

# Modeling of Organic Aerosol during the MEGAPOLI Summer Campaign in the Paris Region

## *CHIMERE - Volatility Basis Set approach*

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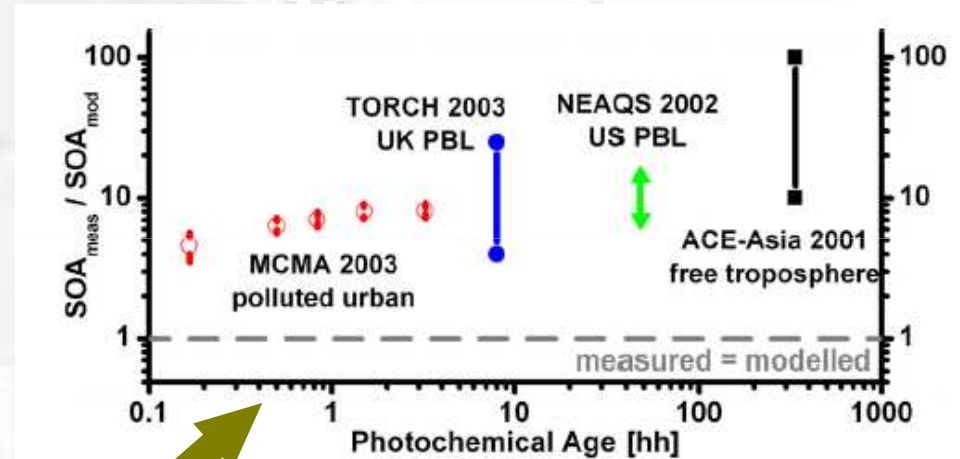
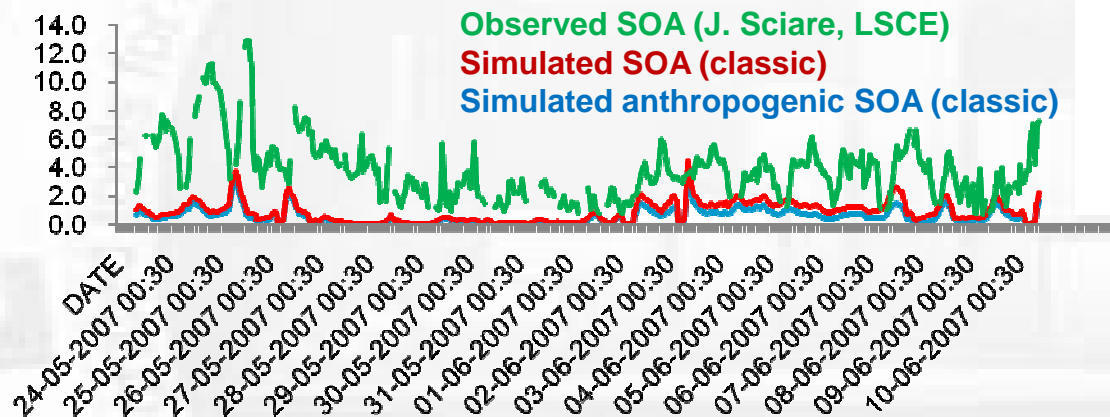
**\* Also Aria technologies**

# Context & Objective

- SOA (Secondary Organic Aerosol):  
under-estimated in Chemistry  
Transport Models

Comparison Model / Measurement, 05/2007-06/2007

LHVP, (urban MEGAPOLI site)



