

Impact of fuel composition on primary and secondary aeronautic emissions: gaseous and particulate chemical characterization at molecular level

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Projet ANR : Unveiling Nucleation mechanism in aiRcraft Engine exhAust and its Link with fuel composition

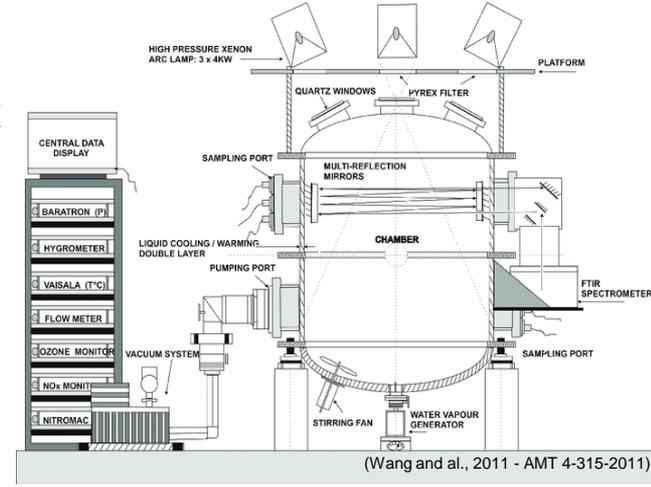
mini CAST burner



ONERA

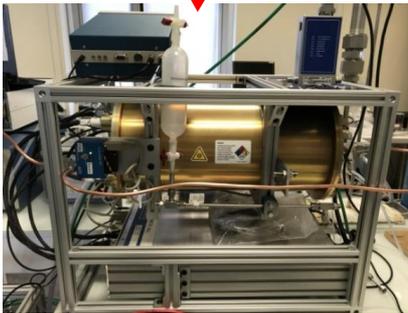
CESAM

lisa
UPEC



INERIS
LSCE

PAM-OFR



- Filters for particulate matter
- Proton Transfer Reaction Mass Spectrometer (PTR-MS)
 - Aerosol Mass Spectrometer (HR-AMS)
 - Aerosol Chemical Speciation Monitor (ACSM)

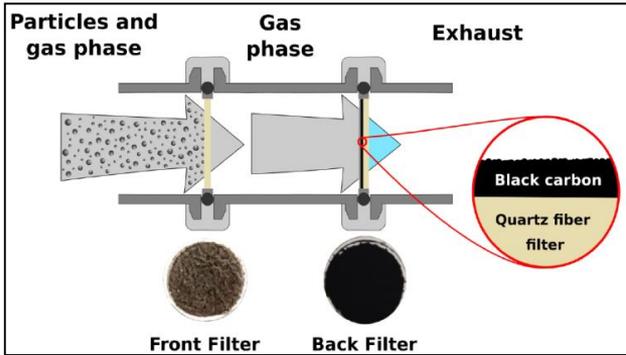
→ objective : study and compare chemically, at a molecular level, gaseous and particulate phases of primary and secondary emissions from various aircraft fuels

Sampling Method

- Quartz filters
- Flow=2.5L/min
- Injection time CESAM: 1min-8min
- Sampling time CESAM: 1h
- Sampling time PAM: 25min
- Sampling time CAST: 30sec



Quartz filter with black carbon for particle phase on the left and filter for gas phase on the right before sampling



(Ngo and al., 2020 - AMT 951-967)

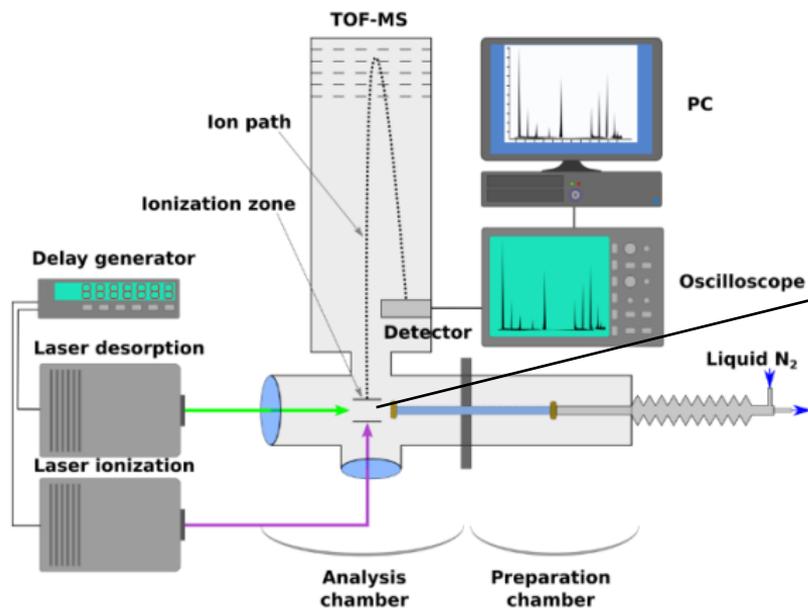


Experimental sampling device

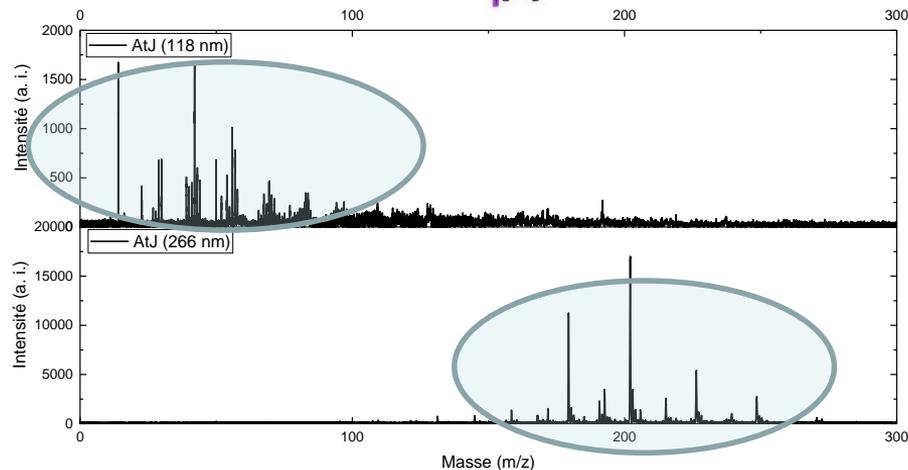
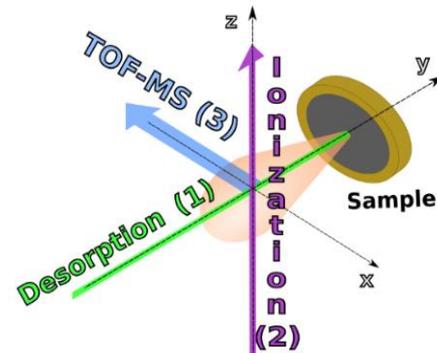


