

Primary Emissions and Secondary Organic Aerosol Formation from Two Heavy Duty Trucks

Zardini AA¹, Suarez-Bertoa R¹, Platt SM², El Haddad I², Pieber S², Hellebust S³, Temime B³, Marchand N³, Jezek I⁴, Mocnik G⁴, Drinovec L⁴, Slowik JG², Baltensperger U², Prevot ASH², Astorga C.¹

¹*European Commission - Joint Research Centre, Institute for Energy and Transport, Sustainable Transport Unit, 21027 Ispra (Va), Italy.*

²*Paul Scherrer Institute, Laboratory for atmospheric Chemistry, CH-5232 Villigen, Switzerland.*

³*Laboratoire Chimie et Environnement, Universit de Provence, Marseille, France.*

⁴*Aerosol d.o., Ljubljana, Slovenia.*

Rationale. Atmospheric aerosol particles have significant effects on climate, human health and air quality in general. The largest uncertainties in quantifying the Earth radiative forcing are connected to atmospheric aerosols [1]. Organics have been identified as important constituents of the atmospheric particulate matter, especially over continental regions and include thousands of species from non-toxic to carcinogenic and mutagenic ones. Secondary organic aerosol (SOA), formed in the atmosphere by photo-oxidation of some volatile organics and consequent conversion to particle phase, represents a large fraction of the total fine particle mass (PM) [2]. Even though SOA has been the focus of several studies in the last decade, many aspects remain unexplained, e.g., gas precursors and nucleation mechanisms, detailed yields, aging paths, and toxicity. In particular, we noticed a lack of documentation regarding SOA formation from internal combustion engine emissions. For these reasons we designed experiments where the primary emissions from two heavy-duty vehicles (HDV) are photochemically aged to produce SOA.

Experimental. A mobile smog chamber (Paul Scherrer Institute, see [3] for details) was hosted inside the climatic cell for chassis dynamometer tests on HDVs at the Vehicle Emission Labs of the European Community – Joint Research Centre (JRC). Emission tests were run at 22°C and -7°C for two in-use Euro V trucks. One truck was fuelled either with standard diesel or a mixture of liquid petroleum gas (LPG) and diesel. Some details about the JRC test cell for HDVs can be found in [4]. Gaseous and particulate analysis of primary and photochemically aged exhaust emissions was performed over a legislative European Transient Cycle (ETC, see Fig. 1 and Fig. 2). Besides regulated compounds (CO, HC, NO_x, PM), we monitored a range of exhaust constituents, both in the gas and particle phase, with online and offline state of the art techniques: aerosol (HR-ToF-AMS, Aerodyne) and proton transfer reaction (HR-ToF-PTR-MS, Ionicon) mass spectrometers;

Fourier transformed infrared spectroscopy (MKS-2030-HS); gas and liquid chromatography. Details on the PSI mobile smog chamber, AMS and other instruments can be found at:

<http://www.psi.ch/lac/instruments-and-tools>. Details on the Vehicle Emission Laboratories of the European Community can be found at:

<http://iet.jrc.ec.europa.eu/clean-and-efficient-vehicles-cleeve>.

Preliminary Results. Preliminary results can be summarized as follows:

- HDVs emissions are in general more stable against temperature changes than passenger cars;
- Large emissions of PM and total hydrocarbon are observed for the mixture LPG/Diesel in the cold phase (Urban phase, see Fig. 1) of tests at -7°C ($\text{PM} \geq 1.5\text{g/km}$; $\text{HC} \geq 15\text{g/km}$);
- Considerable amount of SOA is produced from the diesel truck at -7°C \Rightarrow Large Impact on ambient PM (25-50%);
- SOA from diesel trucks at 22°C does not seem to be of concern when compared to passenger cars and scooters;
- More tests are needed to better constrain the vehicle to vehicle variability.

Acknowledgements. This work was supported by the Swiss Federal Office for the Environment (FOEN), the Federal Roads Office (FEDRO), The French Environment and Energy Management Agency (ADEME, Grant number 1162C00O2). Operation partly financed by the European Union, European Social Fund. The VELA staff is acknowledged for its skillful technical assistance, in particular Franz Muehlberger, Urbano Manfredi, and Philippe Le Lijours.

References

- [1] IPCC Working Group I: <http://www.ipcc.ch/>
- [2] Zhang et al. GRL, **34**, 2007.
- [3] Platt et al. ACPD, **12**, 2012.
- [4] Adam et al., Anal. Chem., **83**, 2011.

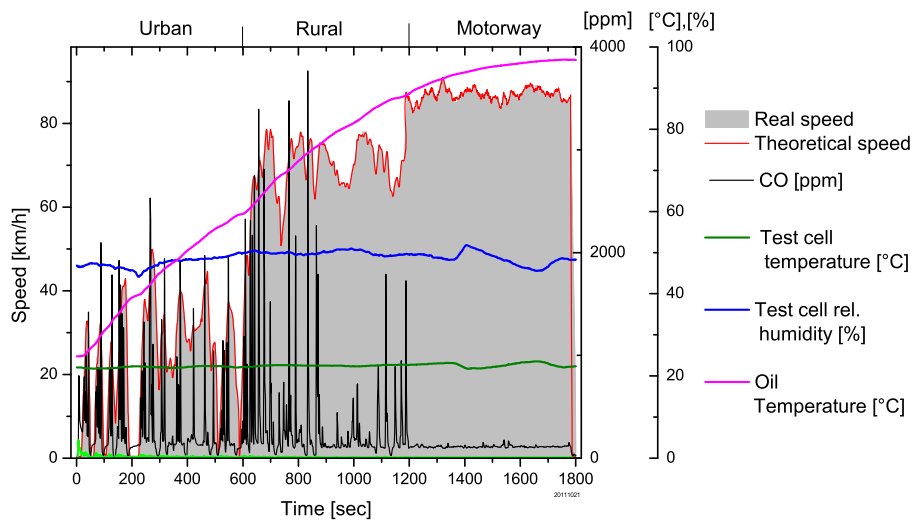


Figure 1: ETC driving cycle. Actual speed and theoretical speed are plotted along with tailpipe CO concentration, test cell ambient conditions (controlled temperature and relative humidity), and engine oil temperature (used to qualify "cold starts", i.e., when initial oil T is close to ambient T) during a typical test on a diesel Euro V HDV.

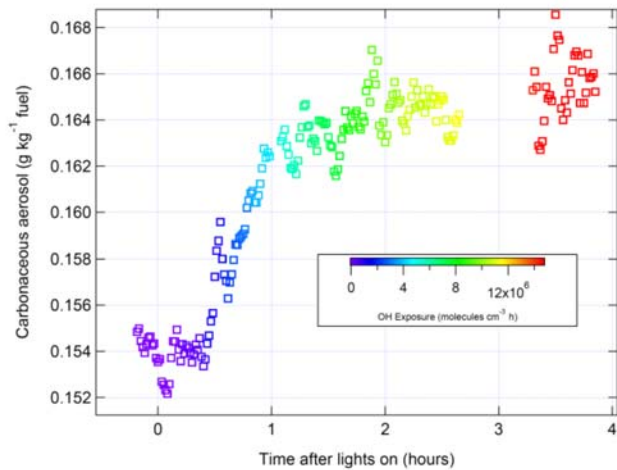


Figure 2: Photochemical aging after an ETC driving cycle. Carbonaceous aerosol (organic aerosol + black carbon) as a function of time after lights on in the smog chamber, and OH exposure (color-coded) for a diesel Euro V HDV.



Joint Research Centre

The European Commission's in-house science service

www.jrc.ec.europa.eu

*Serving society
Stimulating innovation
Supporting legislation*



Joint
Research
Centre



Primary emission and secondary organic aerosol formation from two heavy-duty trucks

Alessandro A. Zardini

**IET-Institute for Energy and Transport
"New pollutants", Sustainable Transport Unit
EC-JRC-Ispra**

Project



Frame

Collaboration agreement JRC/Swiss Federal Office for the Environment/Paul Scherrer Institute

Scope

Formation of **secondary organic aerosol particles** from primary exhaust emissions of vehicles

Method

Combined use of JRC facilities (controlled driving tests) and PSI smog chamber (photochemistry)

Duration

2 sessions of two months

Terminology: POA, SOA, aged POA



Primary

Directly emitted in particulate form at the source.

Secondary organic

Exclusively for aerosol constituents that **enter the particle phase from the gas phase as a result of chemical transformation processes**.

NB

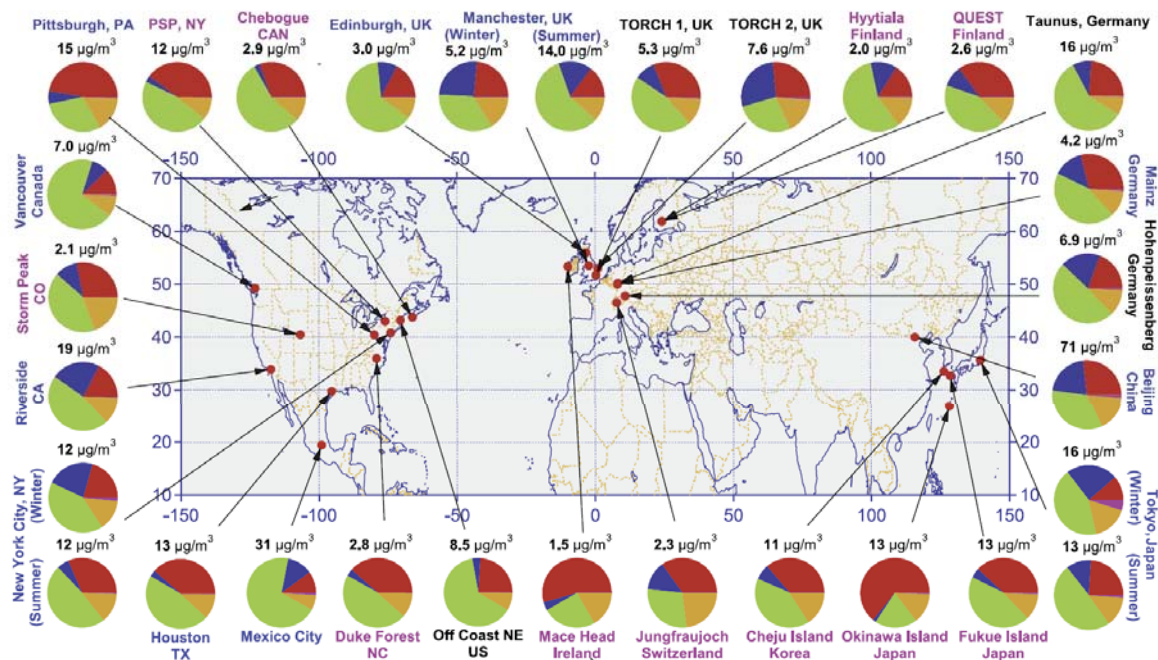
Potential confusion arises in traffic emissions.

T exhaust decrease → fine particles are formed without modification of gaseous precursors by chemical reaction → **primary aerosol, not secondary**

Ambient concentration



Organics are everywhere, and are a lot



Typically 20%-60% of the fine aerosol mass is organic depending on geographical location (up to 90% for forested aereas)

Figure 1. Location of the AMS datasets analyzed here (data shown in Table S1 in the auxiliary material). Colors for the study labels indicate the type of sampling location: urban areas (blue), <100 miles downwind of major cites (black), and rural/remote areas >100 miles downwind (pink). Pie charts show the average mass concentration and chemical composition: organics (green), sulfate (red), nitrate (blue), ammonium (orange), and chloride (purple), of NR-PM₁.

(Zhang et al. 2009)

Organic aerosols are SOA



Deconvolution of OA (Aerosol Mass Spectrometer)

- hydrocarbon-like OA (HOA)
- oxygenated OA (OOA)

HOA \leftrightarrow primary combustion emissions
(mainly from fossil fuel, peaks on rush hours)

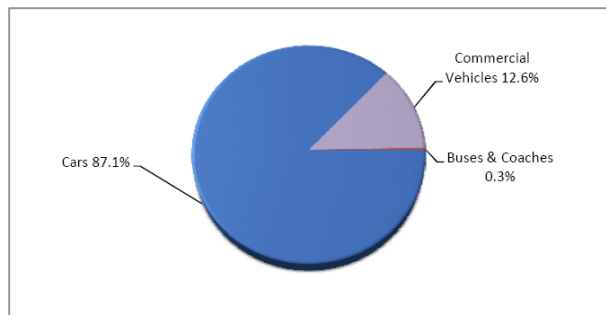
OOA **64%-95% of the total OA** (flat profile)

OOA concentration \gg advected oxidized HOA

1. HOA oxidation is not an important source of OOA
- 2. OOA are mainly SOA**

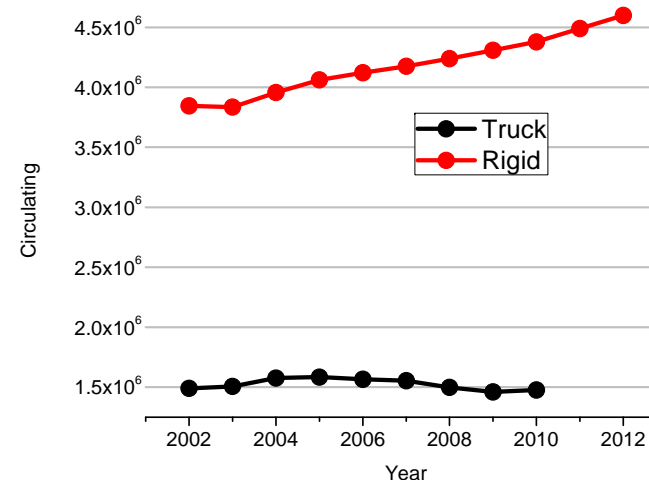
→ Organics are mainly SOA

Motivations – Air quality



Source: Eurostat - 2010

Heavy duty are 13% of EU vehicle fleet



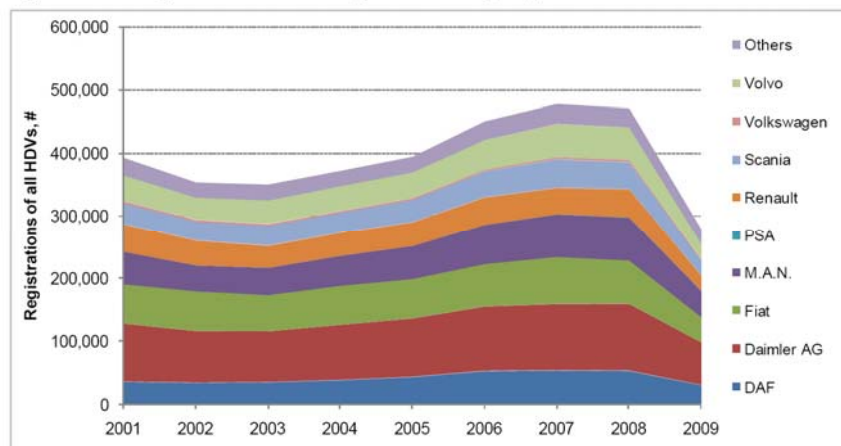
...but circulating HD increased

► Heavy duty vehicles are the **second-biggest source of emissions within the transport sector**, i.e. larger than both international aviation and shipping.

