configured for speciated tests. Finally, six of the eleven tests conducted during APEX-3 were also speciated. Note, however, that not all speciated tests provided useful data and thus certain results are not reported. End-of-runway sampling was also attempted in APEX-3 but was unsuccessful due to poor wind conditions. Detailed information on the plume and background sampling conducted during all three APEX sampling campaigns is provided in Reference 13 of the main text.



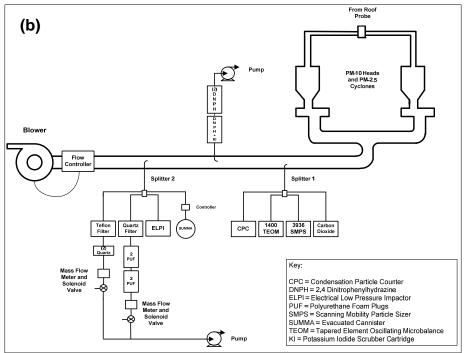


Figure S1-Representative equipment configuration for speciated testing of: (a) engine exhaust plume; and (b) ambient background. Note that the ambient background was affected by crosswinds during some tests.

Table S1-Measurements performed by the DEAL during APEX-1, -2, and -3.

parameter	sampling location	measurement technique	type of sample	instruments and sampling media
PM-2.5 mass concentration	background	microbalance	continuous	Rupprecht and Patashnick (now Thermo Electron) Series 1400a TEOM
	background	gravimetric analysis	time-integrated	47-mm Teflon filter with double quartz backup filters for collection of gas-phase "blow off" ^a
	plume	microbalance ^h	continuous	Rupprecht and Patashnick Series 1105a TEOM
	plume	APEX-2 & -3: QCM ^h	continuous	SEMTECH Model RPM-100 particulate monitor + diluter
	plume	gravimetric analysis	time-integrated	47-mm Teflon filter with double quartz backup filters ^a
particle size distribution	background	low pressure cascade impactor (aerodynamic diameter)	continuous / time-integrated	Dekati ELPI
	background	electrical mobility classifier/condensation nuclei counter (electrical mobility diameter)	continuous	APEX-1: TSI Model 3934 SMPS, Model 3071 A classifier, Model 3010 CPC
				APEX-2 & -3: TSI Model 3936 SMPS (long), Model 3080 classifier, Model 3025a CPC, Model 3081 DMA
	plume	low-pressure cascade impactor (aerodynamic diameter)	continuous / time-integrated	Dekati ELPI
	plume	electrical mobility classifier/condensation nuclei counter (electrical mobility counter)	continuous	TSI Model 3936 SMPS (Nano). Model 3080 classifier, Model 3025a CPC, Model 3085 DMA
	plume	APEX-1: electrical mobility classifier/condensation nuclei counter (electrical mobility counter)	continuous	APEX-1: TSI Model 3936 SMPS (long), Model 3080 classifier, Model 3025 CPC, Model 3081 DMA
		APEX-2 & -3: electrical mobility classifier/electrometers (electrical mobility counter)		APEX-2 & -3: TSI Model 3090 EEPS + diluter
PM-2.5 number concentration ^c	background	condensation nuclei counter	continuous	Model 3025a CPC
	plume	condensation nuclei counter	continuous	Model 3025a CPC + diluter
elemental carbon/organic carbon	background	thermo-optical analysis (NIOSH Method 5040)	time-integrated	prefired 47 mm quartz filter
(EC/OC)	plume	thermo-optical analysis (NIOSH Method 5040)	time-integrated	prefired 47 mm quartz filter
	plume	optical attenuation/UV absorption (black carbon)	continuous	TSI 3302a Diluter +Magee Model AE-2 Aethalometer ^d
PM semivolatile organic	background	GC/MS	time-integrated	prefired 47 mm quartz filter with 4 backup PUF plugs. ^a
compounds (SVOCs)	background	low-pressure cascade impactor	time-integrated	12 aluminum foil ELPI stages + prefired quartz back-up filter ^b
	plume	GC/MS	time-integrated	prefired 47 mm quartz filter with 4 backup PUF plugs. ^a
	plume	low-pressure cascade impactor	time-integrated	12 aluminum foil ELPI stages + prefired quartz back-up filter ^b
	plume	UV analyzer (particle surface PAHs)	continuous	EcoChem Model PAS 2000