Particle phase after CAST for different combustion conditions

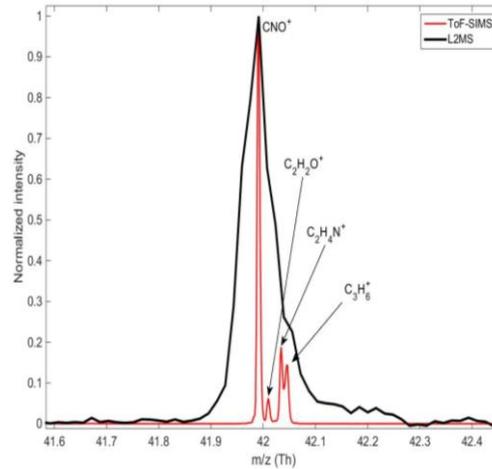
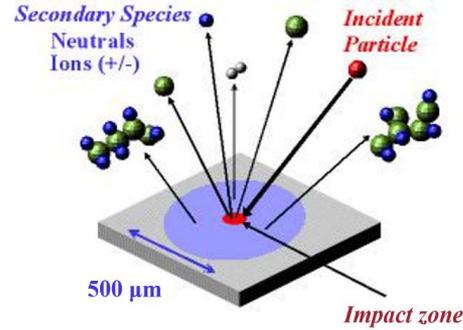
Mass Spectrometry techniques : Laser Two-Step Mass Spectrometry (L2MS)



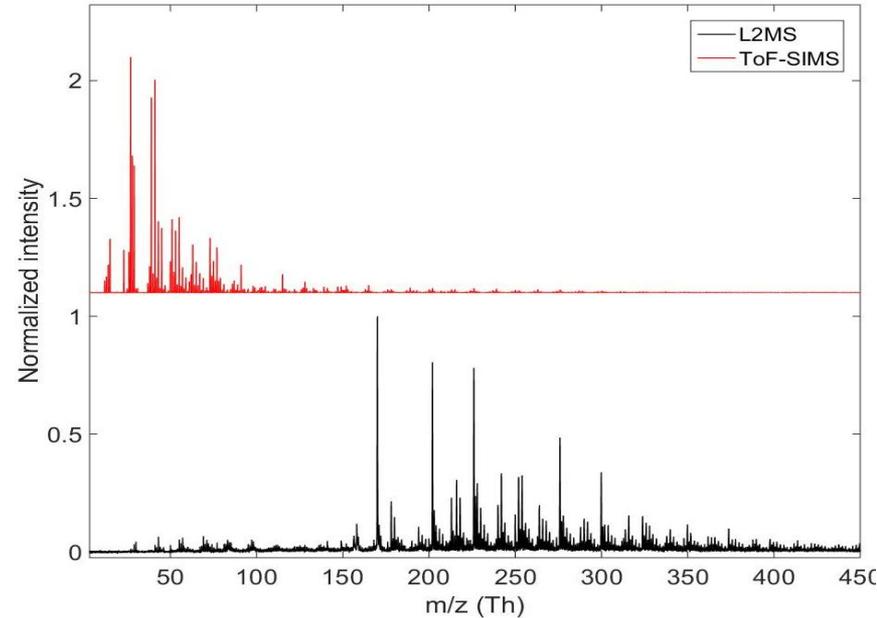
Desorption : 532nm or 266nm
 Ionization : 266nm



Mass Spectrometry techniques : Secondary Ions Mass Spectrometry (SIMS)



- 4-5 areas per sample
- High fragmentation
- High resolution (depends on substrate)

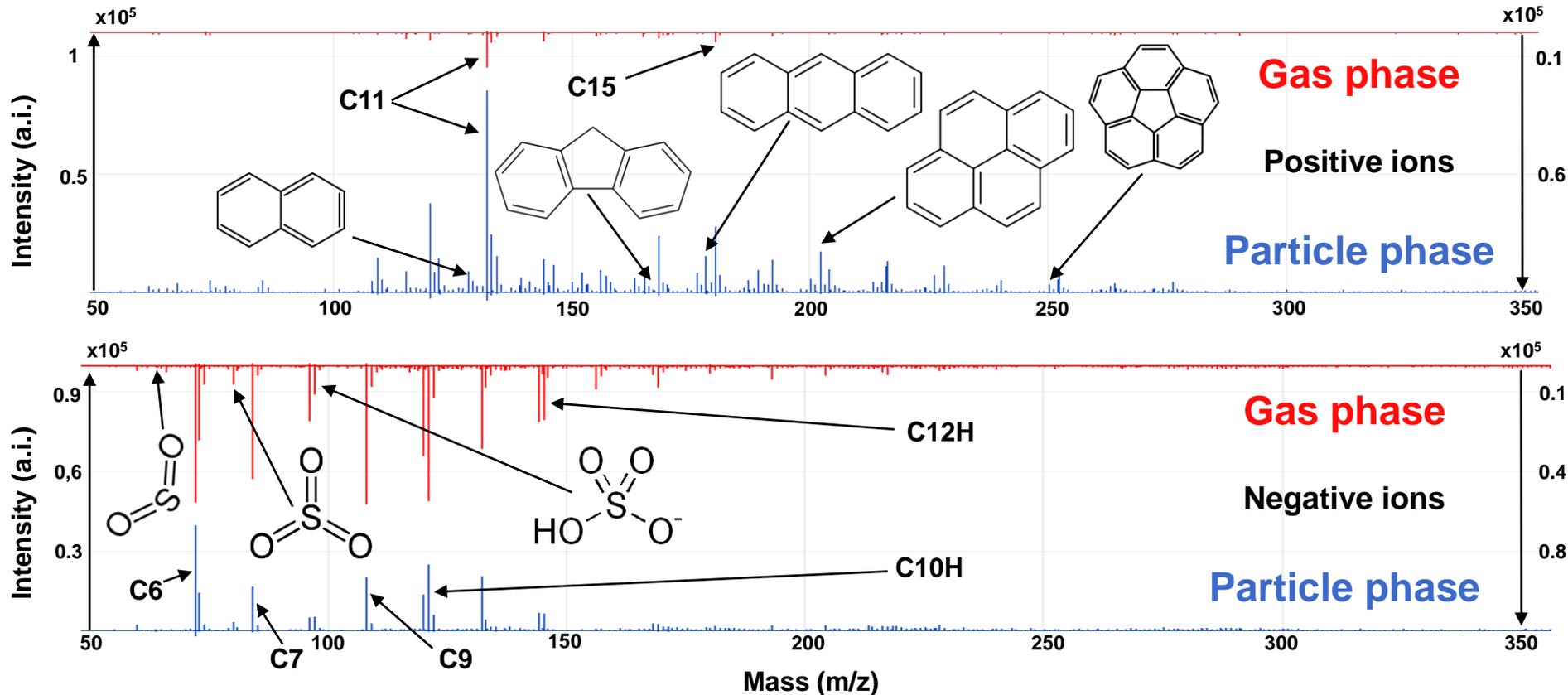


UNREAL campaign - Fuel Matrix

Fuel	Aromatic content (%)	Sulfur content (ppm)
Jet A1 reference	16	4
Jet A1 High aromatic compounds	23	4
Jet A1 High Sulfur compounds	16	3000
Jet A1 High aromatic compounds & Sulfur compounds	23	3000
Jet A1	15.5	200
AtJ	0	0
Jet A1/AtJ blend	10.8	140

