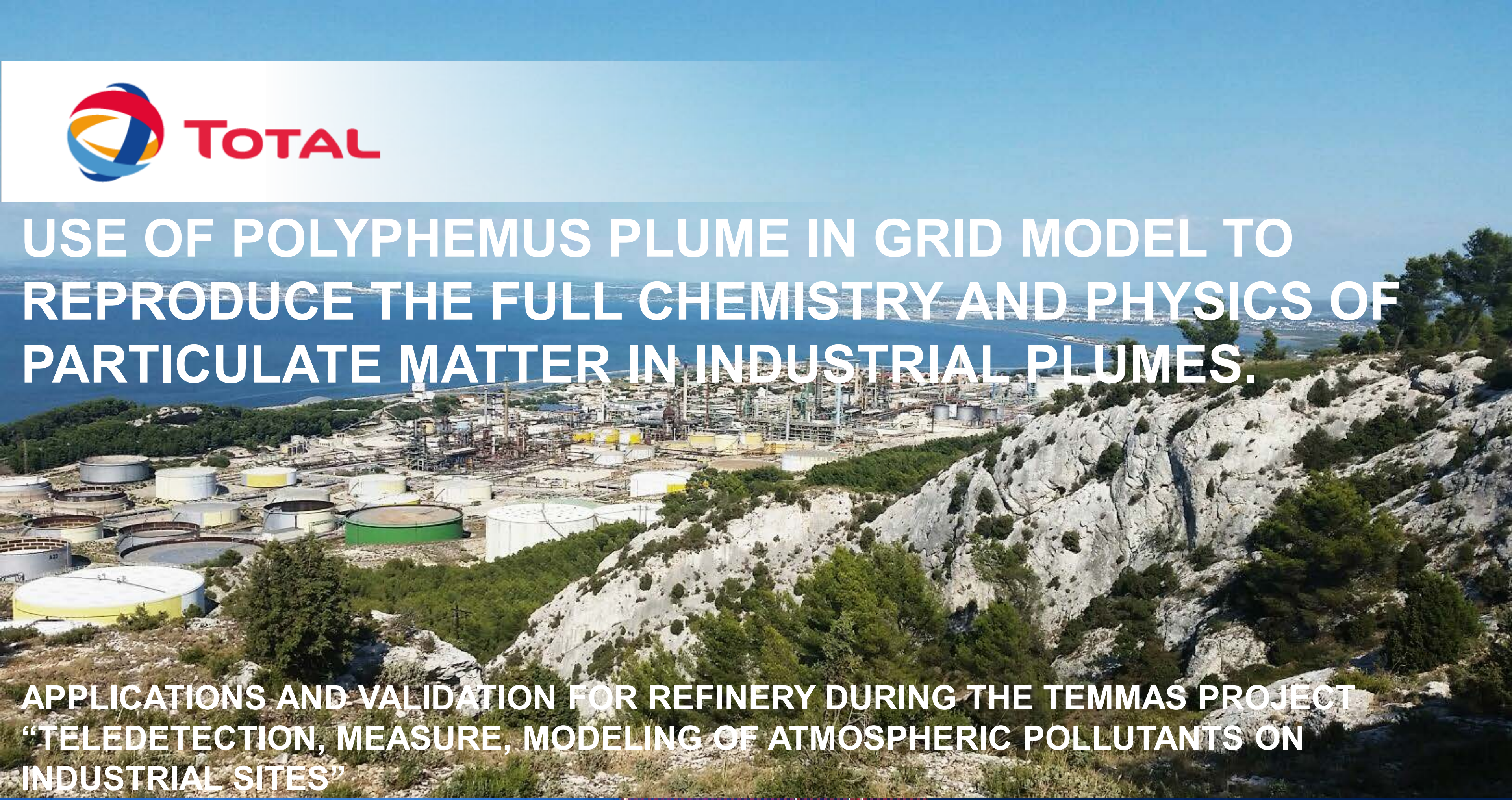


TOTAL

USE OF POLYPHEMUS PLUME IN GRID MODEL TO REPRODUCE THE FULL CHEMISTRY AND PHYSICS OF PARTICULATE MATTER IN INDUSTRIAL PLUMES.

APPLICATIONS AND VALIDATION FOR REFINERY DURING THE TEMMAS PROJECT "TELEDETECTION, MEASURE, MODELING OF ATMOSPHERIC POLLUTANTS ON INDUSTRIAL SITES"

ADEME Agence de l'Environnement et de la Maîtrise de l'Energie

Aix*Marseille université

Laboratoire Chimie Environnement

Airpaca Observatoire Régional Qualité de l'Air

ONERA THE FRENCH AEROSPACE LAB

Université Paul Sabatier TOULOUSE III

LA

TOTAL

cerea

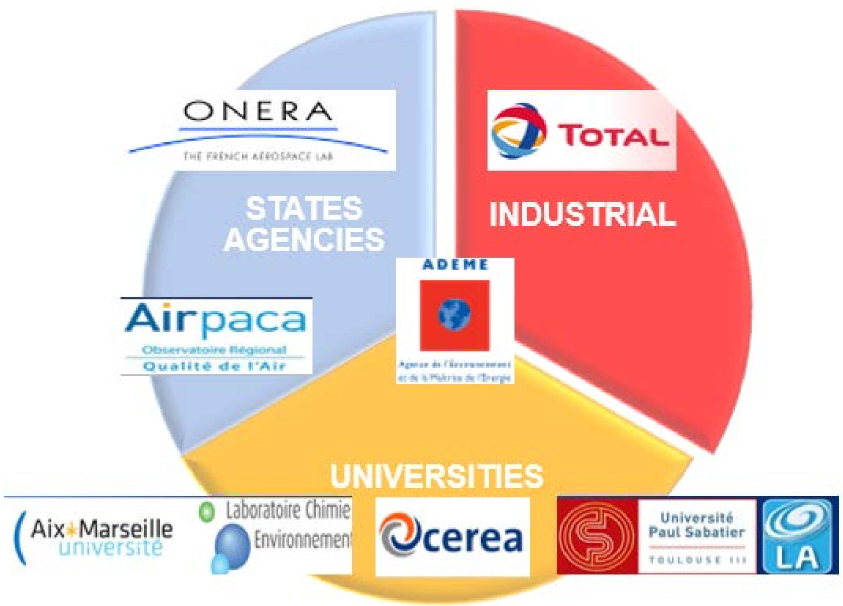
PM PROBLEMATIC : HUGE HEALTH COST, MAIN DRIVER OF THE EUROPEAN POLICY IN AIR QUALITY

- European strategy of pollution reduction **Clean Air For Europe (2000) :**
  - 2020 goal was to reduce the impact (-47%) vs 2000.
- **Focus on PM reduction, but PM is a complex pollutant**
  - PM is primary (directly emitted in atmosphere) and secondary (formed by gas reactions in the atmosphere). 80 % of PM 2.5 is secondary.

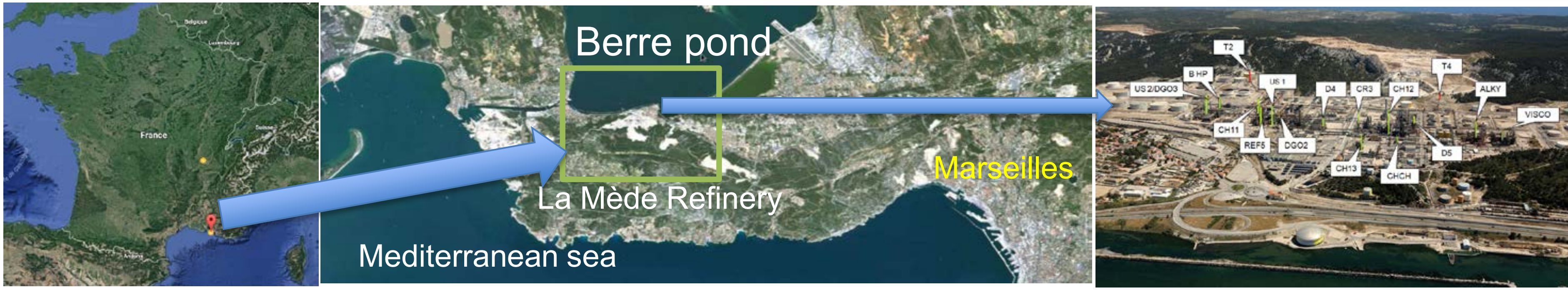
- **TEMMAS** project

Teledetection, **M**easure, **M**odeling of **A**tmospheric pollutants on industrial **S**ites **:**

- **Objective :** evaluate the PM impact of an industrial site
- Consortium of teams specialized in measurements and modeling
- Project supported by the French Agency for the Environment and Energy Management (ADEME)