Volkamer et al., GRL, 2006

**MEGAPOLI Paris Campaign:** Quantify primary and secondary sources of organic aerosols, in urban and in plume

**Objective:** Improve simulation of SOA in CHIMERE (regional CTM)

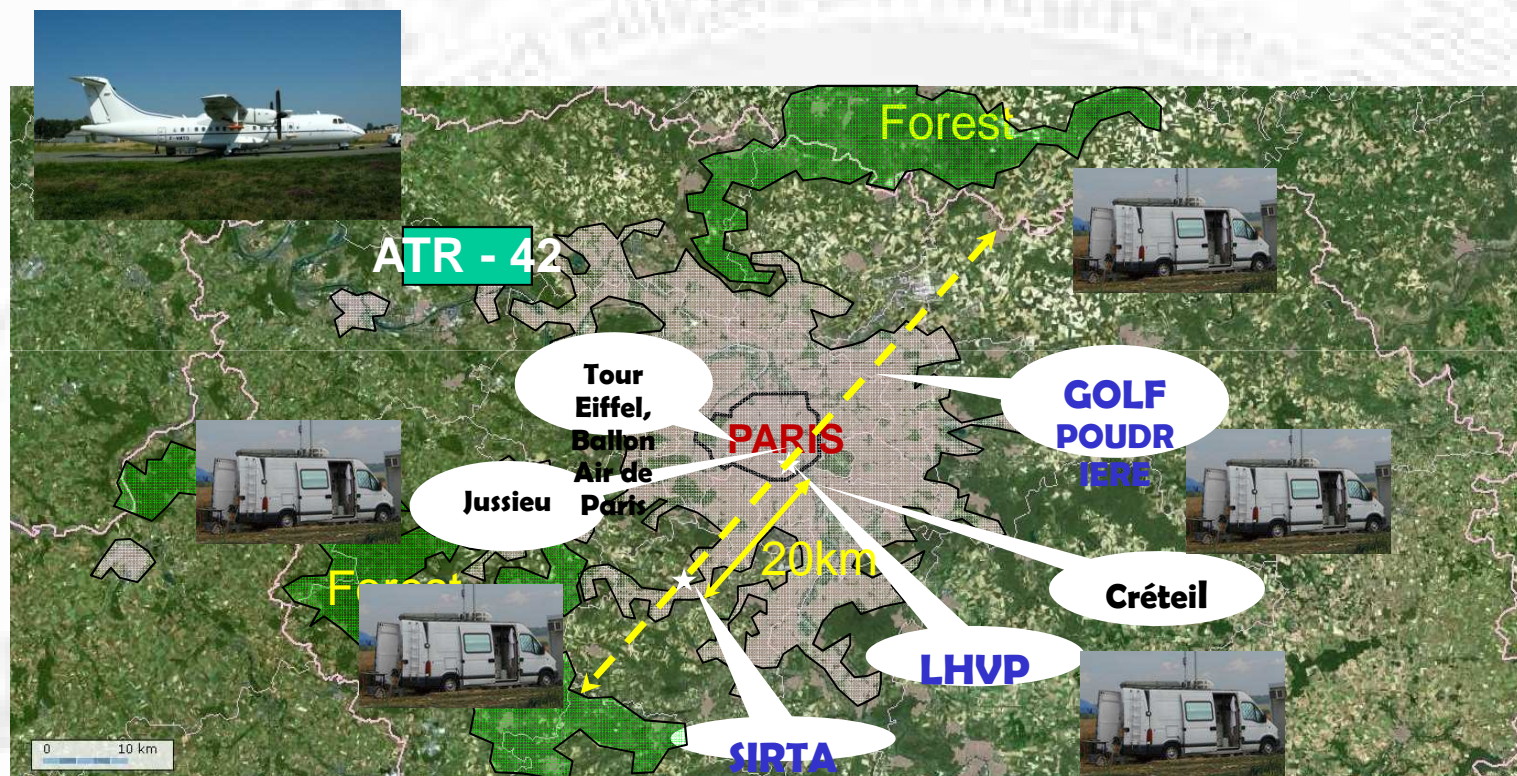


**Volatility Basis Set approach (VBS)**

Robinson et al., 2007      Lane et al. 2008

**Compare with MEGAPOLI measurements**

# MEGAPOLI Campaign - Measurements



Matthias.BEEKMANN  
(Tuesday 14h,  
Harmo13)

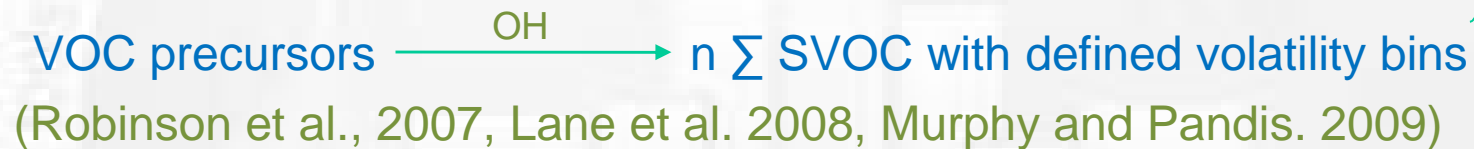
- 3 primary sites** => suite of *in situ* measurements / + meteo at SIRTA.
- 3 secondary sites** => lidar and spectroscopic measurements / or in situ
- 3 mobile labs** => full in situ measurements (PSI + MPI) + Univ Duisburg
- 1 mobile lab** => lidar measurements (CEA)    **1 mobile lab** => MAXDOAS (MPI)
- 1 aircraft ATR-42** => full in situ measurements (SAFIRE, CNRS, MPI)