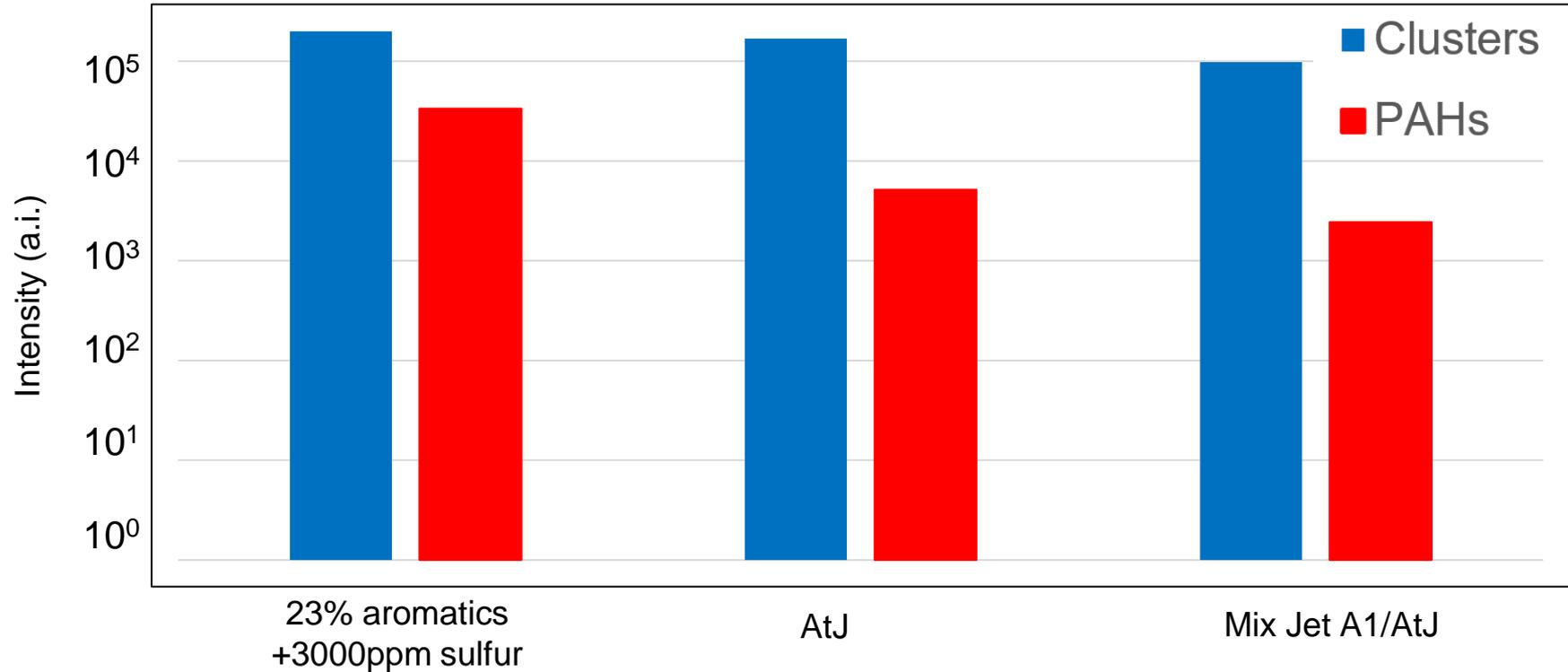
Mass Spectrometry L2MS: CAST sample

- Fuel : [23% aromatics compounds + 3000ppm sulfur]
- $F_{\text{des}} = 46\text{mJ/cm}^2$
- $F_{\text{ion}} = 2.9\text{mJ/cm}^2$
- Carbon cluster and hydrocarbons
- Sulfur content
- PAHs



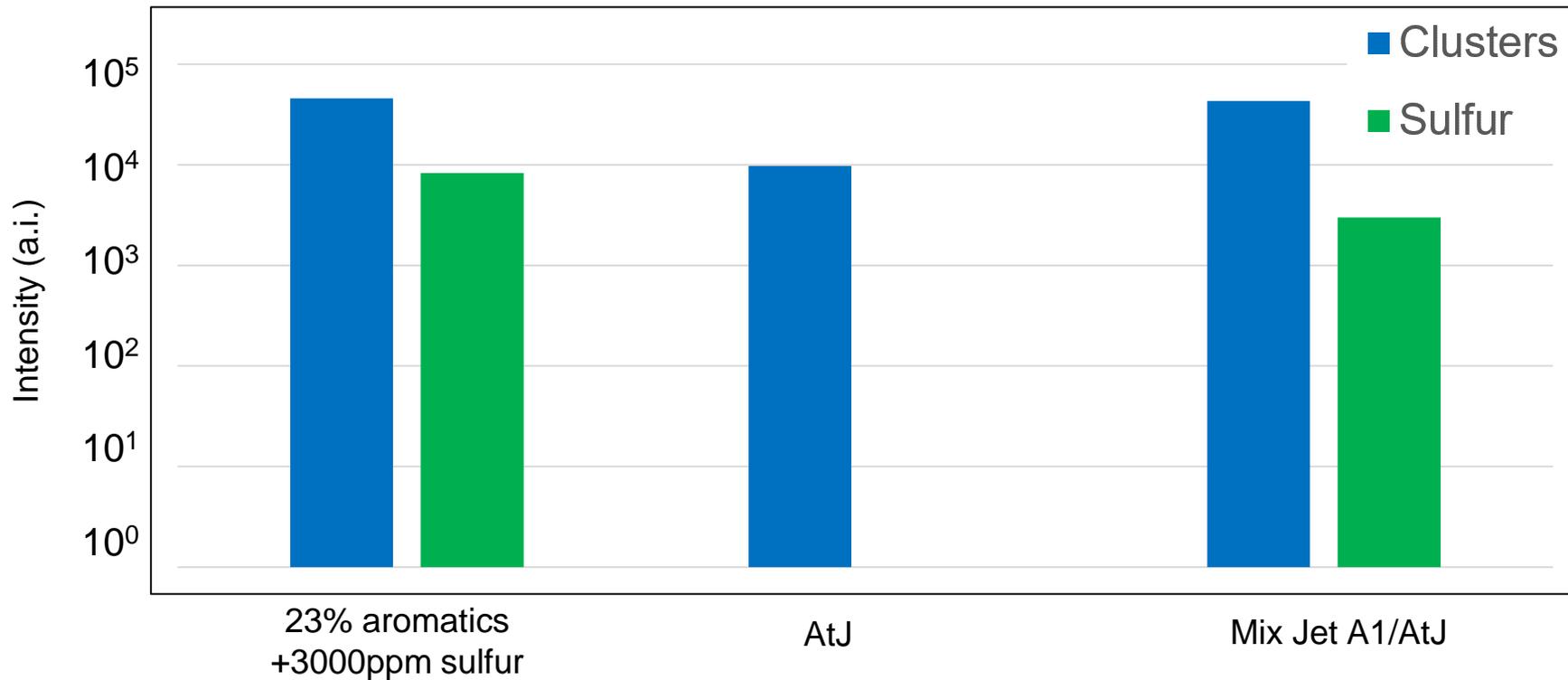
Mass Spectrometry L2MS: Fuel composition CAST comparison