► <EU car annual distance> = 14 000 km/year
Trucks: **x10**
Fuel consumption: **x5**

► Heavy-Duty Vehicles (HDV) represent about a quarter of EU road transport CO₂ emissions and some **6% of the total EU** emissions.

Figure 2-7: EU registrations of all HDVs by manufacturer group, 2001-2009



Source: ACEA, 2010.

Registrations declined (...the crisis)

Motivations - Climate

Aerosols

Direct effect on climate:

Scattering and absorption of radiation

Low impact

Understanding: Very low.

Uncertainty: High

Indirect effect on climate:

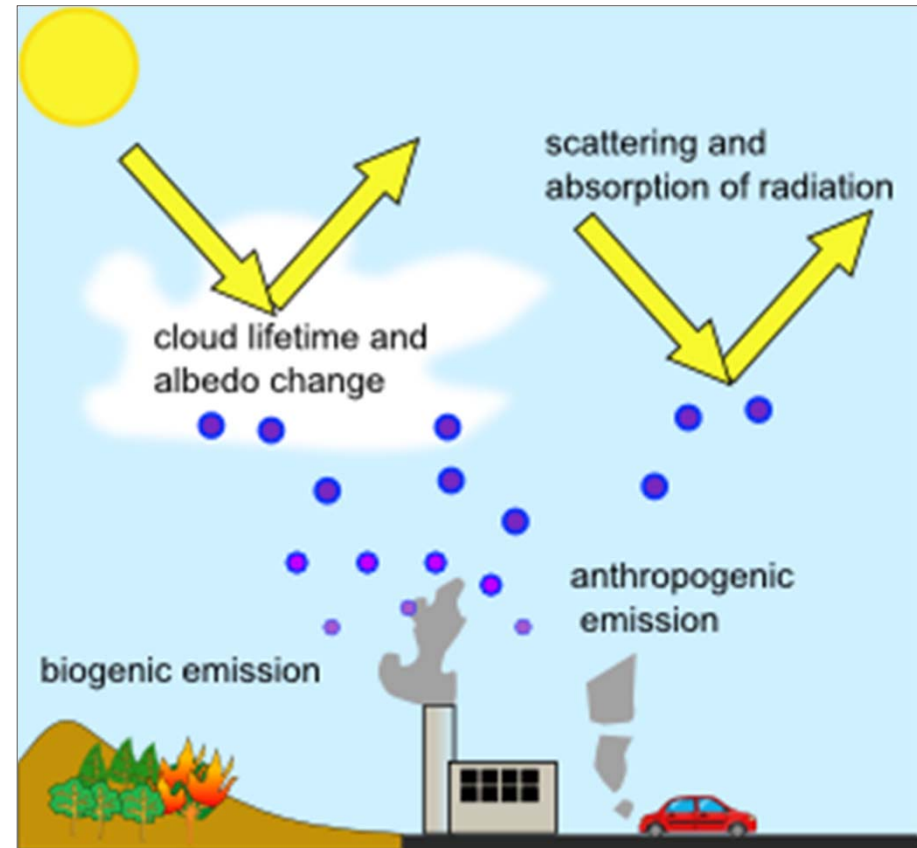
Modification of the cloud/fog/haze parameters.

Huge impact, as big as CO₂

Up to **-1.8 W/m²** (IPCC)

Understanding: Very low.

Uncertainty: Total



Vehicles



	Model	Year	Power	After-treatment	Category	Fuel	Mileage
Truck 1	DAF XF105 12.9L 19.5 ton	2007	340kW	SCR (Urea) DOC (THC,CO) Without DPF	Euro V	Diesel B5 Diesel/LPG, 50%	350000 km Ca.
Truck 2	MAN TGX 12.4L 19 ton	2009	324kW	DPF SCR DOC	Euro V	Diesel B5	250000 km Ca.

Emission Standards



Stage	Date	Test	CO	NMHC	CH ₄ ^a	NOx	PM ^b	PN ^e
			g/kWh					
Euro III	1999.10 <i>EEV only</i>	ETC	3.0	0.40	0.65	2.0	0.02	
	2000.10		5.45	0.78	1.6	5.0	0.16 ^c	
Euro IV	2005.10		4.0	0.55	1.1	3.5	0.03	
Euro V	2008.10		4.0	0.55	1.1	2.0	0.03	
Euro VI	2013.01	WHTC	4.0	0.16 ^d	0.5	0.46	0.01	6.0×10 ¹¹

a - for gas engines only (Euro III-V: NG only; Euro VI: NG + LPG)
 b - not applicable for gas fueled engines at the Euro III-IV stages
 c - PM = 0.21 g/kWh for engines < 0.75 dm³ swept volume per cylinder and a rated power speed > 3000 min⁻¹
 d - THC for diesel engines
 e - for diesel engines; PN limit for positive ignition engines TBD

- Limits refer to **engine bench tests**
"Real" driving tests (either on-road or roller bench) are not considered.
- Euro VI: WHTC cycles, OBD, PEMS (real driving)
Also PN, Max(NH₃) = 10ppm, NO₂ ongoing

VELA7 climatic test cell



Features

Dimension 22 x 8 x 7m

Temperature: -30° +50° C
(± 1k in time & ± 3k space)

RH: 15% - 95% (± 5%)

Chassis dyno: 1.82 m, Zoellner GmbH

Analyzer: AVL AMA 4000 Advanced

VELA7 climatic test cell



VELA7

Diluted exhaust and filtered ambient air (150 m³/min; 30-40°C CVS)

→ Automated Tedlar bags sampler

→ Legislated methodology for regulated compounds

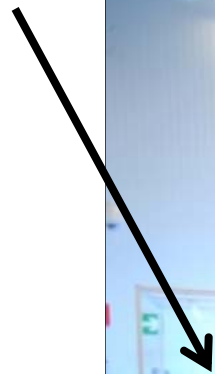


Smog chamber instruments
HR-ToF-AMS (Organic particles)
PTR-ToF-MS (VOCs)
Aethalometer (BC)
Monitors (NO_x, CH₄, THC, O₃, NH₃)
SMPS-CPCs