# SOA scheme in CHIMERE

- **Classic scheme based on “two-product” approach of Odum et al. 1996**

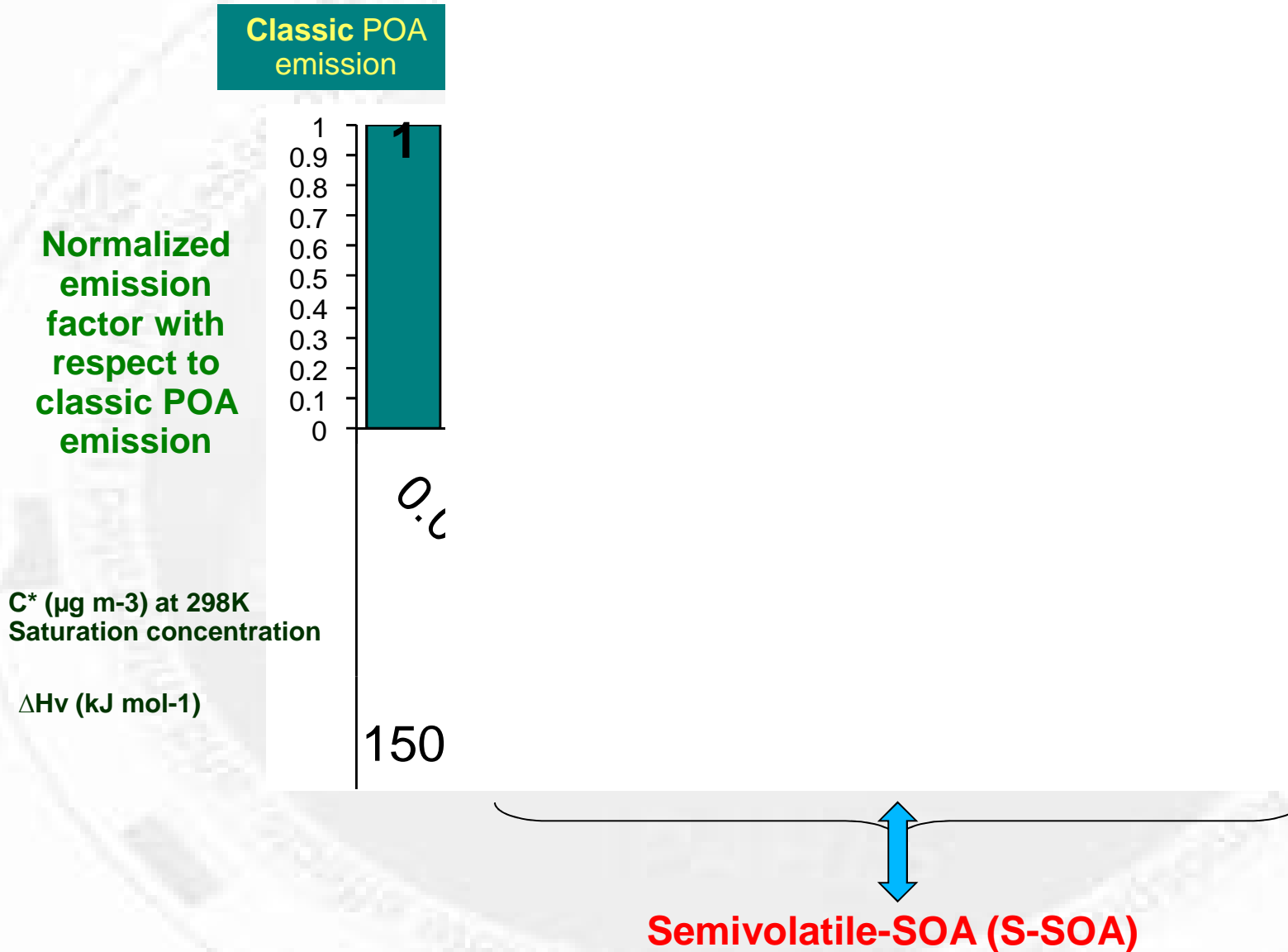


- **VBS « Volatility Basis-Set » approach**

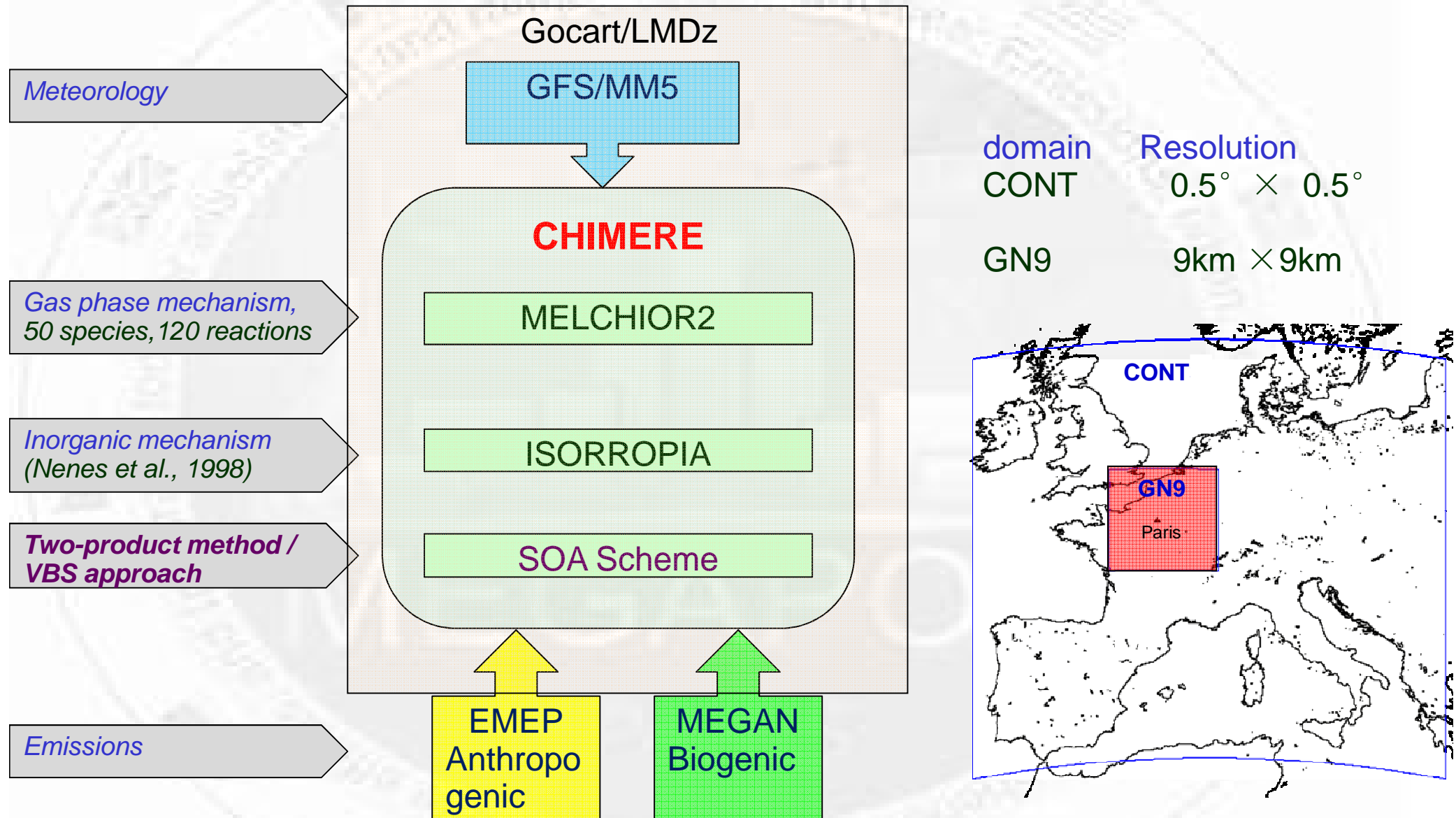


Phase transfer → Aerosol

# VBS approach main features



# Model configuration



# Model simulations

- × Simulations with classic scheme (POA non-volatile)
- × Simulations with VBS

**Total SOA=Oxygenated OA**

<b>Semivolatile-SOA</b>	<b>Anthropogenic SOA</b>	<i>Biogenic SOA (BSOA)</i>
<b>VBS</b>	<b>VBS</b>	<b>Classic</b>
Partitioning of POA emissions (SVOC) + additional IVOC	Lumped VOC (Aromatics, Higher Alkanes, etc.) according to SAPRC □ 4 volatility bins	Isoprene, Terpene, $\alpha$ -pinene, $\beta$ -pinene, Limonene, Ocimene, Humunene
Chemical aging	Chemical aging	

(Robinson et al., 2007, Murphy and Pandis. 2009)

(Lane et al. 2008)

(Pun and Seigneur, 2006; Bessagnet al. 2008)

# AMS measurements

## Aerodyne aerosol Mass spectrometer (AMS) → Organic Aerosol (OA=POA+SOA)

LHVP: by IFT (urban site)

Preliminary simplified PMF (Positive Matrix)

Factorization (Poor man's PMF)

→ Hydrocarbon-like Organic Aerosol (HOA)

→ Biomass Burning Organic Aerosol (BBOA)

HOA+BBOA ⇔ Primary Organic Aerosol (POA)

→ Oxygenated Organic Aerosol (OOA)

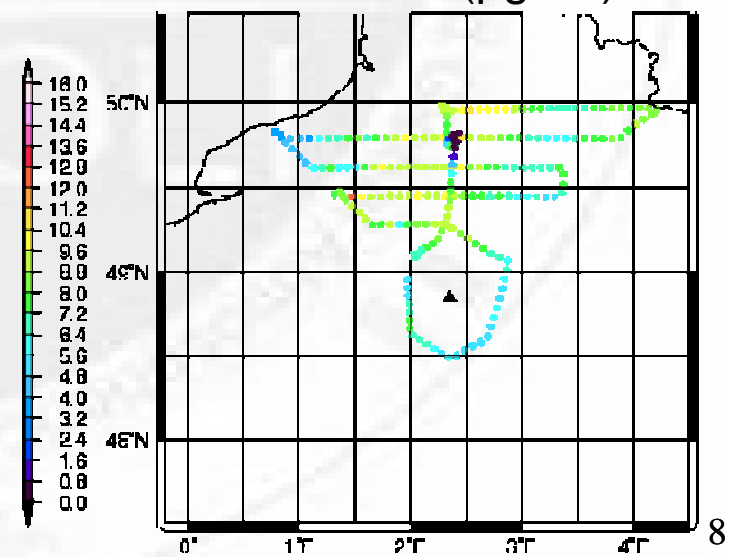
OOA ⇔ SOA(S-SOA+ASOA+BSOA)

