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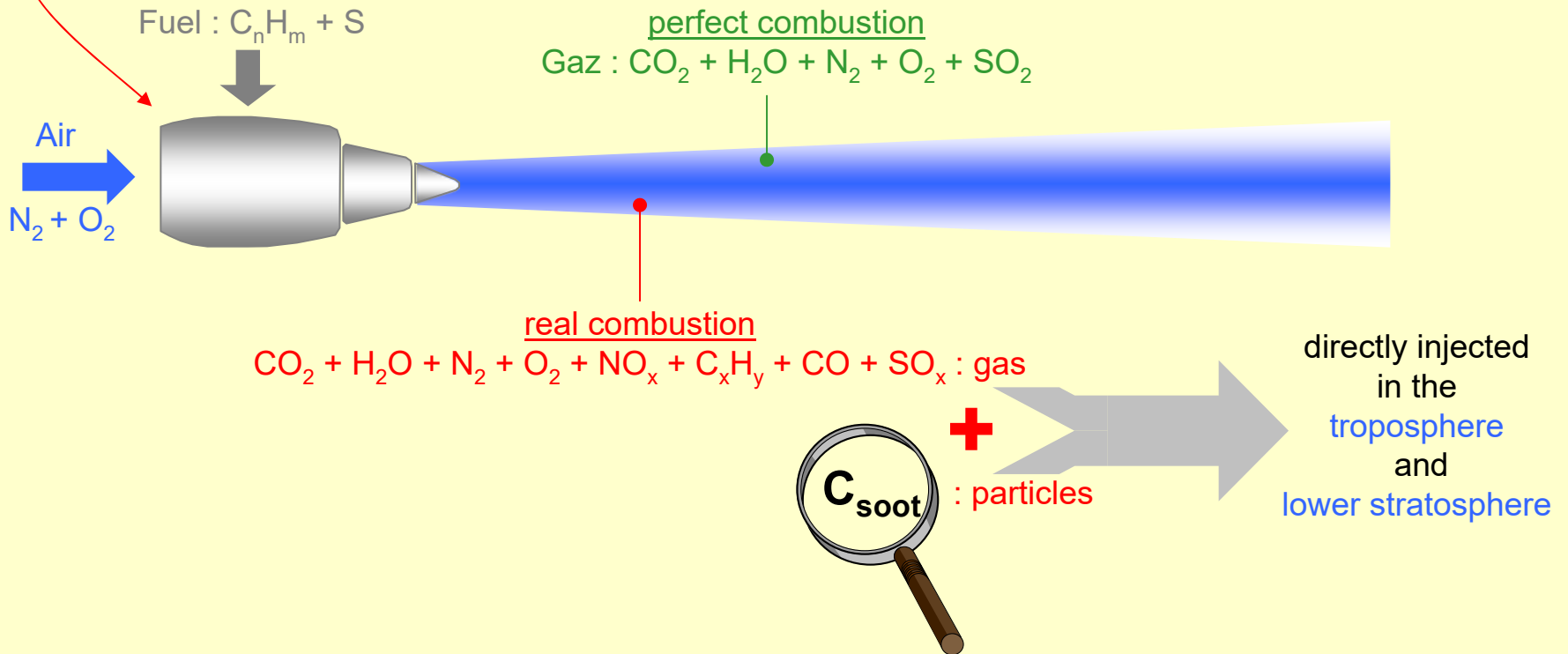
Moscow State University