parameter	sampling location	measurement technique	type of sample	instruments and sampling media
total volatile PM + EC/OC	plume	gravimetric/thermo-optical analysis	time-integrated	Dekati Model EKA-111 thermal denuder with parallel Teflon and double prefired quartz filters
PM inorganic water-soluble ions	background	ion chromatography	time-integrated	Teflon filter
	plume	ion chromatography	time-integrated	Teflon filter
PM elemental composition	background	XRF	time-integrated	Teflon filter
	plume	XRF	time-integrated	Teflon filter
APEX-1 CO, CO ₂ , total VOCs	background	IR absorption	Integrated bage	Brüel & Kjær Model 1302 Photoacoustic Analyzer
	plume	IR absorption	continuous	Brüel & Kjær Model 1302 Photoacoustic Analyzer
APEX-2 & -3 CO ₂	background	IR absorption	continuous	Milton-Roy (CA Analytical) Model 5300A
	plume	IR absorption	continuous	Milton-Roy (CA Analytical) Model 5300A
gas-phase NMOCs	background	GC/MS/FID	time-integrated	SUMMA-passivated canister
	plume	GC/MS/FID	time-integrated	SUMMA-passivated canister
gas-phase carbonyl compounds	background	HPLC	time-integrated	DNPH impregnated silica gel cartridges with KI ozone scrubber cartridge
	plume	HPLC	time-integrated	DNPH impregnated silica gel cartridges with KI ozone scrubber cartridge
sample temperature ^f	plume tunnel	thermocouple	continuous	K-Type thermocouples; T-Type only on APEX-2 sampling probes
APEX-2 plume temperature	plume	thermocouples	continuous	multiple T-type thermocouples
APEX-2 plume velocity	plume	pitot tube	continuous	standard pitot tube plus differential pressure cell
APEX-2 meteorological parameters ^g	background	propeller anemometer & wind vane	continuous	Vaisala MAWS weather station

^a Filter holder design per Federal Test Procedure (FTP) published in 40 Code of Federal Regulations (CFR), Part 86.1065. "Blow off" are gas-phase semivolatile species that have been released from the particulate deposited on the primary filter by the air flow passing through the medium.

PAH = Polycyclic Aromatic Hydrocarbon

SMPS = Scanning Mobility Particle Sizer

TEOM = Tapered Element Oscillating Microbalance

QCM = Quartz Crystal Microbalance

PUF = Polyurethane Foam

UV = Untraviolet

^b Aluminum foil substrates from the ELPI were not analyzed due to insufficient mass.

^c These measurements were redundant and the data were not used.

^d The aethalometer measures "black" carbon which approximates elemental carbon content as determined from diesel engine testing (1).

^e Post-test analysis of time-integrated Tedlar bag sample collected over the entire test period.

^f Temperature was not monitored in sampling lines.

^g Meteorological data provided by collaborators during APEX-1 and -3.

^h Data from these instruments are generally of low reliability and thus not reported in this paper. NMOC = Nonmethane Organic Compound

CPC = Condensation Particle Counter

DMA = Differential Mobility Analyzer	
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DNPH = 2,4-Dinitrophenylhydrazine

- EEPS = Engine Exhaust Particle Sizer
- ELPI = Electrical Low Pressure Impactor
- FID = Flame Ionization Detector