CAST – Particle phase – positive ions : Carbon Clusters/PAHs

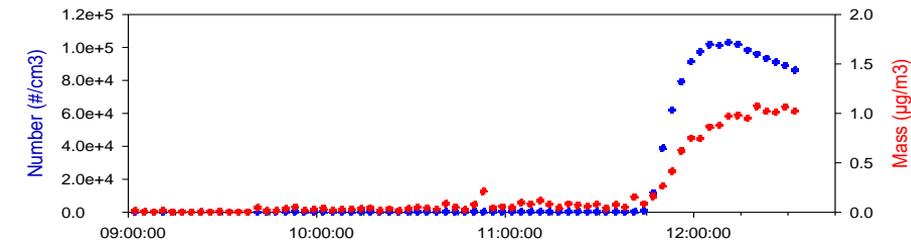
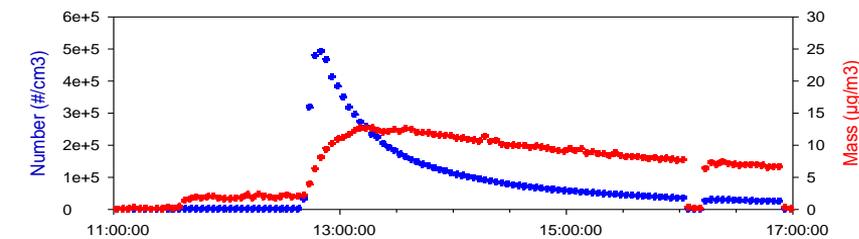
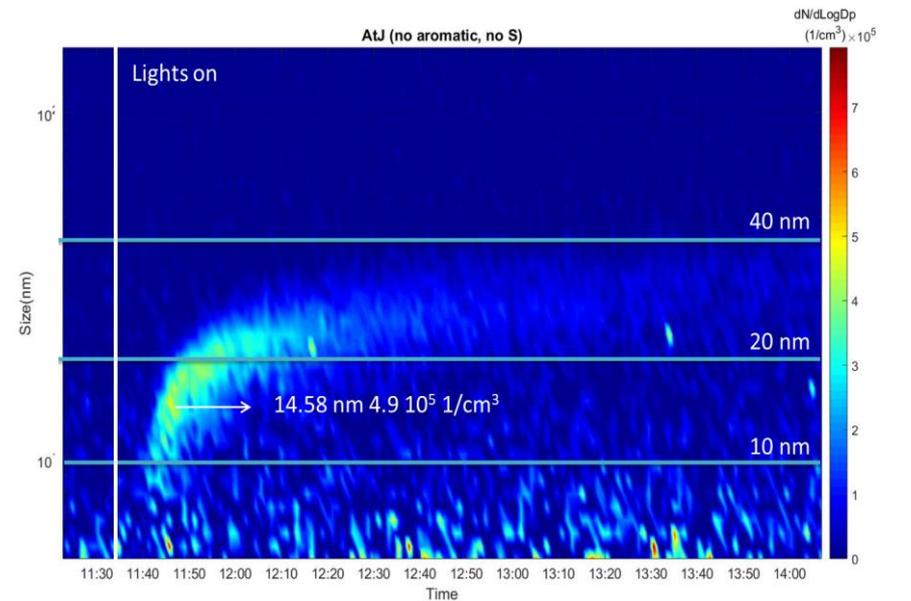
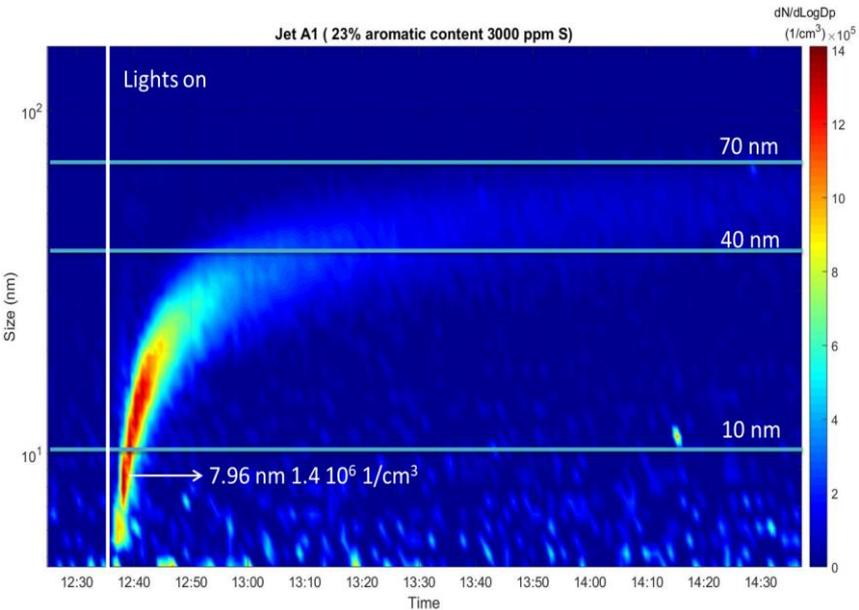


Mass Spectrometry L2MS: Fuel composition CAST comparison

CAST – Particle phase – negative ions : Carbon Clusters/ Sulfur compounds



CESAM first observations

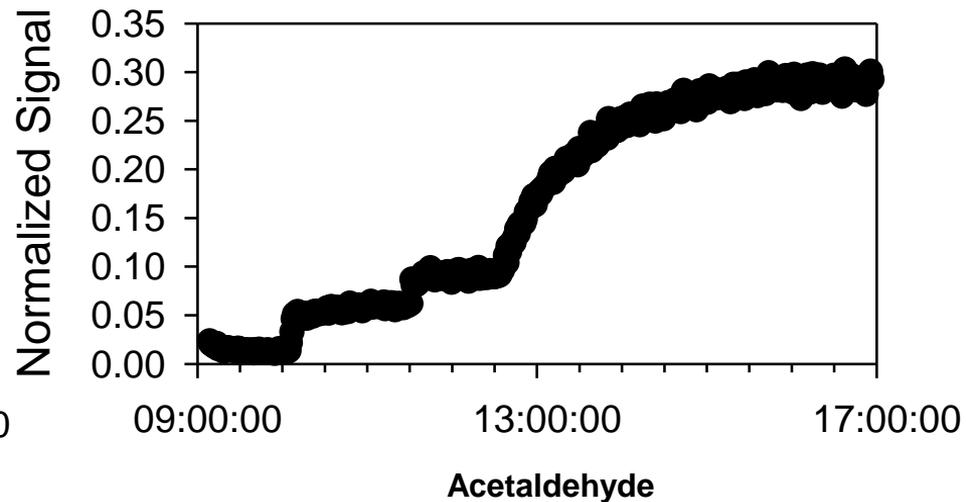
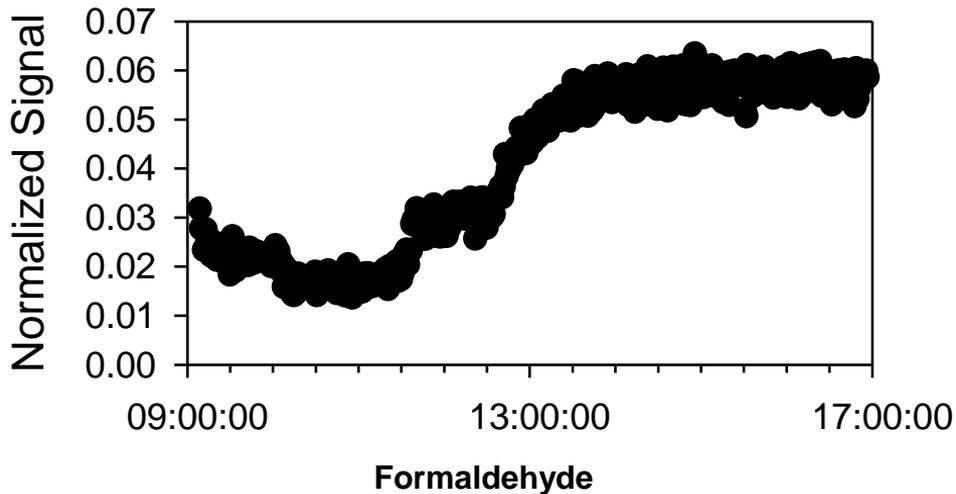


→ New particle formation event representing the evolution of volatile particles in the CESAM chamber with time