# **Aircraft engine soot as ice nuclei in contrails and cirrus formation**

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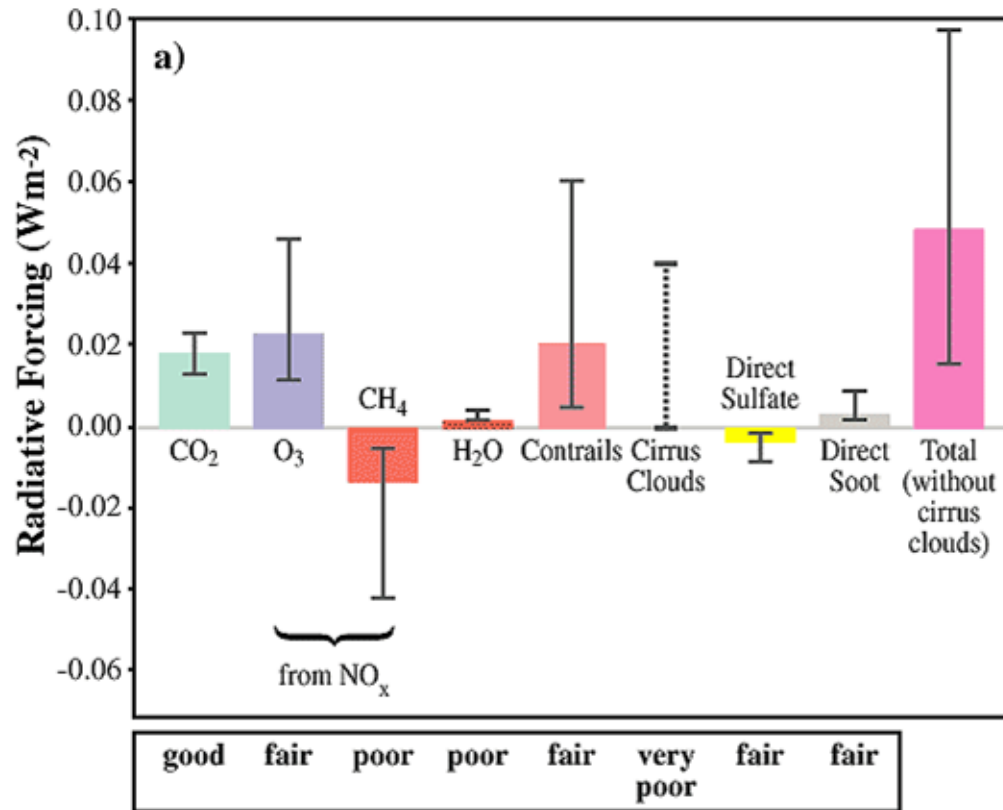
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# WATER - SOOT INTERACTION

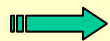
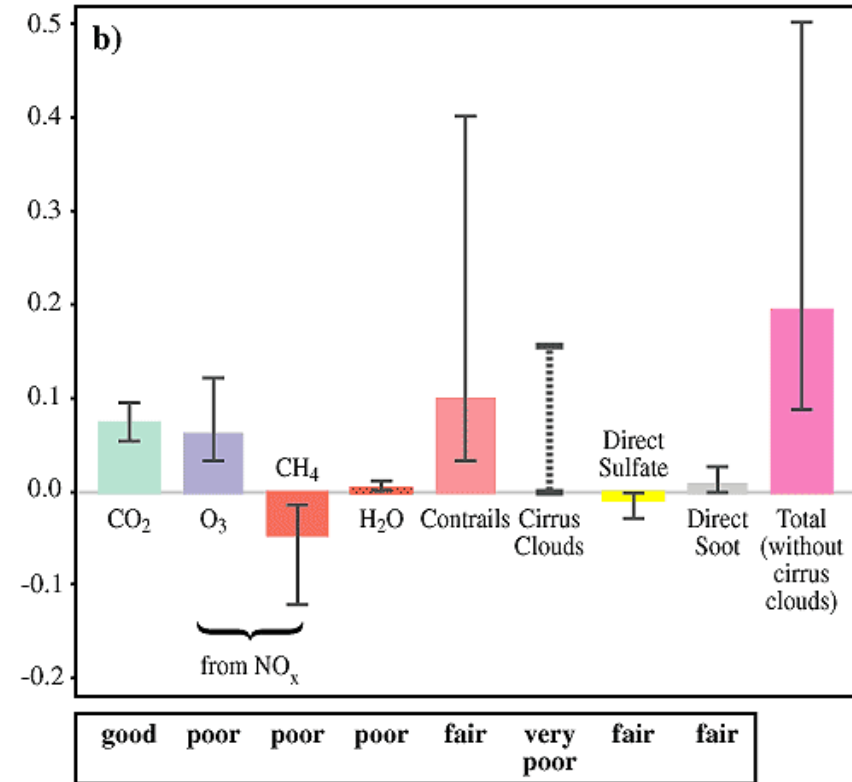


# INFLUENCE OF SOOT ON THE CLIMATE CHANGE

## Radiative Forcing from Aircraft in 1992



## Radiative Forcing from Aircraft in 2050



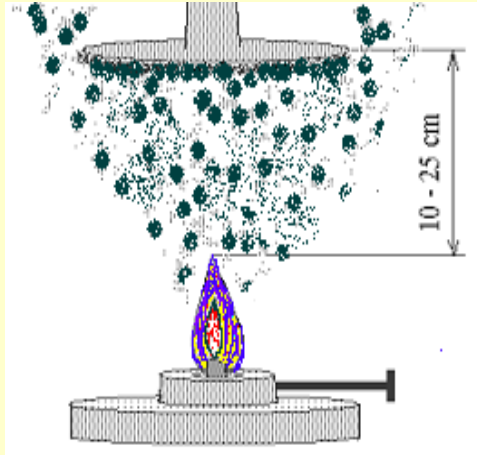
- Significant role of aircraft black carbon (BC) emission on contrail and cirrus formation leading to a positive radiative forcing and climate changes
- An increased concentration of aircraft-generated soot particles may initiate heterogeneous reactions influencing atmospheric chemical composition