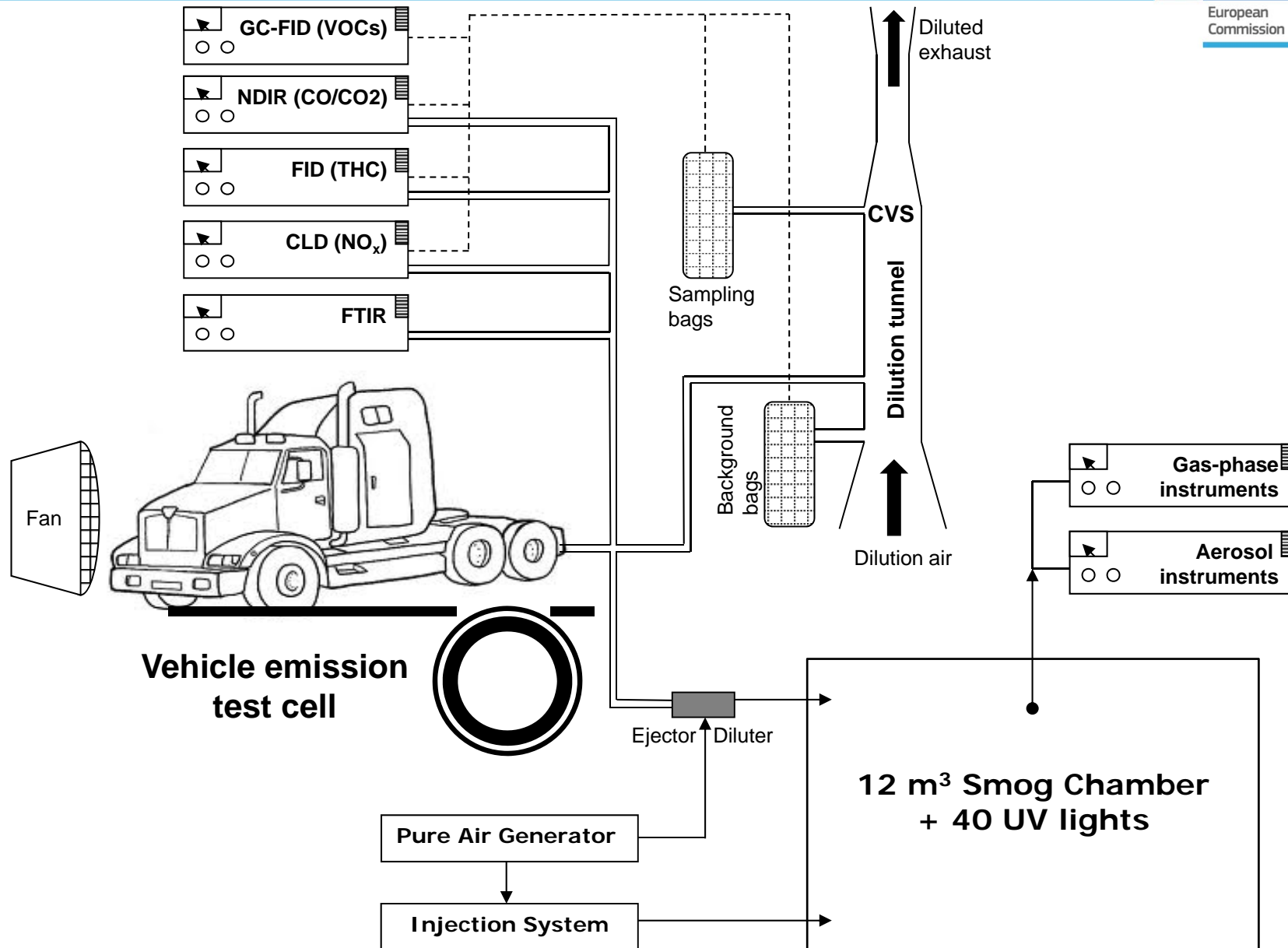
VELA7 climatic test cell



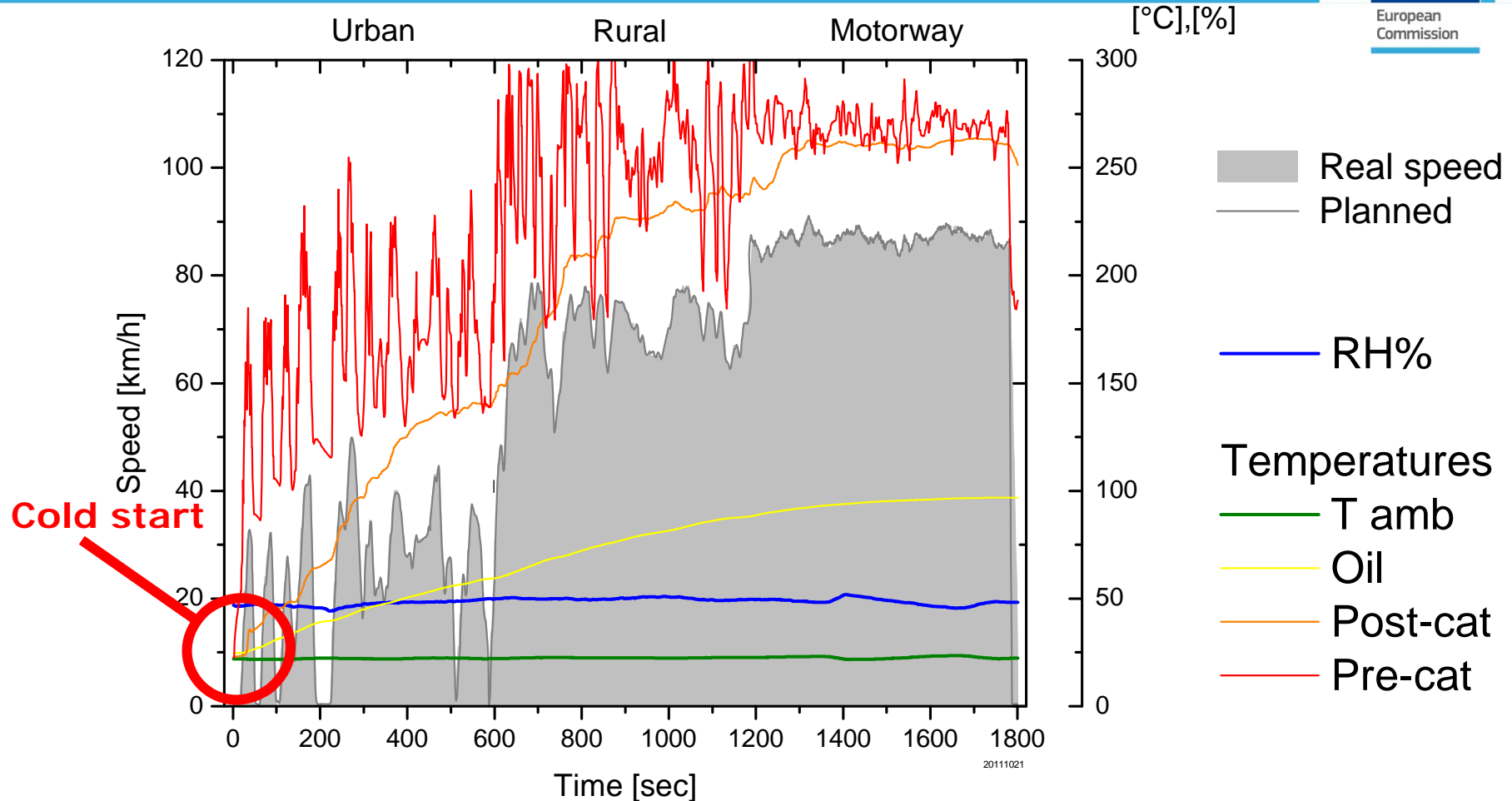
SOA



Schematic

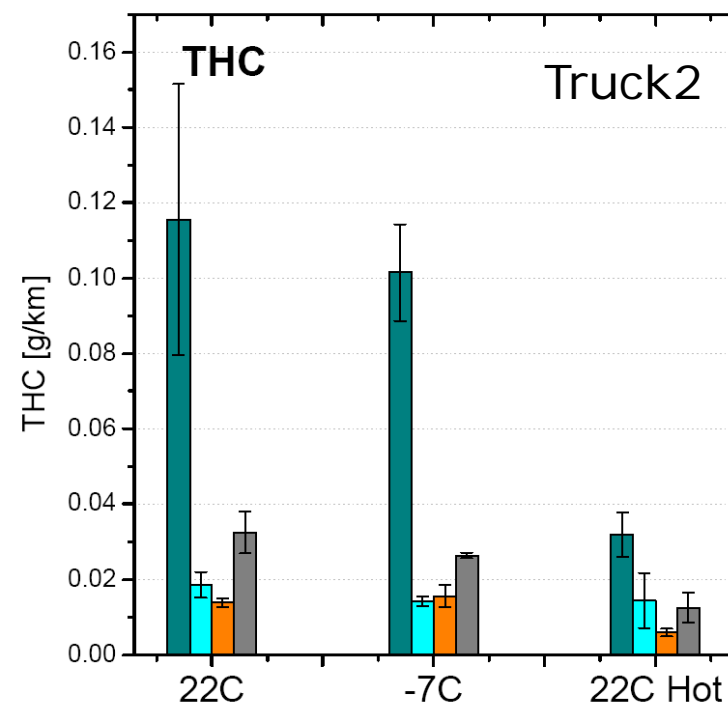
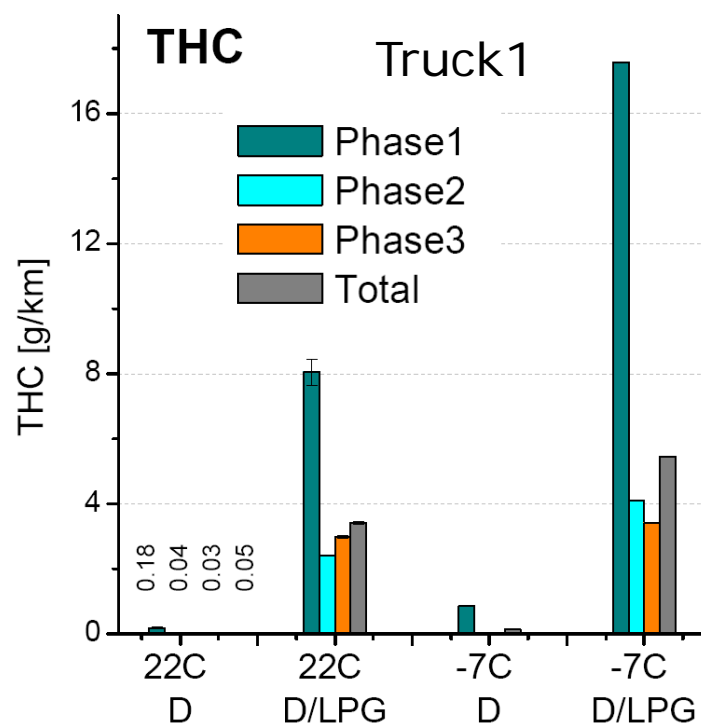


European Transient Cycle (ETC)



- 29km. Urban: max 50 km/h (3.7km). Rural $\langle \text{speed} \rangle = 72$ km/h (10.9km). Motorway: $\langle \text{speed} \rangle = 88$ km/h (14.8km)
- Oil Temperature used to define **cold starts**
- Controlled ambient conditions: **constant T (22C & -7C) and RH=50%**
- Soaking time **>12h (>6h legislated)**

Regulated - THC



22C

Diesel: Better than a Euro VI (not shown).

Best when **HOT started**

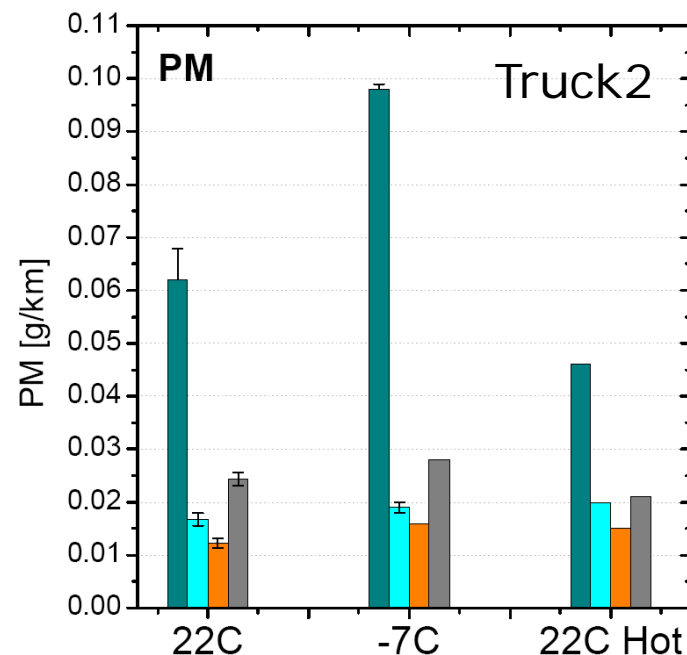
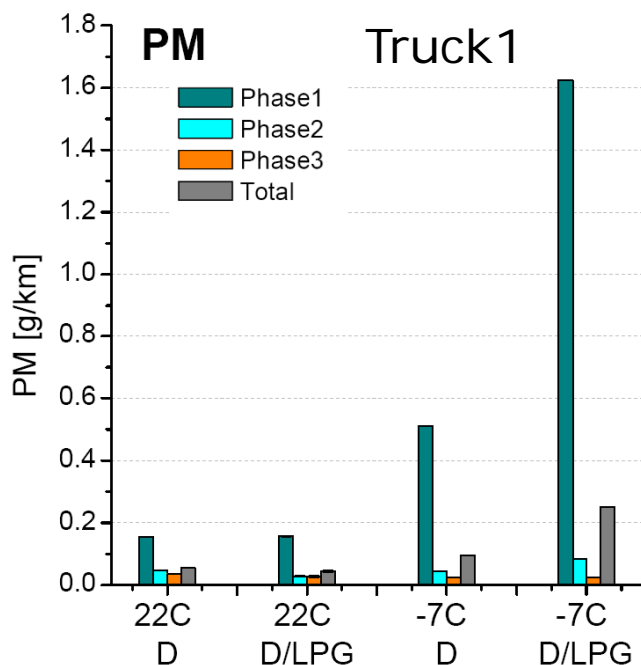
LPG/D: Worse than a Euro III (engine)

-7C

Good performance for Diesel; Bad performance for LPG/D

Dramatic for Phase1 $\times 30 > \text{limit}$ \rightarrow don't use for short distance delivery

Regulated - PM



22C

Diesel: Close to EuroV (engine)

HOT start has limited effect on the entire cycle

LPG/D: Close to (engine) EuroV limit

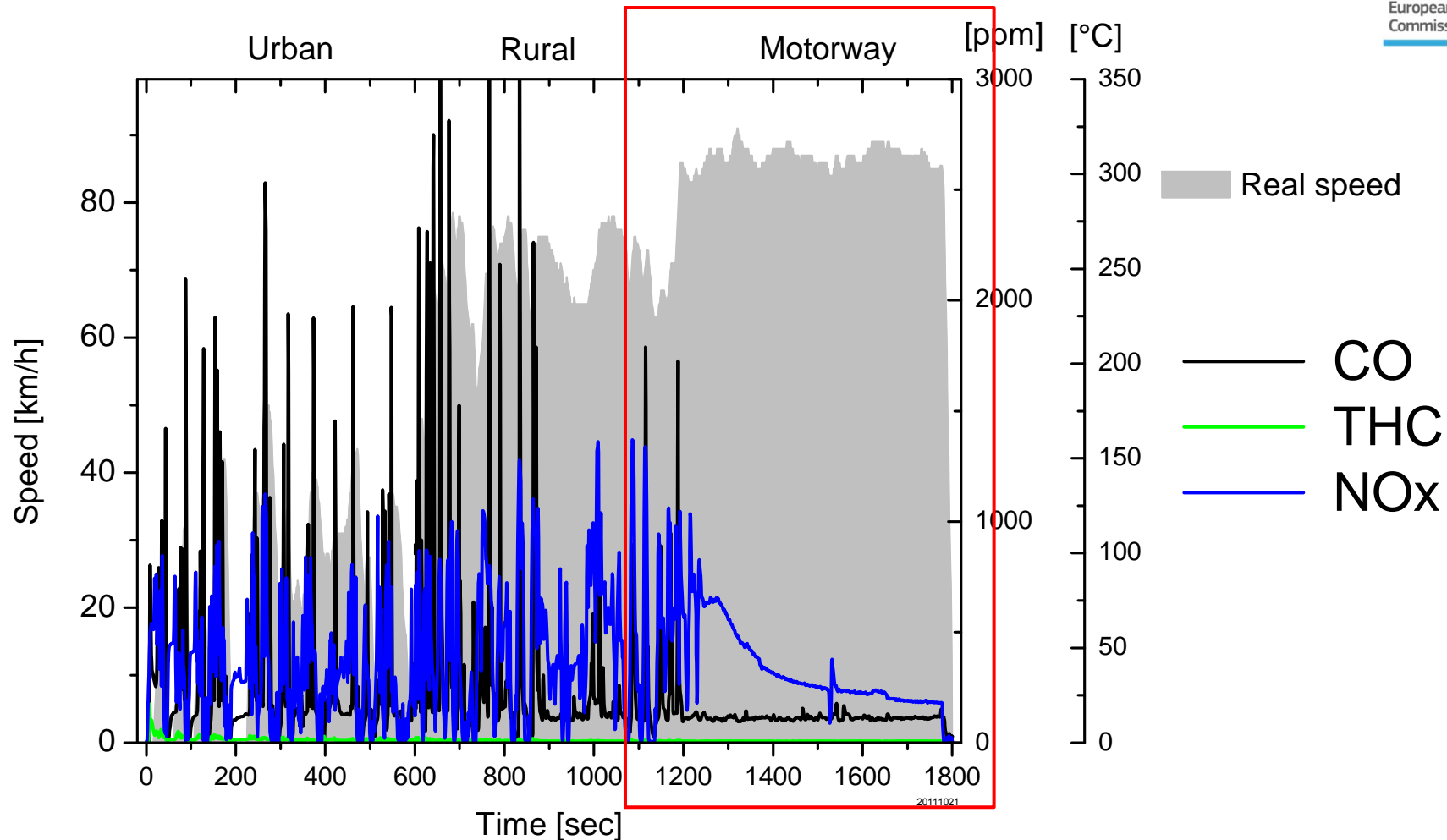
-7C

Good performance for Diesel (mainly 1st phase issue).

Bad performance for LPG/D:

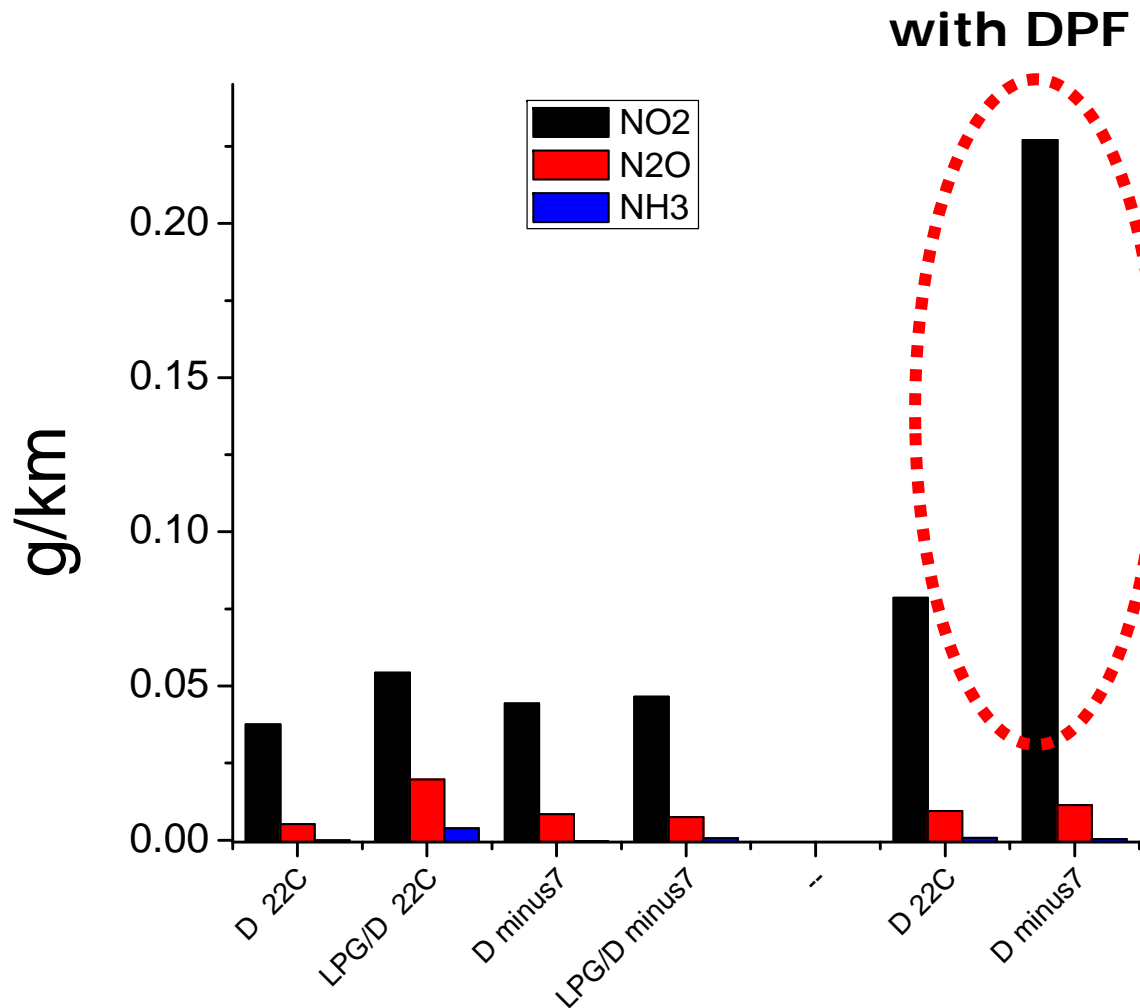
Dramatic for Phase1 $\times 50 >$ limit \rightarrow don't use for short distance delivery

Abatement conditions



Typically, only motorway conditions are followed by emission reduction
Fantastic aftertreatment which **does not work** except for motorways

N-compounds



NH3

See poster 25, Suarez et al.