GC/MS = Gas Chromatography/ Mass Spectrometry

HPLC = High Performance Liquid Chromatography IR = Infrared

XRF = X-ray Fluorescence

NIOSH = National Institute for Occupational Safety and Health

Sampling Media

All sampling media (Table S2) were prepared at the EPA analytical laboratories before leaving for the field. Prior to and after sampling, the pre-fired quartz filters were stored in aluminum-foil lined, plastic petri dishes inside a laboratory freezer maintained at -50 °C. The Teflon filters were stored inside plastic petri dishes, also in the -50 °C freezer. The PUF plugs were stored and transported to the field in glass jars with Teflon-lined screw caps. During transport and in the field laboratory, all sampling media were stored in a small portable freezer at roughly -20 °C. This freezer was also used as the primary shipping container for the sampling media to and from the field site (the freezer was operated on generator power en route).

type of analysis PM mass PM elemental and organic carbon (EC/OC)	sampling media 47-mm Teflon filters 47-mm prefired quartz filters (primary and behind Teflon filters)	analytical method gravimetric NIOSH Method 5040
PM semi-volatile organic compounds (SVOCs)	47-mm prefired quartz filters	multisolvent extraction, GC/MS or thermal desorption, GC/MS
gas-phase SVOCs	PUF plugs behind quartz filters	multisolvent extraction, GC/MS
PM water-soluble ions PM elemental composition	47-mm Teflon filters 47-mm Teflon filters	ion chromatography (IC) XRF spectroscopy

Table S2-Media for Time-Integrated Sampling^a

^a CFR = Code of Federal Regulations; NIOSH = National Institute for Occupational Safety and Health; GC/MS = gas chromatography/mass spectrometry; PUF = polyurethane foam; XRF = X-ray fluorescence.

Detailed Analytical Procedures

The PM_{2.5} gravimetric analysis (Table S2) was performed by weighing the individual Teflon filters before and after sampling on a Sartorius microbalance with a precision of $\pm 3 \mu g$. The filter weighing was done in accordance with the guidelines described in Title 40 of the Code of Federal Regulations (40CFR), Part 50, Appendix L for ambient sampling. The method requires that before weighing, the filter samples are conditioned for a minimum of 24 hr in an environmental chamber at 20 to 23 °C and a relative humidity of 30 to 40%. To eliminate possible electrical charge from accumulating on the filter surface, both sides of each Teflon filter were exposed to polonium strips for at least 20 seconds before placing on the balance. For APEX-2, lab personnel did not follow the procedure to adequately eliminate the effect of electrostatic charge while gathering the blank Teflon filter tare weights, thus PM_{2.5} gravimetric data are not available for this test series.

Following gravimetric analysis, the Teflon filters were analyzed using XRF to quantitatively determine PM_{2.5} elemental composition. In the XRF analyses performed for APEX-1, each Teflon filter was covered with a 4.0-µm thick Prolene film that was attached using glue. The glue was placed on the outer rim of the filter and did not interfere with the analysis. A Philips 2404 wavelength-dispersive XRF spectrometer, running the UniQuant7 program, was used to determine elements greater than atomic number 9 present in the PM_{2.5} sample. For APEX-2 and -3, the analyses were conducted using a commercially available Kevex EDX-771energy dispersive XRF which utilized secondary excitation from selectable targets or fluorescers. Up to seven spectra were acquired per sample depending on how many secondary excitation targets were selected. Although the net sample weights for the APEX-2 Teflon filters could not be determined, the samples were still valid and an XRF analysis was performed on these filters since the net sample weight is not needed for these analyses.

After performing non-destructive analyses (weighing and XRF), the Teflon membrane filter samples were further analyzed using ion chromatography [(IC) DX-120; Dionex Inc.] Teflon filter sample extractions were performed in high pressure liquid chromatography-grade, low-conductivity water aided by sonication (30 min). The extract was injected onto an ion-exchange resin column, on which an isocratic separation of water-soluble cations (K^+ , NH_4^+ , Mg^{+2} , and Ca^{+2}) and anions (NO_3^- , SO_4^{-2} , NO_2^- , and Cl^-) was performed with methanesulfonic acid– and $Na_2CO_3/NaHCO_3$ –buffered water, respectively The ions in the sample were measured with a conductivity detector and quantified using an external standard method.