# THE SCIENTIFIC BACKGROUND

- However, current ability to predict climatic consequences is limited to qualitative estimates due to the paucity of data about the physicochemical properties of aircraft engine soot.
  - Most of studies, based on laboratory-generated soot particles, show a large variation in their nucleation properties and reactivity.
  - There remains a need for research on the interactions of water and engine soot, especially related to the ability of soot to form cloud condensation nuclei (CCN)
- This work is devoted to a comprehensive characterization of the morphology, microstructure, chemical composition, and the surface nature of aircraft engine soot with the aim to identify the mechanisms responsible for both its high hydrophilicity and its ability to act as contrail nuclei in the aircraft plume

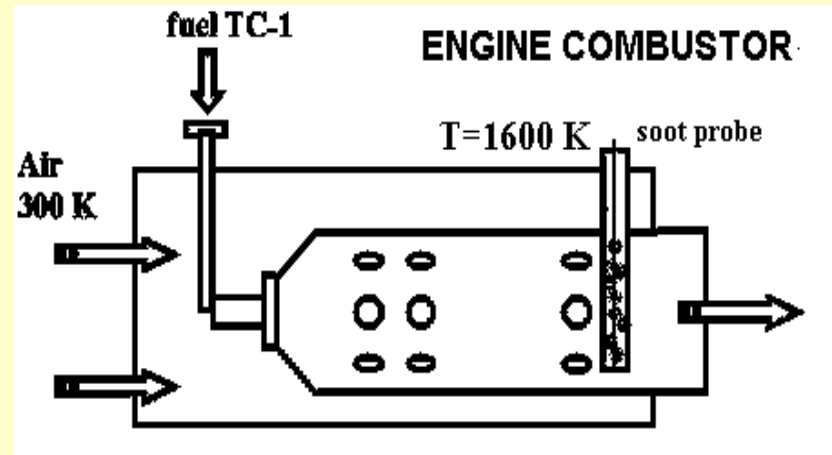
# SOOT PRODUCTION

TC1 laboratory surrogate soot



Laboratory oil lamp

TC1 engine soot

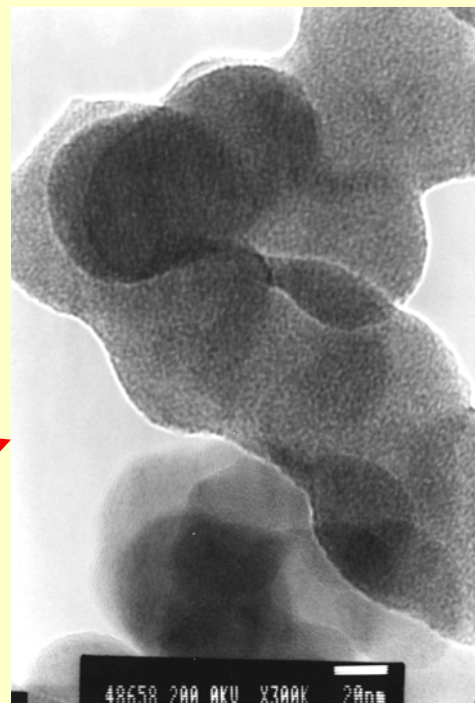
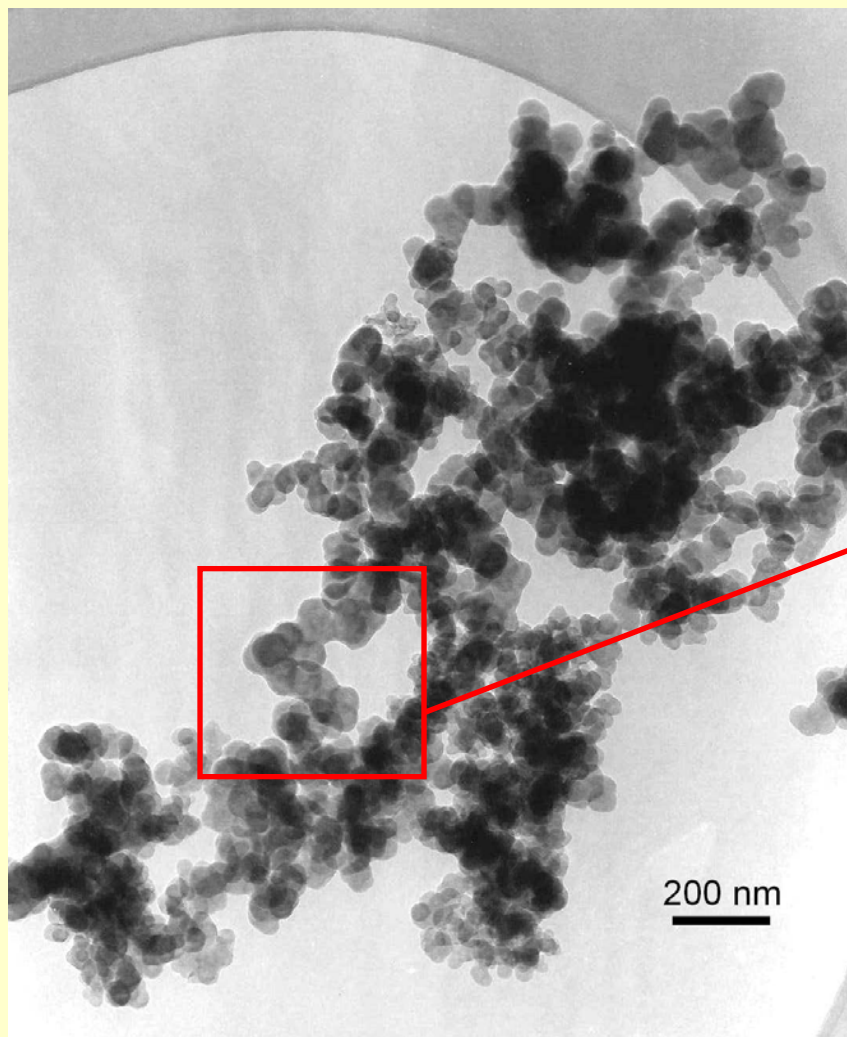