NO2

← NO+aftertreatment

0.05-0.2 g/km

VS

5 g/km of NOx

Max for Diesel with DPF at -7C

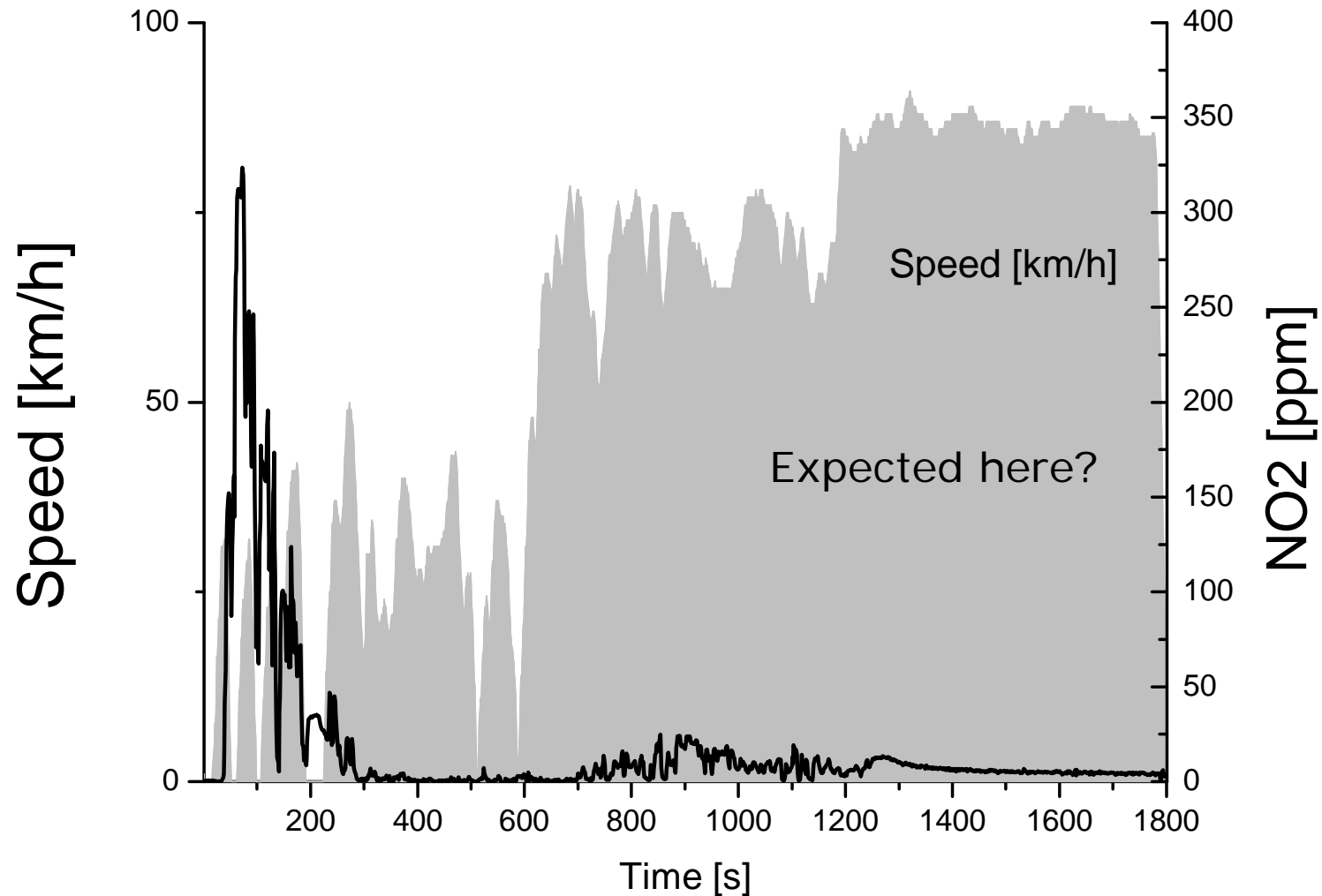
When is it produced?



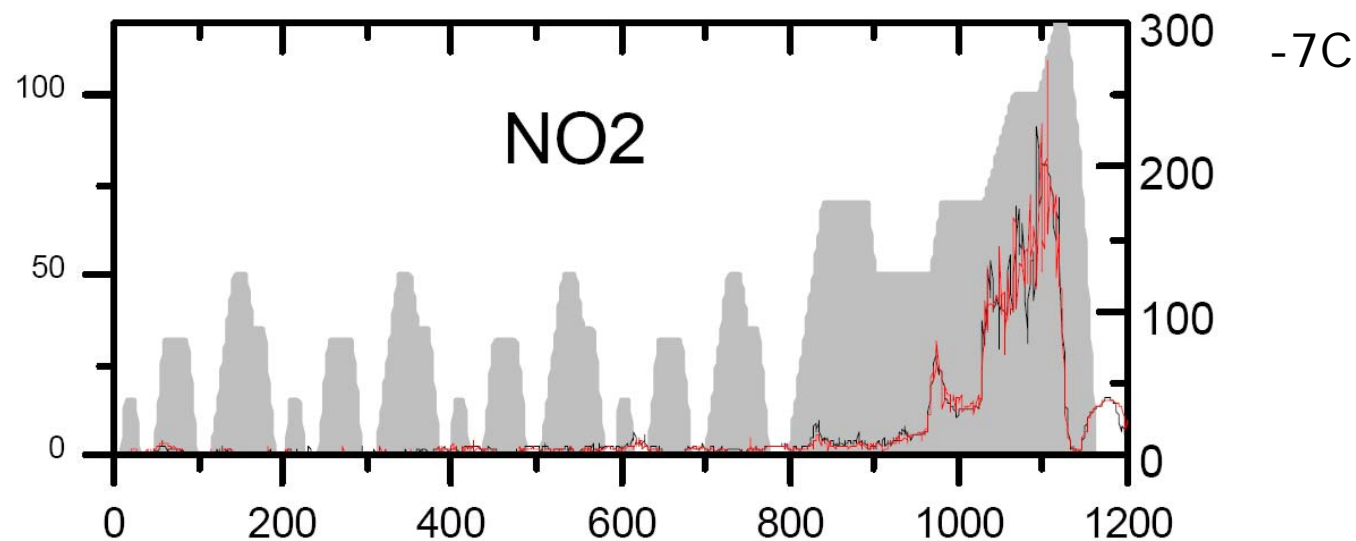
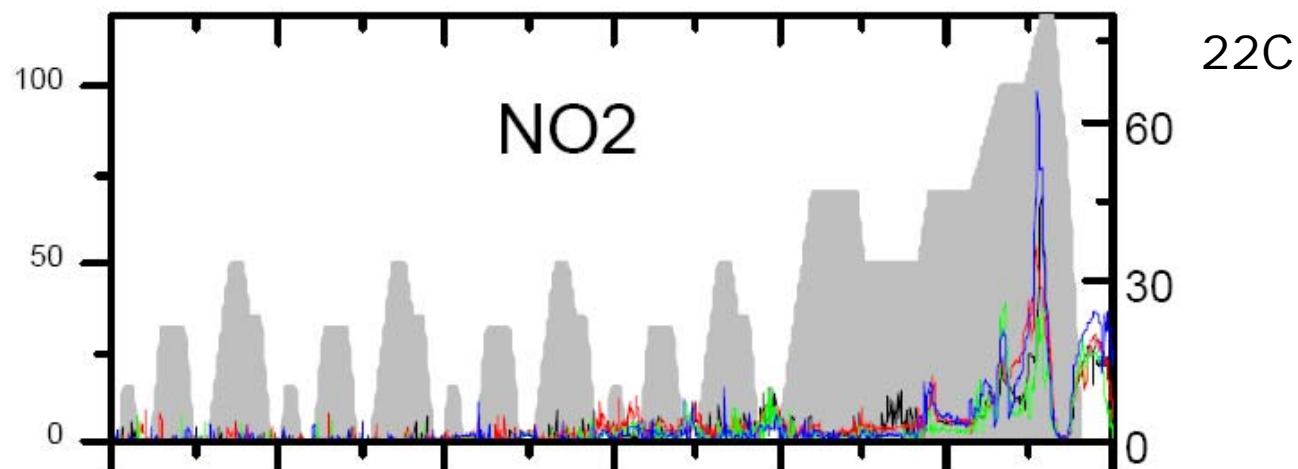
NO2 – Diesel @-7C (with DPF)



mainly in the cold phase of a -7C test



FTIR – Tailpipe - DLDV



Peak: 3x
EF: 10x

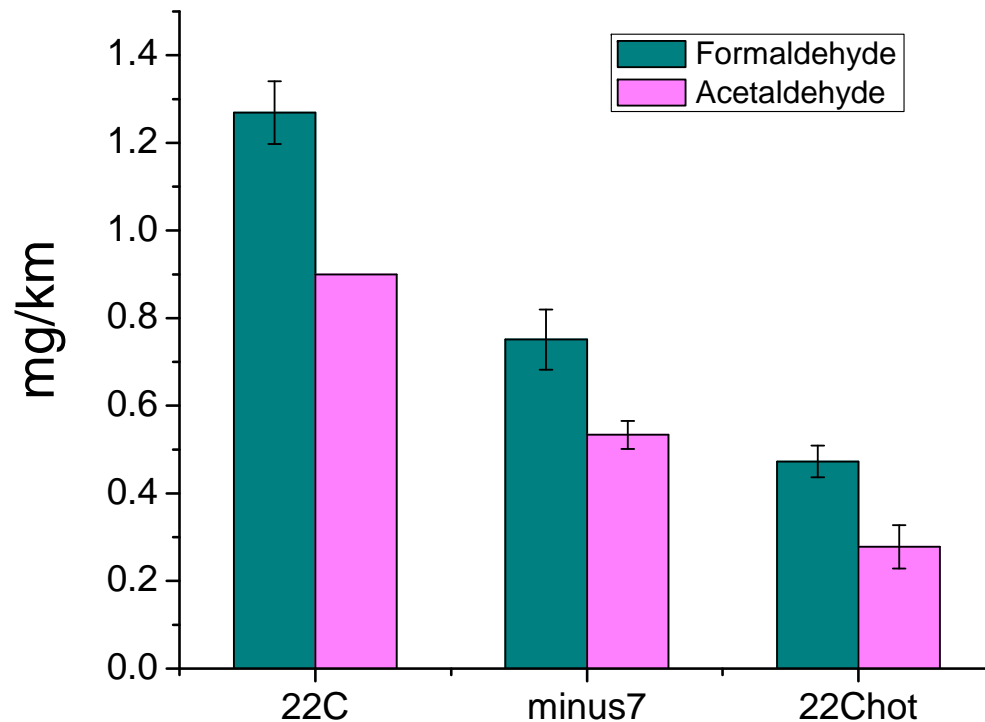
Unregulated - Aldehydes



Tailpipe → CVS → DNPH → HPLC

Methodologies for **ambient air** from CARB and EPA
SOP MLD022 by CARB & EPA/625/R-96/-1-b

Truck 2 - DNPH cartridges - HPLC - CVS diluted - EPA directive



Aldehydes are related to health effects and SOA

For comparison:

Euro 5 Passenger car
1 mg/km @22C
0.5 mg/km @-7C

Similar amounts and T response

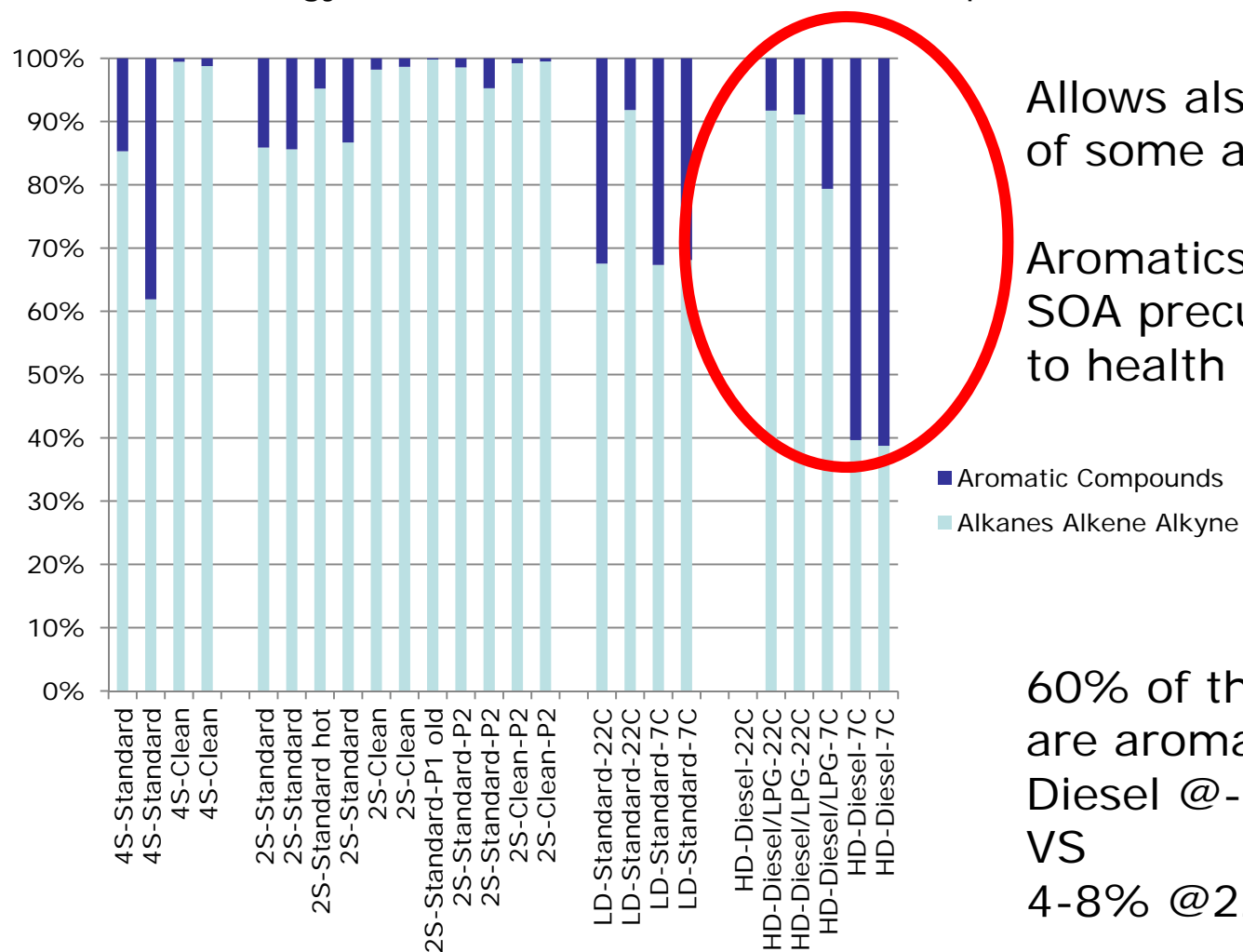
Best: hot engine in cold ambient conditions