SIRTA: upwind of Paris agglomeration, by PSI  
(suburban site)

Flight: by LaMP



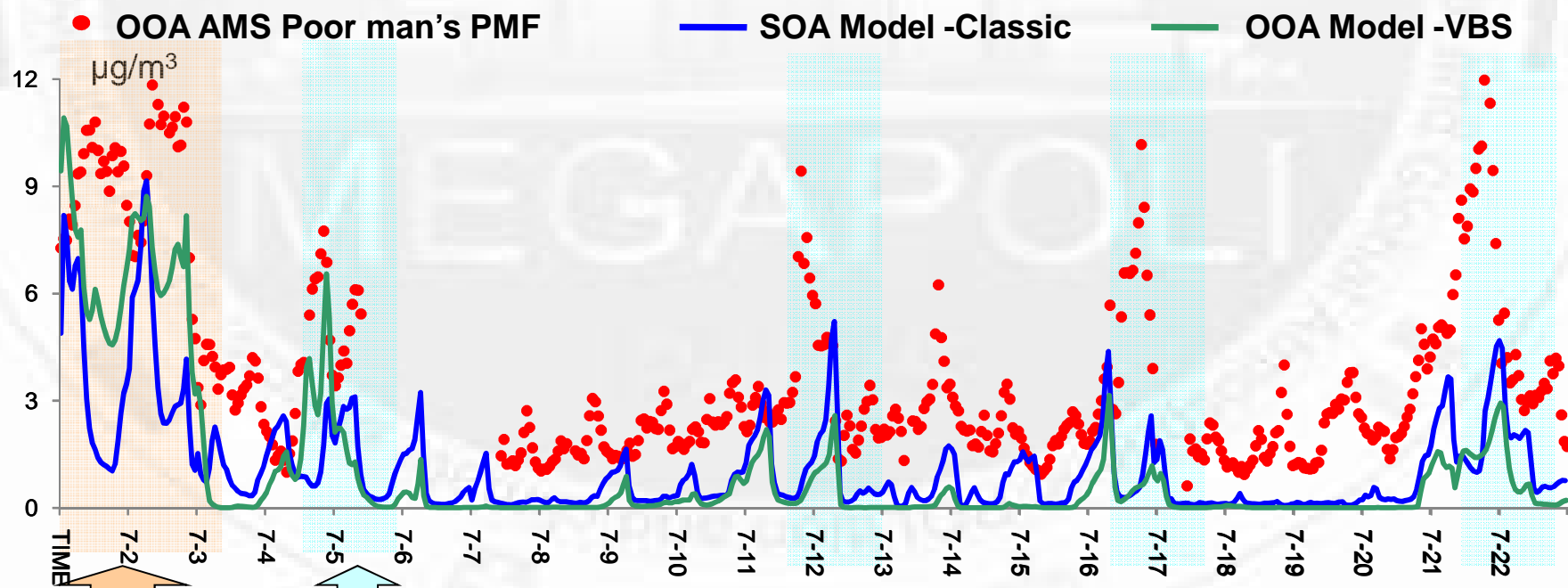
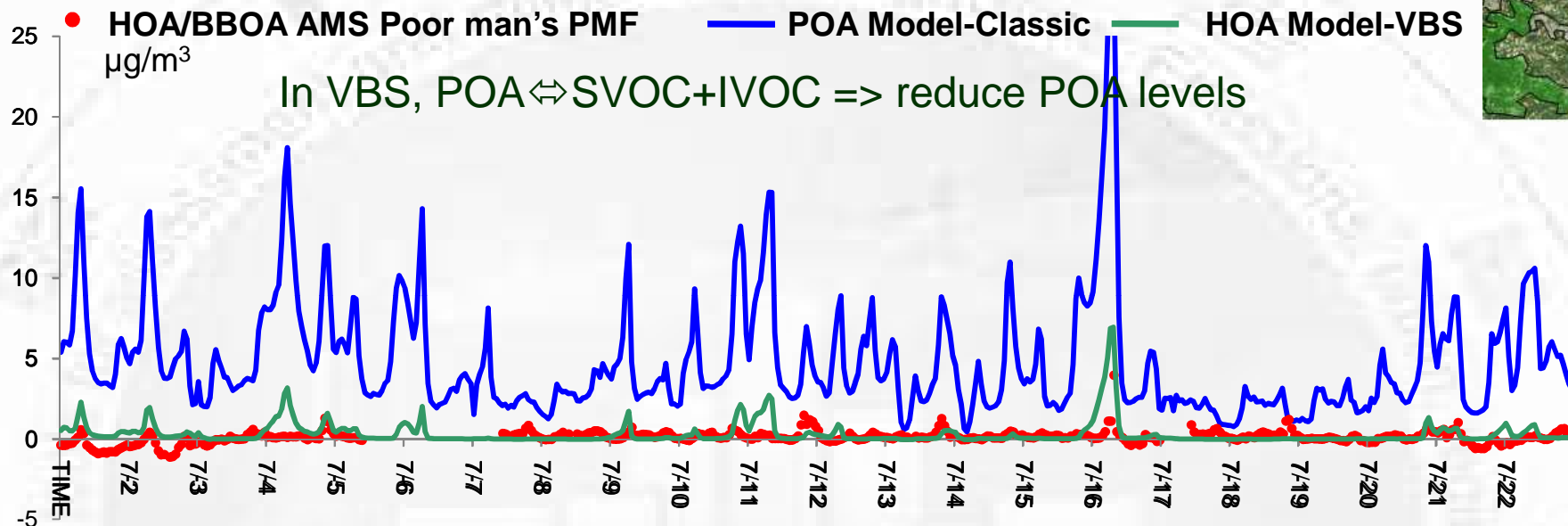
OA - LaMP ( $\mu\text{g}/\text{m}^3$ )