Engine operates so as to simulate the cruise conditions

Engine combustor	$T_{inlet}$ (K)	$T_{outlet}$ (K)	Air-to-fuel ratio	Pressure (atm)	Comment
D30-KU	300	1250-1450	4 - 4.5	3 - 5	Old engine operating on Tu-134

Aviation kerosene TC1 sulfur content:  $1100 \mu\text{g}\cdot\text{g}^{-1}$

# SOOT MORPHOLOGY AND STRUCTURE: TC1 SURROGATE SOOT

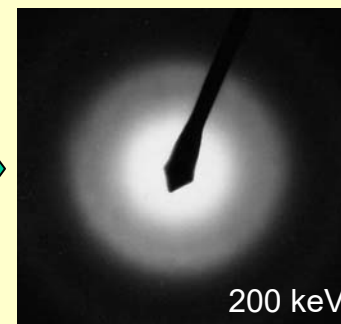


spherical particles



size distribution :  
d ~ 40-50 nm

Diffraction



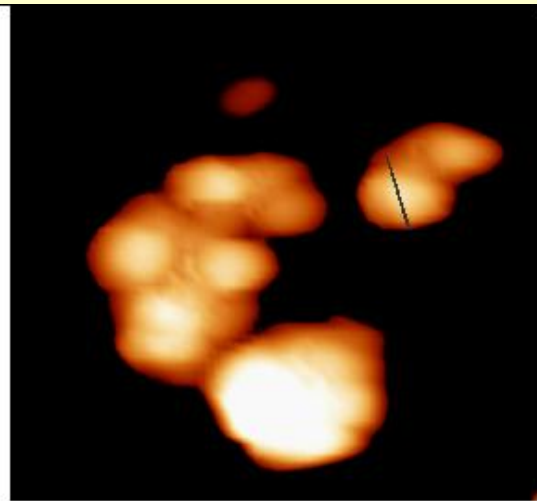
diffuse rings



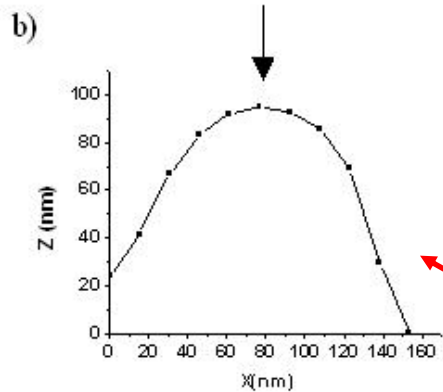
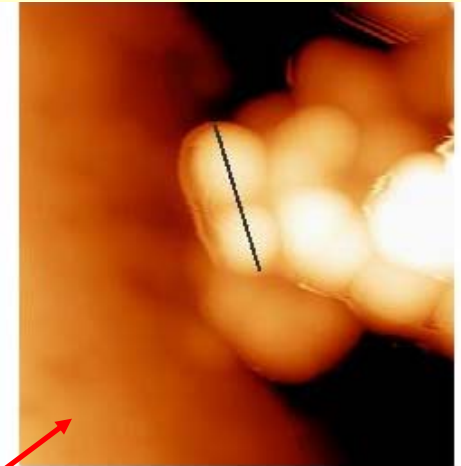
- amorphous carbon  
- not well cristallized