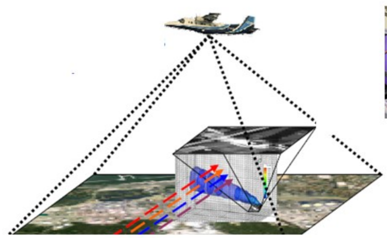
TEMMAS PROJECT : MEASUREMENT CAMPAIGNS



- **2 Measurements campaigns** (Summer Sept.2015, Winter Feb. 2016)**:** Measurements of PM mass, number and chemical composition, in the vicinity of a refinery

TEMMAS FOLLOWS THE PM LIFE

FROM THE STACK … IN THE AIR … TO THE GROUND



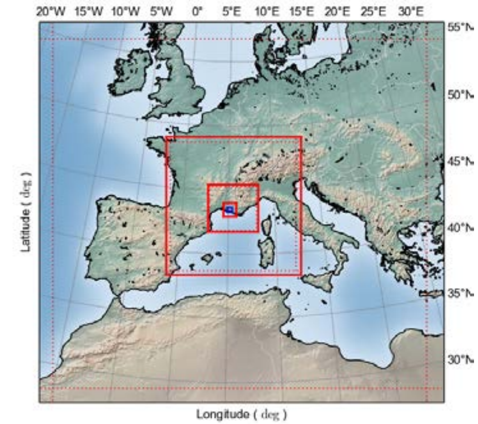
Complete description : P.Y. Foucher et al. ICAC 2017 & ADEME report (www.ademe.fr/mediatheque)

DATA ANALYSIS WITH MODELING, TWO MODELS APPROACH

- Chemical Transport Model to reproduce refinery plume and interaction with other pollutants
- A local dispersion model, to simulate at local scale & short term plumes dispersion.
- According to the type of information measured (punctual or optical), confrontation with model result needs to be adapted or corrected.

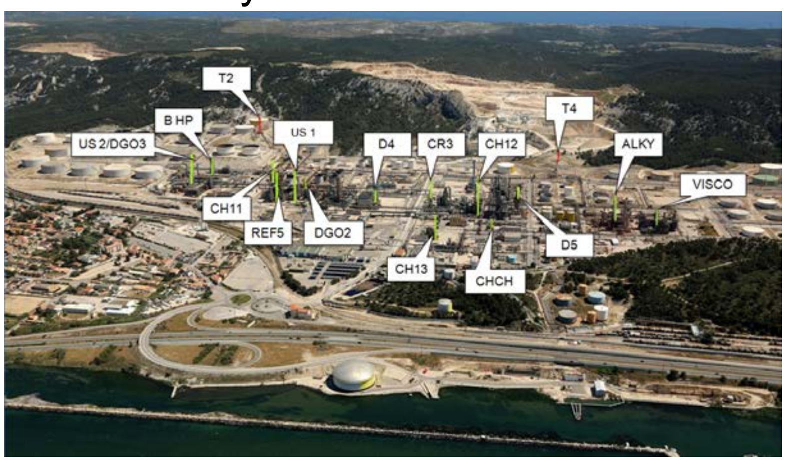
CHEMICAL TRANSPORT MODEL : METHODOLOGY

- **Meteorology**:
- WRF meteorological fields computed over 4 domains, using one-way nesting
- Simulations nudged with local meteorological stations and wind-Lidar measurements in the vicinity of the refinery



- **Emission inventory :**
- Europe: Emep inventory at 50 km * 50 km horizontal resolution
- Bouche-du-Rhône: Airpaca inventory at 1km*1km horizontal resolution
- Refinery: Daily SO_2, No_x, and PM daily emission rates estimated at each stacks

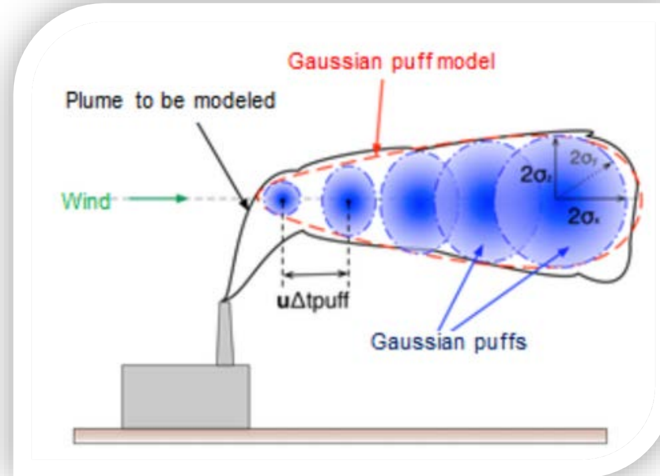
Airpaca emissions inventory



CTM MODEL : POLYPHEMUS PLUME-IN-GRID

Plume-in-Grid

- Background 3D model: Chemistry and transport of background pollutants
- Gaussian Puff model: Chemistry and transport of industrial emissions, in interaction with the background
- Recently updated to include particles number computation (K. Sartelet not curently published)



PM2.5 Refinery contribution

(Eulerian) without PinG **with PinG**

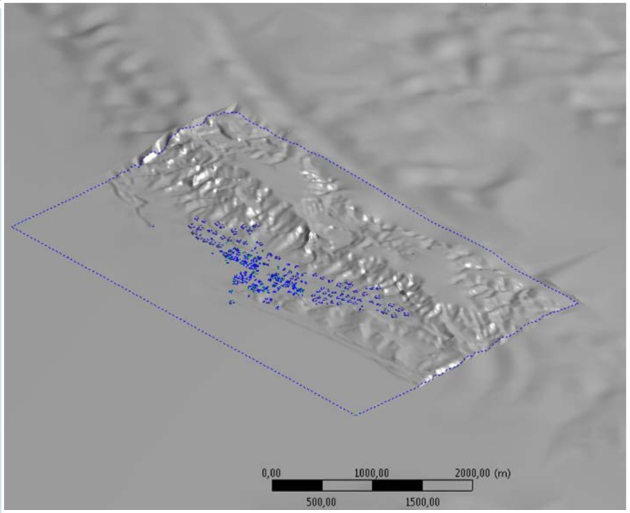
LOCAL DISPERSION MODEL : LAGRANGIAN MODEL "SLAM".

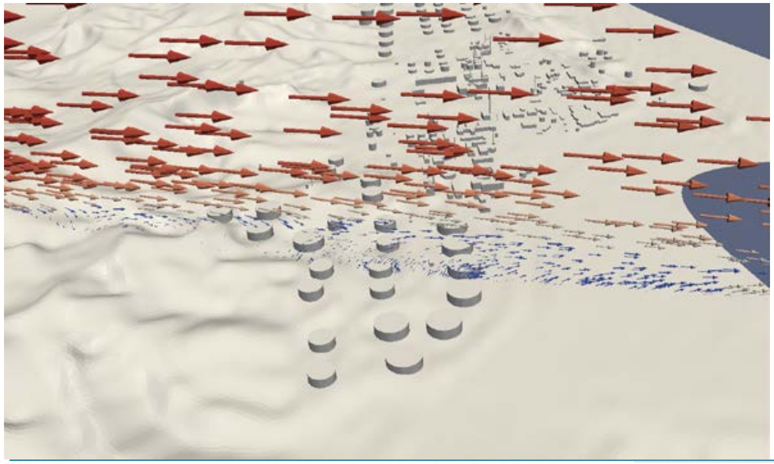
ÉCOLE CENTRALE LYON

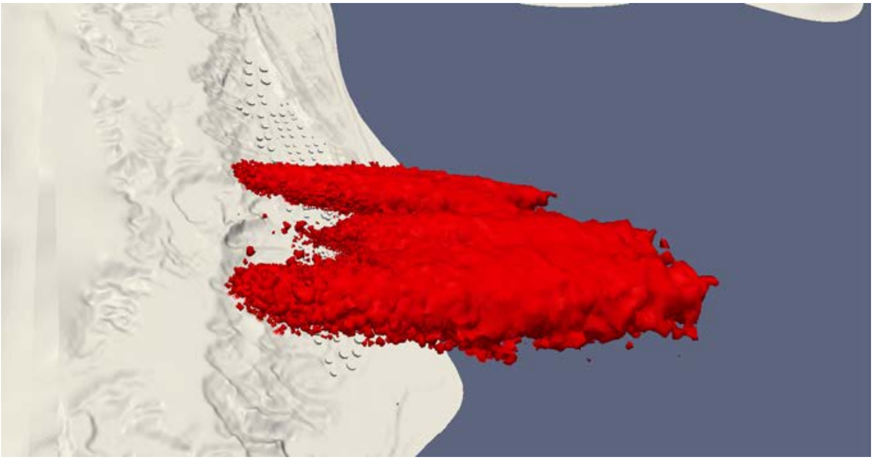
Safety Lagrangian Atmospheric Model (SLAM)

Safety Lagrangian Atmospheric Model

- On site resolution : 1 * 1m with description of buildings/ stacks
- Meteorological input : wind & turbulence measurements
- Flow computation : Computational Fluid Dynamic (FLUENT)
- Dispersion : lagrangian & passive (gas or PM) (SLAM)