The pre-fired quartz fiber filter samples were examined for OC-EC content with a thermal-optical carbon analyzer (Model 107-A, Sunset Laboratory Inc.) using NIOSH Method 5040, subsequent to being analyzed for SVOCs. The method is a two stage thermal-optical method with a detection limit on the order of $0.2 \,\mu$ gC/cm². To remove the background OC, the

quartz filters and aluminum foil petri dish liners were pre-fired in a kiln at 550 °C for 12 hr before use. The filters and liners were handled with Teflon forceps to avoid contamination.

Semi-volatile organic compounds partition between the gas- and particle-phases. Their phase distribution depends on thermodynamic equilibrium, the dynamic sampling conditions, and other factors related to particle composition. As a result, there is no clearly defined cut between the gas and particle phase emissions. Therefore, PUF plugs were installed directly downstream of the quartz filters for collecting the SVOC gases not adsorbed by the quartz filters. However, as stated in the main text, these proved to be unsuitable for this type of research and thus no PUF data are reported.

The identification and quantification of trace organic compounds collected on the APEX quartz filter (Q_f) samples were conducted using either SE- or TE-GC-MS. Studies have shown that the SE- and TE-GC-MS techniques furnish accurate quantitative information for PAH and *n*-alkane constituents in PM (*2 and refs. therein*). The roughly 100-fold greater sensitivity of TE-GC-MS marks a substantial difference between these two methods. If test Q_f composites contained less than the roughly 1 mg of OC normally required for SE, a TE-GC-MS analysis was performed. Following this criterion, filter samples from APEX 1 and 3 were analyzed using TE-GC-MS, and APEX 2 filters were composited and analyzed with SE-GC-MS. Thus, the corresponding samples from T2 and T3 tests for the CFM56-3B tests and T1 and T4 for the -7B24 model CFM56 were combined and labeled as such.

Test Matrix, Engines, and Fuels

A total of 24 tests were conducted during the three APEX sampling campaigns. Table S3 provides the specifications for each engine tested including whether the turbine core flow was mixed with the bypass air before (internally mixed flow) or after (externally mixed flow) being discharged to the atmosphere. Table S4 details each experiment conducted including the test number, fuel type, and engine operating points and also identifies tests during which time-integrated samples were collected for chemical speciation.

Several factors should be noted with respect to the information provided in Table S3 and S4. First, as with most technology, engine compressor, combustor, and turbine design improve over time to meet both fuel burn and emissions reduction requirements. Maintaining the finite balance of high combustion efficiency and low emissions requires focus on a multitude of

Table S3-Engines Tested in APEX 1 to 3

engine model ^a	airframe	bypass ratio ^b	engine	rated thrust ^b	I	CAO smo	ke numbe	test campaign/test number		
		rauo	pressure ratio ^b	(kN)	T/O	C/O	Арр	Idle		
CFMI CFM56-2C1	Boeing DC-8	6	23.5	97.86	6.0	3.0	2.6	2.2	APEX 1 / All Tests	
CFMI CFM56-7B24	Boeing 737-700	5.2	25.8	107.7	12.6 ^d	NA	NA	NA	APEX 2 / Test # 1 and 4	
CFMI CFM56-3B1	Boeing 737-300	5.1	22.4	89.41	4.0	2.5	2.5	2.2	APEX 2 / Test # 2; APEX 3 / Test # 1 and 11	
CFMI CFM56-3B2	Boeing 737-300	5.1	24.1	98.30	6.0	3.0	2.5	2.2	APEX 2 / Test # 3	
General Electric CJ610- 8ATJ (turbojet) ^f	Lear Model 25	na	~ 7	13.12	NA	NA	NA	NA	APEX 3 / Test # 2 and 5	
Rolls Royce AE3007A1E ^e	Embraer ERJ145	4.8	17.8	33.70	1.0	0	0	0	APEX 3 / Test # 3 and 4	
Pratt & Whitney 4158	Airbus A300	4.6	30.7	258.0	8.1 ^d	NA	NA	NA	APEX 3 / Test # 6 & Test #7	
Rolls Royce RB211- 535E4B ^e	Boeing 757-324	4.1	27.9	191.7	7.3 ^d	NA	NA	NA	APEX 3 / Test # 8 and 9	
Rolls Royce AE3007A1/1 ^{e,f}	Embraer ERJ145	4.8	17.9	34.74	1.0	0	0	0	APEX 3 / Test # 10	