Unregulated - VOCs



Tailpipe → CVS → Tedlar bags → GC-FID

Methodology: EU-Directive (2003) on Ozone 29 precursors in **ambient air**

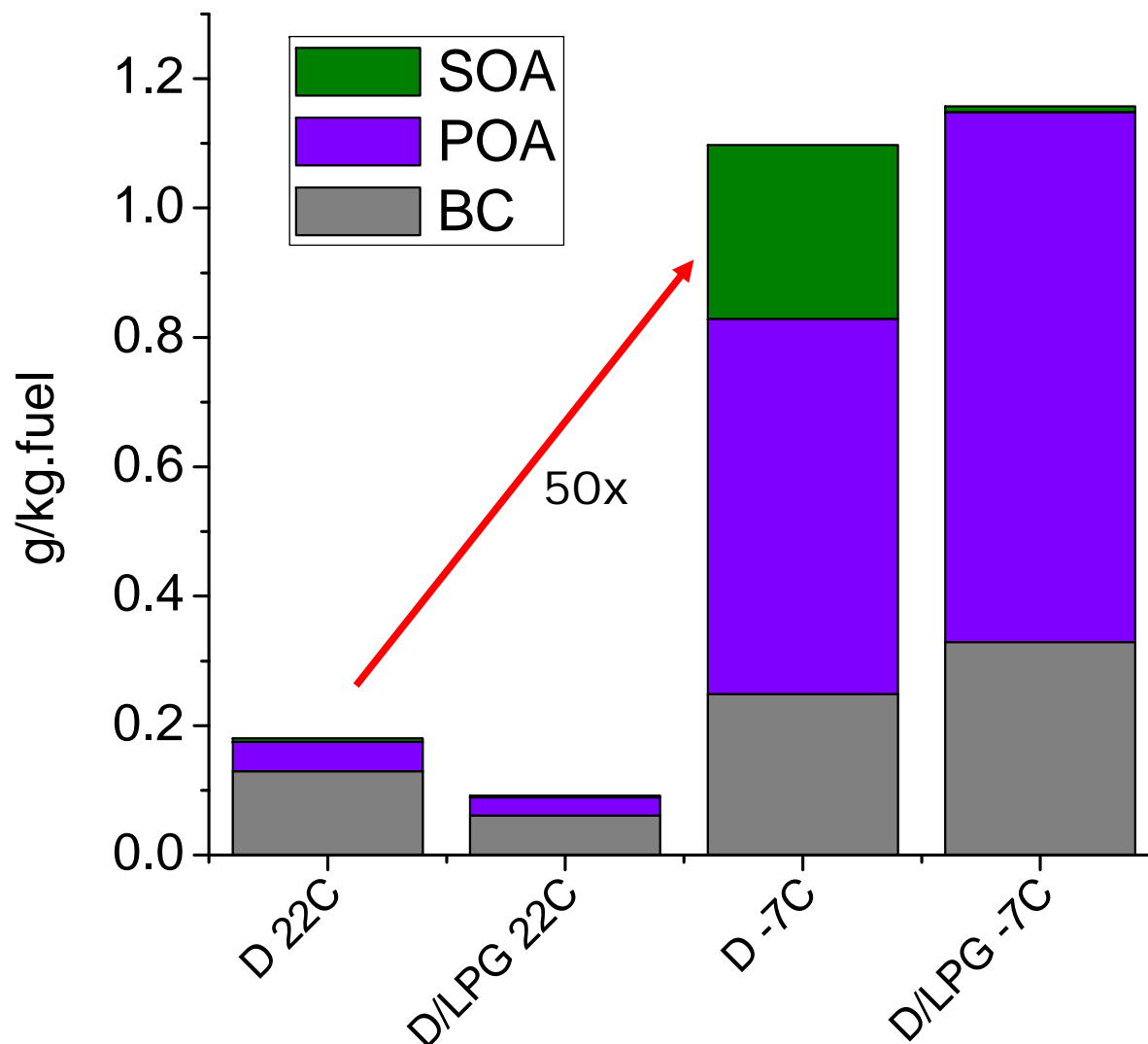


Allows also the measurements of some aromatic compounds.

Aromatics are known to be SOA precursors and related to health effects.

60% of the measured VOCs are aromatics in the case of Diesel @-7C
 VS
 4-8% @22C

SOA - Truck1



Secondary organic aerosol is formed

UV exposure: 6-hours ca.

Diesel:

➤ Strong temperature effect: x50

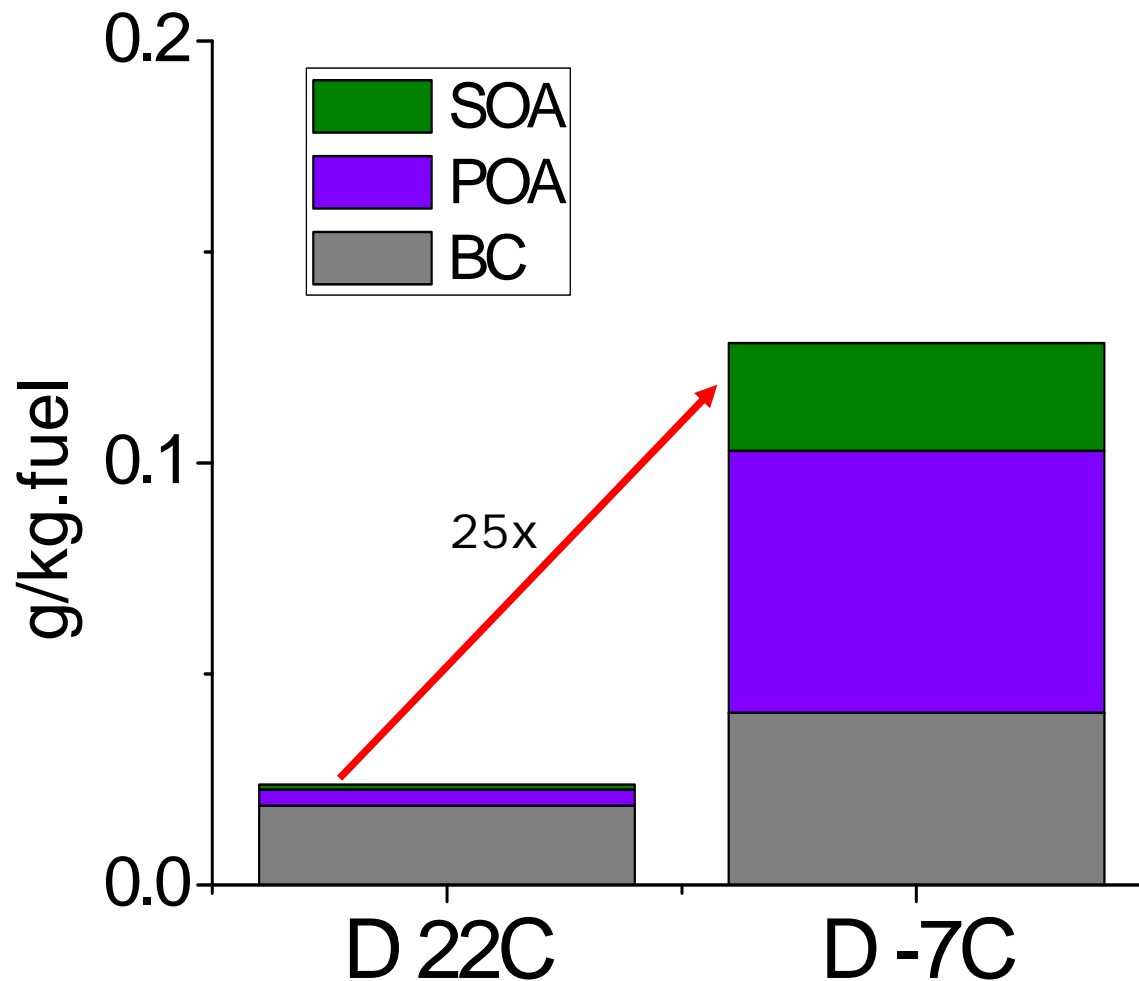
➤ **SOA(-7C, Diesel) = 30% of primary**

→ **SOA should be considered** when comparing PM ambient levels to emissions.

→ 70 mg/kWh

Vs 30 mg/kWh of Euro V

SOA - Truck2



Secondary organic aerosol is formed

UV exposure: 6-hours ca.

Diesel:

➤ Temperature effect: x25, still consistent

➤ **SOA(-7C, Diesel) = 25% of primary**

→ **SOA should be considered** when comparing PM ambient levels to emissions

→ 7 mg/kWh
Vs 30 mg/kWh of Euro V

Conclusions



Regulated emissions

- HDV in general stable wrt temperature changes (more than cars)
- Some problems for LPG/Diesel, especially in the cold phase of cold tests (-7C) → more tests needed (vehicle to vehicle variability)

SOA

- Diesel trucks at 22C do not seem to be of concern when compared to cars, scooters and diesel cars
- Considerable amount of **diesel truck SOA at -7C**
→ **Large Impact on ambient PM (25-50%**, vehicle to vehicle variability)

Contributors



PSI (Villigen, CH): Mobile Smog Chamber

S. Platt, I. El Haddad, S. Pieber, J. G. Slowik,
R. Wolf, F. Klein, R. Richter, A. Prevot, U. Baltensperger

Univ. Marseille (France): VOCs online measurements

S. Hellebust, B. Temime-Roussel, N. Marchand

Aerosol d.o.o. (Ljubljana, Slovenia): Black carbon measurements

I. Jezek, L. Drinovec, G. Mocnik

JRC-EC (Ispra, Italy): Heavy duty Test cell (VELA7)