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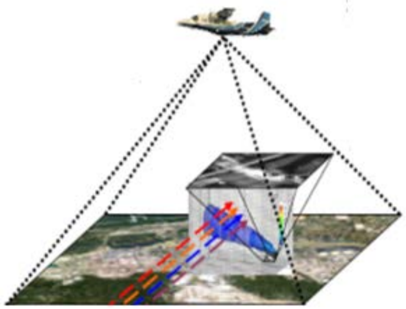
COMPARISON OF PM MEASUREMENT : FOLLOW THE PARTICLES LIFE

- Stack level : Focus on a specific emitter (Boiler) :
  - In stack measurement : Mass, primary and condensable PM

- In the Air : Focus on a specific emitter (Boiler) :
  - Mass quantification : Remote Optical measure with airborne H camera



- Ground impact : Multi source impact
  - Ground measurement : Concentration, Size, Composition

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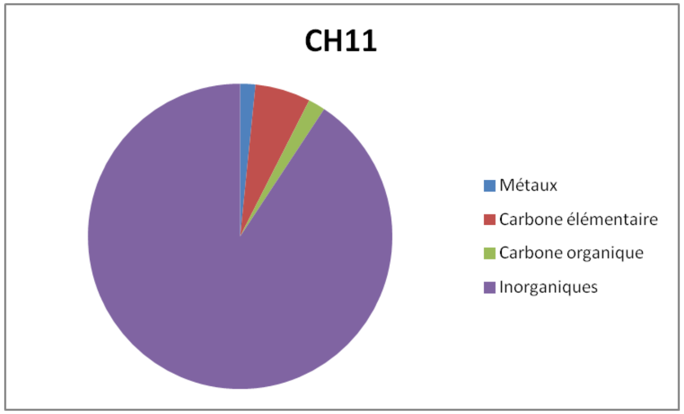
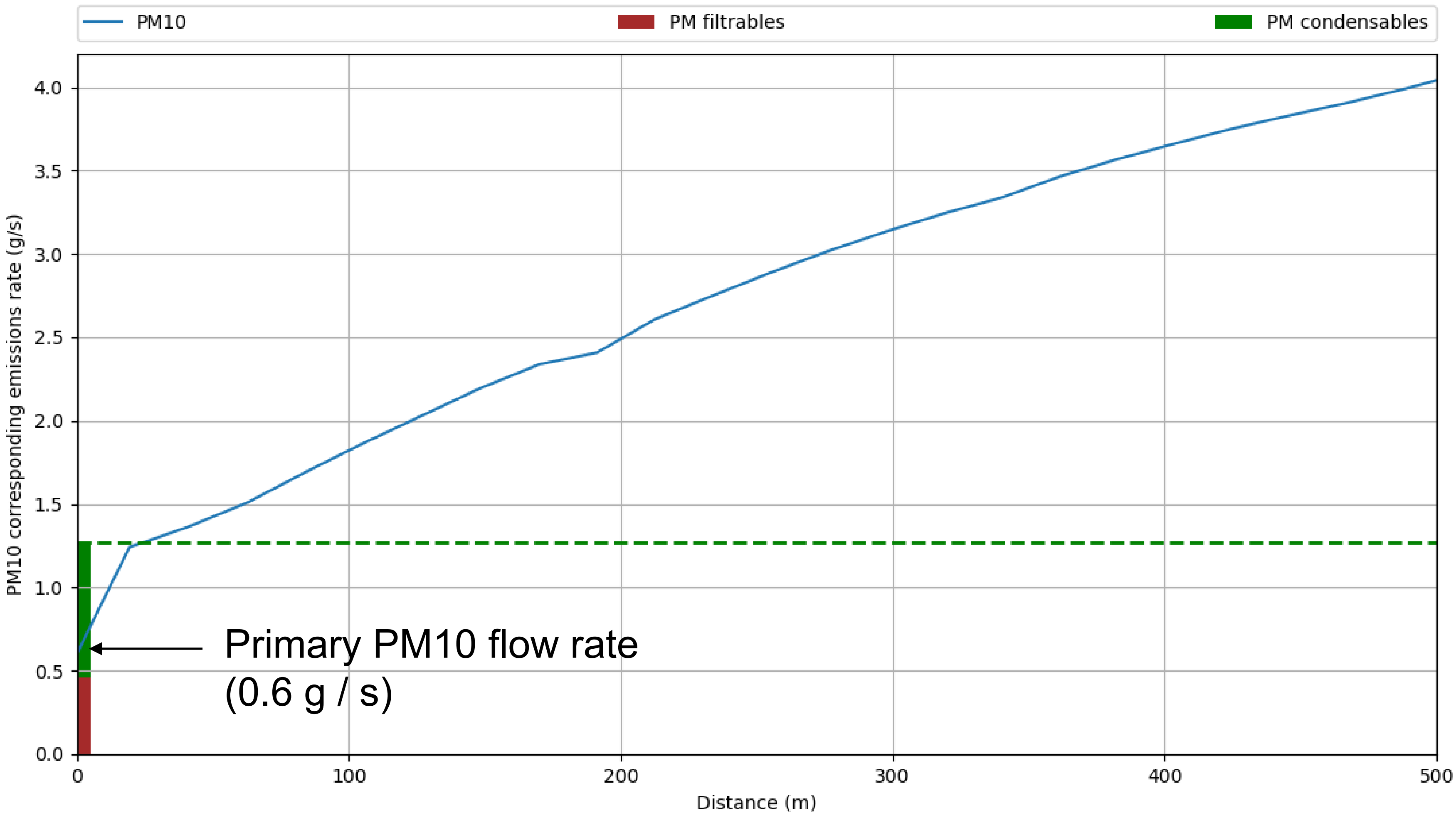
PM FLUX ESTIMATED BY STACK MEASUREMENTS

- In stack Measurements (US EPA Method 202): 39 kg/day filterable and 70 kg/ day condensable = 108 kg/day (1.25 g/s).
- Composition : 90 % sulfate, 8 % Black Carbon, 1 % OM + metals.

Classical PM sampling system
+
Condensation and second filter



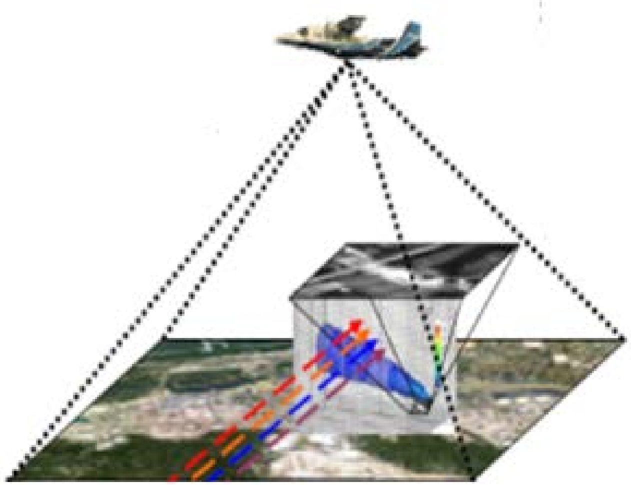
CTM Model Polyphemus PinG - PM10 concentrations + stack measurements



Method 202 measurement : Estimated flow rate at 20 m by model corresponding to the total PM filterable + condensables