^a All engines are turbofan except as noted.

^b Civil Turbojet/Turbofan Specifications <u>http://www.jet-engine.net/civtfspec.html</u> or International Civil Aviation Organization (ICAO) Databank Issue 15-C.

^c New engine certification data taken from ICAO Engine Emissions Databank Issue 15-C. T/O = take-off; C/O = climb-out; App = approach; NA = not available.

^d Maximum SN; no power specified.

^e These are internally mixed flow turbofan engines.

^f No data reported in this paper for these engines.

										non	nina	l per	cent	t rat	ed tl	irus	t			
APEX	test no.	aircraft	engine ^a	test type ^b	fuel type	4	5.5	7	8.4	15	30	40	45	60	65	70	76	80	85	100
1	EPA 1 ^c	DC-8	CFM56-2C1	S	base			Х			Х								Х	Х
	EPA 2			S				Х			Х								Х	Х
	NASA 1 ^c			Ν		Х	Х	Х		Х	Х	Х			Х				Х	Х
	NASA 1a ^c			Ν		Х								Х	Х	Х			Х	Х
	EPA 3			S	high sulfur			Х			Х						Х		Х	Х
	NASA 2			Ν		Х	Х	Х		Х	Х	Х		Х	Х	Х			Х	Х
	NASA 3			Ν		Х	Х	Х		Х	Х	Х		Х	Х	Х			Х	Х
	NASA 4			Ν	high aromatic	Х	Х	Х		Х	Х	Х		Х	Х	Х			Х	Х
	NASA 5			Ν		Х	Х	Х		Х	Х	Х		Х	Х	Х			Х	Х
2	T1	B737-700	CFM56-7B24	S	fleet fuel	Х		Х			Х	Х			Х				Х	
	T4			S		Х		Х			Х	Х			Х				Х	
	T2	B737-300	CFM56-3B1	S		Х		Х			Х	Х			Х				Х	
	T3		CFM56-3B2	S		Х		Х			Х	Х			Х				Х	
3	T1°	B737-300	CFM56-3B1	Ν	fleet fuel	Х		Х		Х	Х		Х		Х				Х	Х
	T11			S		Х		Х		Х	Х		Х		Х				Х	Х
	T2 ^c	Lear 25	CJ610-8ATJ	Ν	fleet fuel			Х		Х	Х		Х		Х				Х	Х
	T5 ^c			Ν				Х		Х	Х		Х		Х				Х	Х
	T3	ERJ145	AE3007A1E	S	fleet fuel				Х	Х	Х		Х		Х				Х	Х
	T4			S					Х	Х	Х		Х		Х				Х	Х
	T10 ^c		AE3007A1/1	Ν					Х	Х	Х		Х		Х				Х	Х
	T6	A300	P&W 4158	S	fleet fuel			Х		Х	Х		Х		Х			Х		
	T7			S				Х		Х	Х		Х		Х			Х		
	T8 ^c	B757	RB211-535E4-B	Ν	fleet fuel	Х		Х		Х	Х		Х		Х				Х	
	Т9			S		Х		Х		Х	Х		Х		Х				Х	Х
	End-of- runway (aborted) ^c	N/A	N/A	S	N/A															

Table S4-APEX Experimental Matrix

^a All engines were turbofan except the CJ610-8ATJ which was a turbojet engine.

^b S = speciated test; N = non-speciated test.