*Transmission Electron Microscope : JEOL JEM 2000 FX ; resolution: 2.8Å at 200 keV*

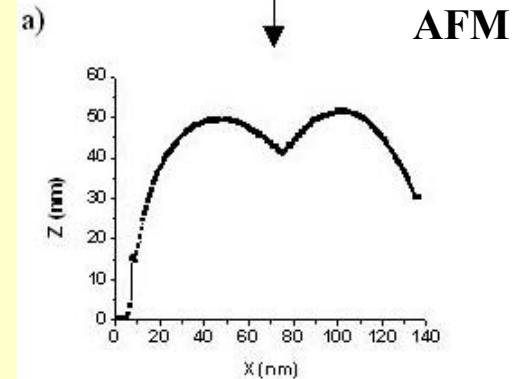
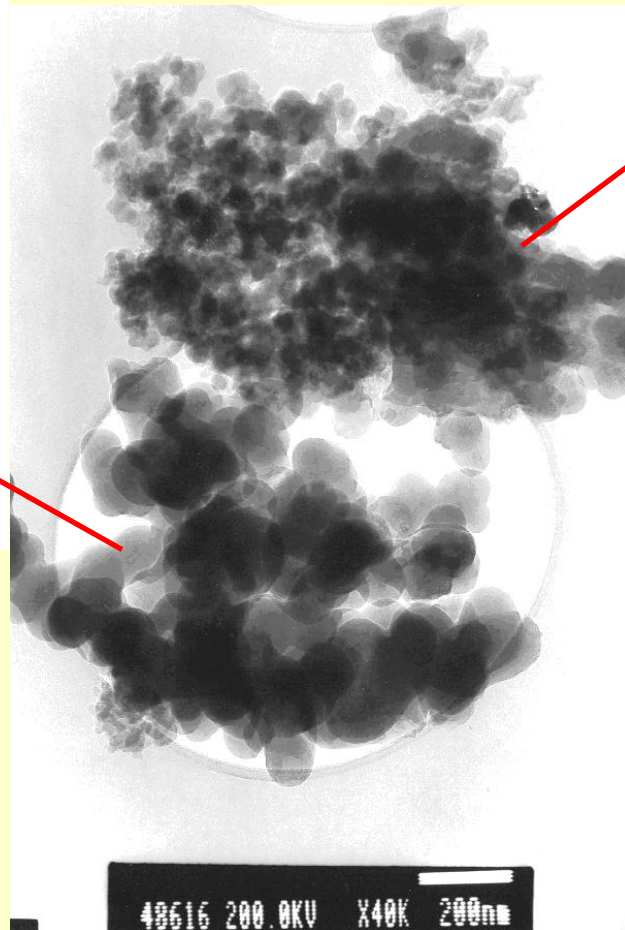
# SOOT MORPHOLOGY AND STRUCTURE: ENGINE SOOT