COMPARISON OF MODEL RESULTS WITH AIRBORNE OPTICAL MEASUREMENT

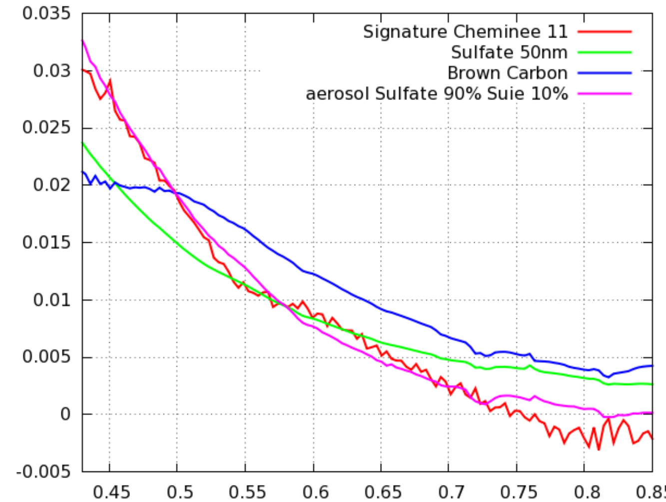
ONERA
THE FRENCH AEROSPACE LAB



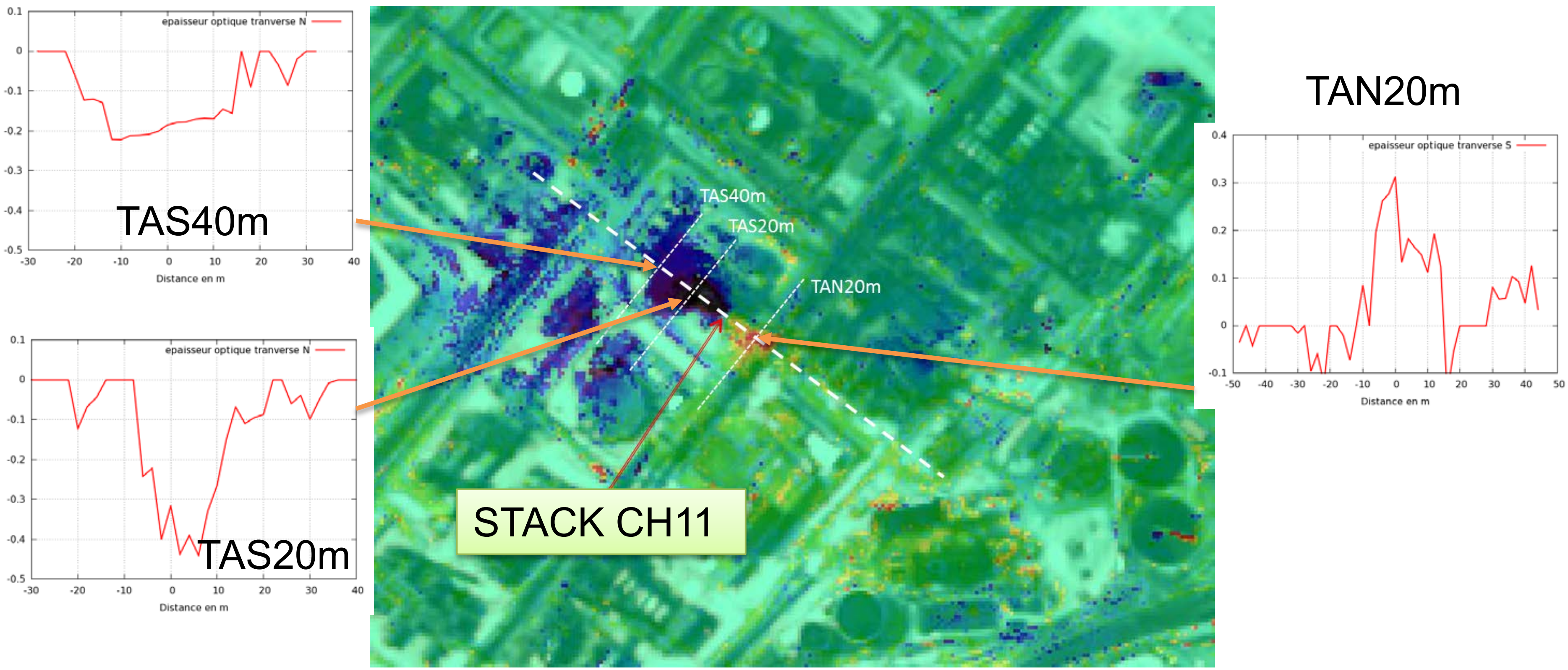
- Airborne hyperspectral measurements
- 3 flights per (sunny) day

Characteristics	HySpex VNIR	HySpex SWIR
Type of acquisition	Push-broom	Push-broom
Number of pixels	1600	320
Field of view	17°	14°
Spectral Interval	0,4-1 µm	1-2,5 µm
Number of spectral bands	160	256
Bandwidth	3,7 nm	6 nm
step on the ground (@ 2667m) perpendicular to the direction of flight	0,50 m	2,00 m
step on the ground (@ 2667m) parallel to the direction of flight	1,00 m	2,00 m
Swath at 2667m (height / ground)	800 m	640m

OPTICAL THICKNESS MEASUREMENTS OF BOILER PLUMES (CH11), 8/9 11H40



Selection of several plume transects for quantification : flux = mass * perpendicular wind at plume height



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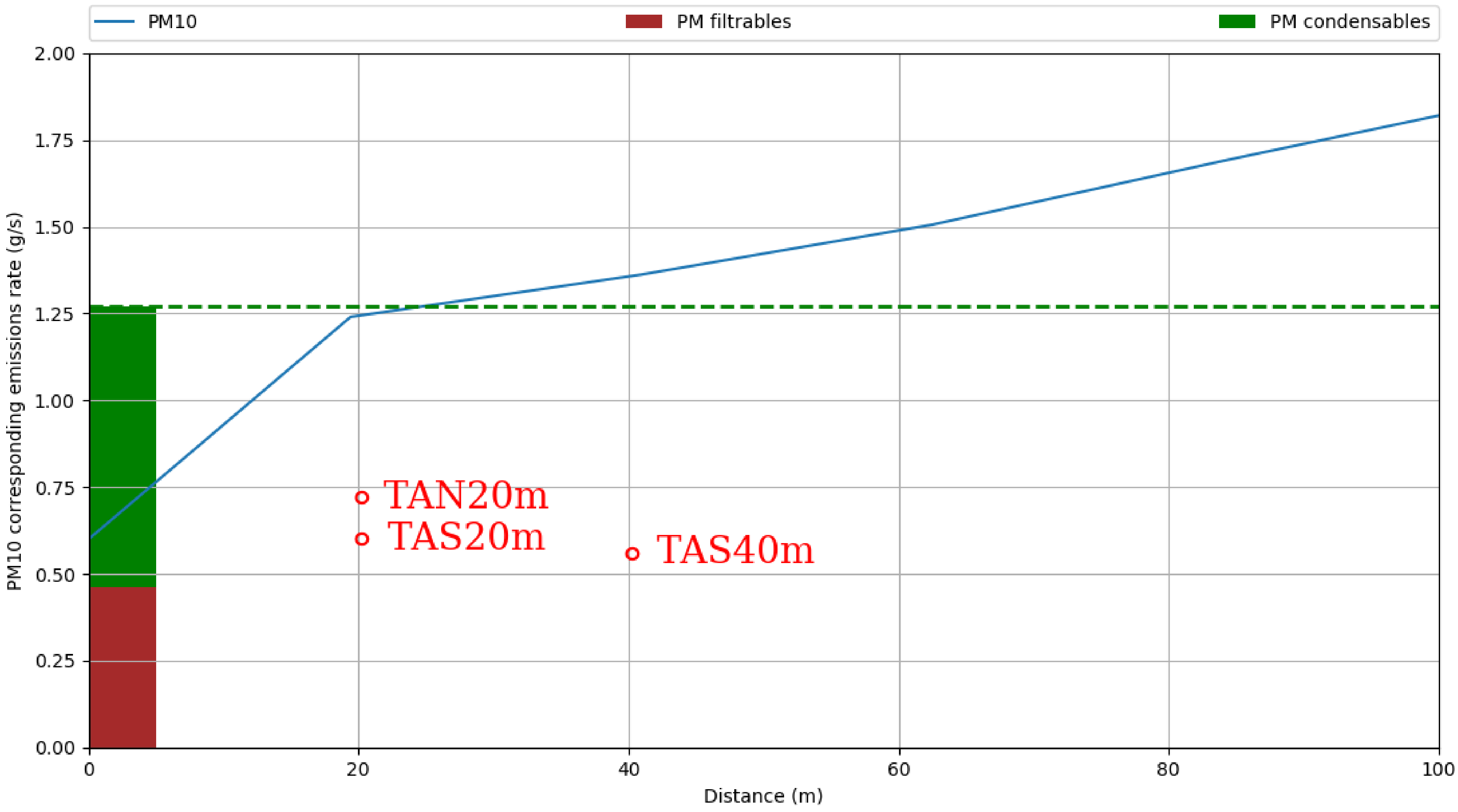
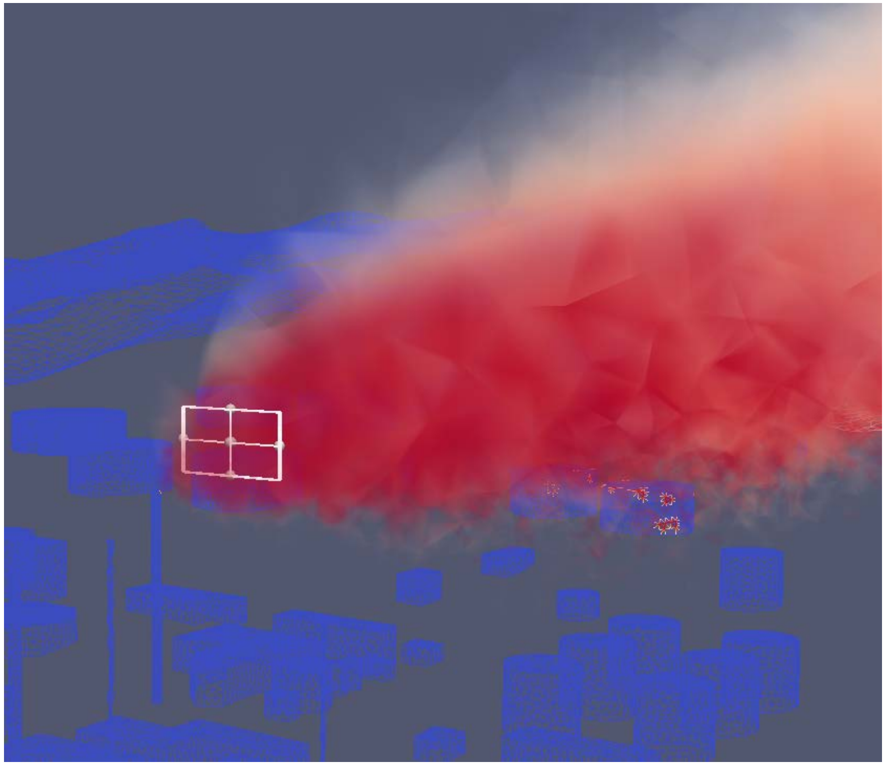
CTM Model Polyphemus PinG - Concentration in PM10 + measurement chimney + estimation flow by hyperspectral camera