# Simulation results (LHVP-Urban site)

## vs. ground based AMS measurements



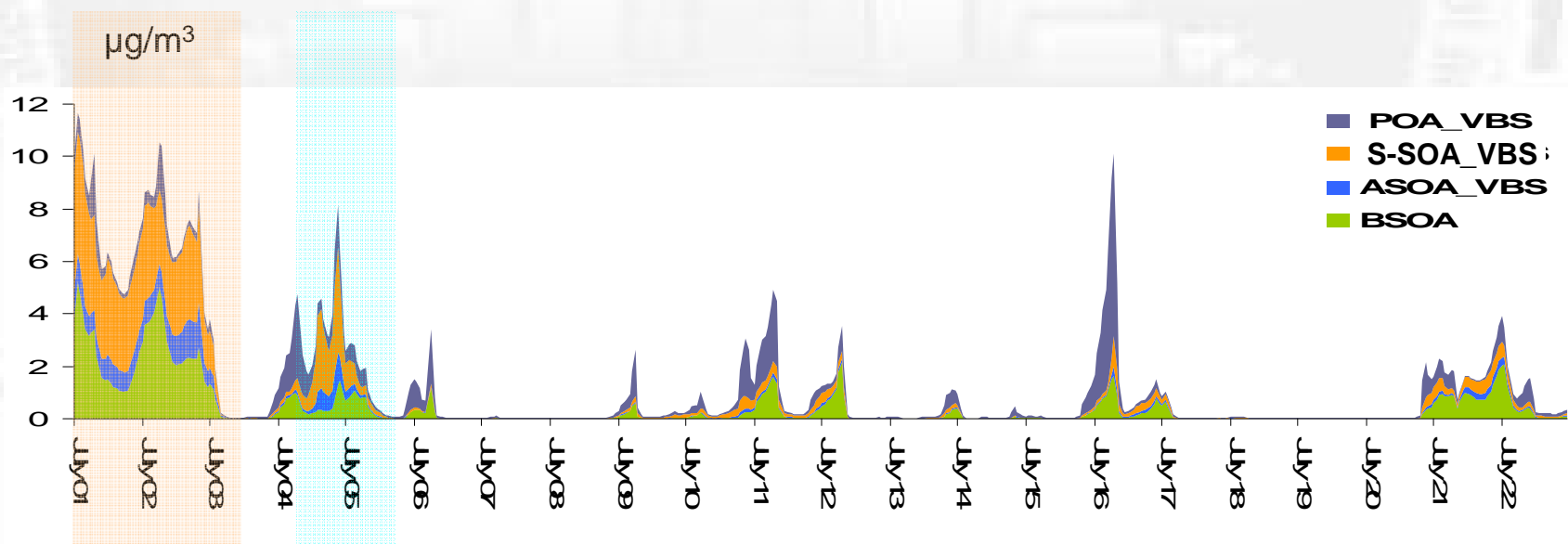
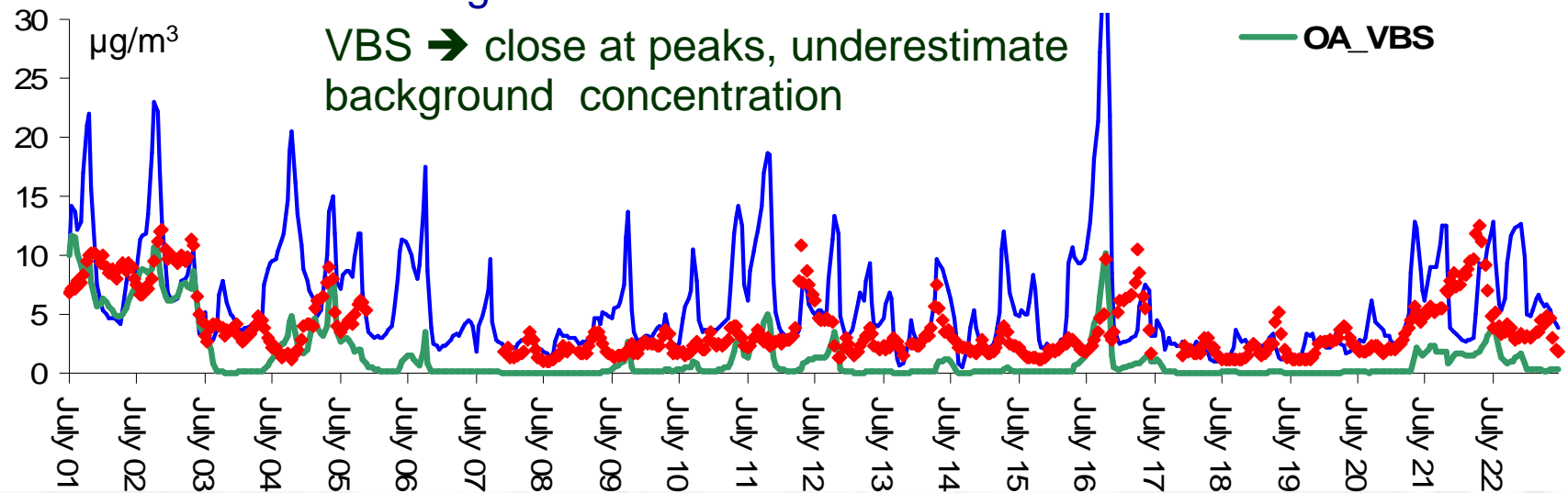
# OA = HOA+OOA

(LHVP-Urban site)