Spherical and amorphous particles



size distribution :  
 $d \sim 100$  nm



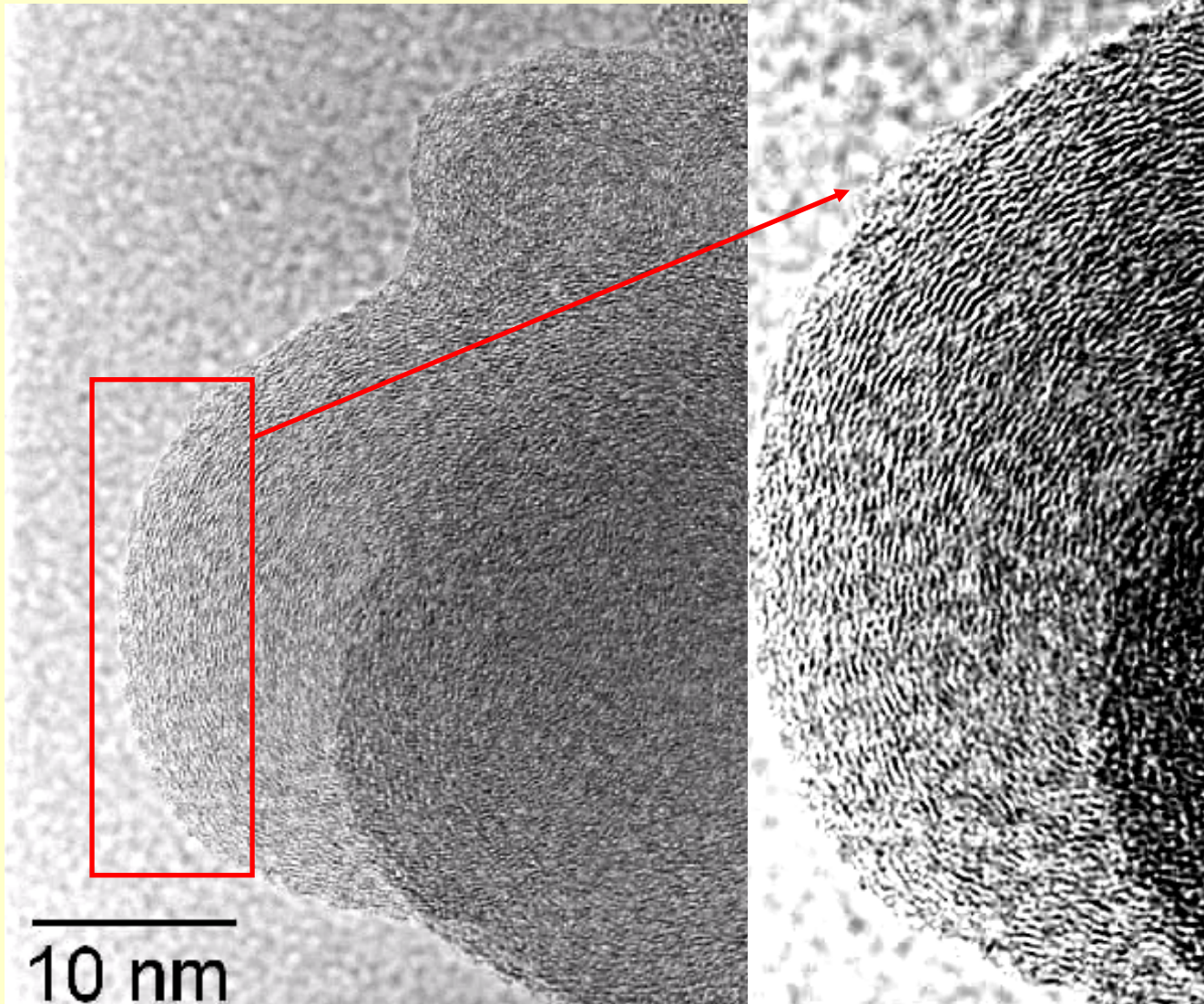
size distribution :  
 $d \sim 40-50$  nm

AFM: Nanoscope III: Digital Instruments

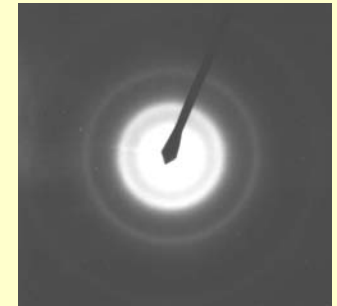
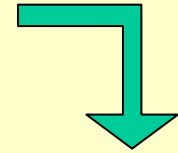
TEM: JEOL JEM 2000 FX



👉 Engine soot : some particles show a microstructure



Onion like-structure



graphitic structure  
 $d_{100} = 2.03 \text{ \AA}$   
 $d_{002} = 3.36 \text{ \AA}$

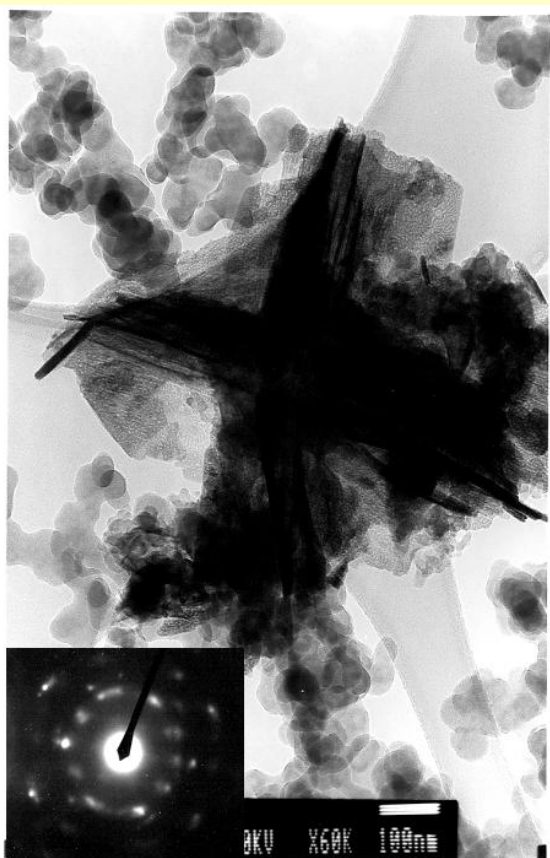


 X-Ray Energy Dispersive Spectroscopy: chemical composition

	C (weight %)	O (weight %)	S (weight %)
TC1 surrogate soot	98-99	1-2	-
TC1 engine soot	98	1.6	0.2



for both soot, the main fraction is essentially composed of amorphous spherical carbon particles