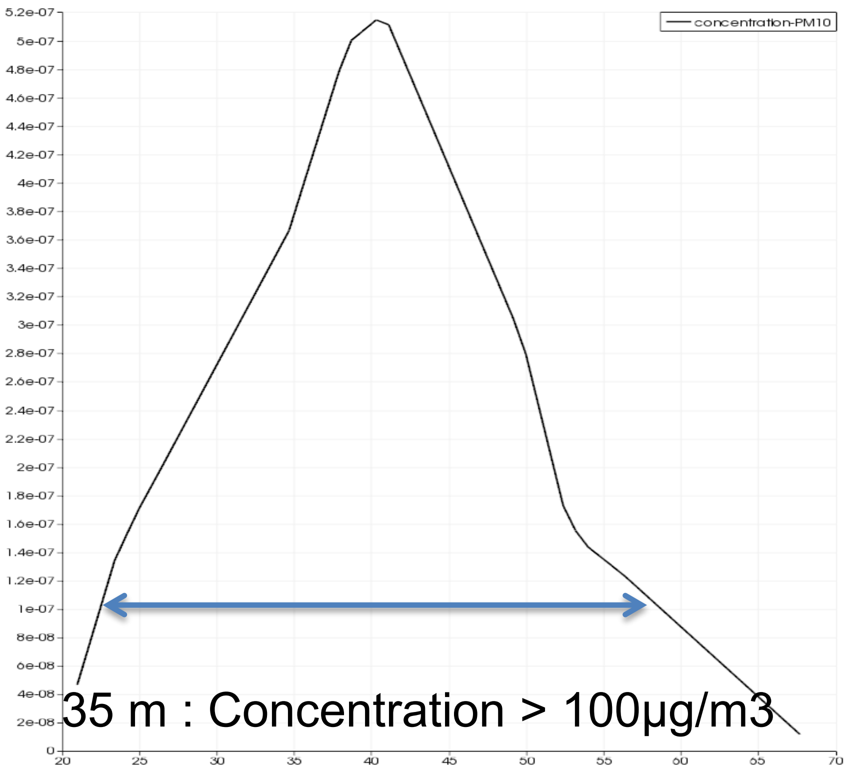


Aircraft Flight Measurements: Estimated Flow Rates Below Model Results and Filters, decrease with distance is related to baseline correction error.

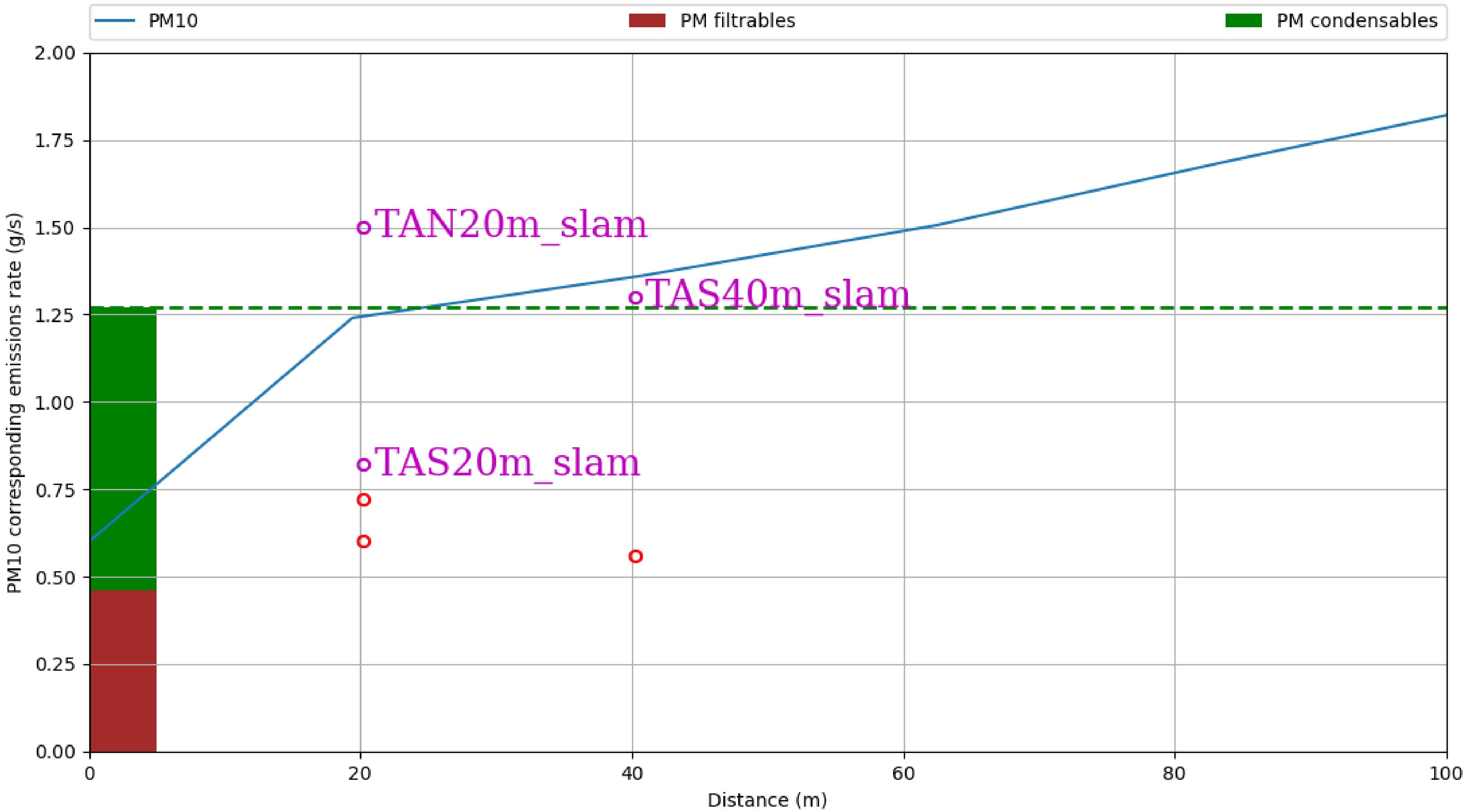
IMPROVEMENT OF OPTICAL MEASUREMENT WITH THE USE OF LOCAL MODEL

- In the Ping model, the plume is represented by gaussian puffs, which is correct except in the first 100 meters (too simple).
- The lagrangian model SLAM is used to reproduce the initial plume shape.
- SLAM does not reproduce the chemistry, only the dispersion of primary PM