R. Suarez-Bertoa, F. Muehlberger, U. Manfredi, M.
Cadario, P. Le Lijours, M. Sculati, R. Colombo, C. Astorga

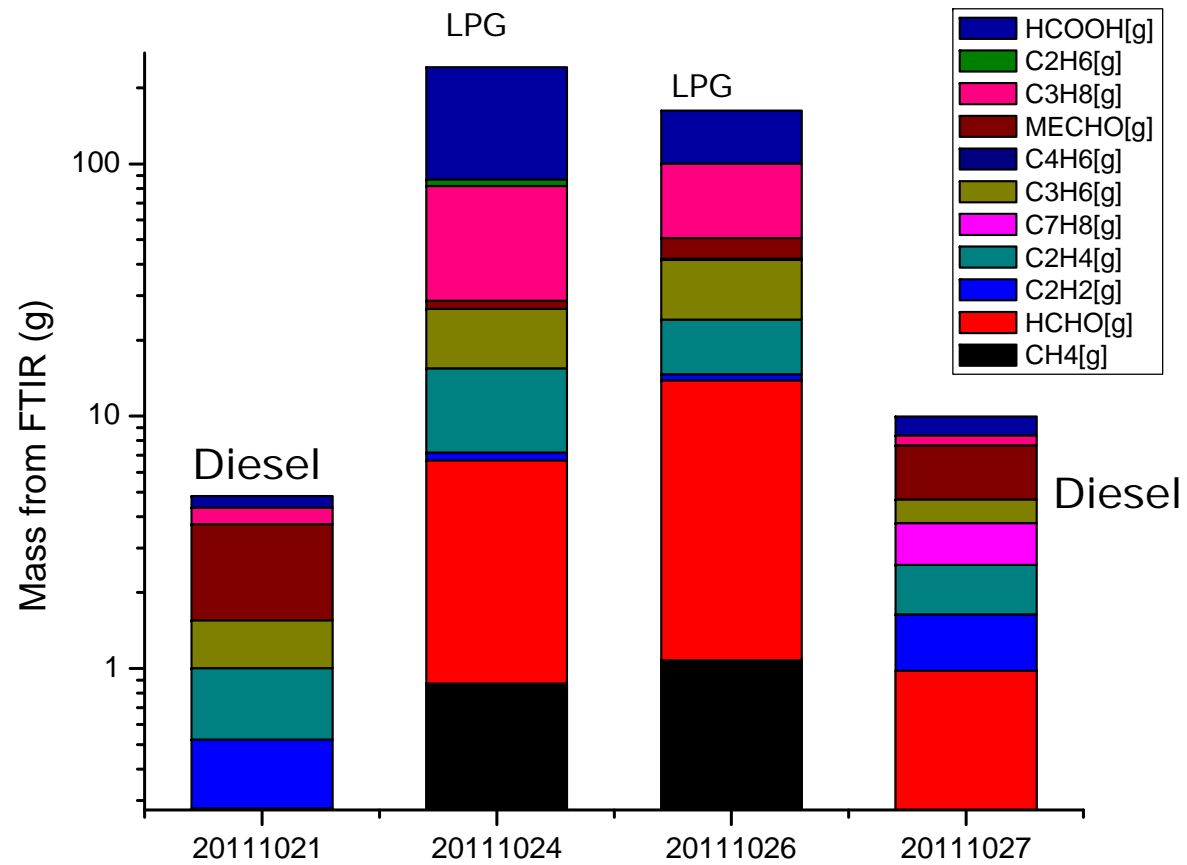
Unregulated



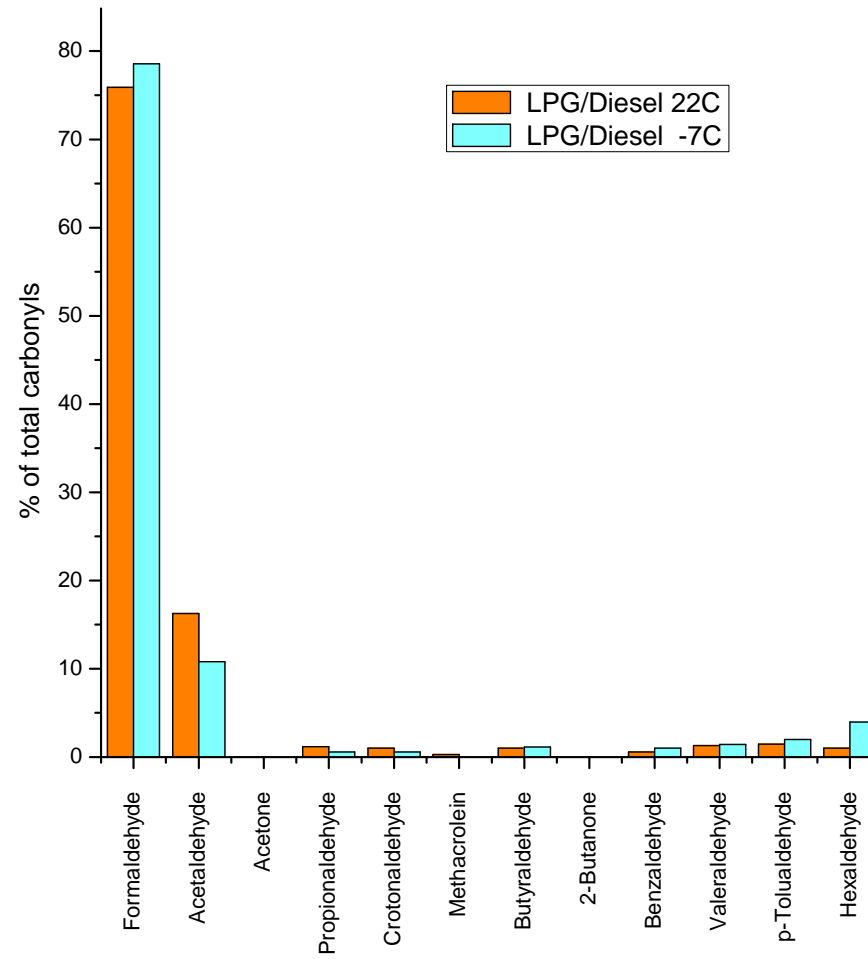
22C

-7C

FTIR
oxygenates
formic
acet
formal



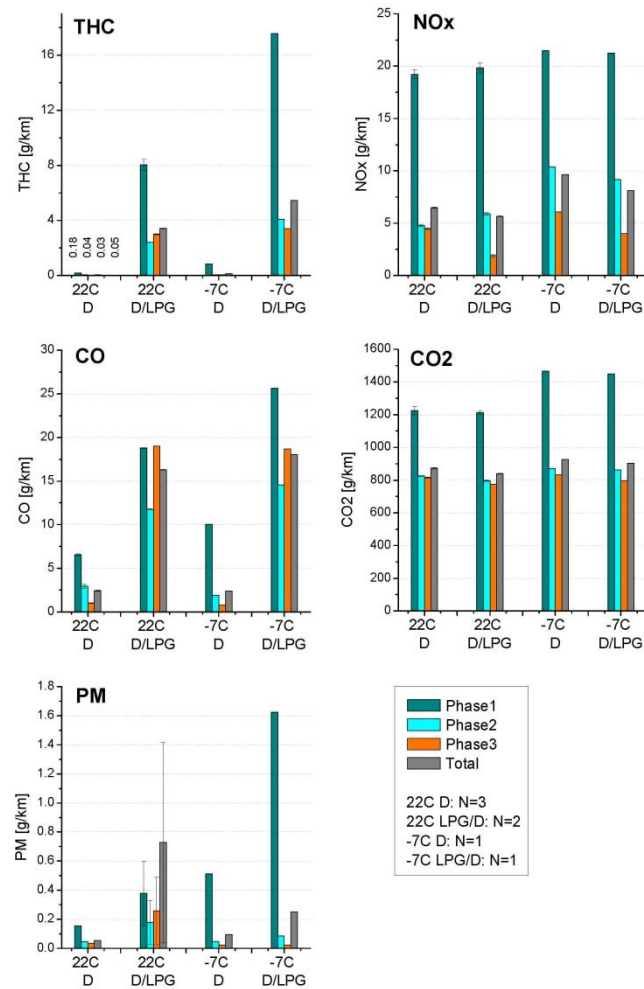
Outline



Regulated



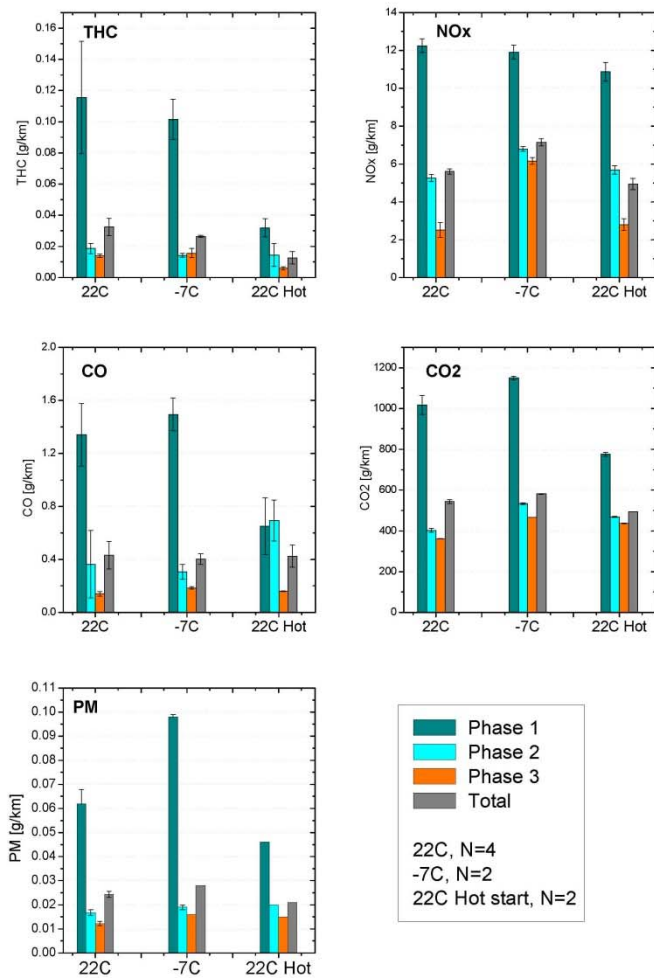
Truck 1 - Regulated emissions



Regulated



Truck 2 - Regulated emissions



Diesel Certificate



17/07/2010 13:08 +39 02 ENI SPA RHO ENI MARKETING NR. 859 P. 13/05/2010
 Data 13-05-2010
 Pag. 1/1

Raffineria di Sannazzaro
 VIA CANTIERI 46
 27089 Sannazzaro (PV)

Bollettino di analisi
 N° 28946

Prodotto
GASOLIO AUTO 0.001%S (N.C. = 51)
 Codice prodotto : 1311

Data Campionamento 12-05-2010
 Serbatoio 4159
 Camioncino 200170640

Voce doganale: 2710.1941

STAGIONALTA'	ESTIVA				
Analisi	Note	Risultato	U. di M.	Metodo	
densità a 15°C (1)		836.5	kg / m ³	EN ISO 3675:1998	
colore esm		1.5		ASTM D 1500-02	
aspetto a temperatura ambiente		clear/bright		ASTM D 4176/2-02	
punto di interpidamento		1	°C	EN 13015:1994	
c.f.p.p.		-2	°C	EN 116:1997	
punto di infiammabilità		89	°C	EN ISO 2719:2002	
zolfo totale		5.9	mg / kg	EN ISO 20848:2004	
Inc. di cetano		60.0		EN ISO 4264:1996	
numero di cetano		32.0		EN ISO 5165:1998	
viscosità a 40°C		3.666	mm ² / s	EN ISO 3104:1996	
residuo carb. Conradson (su res.10%)		<0.10	% m / m	EN ISO 10370:1995	
contenuto di acqua		90	mg / kg	EN ISO 12937:2000	
cenere		< 0.001	% m / m	EN ISO 6245:2002	
corrosione rame (3h a 50°C)		1	Indice ASTM	EN ISO 2160:1998	
numero di acidità		<0.10	mg KOH / g	ISO 6618:1997/C1:99	
contaminazione totale		4.5	mg / kg	EN 12662:1998	
stabilità all'ossidazione		1	g / m ³	EN ISO 12205:1996	
poliaromatici (2 anelli +)		4.0	% m / m	EN 12816:2000	
potere lubrificante		230	µm	EN ISO 12156-1:2000	
conduttività elettrica		68	pS / m	IP 274/99	
alla temperatura di:		21	°C	IP 274/99	
contenuto di biodiesel		< 7	% v / v	EN 14078:2003	
distillazione iso 3405					
95% v/v		300.0	°C	EN ISO 3405:2000	
recup. a 150°C		0.0	% v / v	EN ISO 3405:2000	
recup. a 250°C		12.9	% v / v	EN ISO 3405:2000	
recup. a 350°C		91.3	% v / v	EN ISO 3405:2000	

(1) Valore determinato in fase di accettazione tecnica.

Il Responsabile del Laboratorio
P. Ho

2009.01: A maximum sulfur limit of **10 ppm** ("sulfur-free") for diesel fuel for highway vehicles.
Our diesel is 5.9 ppm

Unregulated compounds - VOCs



European
Commission

29 VOCs with GC-dual FID (Offline, Tedlar bags)

Main **Ozone precursors** (EC Ozone Directive, 2003)
(Ozone is the biggest problem in air quality:
toxic and GHG)

Two of them are nasty (carcinogenic, mutagenic):

- Benzene (European Fuel Directive, EPA)
- 1-3 Butadiene (EPA)

Mandatory monitor in ambient air, but not in
exhaust emissions.

**EEA (2006, 2007): Emissions from vehicles are
the largest contributors**

Ethane
Ethene 29 VOCs JRC-GC
Propane
Propene
Acetylene
Iso-butane
n-Butane
1-Butene
trans-2-Butene
Isobutene
cis-2-Butene
Propyne
isoPentane
1,3-Butadiene
n-Pentane
trans-2-Pentene
Cis-2-Pentene
Methylpentanes
Isoprene
n-Hexane
n-Heptane
Benzene
Toluene
Ethyl-benzene
m-Xylene
o-Xylene
1,3,5-Tri-methyl benzene
1,2,4-Tri-methyl benzene

Unregulated compounds C=O



Carbonyls with HP-LC-UV (offline, on DNPH cartridges)

Compounds

Formaldehyde
Acetaldehyde
Acetone
Propionaldehyde
Crotonaldehyde
Methacrolein
Butyraldehyde
2-Butanone
Benzaldehyde
Valeraldehyde
p-Tolualdehyde
Hexaldehyde

Methods

SOP MLD022 by CARB
Determination of Carbonyl
Compounds in Ambient Air
Using High Performance
Liquid Chromatography)

and

EPA/625/R-96/-1-b
Compendium Method TP-
11A:
Determination of
Formaldehyde in Ambient
Air Using Absorbent
Cartridge Followed by High
Performance Liquid
Chromatography (HPLC)

Motivations

- Some are **ozone precursors**
- Others have adverse chronic and acute **health effects** (formaldehyde, acetaldehyde, methyl-ethyl-ketone, acrolein)

The major sources of **directly emitted** carbonyls are (fuel) **combustion**, mobile sources, and process emissions from oil refineries.

LPG is worse?



THC increases with LPG

^ [a](#) [b](#) Zhang, Chunhua; Bian, Yaozhang; Si, Lizeng; Liao, Junzhi; Odbileg, N (2005).

"A study on an electronically controlled liquefied petroleum gas-diesel dual-fuel automobile".

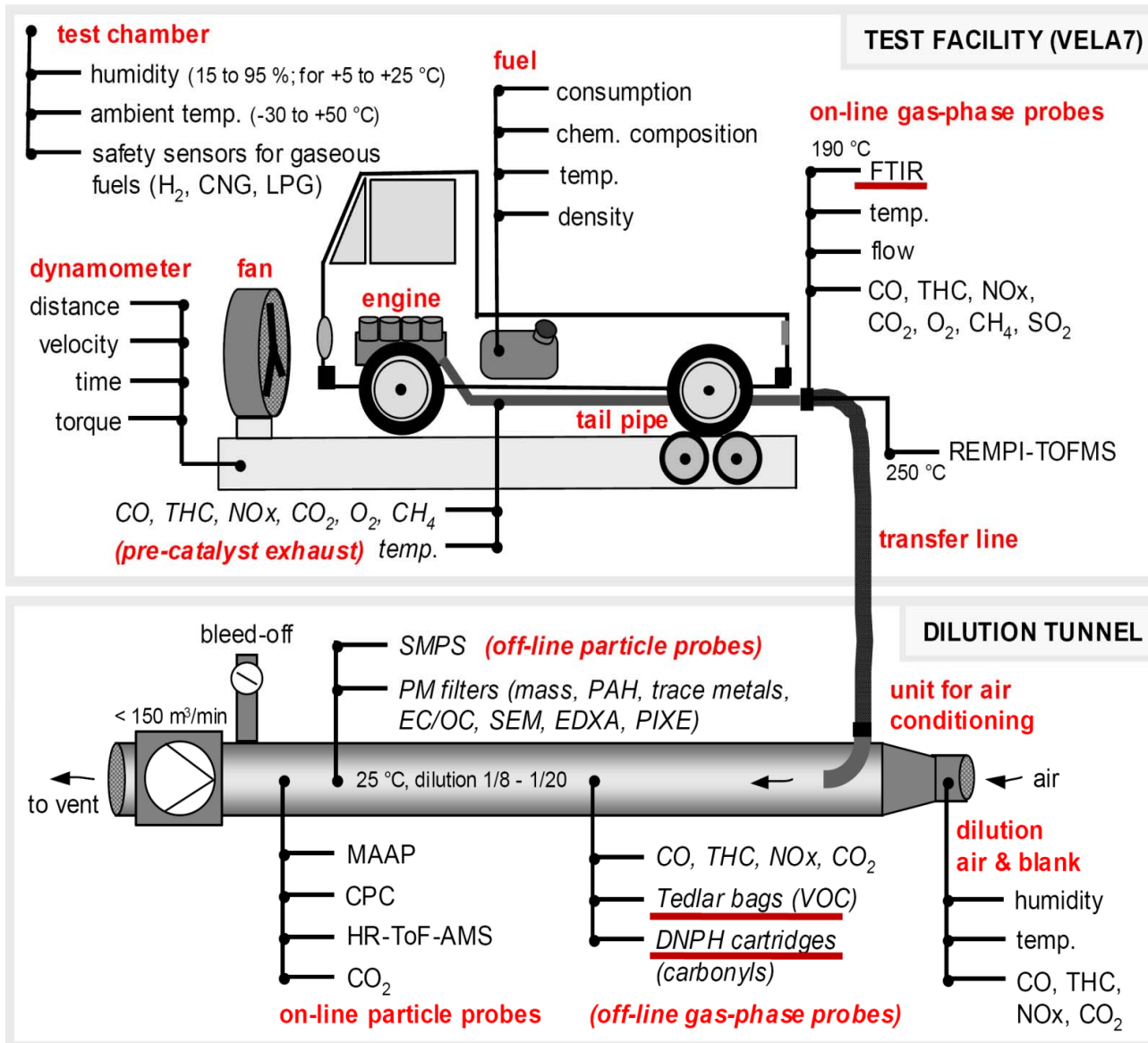
Proceedings of the Institution of Mechanical Engineers, Part D:

Journal of Automobile Engineering **219** (2): 207. [doi:10.1243/095440705X6470](https://doi.org/10.1243/095440705X6470).