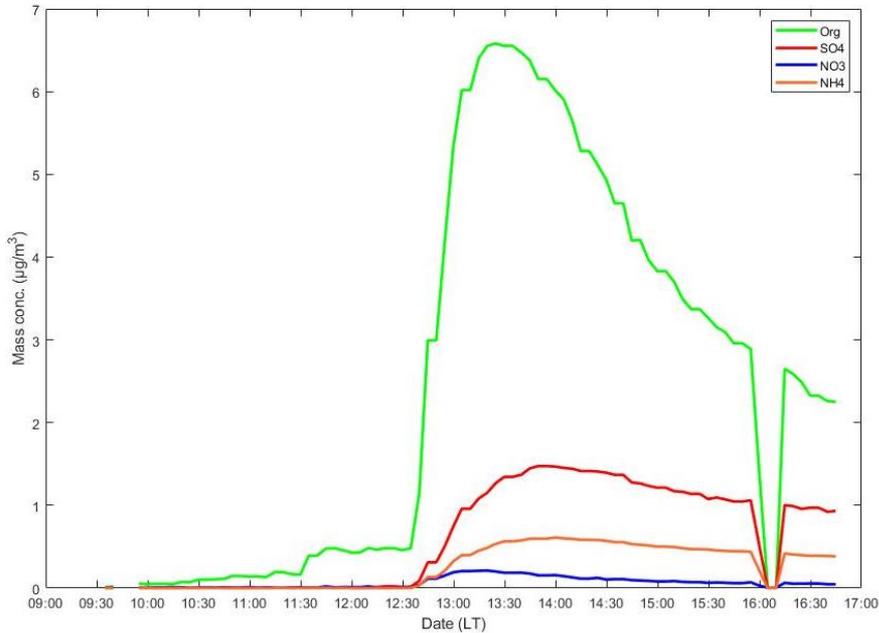
Preliminary Results with PTR-MS : only gas injection CESAM

	23%aromatics+3000ppm sulfur	AtJ
Aromatics compounds	Benzene, Toluene, Xylene, TMB, Naphthalene, <u>Anthracene</u>	Benzene, Toluene, Xylene, TMB, Naphthalene, <u>Acenaphtene</u>
Oxygenated compounds	Formaldehyde, Acetaldehyde, Formic Acid, Acetone, Butanone, <u>3-OH-Butanone</u> , Hexanal, Hexanol	Formaldehyde, Acetaldehyde, Formic Acid, <u>Acetic acid</u> , Acetone, Butanone, Hexanal, <u>Heptanal</u> , Hexanol
Sulfur compounds	<u>Di Ethyl Sulfur and Dimethyl Sulphate</u>	

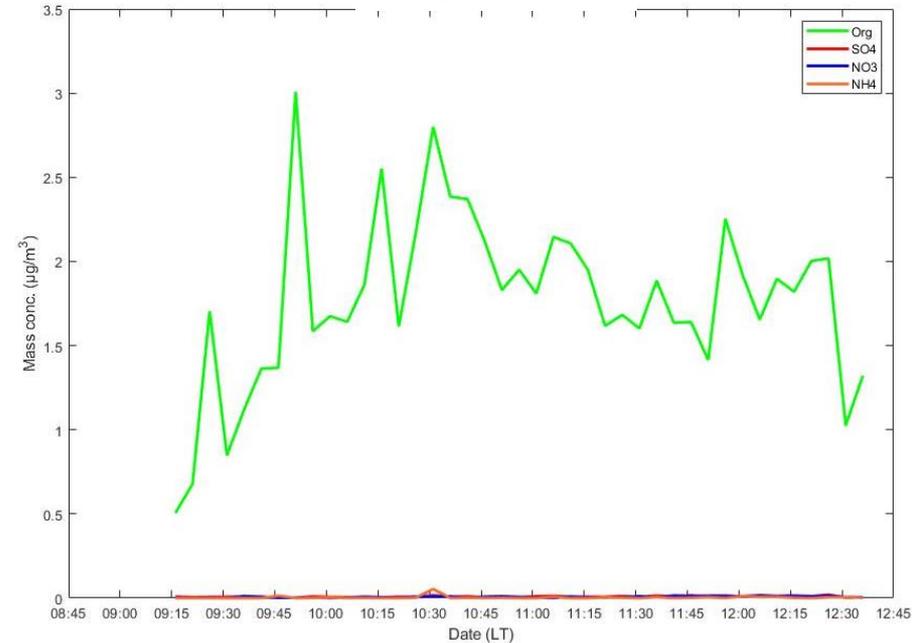


Preliminary Results with HR-AMS : only gas injection CESAM

23% aromatics + 3000 ppm sulfur (19-Nov-2020)



AtJ (24-Nov-2020)



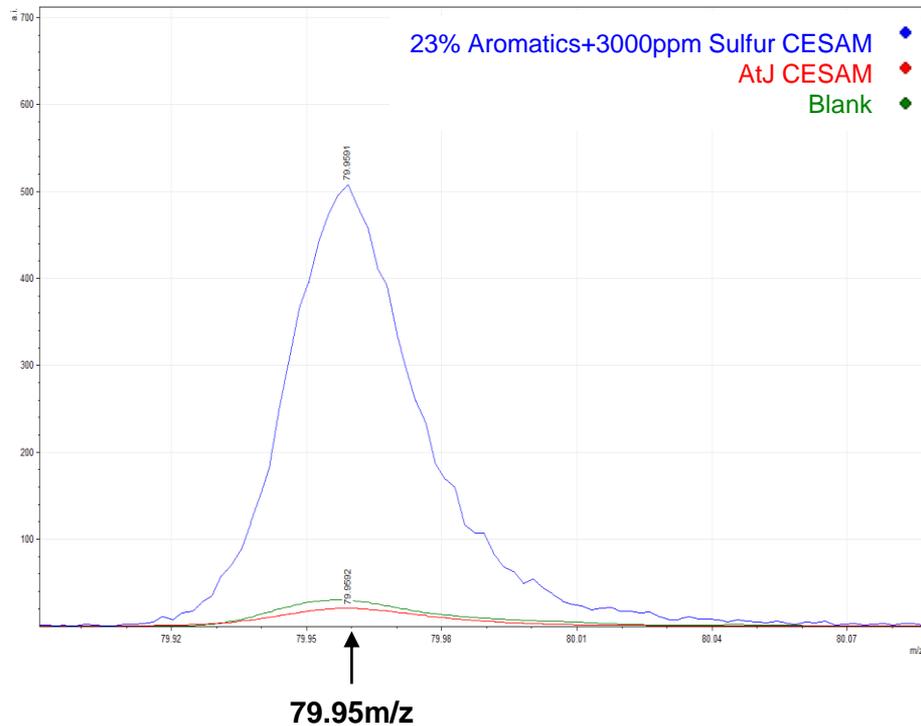
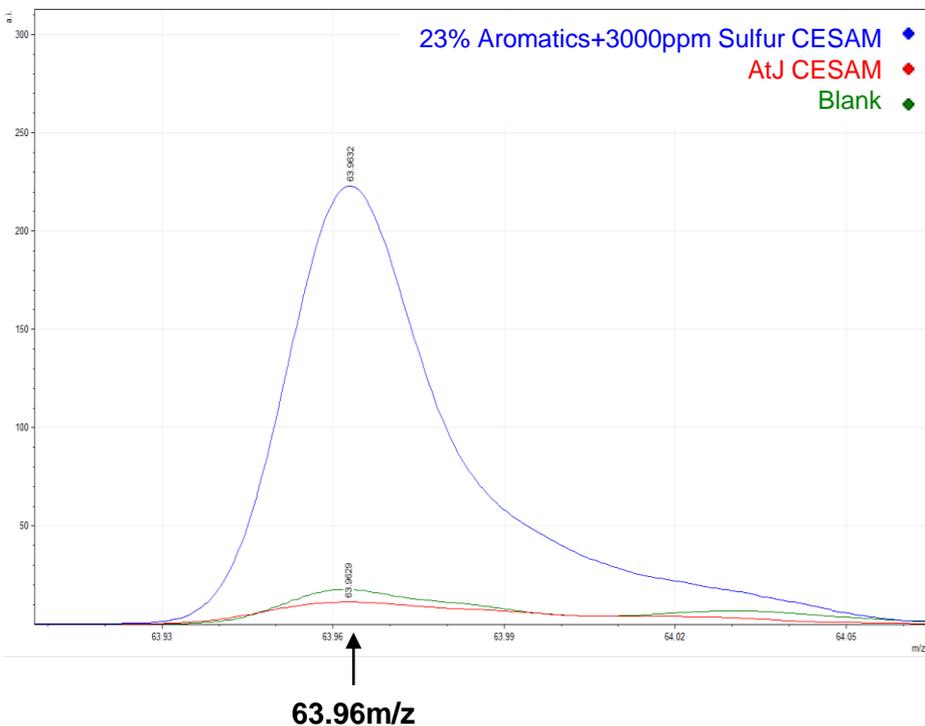
→ Particle chemical composition is dominated by Organics/Sulfates for fuels with Sulfur and by Organics for fuels without Sulfur.