Continental

Classic → over-estimate peaks, close at background concentration

VBS → close at peaks, underestimate background concentration



S-SOA+BSOA

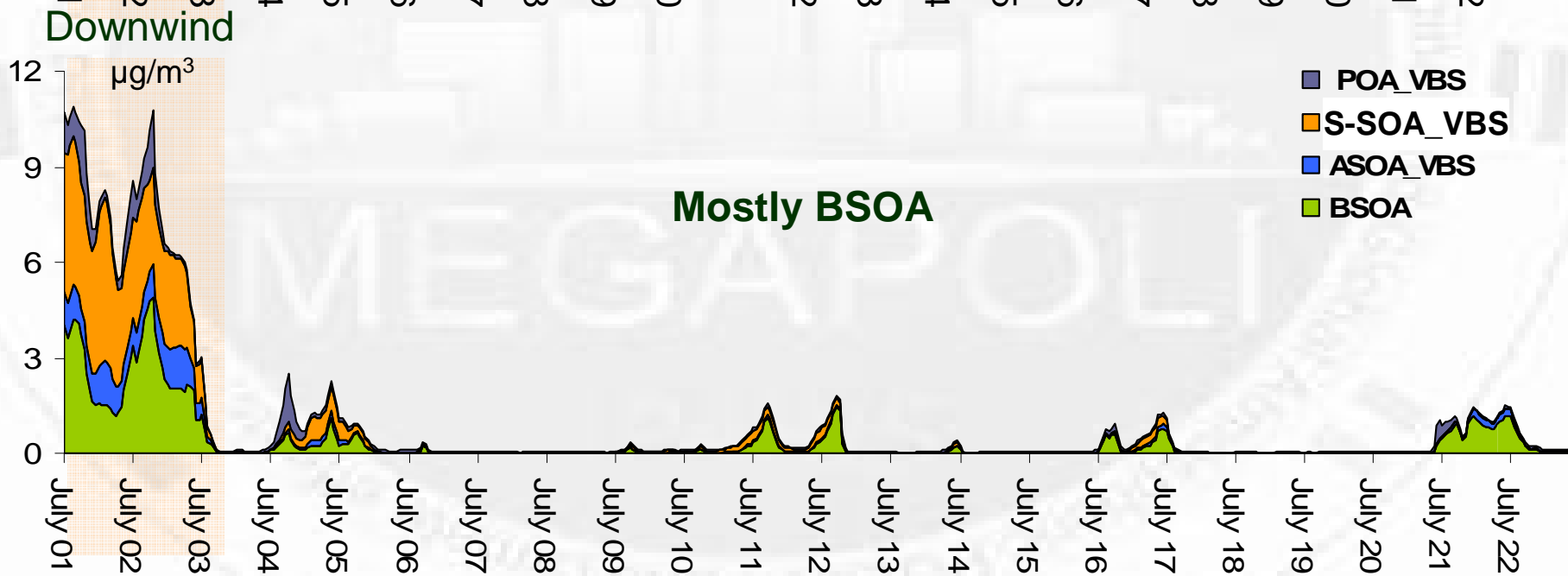
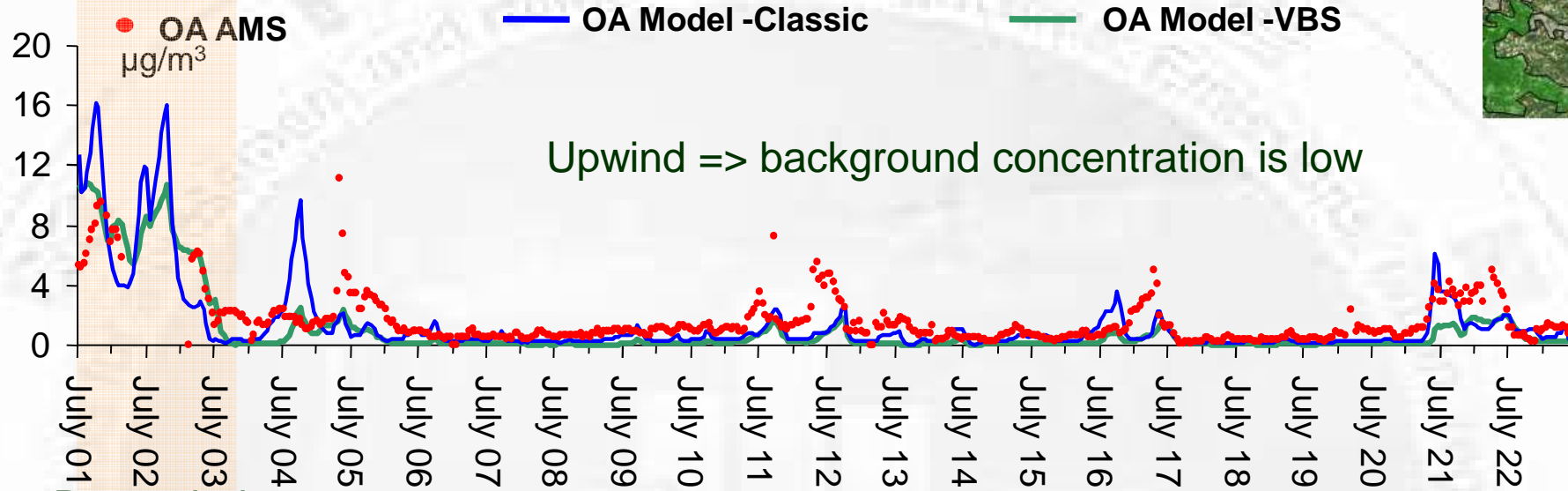
POA+BSOA

# Simulation results

(SIRTA-Suburban site)