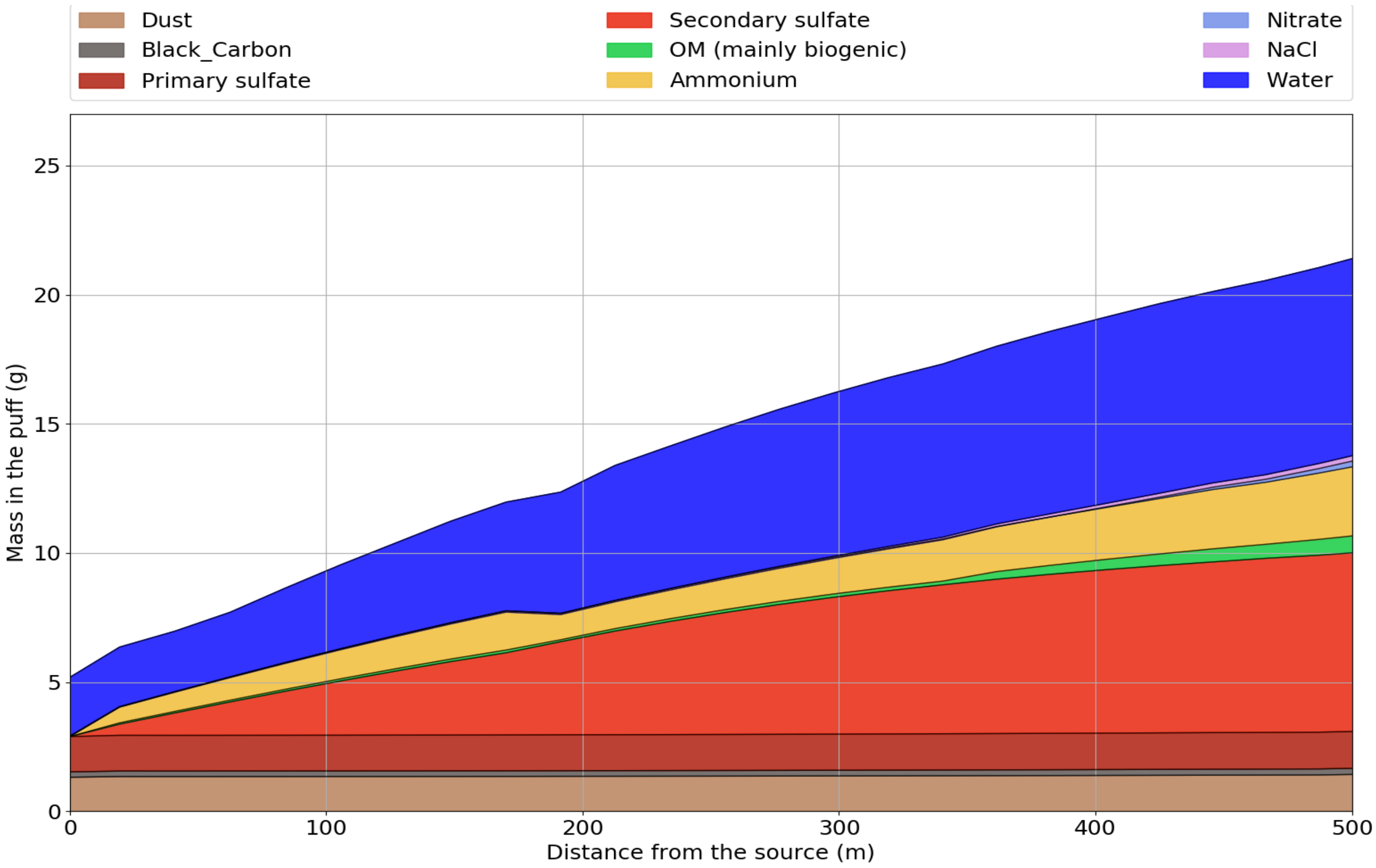


CORRECTION OF HYPERSPECTRAL OBSERVATION USING DISPERSION AND MODELING



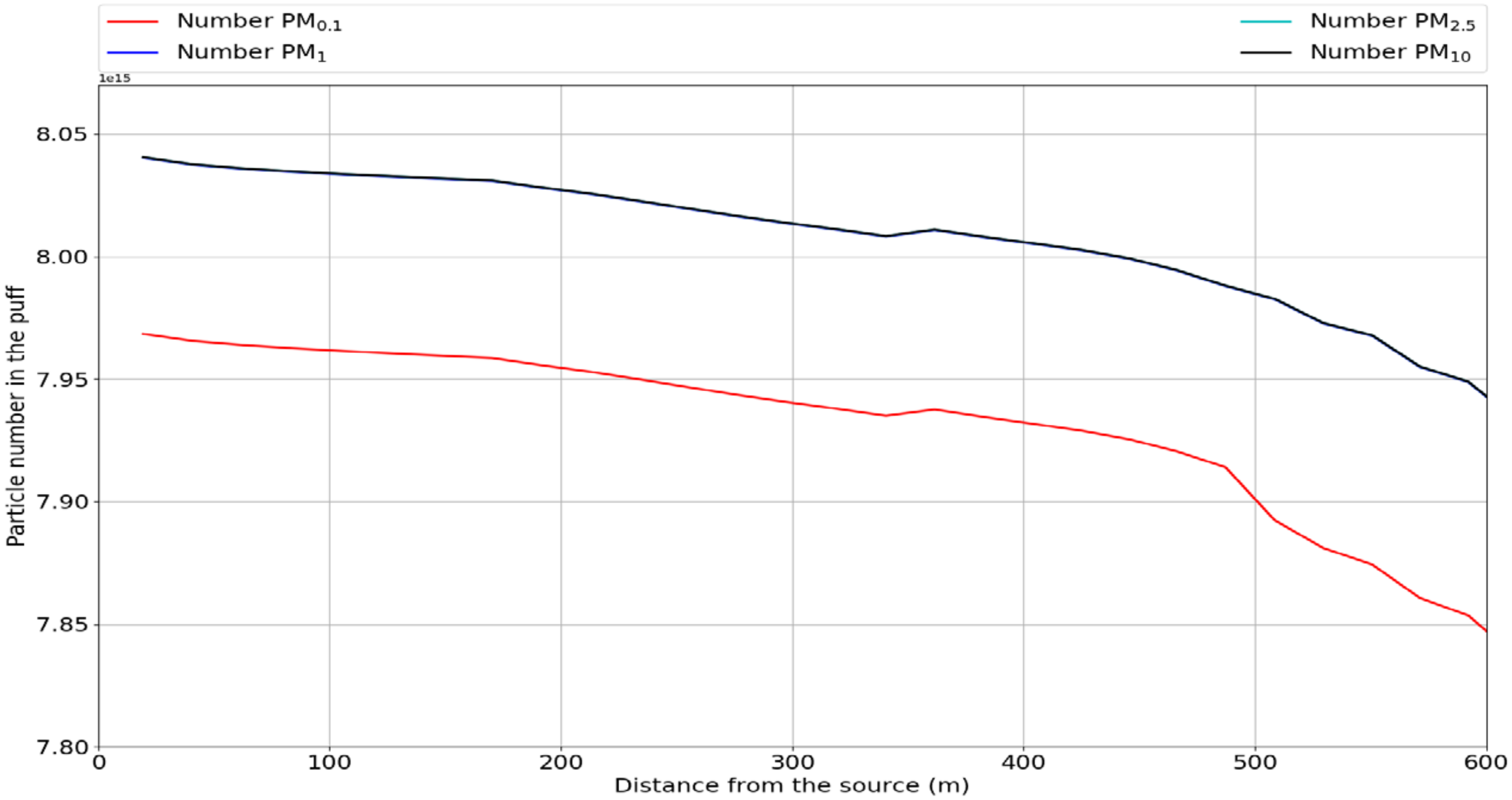
Correction of fluxes with SLAM results: Increased estimated flow with distance, consistent with Polyphemus results and condensable PM measurements

EVOLUTION OF PM COMPOSITION IN THE PLUME



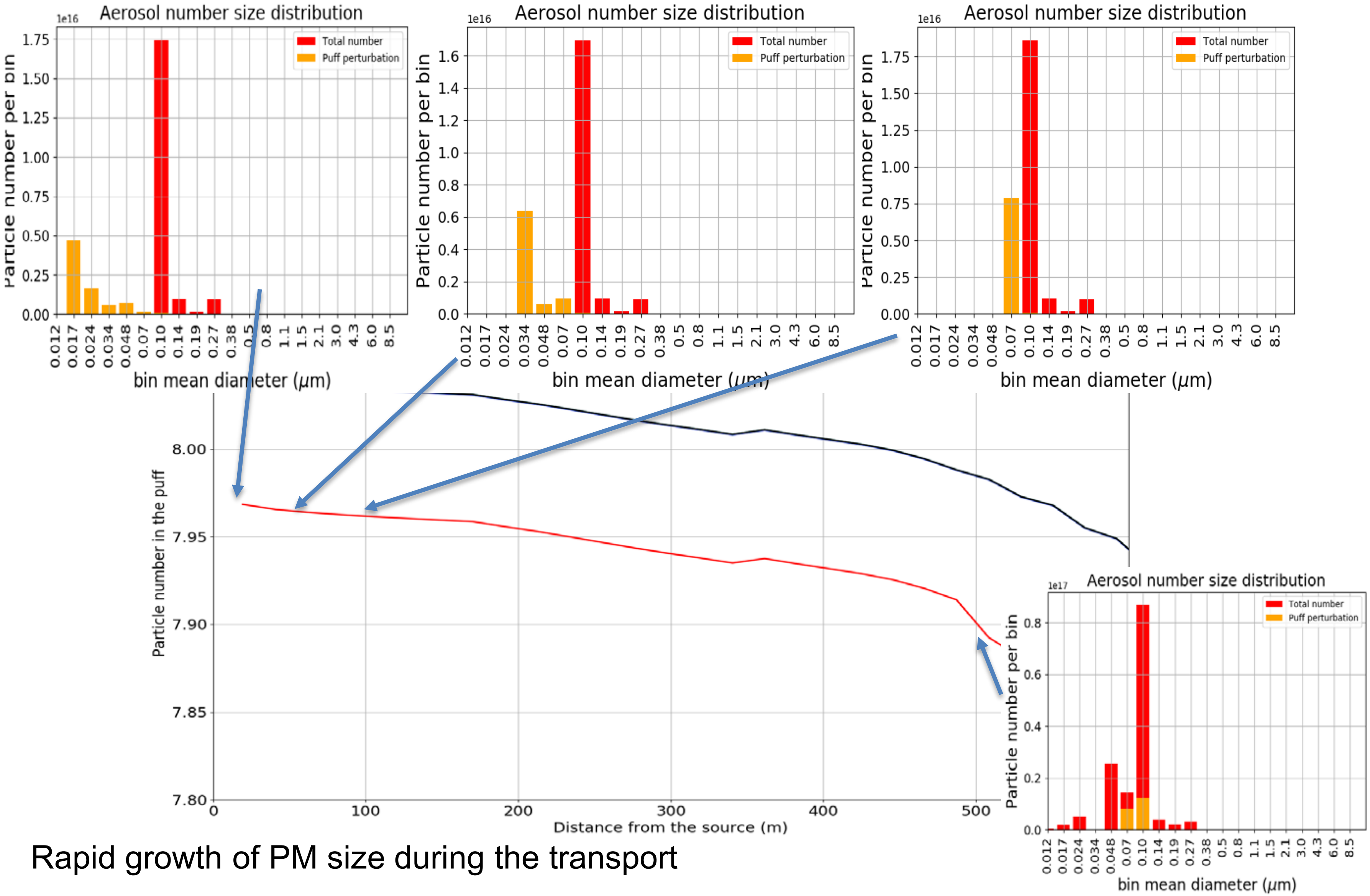
- Emitted PM mainly composed of sulfate : high absorption of water into the PM phase
- First 100m : Formation of ammonium sulfate, reaction between H2SO4 present in the puff and NH3 present in the background
- Low formation of nitrate and OM during the entire plume lifetime