Preliminary results SIMS : only gas injection CESAM - sulfur compounds

SO₂ – 63.96m/z

Particle Phase

SO₃ – 79.95m/z

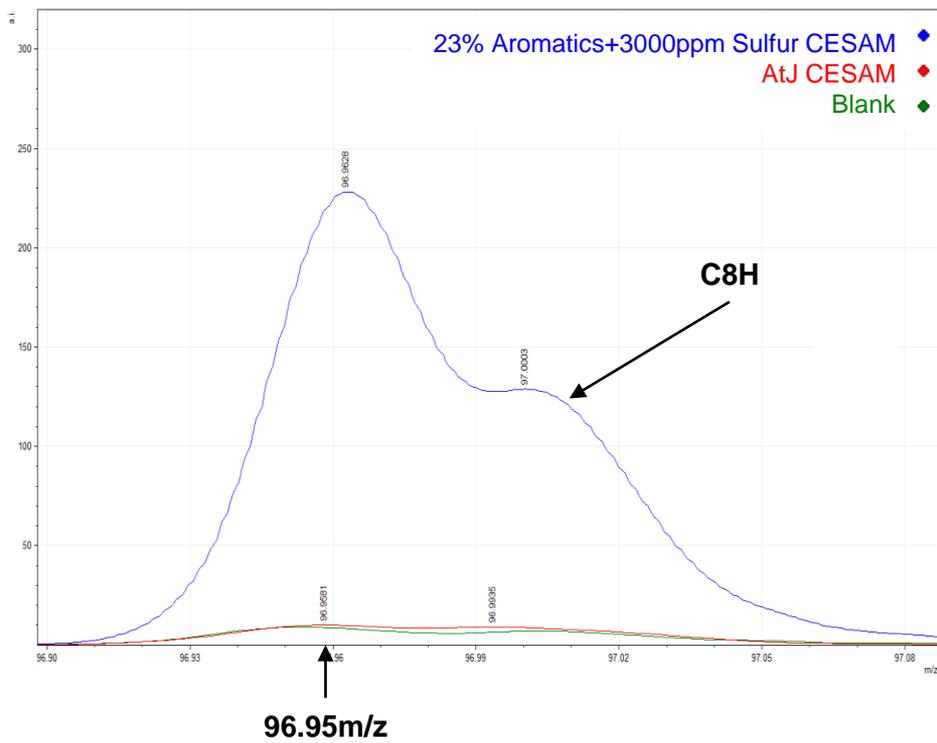
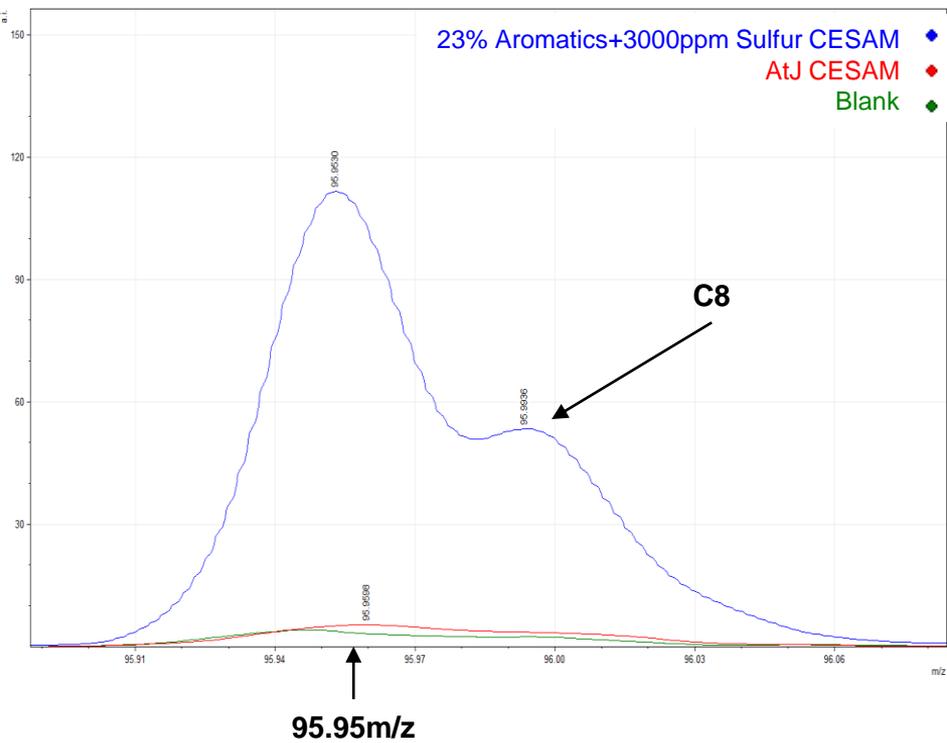


