The NCAR Trace Organic Gas Analyzer with Time of Flight mass spectrometer (TOGA-TOF)

The TOGA-TOF is an in-situ online gas chromatograph mass spectrometer (GC-MS) that provides near-continuous atmospheric mixing ratios of an extensive and growing list of volatile organic compounds (VOCs) in the C_1-C_{10} molecular structure range. The list of species that can be quantified using TOGA-TOG includes alkanes, alkenes, aromatics, halogenated VOCs, nitrates, nitriles, sulfides, alcohols, ketones, aldehydes, esters, and ethers. One hundred or more unique trace gases can be measured, with sufficient sensitivity to measure trace species in the remote background atmosphere and dynamic range to measure in highly polluted regions. Table 1 is a list of species that have been identified and/or quantified using the TOGA-TOF, as well as typical limits of detection where known.

The TOGA-TOF uses a cryogenic preconcentrator, consisting of a custom-built liquid nitrogen (LN2) dewar and a system of traps, for water removal, sample enrichment, and cryofocusing of trace constituents. A high-resolution electron impact time-of-flight mass spectrometer (HR-EI-TOF-MS; Tofwerk, Switzerland) is used to identify and quantify individual compounds, using Igor-based software packages developed by Tofwerk and Aerodyne Research Inc. System calibrations and blanks are performed using a catalytic-clean air generator/dynamic dilution system with accurate (±1%) and precise (±1%) calibration gas delivery. The system operates continuously, allowing for frequent calibrations and zeros during flight. The TOGA-TOF inlet is a recently-designed constant mass flow design to mitigate the intrusion of aerosols and allow for calibrations and system blanks through the inlet and associated tubing. The TOGA-TOF is contained in an elongated HIAPER rack standard DC-8 rack, weighs less than 200 kg and consumes ~1 kW of power. More information on the TOGA and TOGA-TOF can be found here: https://www2.acom.ucar.edu/voc-measurements/measurement-instrumentation.

Table 1. Chemical species identified using the TOGA-TOF and limits of detection (LOD) where known.

NMHCs	Formula	LOD; ppt
Alkanes		
Propane	C_3H_8	5
Isobutane	C_4H_{10}	1
n-Butane	C_4H_{10}	1
Isopentane	C_5H_{12}	1
n-Pentane	C_5H_{12}	1
2-Methylpentane	C_6H_{14}	0.5
3-Methylpentane	C_6H_{14}	0.5
n-Hexane	C_6H_{14}	0.5
n-Heptane	C_7H_{16}	1
2,2,4-Trimethylpentane	C_8H_{18}	0.5
n- Octane	C_8H_{18}	0.5
Alkenes		
Propene	C_3H_6	5
1-Butene/Isobutene	C_4H_8	1
cis-2-Butene	C_4H_8	1
trans-2-Butene	C_4H_8	1
Isoprene	C_5H_8	1
α-Pinene	$C_{10}H_{16}$	1
β-Pinene/Myrcene	$C_{10}H_{16}$	1
Camphene	$C_{10}H_{16}$	1
Limonene/3-Carene	$C_{10}H_{16}$	1
Tricyclene	$C_{10}H_{16}$	1
Aromatics		
Benzene	C_6H_6	0.3
Toluene	C_7H_8	0.3
Ethylbenzene	C_8H_{10}	0.2
p-/m-Xylene	C_8H_{10}	0.2
o-Xylene	C_8H_{10}	0.2
Styrene	C_8H_8	0.1
Ethynylbenzene	C_8H_6	TBD

OVOCs	Formula	LOD; ppt
Aldehydes		
Formaldehyde	CH_2O	20
Acetaldehyde	C_2H_4O	5
Propanal	C_3H_6O	2
Isobutanal	C_4H_8O	TBD
Butanal	C_4H_8O	1
Acrolein	C_3H_4O	1
Methacrolein	C_4H_6O	1
2-Butenal	C_4H_6O	2
Furfural	$C_5H_4O_2$	TBD
3-Furaldehyde	$C_5H_4O_2$	TBD
Ketones		
Acetone	C_3H_6O	5
MEK	C_4H_8O	0.5
MVK	C_4H_6O	0.5
2,3-Butanedione	$C_4H_6O_2$	TBD
Alcohols		
Methanol	CH_4O	5
Ethanol	C_2H_6O	2
2-Propanol	C_3H_8O	4
Ethenol	C_2H_4O	TBD
MBO (2-Methyl-3-Buten-2-ol)	$C_5H_{10}O$	1
Esters		
Methyl formate	$C_2H_4O_2$	TBD
Methyl acetate	$C_3H_6O_2$	TBD
Methyl propionate	$C_4H_8O_2$	TBD
Ethyl acetate	$C_4H_8O_2$	TBD
Ethers/Furans		
MTBE (Methyl t-butyl ether)	$C_5H_{12}O$	0.3
Furan	C_4H_4O	1
THF (Tetrahydrofuran)	C_4H_8O	TBD