But, in some areas of the engine soot sample:

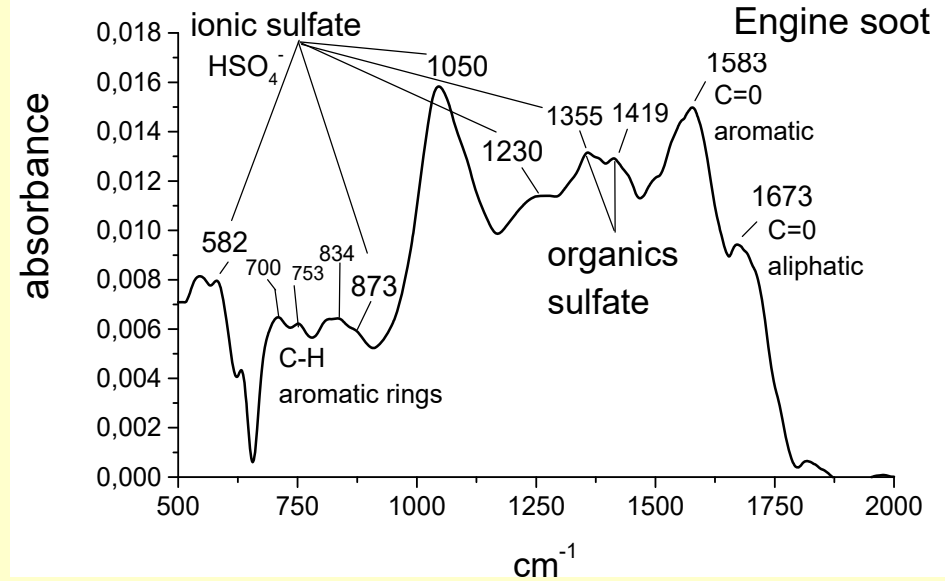
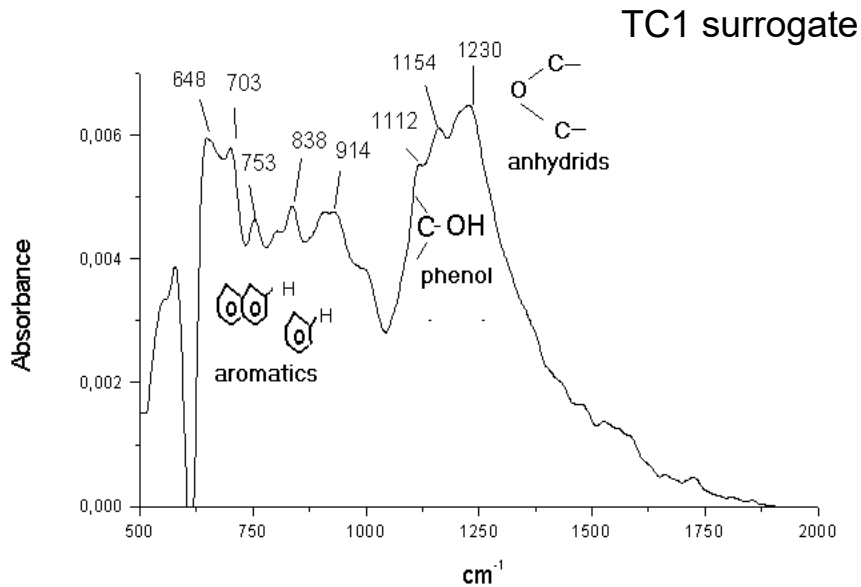
- Presence of dark and well-crystallised impurities
- Diffraction pattern analysis → Iron oxide
- Chemical composition:

	C (wt %)	O (wt %)	<b>S (wt %)</b>	Fe (wt %)
engine soot (with impurities)	43-54	<b>11</b>	<b>2</b>	<b>33-43</b>

# SOOT CHEMICAL COMPOSITION



FTIR: surface functional groups



## SURROGATE ; ENGINE

Bands (cm<sup>-1</sup>)

Hydrophilicity

CH deformation, aromatics

650-920

Low

-C-O-C- anhydrides, aryls

1230

Medium

C-OH stretch, phenols

1154,1112

Medium

-O- aromatic ester

1154, 1112

Low

O-H stretch, hydroxyl

3290

High

## ENGINE ONLY

Bands (cm<sup>-1</sup>)