^ [a](#) [b](#) Qi, D; Bian, Y; Ma, Z; Zhang, C; Liu, S (2007).

"Combustion and exhaust emission characteristics of a compression ignition engine using liquefied petroleum gas–fuel-oil blended fuel".

Energy Conversion and Management **48** (2): 500



FID (HC)
NDIR (CO, CO₂)
Chemiluminescence
Microbalance (PM)
MPD (O₂)
CLD (NO_x+NH₃)

FTIR
FID-GC (VOCs)
HP-LC (Carbonyls)

Dataset



Date/FTIR	Vehicle	Code	Cycle	VOC/ Carb L@0C	Vela	Time	Fuel Cycle	Notes
19-20-1002011	move to VELA7	Pre test						
20111021	DAF		ETC	Y/Y	21102011_1	11:30	diesel full 22C	SCR
20111024	DAF		ETC	Y/Y	24102011_1		LPG/Diesel full 22C	
20111025	DAF		ETC	Y/Y	25102011_1		LPG/Diesel full 22C	
20111026	DAF		ETC	Y/Y	26102011_1		LPG/Diesel full -7C	(SCR started later, 3 rd phase)
20111027	DAF		ETC	Y/Y /done	27102011_1		Diesel full -7C	

Date/FTIR	Vehicle Code	Vela	Start	Cycle	Oil Temp (C)	RH %	Press kPa	Temp Cell C
20130405T1	MN003	.1	10:00	ETC	21.3	50±4	97.23±0.01	22.1±0.4
20130408T1	MN003	.1	9:00	ETC	21.6	50±1	98.26±0.01	22.3±0.2
20130408T2	MN003	.2	15:00	S.S. (steady state)	28.1			
20130409T1	MN003	.1	9:15	ETC	23.1	51±3	98.12±0.01	22.2±0.2
20130409T2	MN003	.2	15:00	S.S. (steady state)	28.4			
20130410T1	MN003	.1	10:00	ETC	24.0	49±5	98.32±0.01	22.3±0.2
20130410T2	MN003	.2		S.S 85kmh				
20130410T3	MN003	.3		S.S. Full load				
20130411T1	MN003	.1	9:30	ETC	-1.3	64±2	98.71±0.01	-6.4±0.3
20130411T2	MN003	.2		S.S 85kmh				
20130411T3	MN003	.3		S.S. Full load				
20130412T1	MN003	.1	9:30	ETC	-4.2	67±2	98.10±0.00	-7±1
20130412T2	MN003	.2	15:00	S.s				
20130415T1	MN003	.1	9:30	ETC HOT start	93.4	48±2	99.70±0.01	22.2±0.6
20130416T1	MN003	.2	9:45	ETC HOT start	85.0	47±1	99.59±0.01	22.5±0.2

Outline



- what's an AMS
- what's a PTR-ToF-MS
- PMP protocol on HDV also?
- Urbano: THC for trucks is NMHC, ok, ch4 is low but do we measure THC or NMHC?
- remember density of LPG is different than that of diesel

Motivations - Health



Air Pollution from combustion sources is an **old problem!**

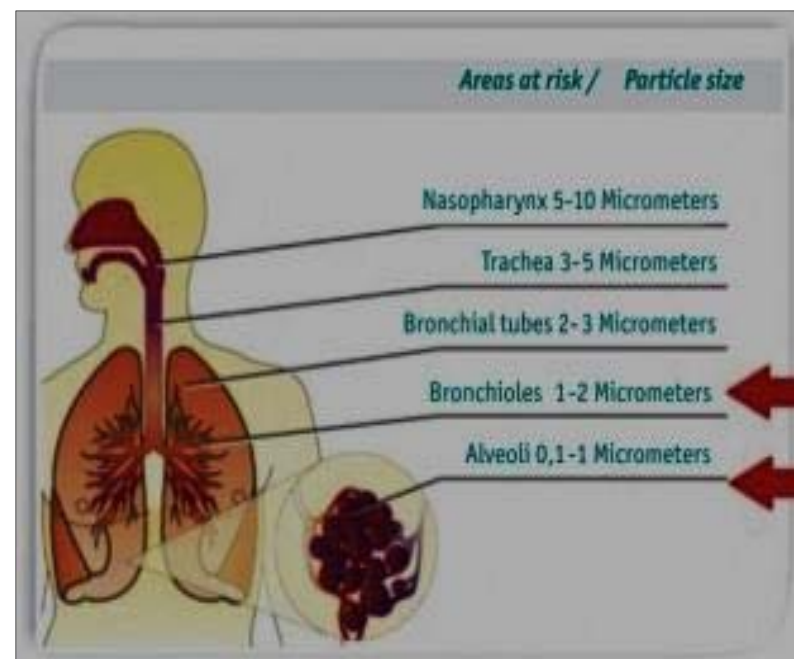
Odyssey wars (fires and brown dust)

First published: Ramazzini (1600, Padua) on miners' lungs disease.

Only recently (last decades), it was proved that fine particles correlate with a number of diseases (WHO reports) and actions were taken.

Poor understanding of the mechanism.

Combination of Size + Chemical composition + Morphology



In secondary organic aerosols:

Thousands of compounds, mainly unresolved.

From non-toxic to carcinogenic/ mutagenic substances (PAH)

Outline



European
Commission

Contaminant	Note
acetaldehyde	IARC Group 2B carcinogens
acrolein	IARC Group 3 carcinogens
aniline	IARC Group 3 carcinogens
antimony compounds	Toxicity similar to arsenic poisoning
arsenic	IARC Group 1 Carcinogens , endocrine disruptor
benzene	IARC Group 1 Carcinogens
beryllium compounds	IARC Group 1 Carcinogens
biphenyl	It has mild toxicity.
bis(2-ethylhexyl)phthalate	endocrine disruptor
1,3-butadiene	IARC Group 2A carcinogens
cadmium	IARC Group 1 Carcinogens , endocrine disruptor
chlorine	
chlorobenzene	It has "low to moderate" toxicity.
chromium compounds	IARC Group 3 carcinogens
cobalt compounds	
cresol isomers	
cyanide compounds	
dibutyl phthalate	endocrine disruptor
1,8-dinitropyrene	Carcinogen ^[citation needed]
dioxins and dibenzofurans	
ethyl benzene	
formaldehyde	IARC Group 1 Carcinogens
inorganic lead	endocrine disruptor
manganese compounds	
mercury compounds	IARC Group 3 carcinogens
methanol	It may cause blindness.
methyl ethyl ketone	It may cause birth defects. ^[citation needed]
naphthalene	IARC Group 2B carcinogens
nickel	IARC Group 2B carcinogens
3-Nitrobenzanthrone	One of the strongest carcinogens known
4-nitrobiphenyl	
phenol	endocrine disruptor ^[citation needed]
phosphorus	
polycyclic organic matter , including polycyclic aromatic hydrocarbons (PAHs)	
propionaldehyde	
selenium compounds	IARC Group 3 carcinogens
styrene	IARC Group 2B carcinogens
toluene	IARC Group 3 carcinogens
xylene isomers and mixtures: o-xylenes, m-xylenes, p-xylenes	IARC Group 3 carcinogens

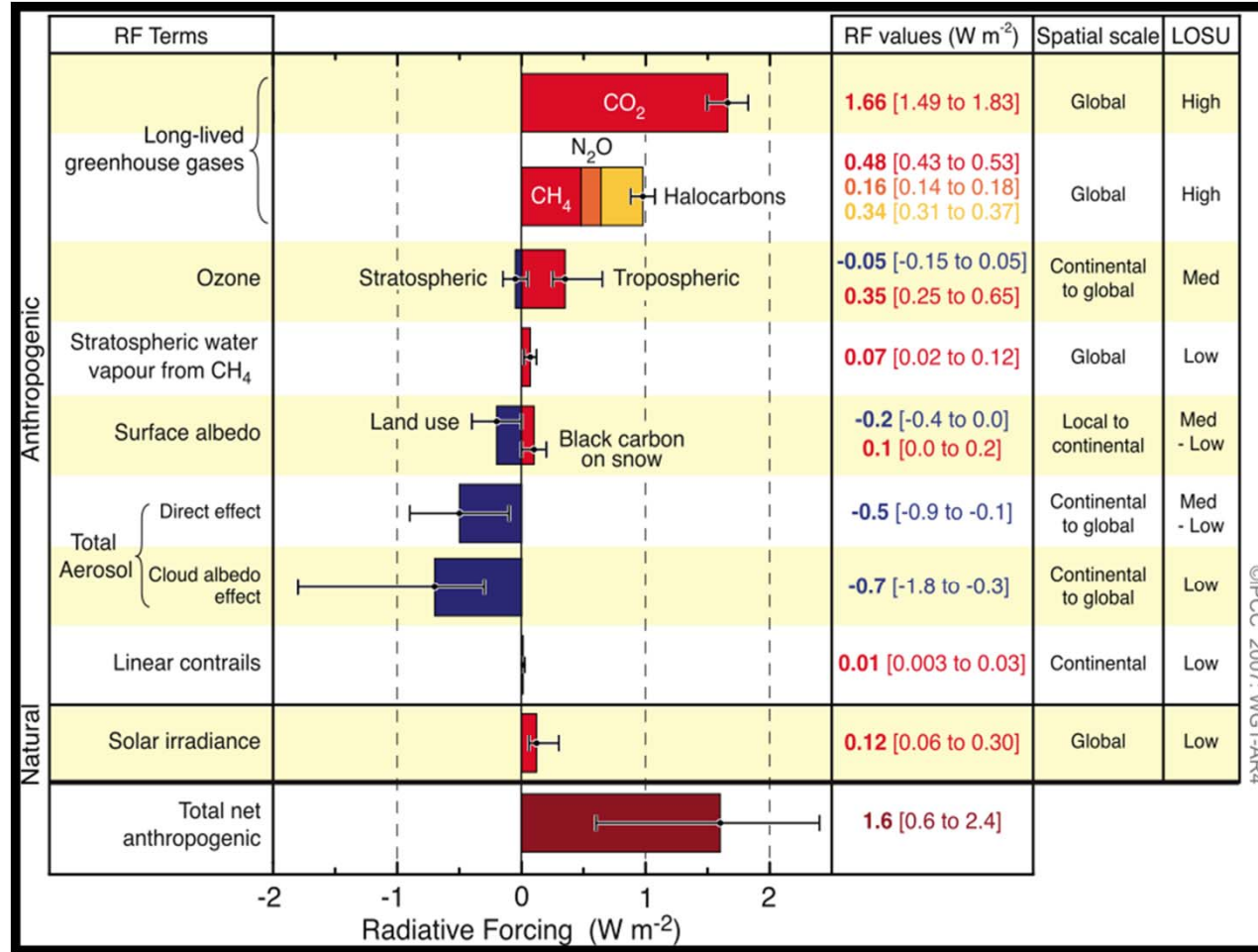
PSI mobile smog chamber



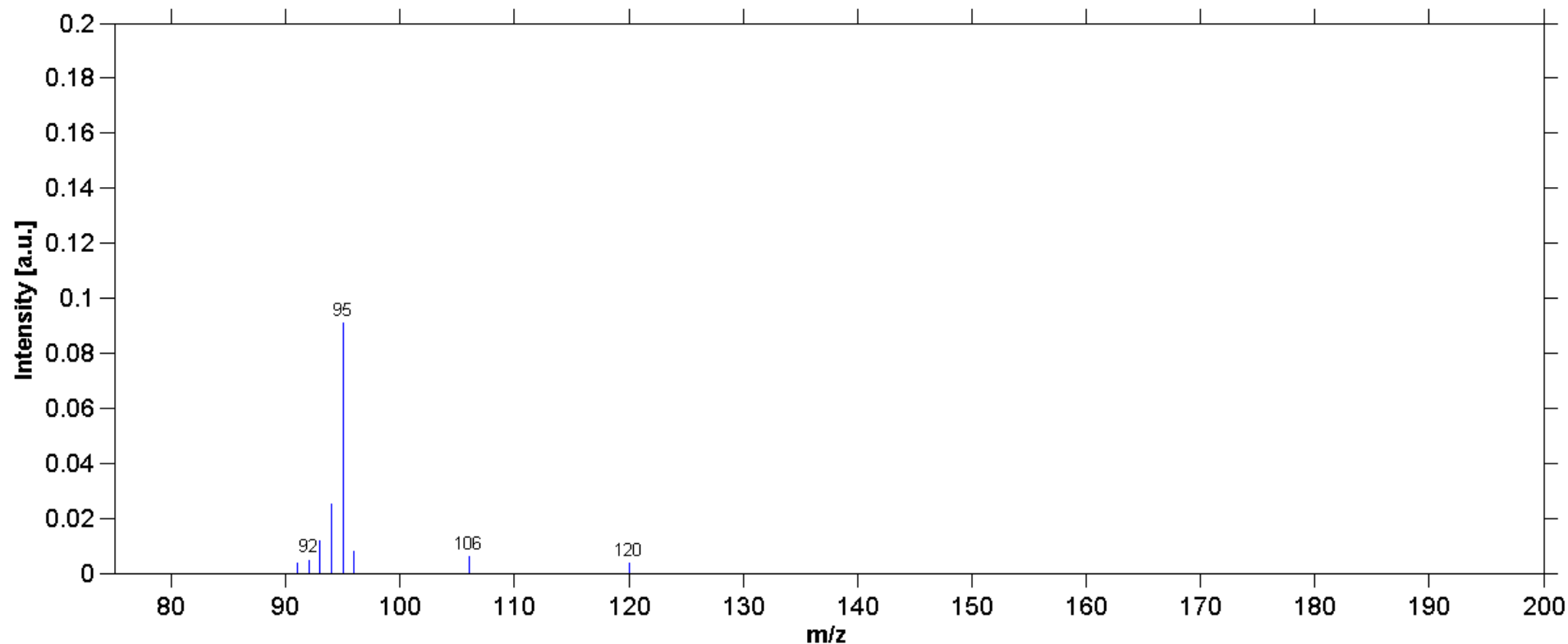
- 12m³ Teflon bag of 40x100W UV lights
- Pure air generator
- NO, NO₂, O₃, H₂O, organic compounds, seeds production