Preliminary results SIMS : only gas injection CESAM - sulfur compounds

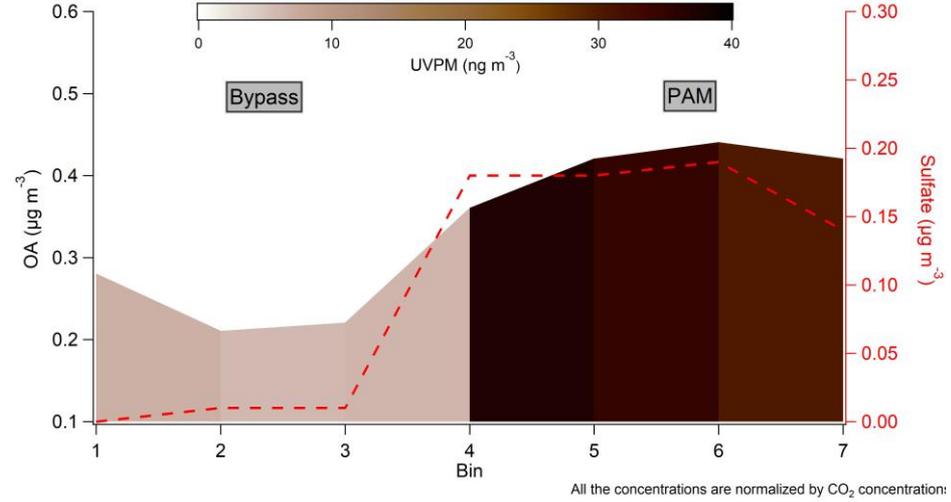
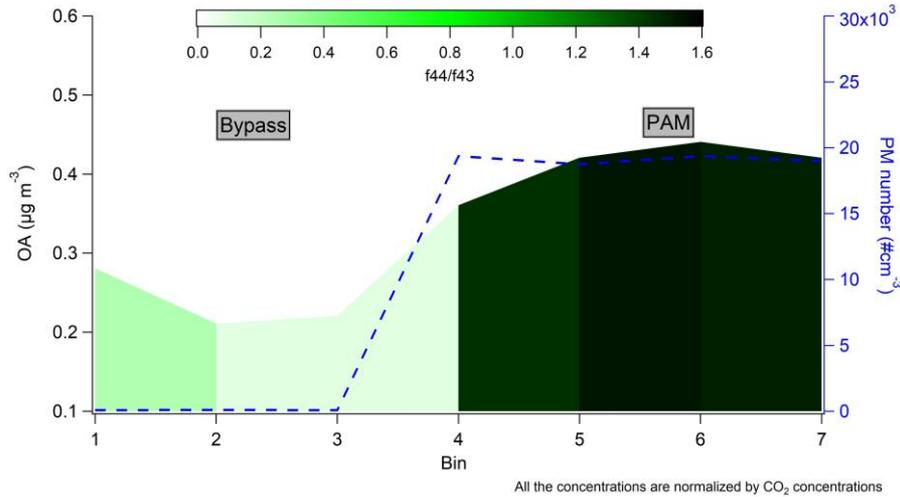
SO₄ – 95.95m/z

Particle Phase

HSO₄ – 96.95m/z



Preliminary Results ACSM: only gas injection PAM



↑
13:51:00

↑
14:11:00

↑
14:26:00

↑
13:51:00

↑
14:11:00

↑
14:26:00

- Fuel : [23% aromatics compounds + 3000ppm sulfur]

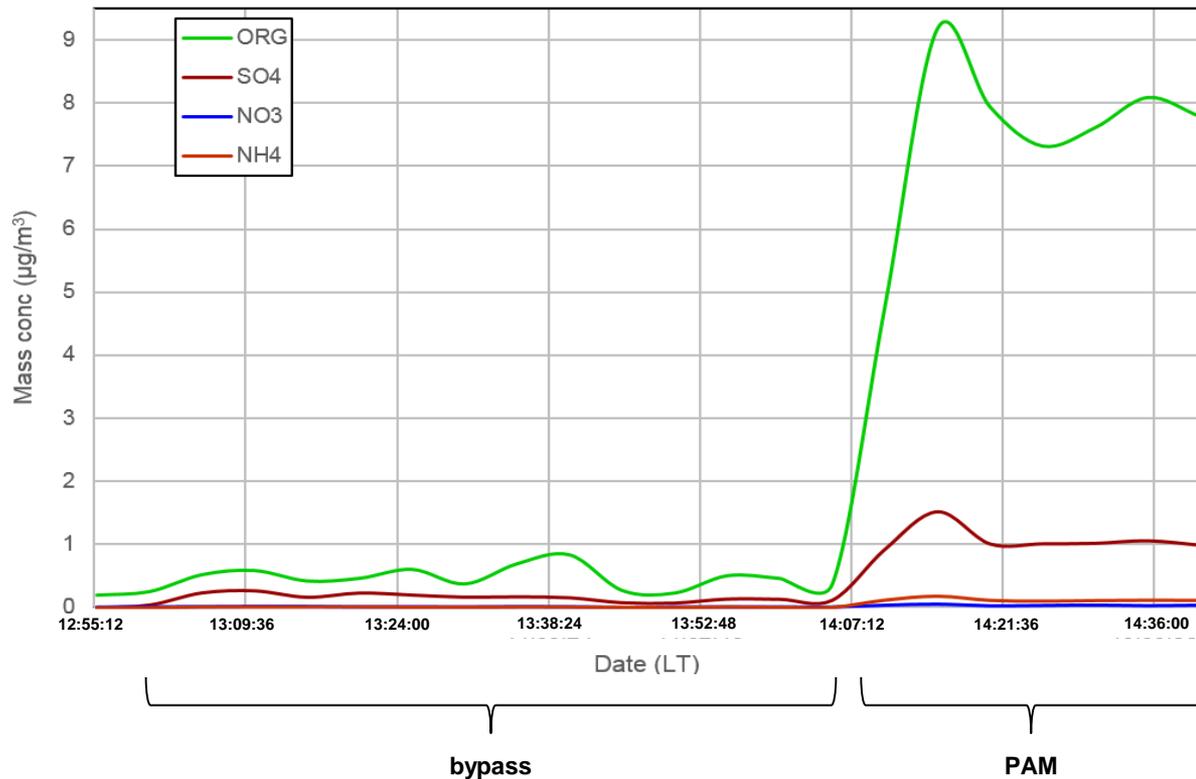
Conclusion and Perspectives

- We observed particle formation with all fuels
- Particle chemical composition is dominated by Organics
- Oxygenated compounds present in the gas phase
- Complete data analysis: extended chemical characterization using mass spectrometry
- Comparison of primary and aged emission chemical fingerprints as well as the ones obtained from smog chamber (CESAM) and PAM-OFR experiments
- New experimental campaign focused on nucleation clusters (API-ToF + PSM)

Back Up

Preliminary Results AMS: only gas injection PAM

23-Nov-2020



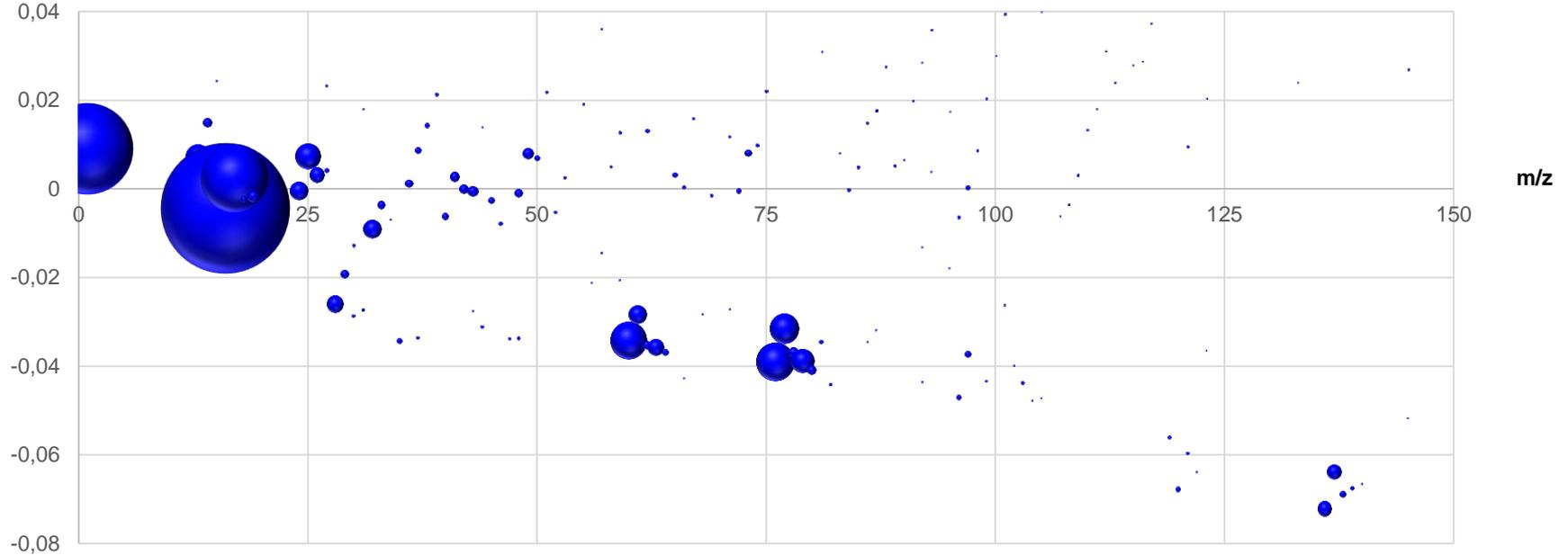
- Fuel : 23% aromatics compounds + 3000ppm sulfur
- Only gas