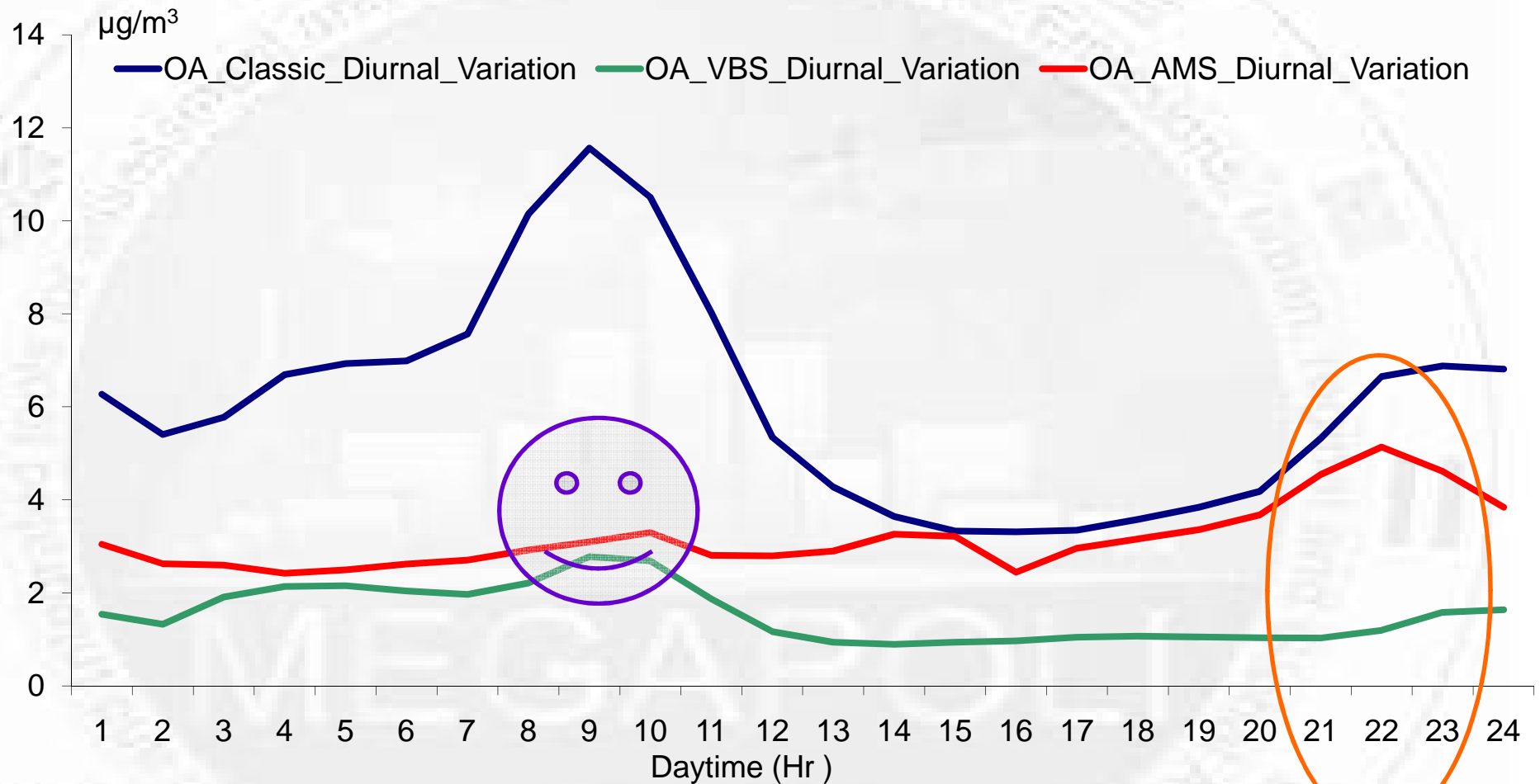


## vs. ground based AMS measurements



↑  
**Continental**

# Diurnal Variation of OA (LHVP-Urban site)



## Classic scheme:

Wrong morning peak due to primary emissions (non-volatile)

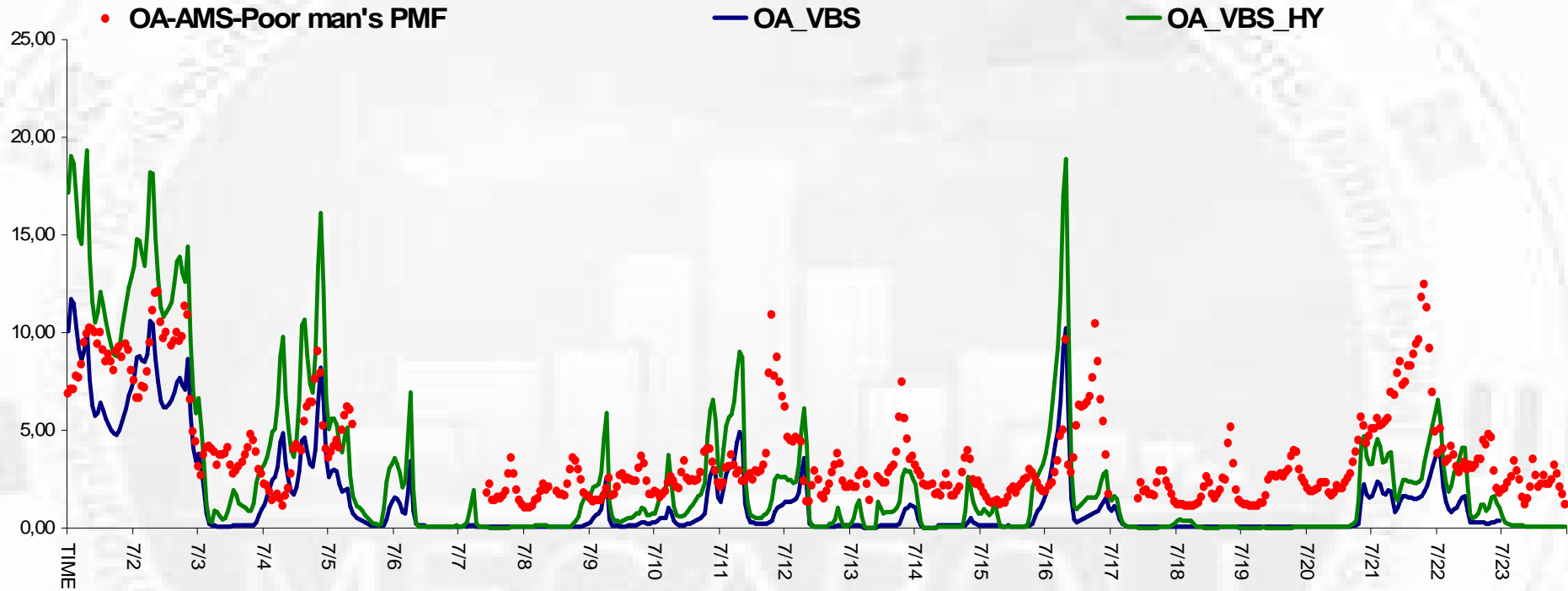
## With VBS scheme:

Peak in the morning corrected  $\Leftrightarrow$  distribution of POA into S/IVOC