EVOLUTION OF PM NUMBER IN THE PLUME



- Decrease on PM number when the distance from the source increases
- PM number is dominated by PM1, with 98% in PM0,1

EVOLUTION OF PM SIZE IN THE PLUME

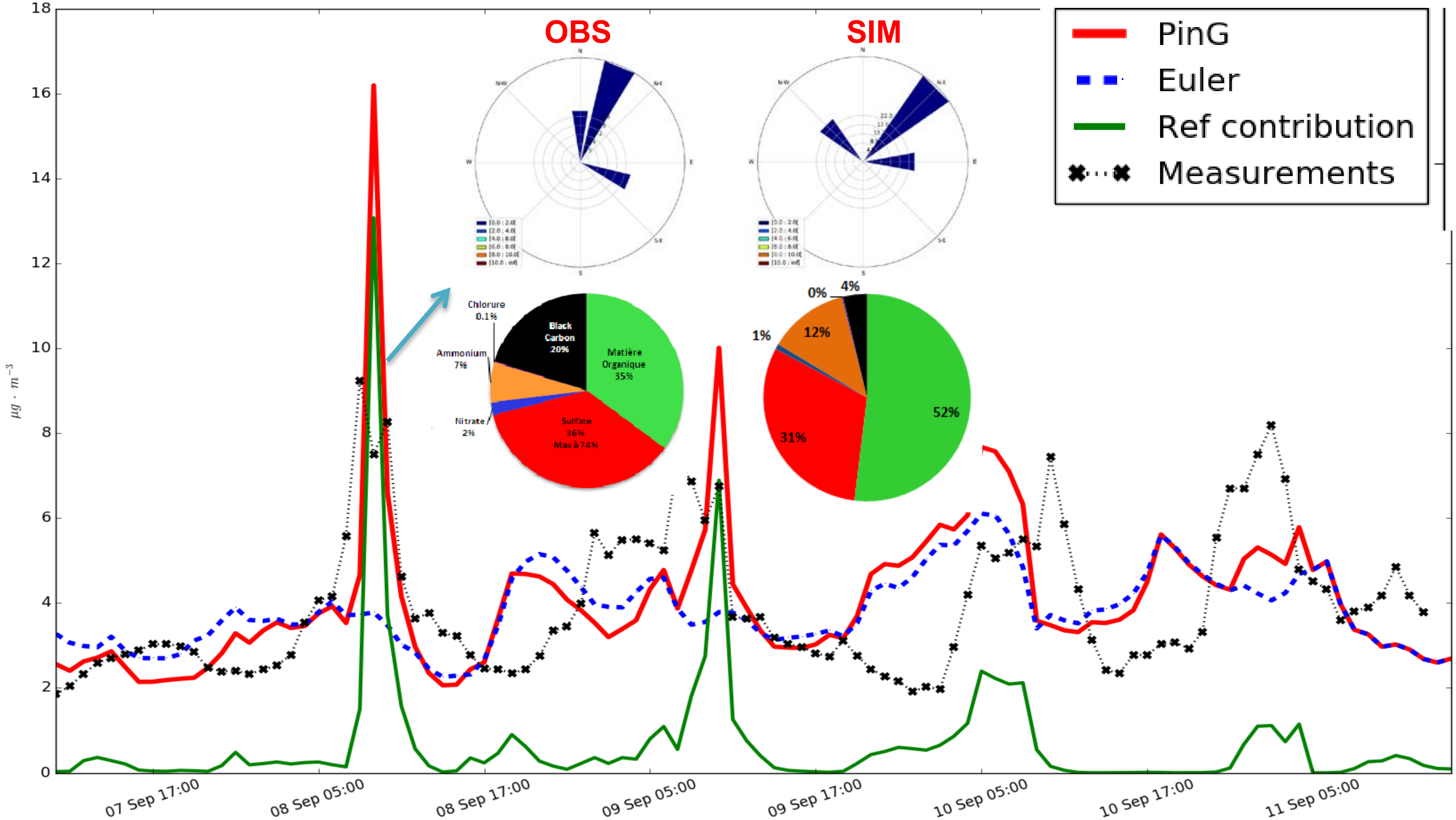


- Rapid growth of PM size during the transport
  - PM sizes in the plume are comparable to the background after 500m of transport

COMPARISON WITH GROUND LEVEL CHEMICAL/PHYSICAL OBSERVATIONS

Instruments	Measurements	Frequency
SMPS Scanning Mobility Particle Sizer	Particles number /cm^3 as a function of granulometry (15 to 660 nm with 106 sizes)	5 min
OPC Optical Particle Counter	Particles number /cm^3 as function of granulometry (0,265 µm to 34 µm with 30 sizes)	1 min
LAAP-TOF Laser Ablation Aerosol Particle with Time of Flight Mass Spectrometry	Size and chemical composition particle by particle between 300 nm - 5 µm diameter	2 min
AMS Aerosol Mass Spectrometer	Chemical composition : sulfate, nitrate, ammonium, organic matter for particles diameter < 450 nm	2 min
MAAP Multi Angle Absorption Photometer	Black Carbon	1 min
PTR-MS (TOF) Proton Transfer Reaction – Mass Spectrometry	VOC SPECIATION	1 min

PM COMPOSITION: POLYPHEMUS COMPARISON TO AMS (< 0,45 µm)