OVOCs	Formula	LOD; ppt
Ethers/Furans (cont'd)		
2-Methylfuran	C_5H_6O	0.5
3-Methylfuran	C_5H_6O	0.5
2,3-Dimethylfuran	C_6H_8O	TBD
2,4-Dimethylfuran	C_6H_8O	TBD
2,5-Dimethylfuran	C_6H_8O	TBD
2-Ethylfuran	C_6H_8O	TBD
3-Ethylfuran	C_6H_8O	TBD
2-Vinylfuran	C_6H_6O	TBD
3-Vinylfuran	C_6H_6O	TBD
1,3-Dioxolane	$C_3H_6O_2$	TBD

Nitrogen-containing VOCs	Formula	LOD; ppt
Nitriles		
Hydrogen cyanide	HCN	5
Chlorine cyanide	ClCN	TBD
Acetonitrile	C_2H_3N	1
Propanenitrile	C_3H_5N	1
Acrylonitrile	C_3H_3N	1
Methylacrylonitrile	C_4H_5N	2
Nitrates		
Methyl nitrate	CH_3NO_3	TBD
Ethyl nitrate	$C_2H_5NO_3$	TBD
Isopropyl nitrate	$C_3H_7NO_3$	2
n-Propyl nitrate	$C_3H_7NO_3$	2
t-Butyl nitrate	$C_4H_9NO_3$	2
2-Butyl+Isobutyl nitrate	$C_4H_9NO_3$	2
n-Butyl nitrate	$C_4H_9NO_3$	2
Other		
Pyrrole	C_4H_5N	TBD
Nitromethane (CH_3NO_2)	CH_3NO_2	TBD

Halogenated VOCs	Formula	LOD; ppt
Methyl chloride	CH_3Cl	1
Dichloromethane	CH_2Cl_2	1
Chloroform	$CHCl_3$	1
Tetrachloromethane	CCl_4	1
Tetrachloroethene	C_2Cl_4	0.1
1,2-Dichloroethane	$C_2H_4Cl_2$	0.5
Methyl chloroform	$C2H_3Cl_3$	0.5
Methyl bromide	CH_3Br	1
Dibromomethane	CH_2Br_2	0.03
Bromoform	$CHBr_3$	0.1
Methyl iodide	CH_3I	0.03
Diiodomethane	CH_2I_2	0.05
Ethyl iodide	C_2H_5I	0.5
Chloroiodomethane	CH_2ICl	0.05
Bromodichloromethane	$CHBrCl_2$	0.05
Dibromochloromethane	$CHBr_2Cl$	0.03
CFC-11	CCl_3F	5
CFC-12	CCl_2F_2	1
CFC-113	$C_2Cl_3F_3$	1
CFC-114	$C_2Cl_2F_4$	1
HCFC-22	CHClF2	1
HCFC-141b	$C_2H_3Cl_2F$	1
HCFC-142b	$C_2H_3ClF_2$	TBD
HFC-134a	$C_2H_4F_4$	1

Sulfur-containing VOCs	Formula	LOD; ppt
Carbonyl sulfide	OCS	1
Carbon disulfide	CS_2	0.2
Methanethiol	CH_4S	TBD
DMS (Dimethyl sulfide)	C_2H_6S	1
Carbon suboxide	C_3O_2	TBD

Measurements:

VOCs

Aircraft:

Gulfstream V – NSF, C-130 – NSF, DC-8 - AFRC

Measurement Characteristics:

Overall estimate of uncertainty: VOC dependent, typically 20%.

Precision: 3% or less.

Response time: typically 35-second samples on a 2-minute cycle, with the option for a shorter, targeted sample.

Instrument Type:

Gas chromatography, Time-of-Flight Mass Spectrometry (in situ)

Point(s) of Contact:

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