^c No data reported in this paper for these engines.

complex driving factors which are beyond the scope of this paper. However, one of the primary factors which dictate overall combustion performance is engine pressure ratio (EPR) (3). With all other factors being equal (or optimized in the overall design) a pressure ratio increase tends to lead to a decrease in direct combustion emission products such as unburned hydrocarbons and CO. An associated decrease in PM emission constituents for engines with a higher EPR was not always found to be the case, however, as shown by the data in the main text.

Also, as noted from Tables S3 and S4, four variants of the CFM International CFM56 engine were tested. The CFM56 is one of the most widely used engine families in commercial service representing approximately 14% of the total engines (assuming an average of two engines per aircraft) worldwide as determined from the Ascend Online Fleets database.

Table S5 summarizes the composition of the fuels used during the APEX campaigns. Three types of jet fuels were used in the APEX-1 campaign: a base fuel, a higher sulfur fuel, and a higher aromatic fuel. The base fuel, which was a typical JP-8 (Jet-A1) jet engine fuel, was used for EPA 1 and 2, and NASA 1 and 1a. The base fuel doped to approximately four times the sulfur content, was used for EPA 3 and NASA 2 and 3 and a higher aromatic fuel, with approximately 25 percent more aromatics than the base or high-sulfur fuels, was used during NASA 4 and 5. During APEX-2 and -3, commonly available Jet-A fleet fuel was used for all engines tested. Table S5 illustrates that although the sulfur content varied in these fuels (ranging from 132 to 700 ppm), they were generally similar to the base fuel used in APEX-1.

Organic Speciation Results

The EIs for various semi-volatile organic compounds as determined from the analyses of the quartz filters are shown in Table S6 by individual chemical species. Also shown in this table is the total EI for all organic species detected by the GC/MS as well as the total EI for each chemical compound class (e.g., PAHs). Table S7 provides the chemical compound abbreviations used in Figure 3a of the main text.

APEX	test no.	airframe	engine ^a	fuel type	carbon (fraction)	hydrogen (fraction)		aromatics (vol%)	density (mg/cm ³)	heating value (MJ/kg)
1	EPA 1 ^c	DC-8	CFM56-2C1	base	0.8627	0.1369	409	17.5	0.8199	43.2
	EPA 2									
	NASA 1 ^c									
	NASA 1a									
	EPA 3			high sulfur	0.8617	0.1367	1639	17.3	0.8194	43.3
	NASA 2									
	NASA 3									
	NASA 4			high aromatic	0.8624	0.1370	553	21.8	0.8114	43.3
	NASA 5									
2	T1	B373-700	CFM56- 7B24	fleet fuel	0.8569	0.1430	132	19.7	0.8254	NA
	T4				0.8525	0.1470	412	20.3	0.8080	NA
	T2	B737-300	CFM56-3B1		0.8587	0.1411	206	20.4	0.8202	NA
	T3		CFM56-3B2		0.8522	0.1474	352	22.7	0.8169	NA
3	T1 ^c	B737-300	CFM56-3B1	fleet fuel	0.8613	0.1380	700	17.4	0.8044	43.2
	T11				0.8616	0.1380	400	16.8	0.8109	43.2
	T2 & T5 ^c	Lear 25	CJ610-8ATJ	fleet fuel	0.8599	0.1401	$0^{\rm b}$	14.5	0.7990	43.3
	T3 & T4	ERJ145	AE3007A1E	fleet fuel	0.8637	0.1360	300	19.9	0.8105	43.1
	T10 ^c		AE3007A1/1	l	0.8638	0.1360	200	18.6	0.8142	43.1
	T6 & T7	A300	P&W 4158	fleet fuel	0.8624	0.1370	600	16.5	0.8048	43.2
	T8 ^c	B757	RB211- 535E4-B	fleet fuel	0.8637	0.1360	300	19.4	0.8096	43.1
	Т9				0.8637	0.1360	300	19.1	0.8090	43.1

Table S5-Composition of Test Fuels for APEX 1 – 3

^a All engines are turbofan except as noted ^b Questionable value as reported by NASA. Actual sulfur content should be similar to other APEX-3 tests.