Hydrophilicity

C=O carbonyl, aliphatic

1673

High

C=O carbonyl, aromatic

1583

High

HSO<sub>4</sub><sup>-</sup> ion

1355,1230

High

1050, 878, 582

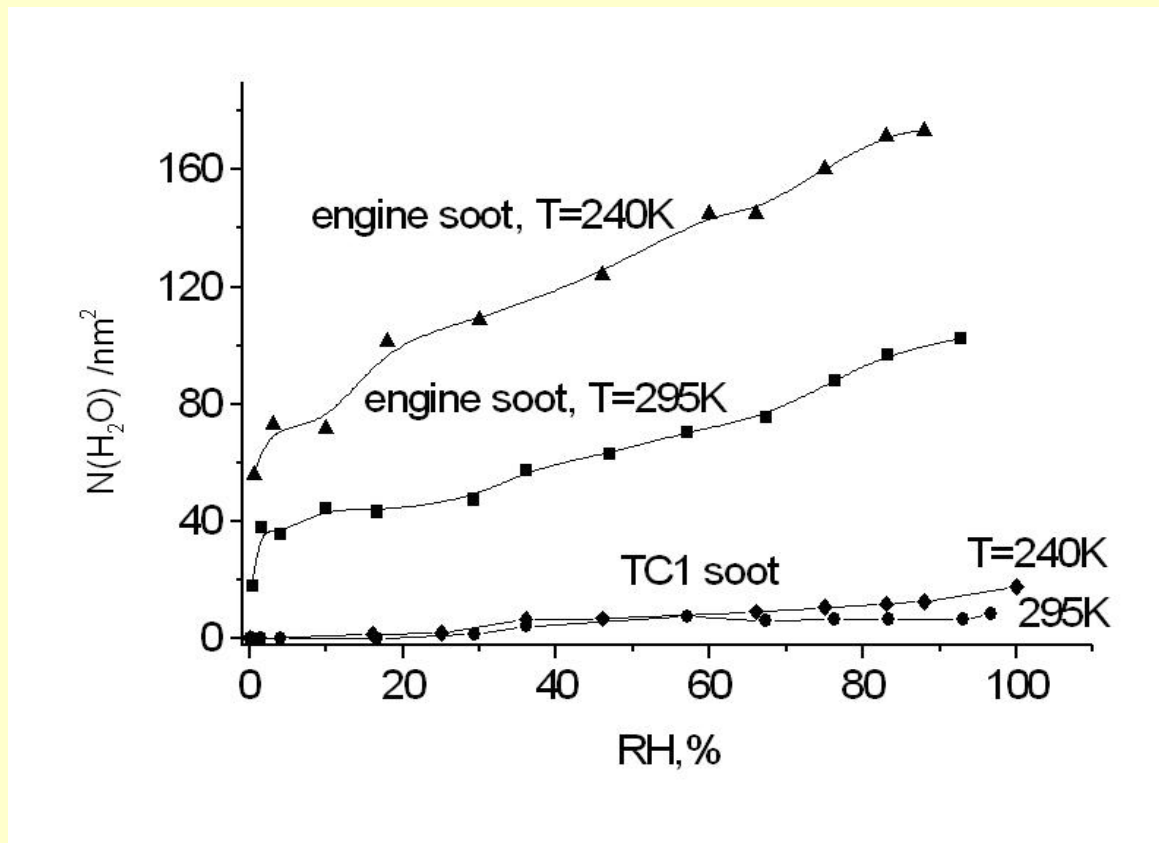
Sulfates, organics

1350, 1420

High

Engine soot has much more hydrophilic surface functional groups than the surrogate soot

# WATER ADSORPTION ISOTHERMS



- surprisingly high level of water adsorption on engine soot at low RH and at  $T = 295 \text{ K}$ 
  - initial adsorption on the strongest active sites (surface ionic and organic sulfates).
- adsorption on engine soot  $\gg$  TC1 surrogate soot. (TC1 isotherm shape corresponds to an hydrophobic mat.)
  - The amorphous carbon main fraction of soot is not responsible of the hydrophilicity
  - Only the fraction of impurities (most hydrophilic) of engine soot can act as Cloud Condensation Nuclei.

## CONCLUSION

- Combustion conditions within an aircraft engine have a dramatic influence on engine soot properties.
- According to its chemical composition and structure, engine soot is a mixture of a relatively hydrophobic main fraction almost free of impurities and a more hydrophilic fraction containing impurities.
- A significant amount of sulfur is accumulated within the aircraft engine on the soot surface as derivatives of sulfuric acid. Together with water soluble organics, they are responsible for the highly hygroscopic nature of the engine soot and for its ability to act as CCN for contrails.

## THANKS TO ...

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