Emissions of Gas-Phase Low-Volatility Organic Compounds from Mobile Sources


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Emissions of organic species

VOC: volatile organic compounds (gas phase)
IVOC: “intermediate volatility” organic compounds (gas phase)
SVOC: semivolatile organic compounds (gas, particle phase)
Emissions of organic species

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High-resolution electron impact mass spectrometer

- Syringe Injection
- PM Filter
- Sampling Inlet
- UHP He
- 2-Stage Turbo Pump
- Electron Impact Ionization
- Liquid N₂
- Ultra Zero Air
- LICOR CO₂
- Time-of-Flight Mass Spectrometer
High-resolution electron impact mass spectrometer
High-resolution electron impact mass spectrometer

Diagram showing a high-resolution electron impact mass spectrometer setup. The diagram includes components such as Syringe Injection, PM Filter, Sampling Inlet, UHP He, Capillary Transfer Line, Pump, Liquid N2, LICOR CO2, Ultra Zero Air, Time-of-Flight Mass Spectrometer, V-Mode, W-Mode, 2-Stage Turbo Pump, Electron Impact Ionization.
HR-EI-MS data

a) mass spectrum (total organic mass)

b) individual ion abundances (elemental ratios)
High-resolution electron impact mass spectrometer

1) Temperature: Volatility
2) EI signal: Total mass
3) Mass spectrum: Composition
4) HR ions: Elemental ratios
Instrument response (n-alkanes)
Calibration (volatility, mass concentration)
Emissions characterization: aircraft

AAFEX II: Alternative Aviation Fuels Experiment II
Dryden Aircraft Operations Facility, Palmdale CA, March-April 2011

DC-8, two turbofan CFM56-2C1 engines (JP-8 and FT fuels)
Measurements: 150 m downwind
Engine power sweep

- Semicontinuous measurements (2 min collection, 10 min desorption/cooling cycle)
- Can detect rapid changes, transients

[Cross et al., *Atmos. Chem. Phys.*, 2013]
Emission factors, I/SVOC contributions

Low powers: I/SVOCs account for 10-20% of organic emissions

High powers: I/SVOCs account for >50% of organic emissions

[Cross et al., Atmos. Chem. Phys., 2013]
Volatility distribution (7% power)

[Cross et al., Atmos. Chem. Phys., 2013]
PMF factors

[Cross et al., Atmos. Chem. Phys., 2013]
PMF factors

Saturated HC Factor
H:C = 2.07
O:C = 0.03

Aromatic HC Factor
H:C = 1.36
O:C = 0.04

Oxygenated HC Factor
H:C = 1.46
O:C = 0.26

[Cross et al., Atmos. Chem. Phys., 2013]
Unsaturated HC factor

[Cross et al., *Atmos. Chem. Phys.*, 2013]
Unsaturated HC factor

[Cross et al., Atmos. Chem. Phys., 2013]
Aromatic HC factor

[Cross et al., Atmos. Chem. Phys., 2013]
Oxygenated HC factor

[Cross et al., *Atmos. Chem. Phys.*, 2013]
Summary: I/SVOCs from aircraft

[1]: Alkanes from unburnt fuel
[2]: Aromatics from unburnt fuel
[3]: Aromatics from pyrolysis
[4]: Oxidized fuel components
[5]: Partially oxidized lubricant(?)

[Cross et al., Atmos. Chem. Phys., 2013]
Trace elements in emitted particles

[Cross et al., J. Eng. Gas Turbines and Power, 2012]
Trace elements in emitted particles

Unambiguous identification of trace metals:
- Exact mass
- Isotopic abundances

[Cross et al., *J. Eng. Gas Turbines and Power*, 2012]
Trace elements in emitted particles

Lubricant components: B, Ca, Mg, P, Zn
Engine-wear markers: Fe, Pb
Others: K, Na, S, Cl

[Cross et al., J. Eng. Gas Turbines and Power, 2012]
Summary/conclusions

- New instrument for measuring amount, volatility, and (ensemble) composition of IVOCs and SVOCs in near-real time

- Aircraft emissions: Emissions, composition (alkane/aromatic/oxygenate), and volatility all strongly power-dependent (fuel $\rightarrow$ pyrolysis)

- Diesel engine emissions: Emissions of 0.2-20 mg/kg fuel, depending on engine power; analysis of volatility and composition still in progress

- Follow-on work: Comparison of multiple IVOC/SVOC techniques on the same engine (May-June 2014)
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