^c No data reported in this paper for these engines.

	APEX-1		APEX-2			EX-3		
	CFM56	5-2C1 high S	CFM56- 7B24	CFM56- 3B1&2	AE3007- A1E	PW 4158	RB211- 535E4-B	CFM56- 3B1
chemical compound	base fuel EPA2	fuel EPA3	fleet fuel T1&4	fleet fuel T2&3	fleet fuel T3&4	fleet fuel T6&7	fleet fuel T9	fleet fuel T11
n-alkanes (total EI)	7.51	10.1	13.0	589	171	20.7	59.0	81.1
n-undecane (n-C11)							3.61	
n-dodecane (n-C12)				3.73			3.01	
n-tridecane (n-C-13)				1.86		0.362	0.24	5.01
n-tetradecane (n-C14)	0.578		6.90	4.28		0.724	7.97	8.58
n-pentadecane (n-C15)	6.93					0.815	14.5	13.7
n-hexadecane (n-C16)					3.43	0.818	14.7	5.92
n-heptadecane (n-C17)						1.31	5.64	
n-octadecane (n-C18)						0.403		
n-nonadecane (n-C19)								11.6
n-heneiicosane (n-C21)		1.01						20.7
n-docosane (n-C22)		1.18	6.12	7.91				
n-tricosane (n-C23)				28.4	23.7		9.32	
n-tetracosane (n-C24)				46.7		7.27		9.41
n-pentacosane (n-C25)				49.9				1.94
n-hexacosane (n-C26)		3.01		56.7	10.8			
n-heptacosane (n-C27)				70.9	15.1			
n-octacosane (n-C28)		4.87		62.7	7.42	5.98		
n-nonacosane (n-C29)				94.5	41.3			
n-triacontane (n-C30)				50.0	0.171			
n-hentricontane (n-C31)				43.5	27.4			
n-dotriacontane (n-C32)				36.3	13.7			1.39
n-tritriacontane (n-C33)				16.5	20.4			2.89
n-tetratriacontane (n-C34)				14.9	2.70	1.27		
n-pentatriacontane (n-C35)					2.54	1.09		
n-hexatriacontane (n-C36)					1.89	0.362		
n-heptatriacontane (n-C37)						0.272		
branched alkanes (total EI)	2.50	9.32				1.63		3.82
2-methylnonadecane		9.32				1.44		3.82
phytane	2.50					0.190		
alkenes (total EI)						8.57		34.2
squalene						8.57		34.2
cyclohexanes (total EI)						2.35		
dodecylcyclohexane						0.416		
nonadecylcyclohexane						1.93		
oxy PAHs (total EI)	19.8	76.5						
9-H-fluoren-9-one		3.03						
anthraquinone		3.80						
naphthalic anhydride	19.8	69.7						
PAHs (total EI)	50.9	32.6	9.97	24.3	123	8.07	115	146
naphthalene	14.0		1.00		6.33		7.58	4.64
1-methylnaphthalene	6.13	5.01			9.10		6.85	9.56
2-methylnaphthalene	12.9	8.25			2.73		6.81	5.13
2,7 dimethylnaphthalene	1.84	2.09						