SIMS mass defect plot : only gas injection CESAM

Mass defect (Δm), u

23% aromatics + 3000ppm sulfur

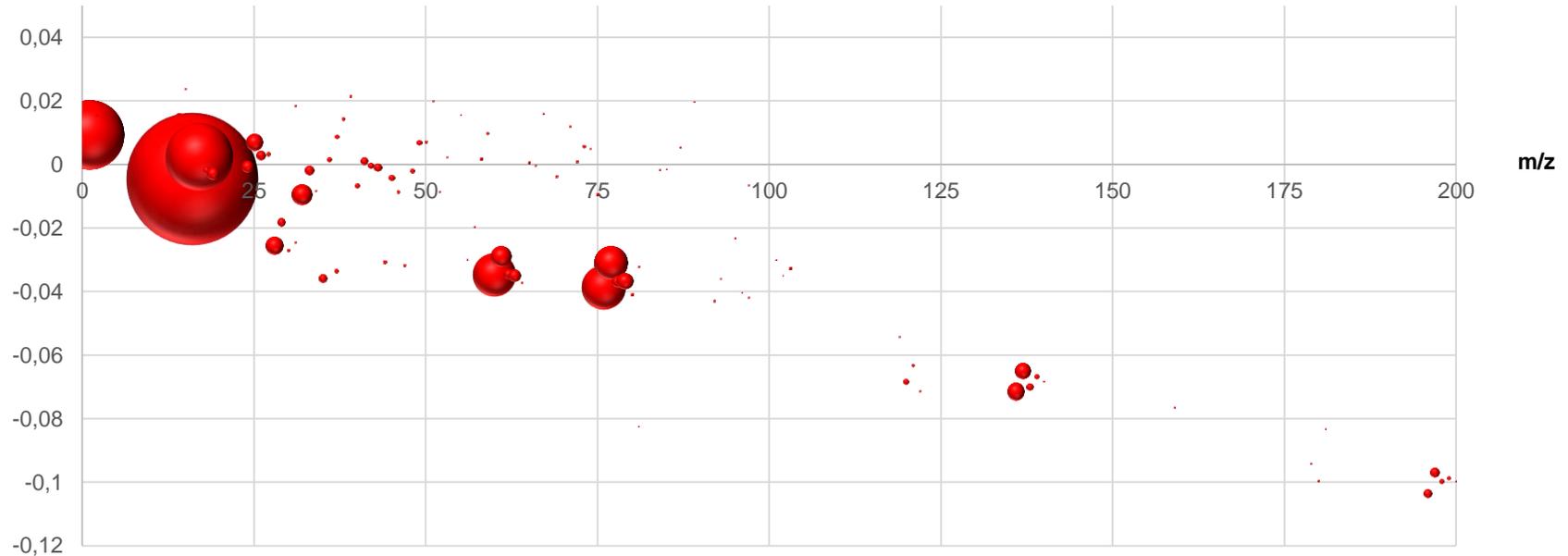


Mass Defect Plot – Particle phase - CESAM sample (gas) - 23% aromatics + 3000ppm sulfur (19-Nov-2020)

SIMS mass defect plot : only gas injection CESAM

Mass defect (Δm), u

AtJ

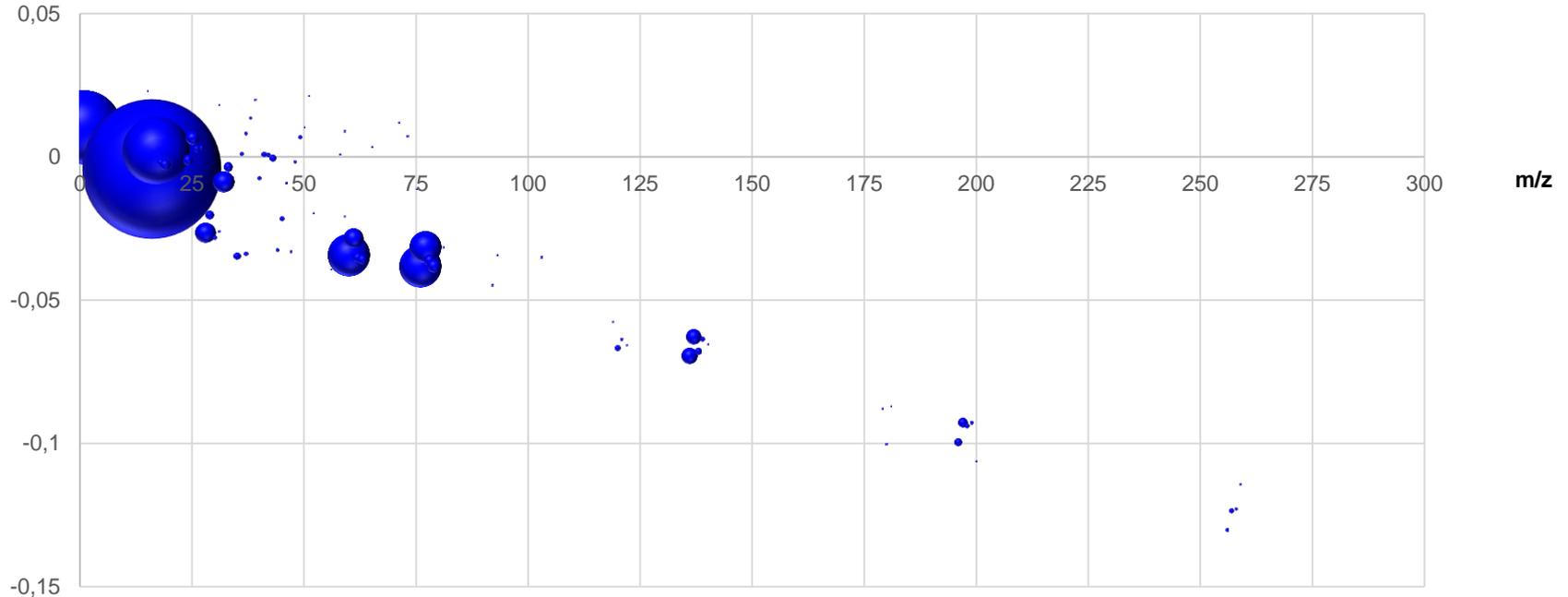


Mass Defect Plot - Particle phase - CESAM sample (gas) – AtJ (24-Nov-2020)

Mass Defect Plot SIMS : only gas injection PAM

Mass defect (Δm), u

23% aromatics + 3000ppm sulfur



Mass Defect Plot – Particle phase - PAM sample (gas) - 23% aromatics + 3000 ppm sulfur (23-Nov-2020)