European Commission



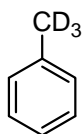
©IPCC 2007: WG1-AR4



Date: April 11th

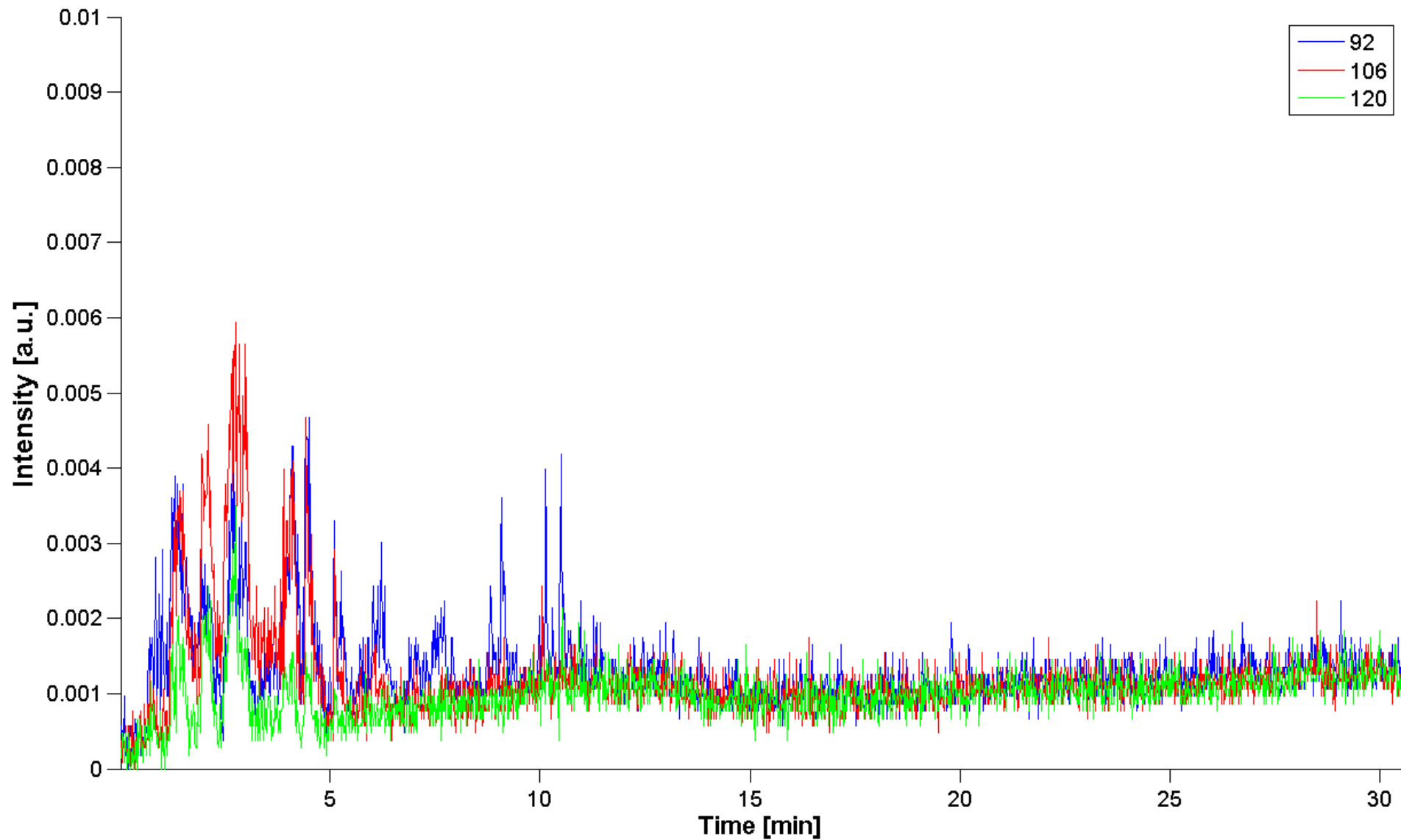
ETC

-7 ° C

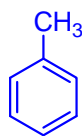


m/z 95 deuterated toluene
1ppm standard

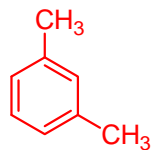
Signal at m/z 91 fragment of alkylated benzenes → Tropylium ion
Signals at m/z 93 and 94 fragments of deuterated toluene
Signal at m/z 96 deuterated toluene with one atom of ¹³C within the molecule



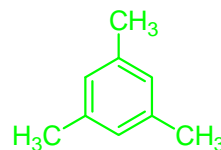
Date: April 11th
ETC
-7 ° C



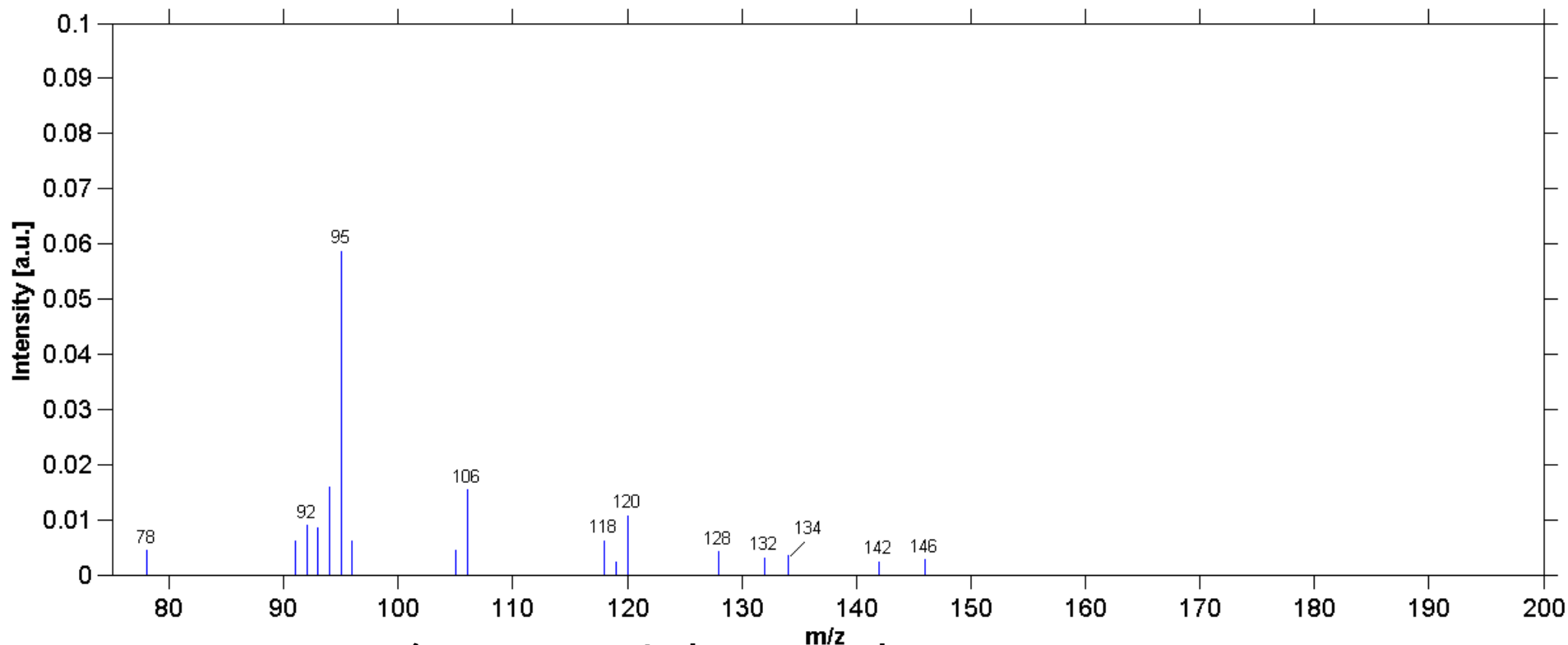
toluene



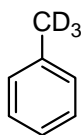
xylene



trimethylbenzene

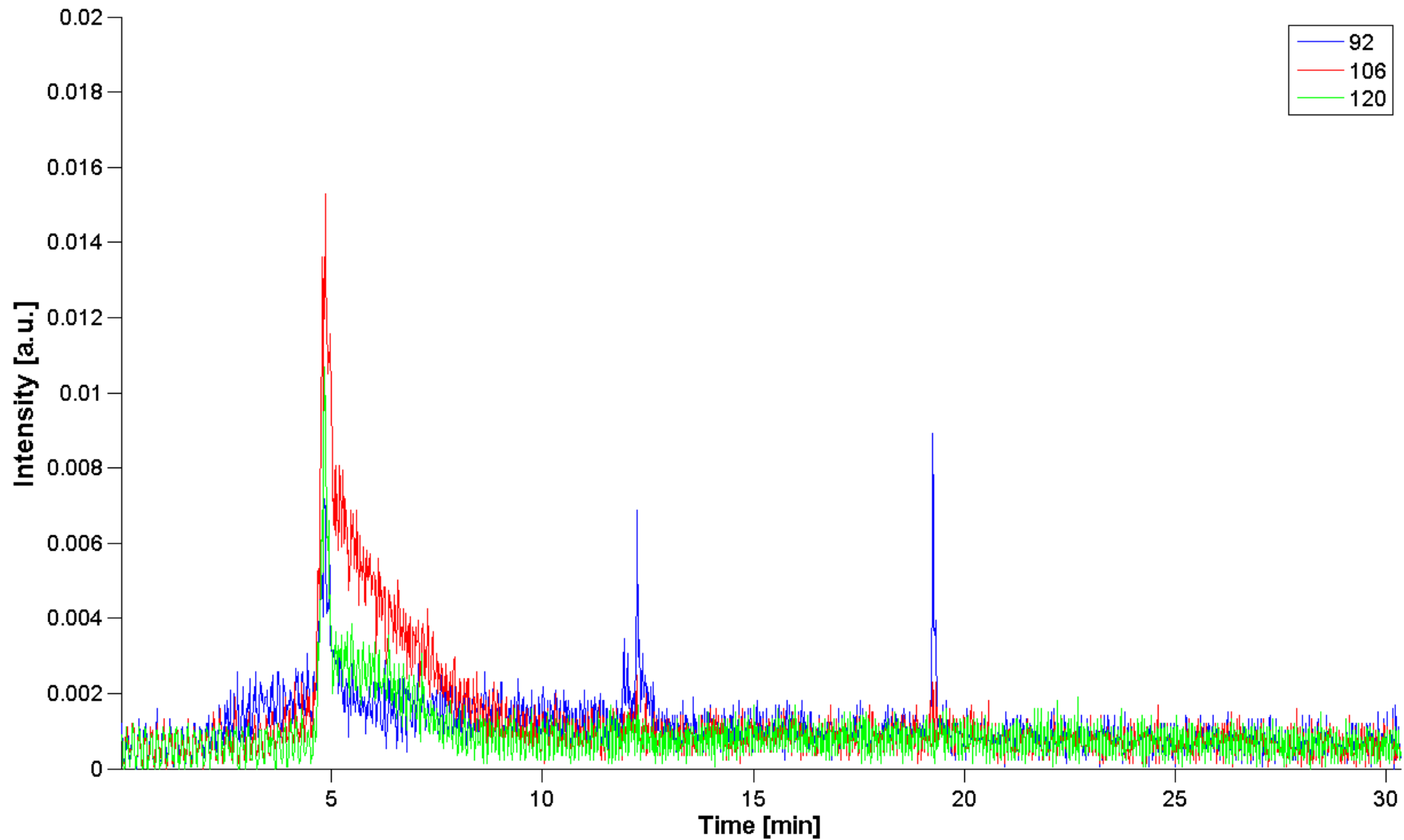


Date: April 12th	m/z	suspected compound
Steady state	78	benzene
-7 ° C	92	toluene (C1-alkylated benzene derivative)
	106	Xylene (C2-alkylated benzene derivative)
	118	indane and/or benzofuran
	120	C3-alkylated benzene derivative
	128	naphthalene
	132	C1-alkylated derivative of Indan and/or Benzofuran
	134	C4-alkylated benzene derivative
	146	C2-alkylated derivative of indane and/or benzofuran

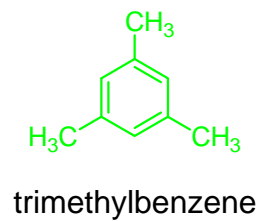
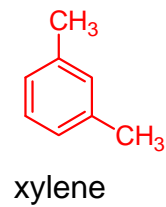
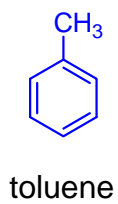


m/z 95 deuterated toluene
1ppm standard

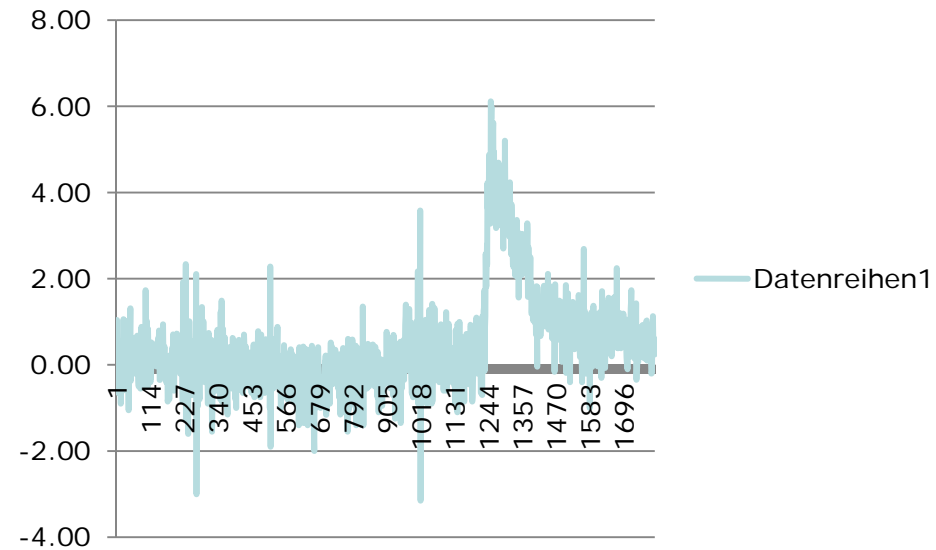
Signal at m/z 91 fragment of alkylated benzenes → Tropylium ion
 Signals at m/z 93 and 94 fragments of deuterated toluene
 Signal at m/z 96 deuterated toluene with one atom of ¹³C within the molecule



Date: April 12th
Steady state
-7 ° C



LPG/D NH3



LPG/D NO2