Table S6-Emissions Index (μ g/kg fuel) by Individual Chemical Compound^a

	APEX-1		API	EX-2	APEX-3					
	CFM5	5-2C1 high S	CFM56- 7B24	CFM56- 3B1&2	AE3007- A1E	PW 4158	RB211- 535E4-B	CFM56- 3B1		
chemical compound	base fuel EPA2	fuel EPA3	fleet fuel T1&4	fleet fuel T2&3	fleet fuel T3&4	fleet fuel T6&7	fleet fuel T9	fleet fuel T11		
PAHs (continued)										
1,3 dimethylnaphthalene	1.97	1.79								
2,6-dimethylnaphthalene	4.02	3.22			3.15		6.81	7.58		
acenaphthylene	2.55				1.65		3.79	1.99		
dibenzofuran					0.135					
fluorene					1.13	0.0720	1.00	1.15		
1-methylfluorene		0.368								
phenanthrene		0.480		3.35	7.12		8.28	7.67		
anthracene		0.0804			1.08	0.0604	0.641	0.625		
fluoranthene		0.992		5.42	62.5			53.3		
retene						2.93				
pyrene	0.757		0.882	5.48	23.7		28.8	9.16		
chrysene	0.496	0.848			2.56		3.93	3.61		
benzo[a]anthracene	0.324	0.210			1.08	0.0905	1.85	0.576		
benzo[k]fluoranthene	1.74	0.518					5.22			
benzo[b]fluoranthene	3.15	2.04					8.83			
benzo(e)pyrene					1.08		6.86	1.26		
indeno[1,2,3-cd]pyrene	0.208	1.59					7.83			
dibenzo[a,h]anthracene		2.27								
benzo[ghi]perylene	0.538	1.95					10.2			
benzo(ghi)flouranthene				5.59						
ABB-20R-C27-cholestane			8.09	4.47		0.604		3.72		
AAA-20S-C27-cholestane						1.30		5.49		
ABB-20R-C28-						0.785		2.35		
methylcholestane ABB-20R-C29-						1.36	0.0151	4.49		
ethylcholestane 17A(H)-22,29,30-						0.875		3.46		
trisnorhopane 17B(H)-21A(H)-30-								9.75		
norhopane 17A(H)-21B(H)-hopane								10.7		
coronene	0.225	0.876								
total organic species detected	80.6	128.5	23.0	613.2	293.9	41.3	174.3	265.3		

^a All data are background and artifact corrected. Data taken from Appendix H of Reference 13 shown in the main text.

Table S7-Abbreviations of Chemical Compounds Used in Figure 3a of Main Text

abbreviation	name of chemical compound
1,3dm-NAP	1,3-dimethylnaphthalene
1m-NAP	1-methylnaphthalene
2,6dm-NAP	2,6-dimethylnaphthalene
2,7dm-NAP	2,7-dimethylnaphthalene
2m-NAP	2-methylnaphthalene
9-H-fluorene-9-one	self explanatory
AAA-chloestane	$\alpha \alpha \alpha$ -20 <i>S</i> -C27cholestane
ABB-chloestane	$\alpha\beta\beta$ -20 <i>R</i> -C27-cholestane
ABB-e-chlorestane	$\alpha\beta\beta$ -20 <i>R</i> -C29-ethylcholestane
ABB-m-chlorestane	$\alpha\beta\beta$ -20 <i>R</i> -C28-methylcholestane
ACE	acenapthylene
ANT	anthracene
anthraquinone	self explanatory
B[a]A	benz(a)anthracene
B[b]F	benzo(b)fluoranthene
B[e]P	benzo(e)pyrene
B[g,h,i]F	benzo(ghi)flouranthene
B[g,h,i]P	benzo(ghi)perylene
B[k]F	benzo(k)fluoranthene
CRY	chrysene
D[a,h]A	dibenzo(a,h)anthracene
FLR	fluorene
FLU	fluoranthene
hopane	$17\alpha(H)-21\beta(H)$ -hopane
I[1,2,3-c,d]P	indeno(1,2,3-cd)pyrene
methyl-C19	methylnonadecane
m-FLR	1-methylfluorene
NAP	naphthalene
napthalic anhydride	self explanatory
n-C11C37	C11 to C37 alkanes
norhopane	17β (H)-21α(H)-30-norhopane
octadecene	self explanatory
PHE	phenathrene
phytane PYR	self explanatory
	pyrene
squalene	self explanatory
trisnorhopane	17 α (H)-22,29,30-trisnorhopane

Supporting Information Literature Cited

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