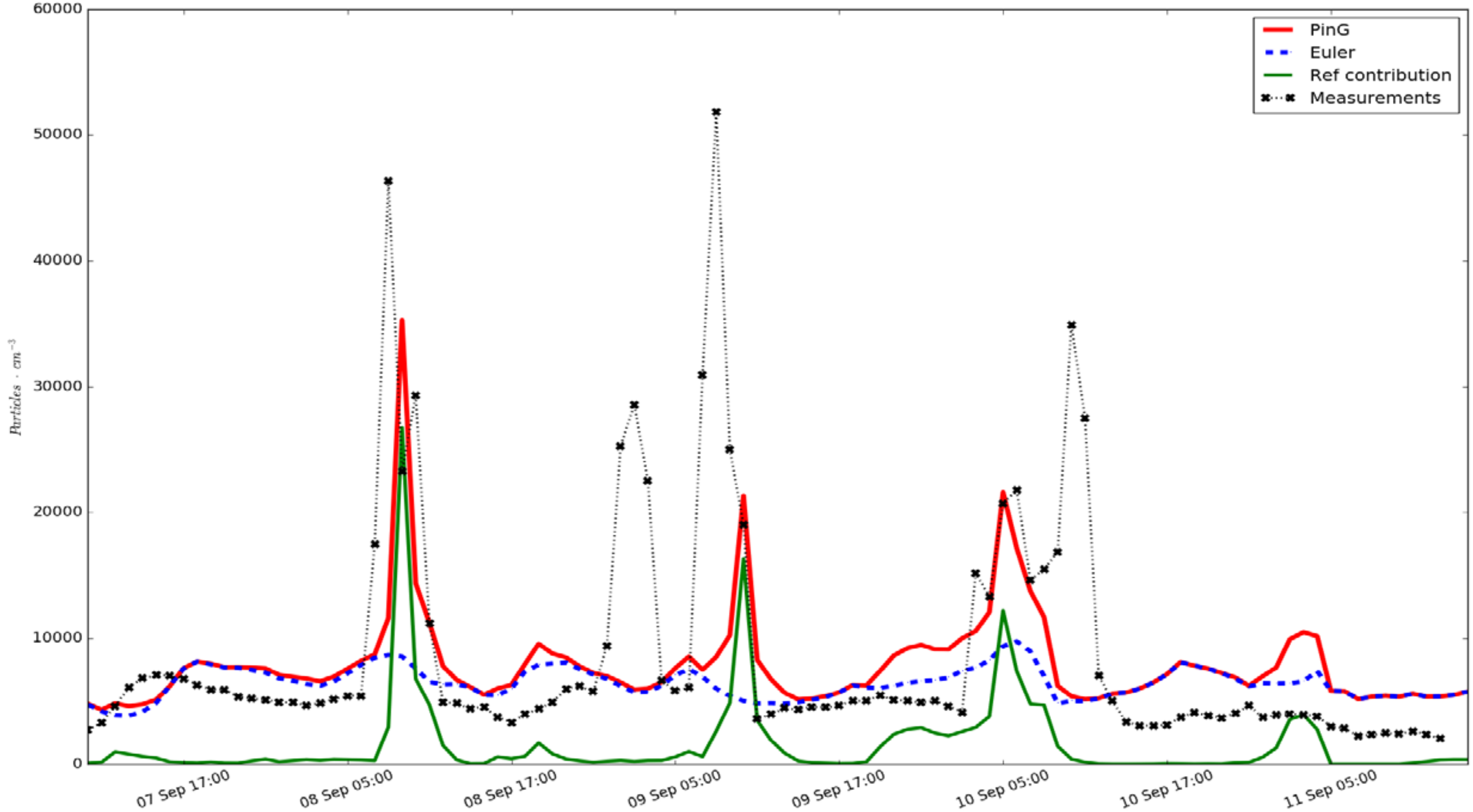


Evaluation of modeled PM compositon:

- Good simulation of the sulfate fraction (characteristic of refining activity)
- OM fraction is over-estimated, and BC is underestimated due to uncertainties in the emission inventory

EVALUATION OF PM NUMBER CONCENTRATION

- Comparison of modeled PM number to SMPS measurements (< 0,16 µm)

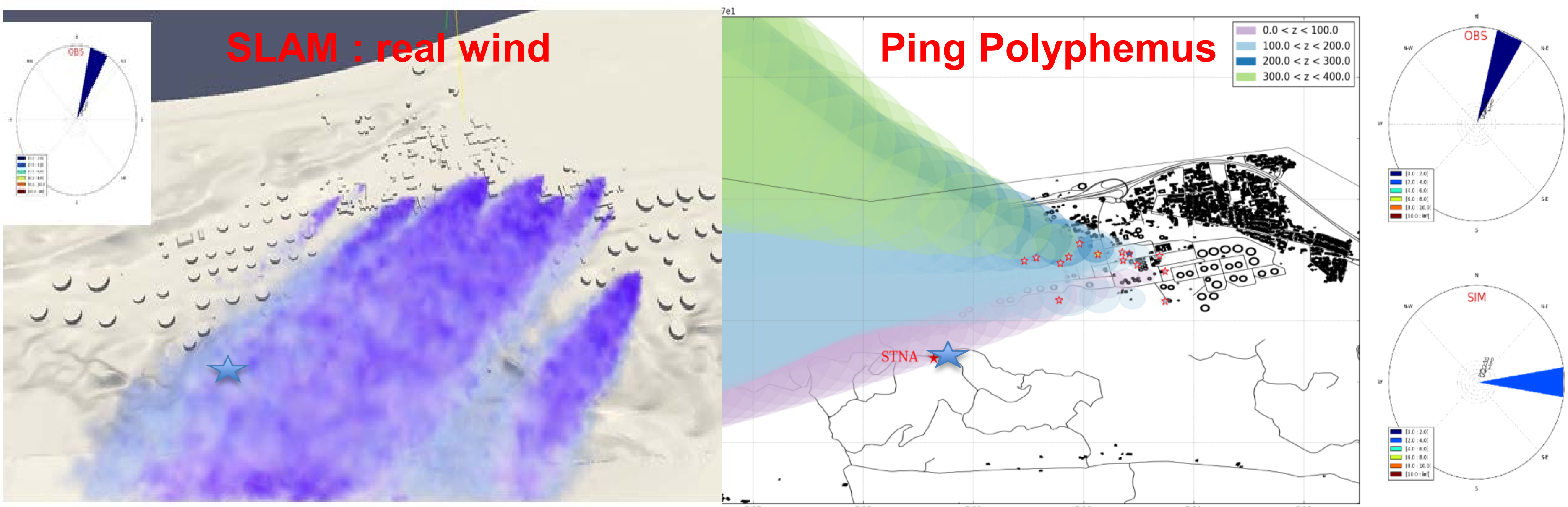


- Good reproduction of PM number in the smallest size sections (15 to 685 nm):
  - Modelled contribution in peak period: 30 000 particles/cm^3
  - Underestimation of measured peaks

IMPROVEMENT OF COMPARISON WITH LOCAL MODEL

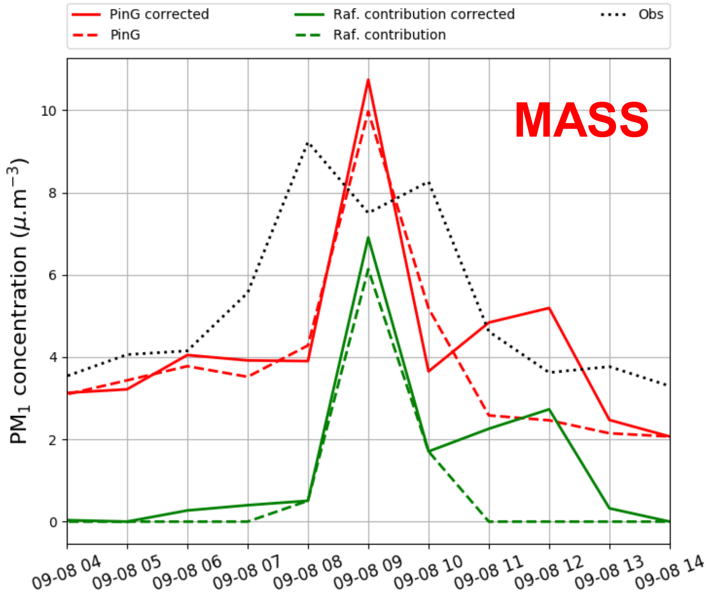
- CTM model uses 3D modeled meteorological field, and despite the assimilation with local stations and wind-Lidar measurements, significant errors in local wind direction represented by the meteorological mesoscale model (WRF) can still be noticed.

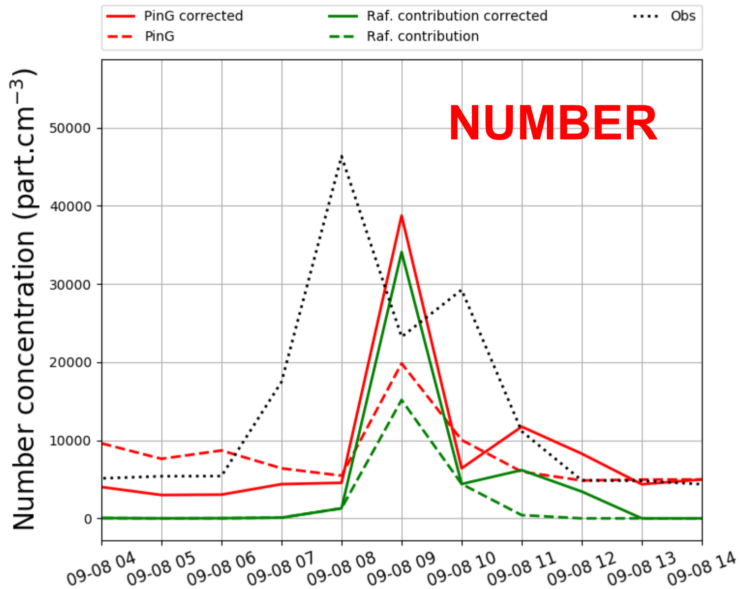
- With SLAM, use of wind measurement allows a more realistic determination of the impacted area : improved comparison with ground measurements.



IMPROVEMENT OF COMPARISON

- Comparison with the correct wind direction (impact of west stacks) gives a better comparison.





- Other improvements in progress : need to change the PM granulometry at emission level : smallest particules …

- Number representation is improved if you simulate the right plume. Classical issue of ground level comparison, not the case with optical measurements

CONCLUSIONS

- In comparison of field measurement, the Polyphemus PING model is able to reproduce mass, composition and size evolutions of Particulate Matter in industrial plumes.

  - PM Flux estimation using hyperspectral measurements gives realistic estimations but requires a complex background correction, especially above industrial sites in case of “moderate” emissions (100 kg/ day).

  - Lagrangian local scale modeling of the plume :
    - Improves remote sensing quantification (instantaneous & background)
    - Avoid Mesoscale model error .

- Refinery boiler plume present a rapid evolution :
  - Decrease of number, size bin comparable to background after 500 m
  - Increase of mass, and composition evolution