But OOA lacks in the evening

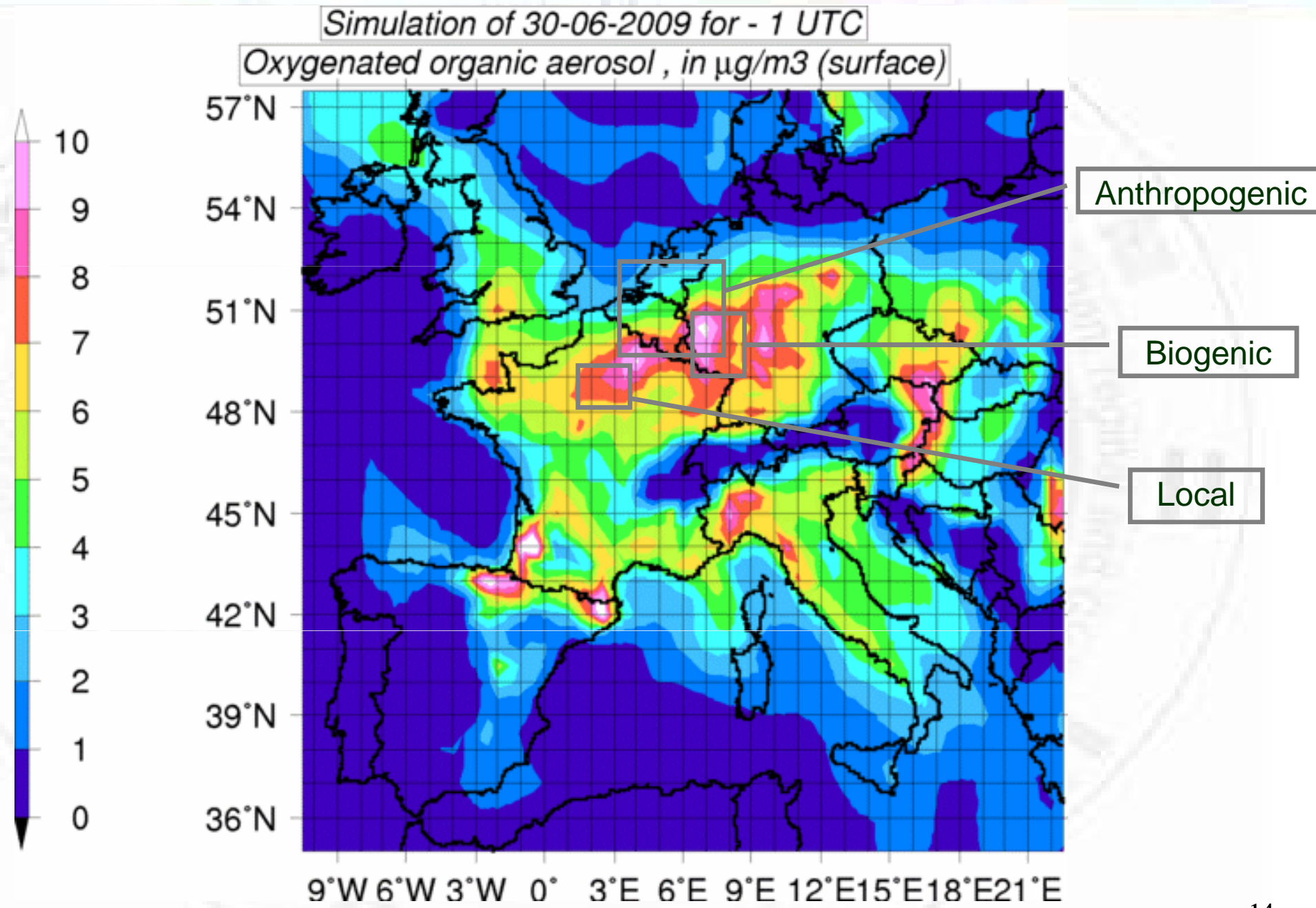
# High yield case (LHVP-Urban site)

- POA-SVOC/IVOC emissions \*2
- Anthropogenic SOA yield \*2



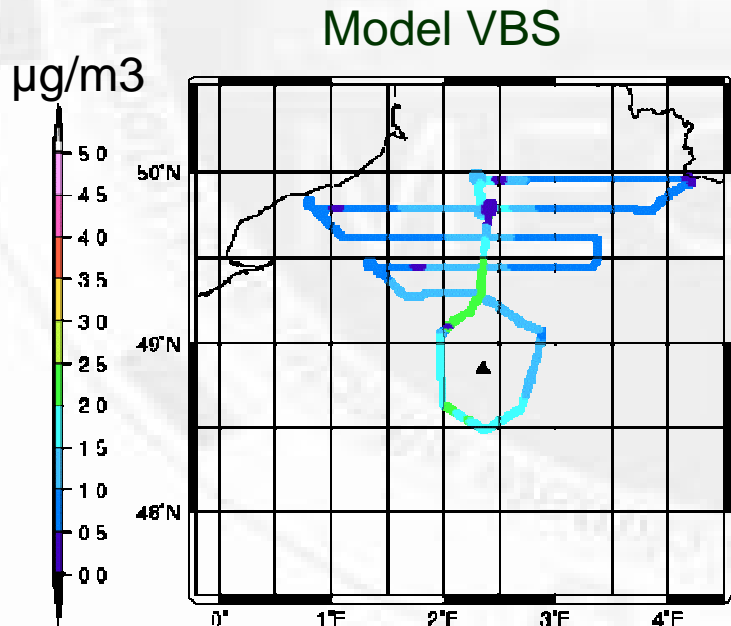
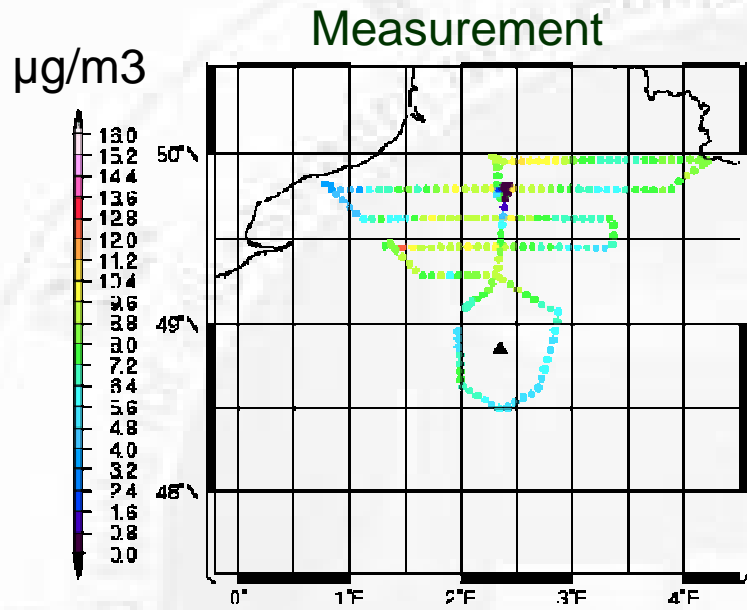
Background concentration underestimated  
Peak overestimated

# Regional influence on OOA plume



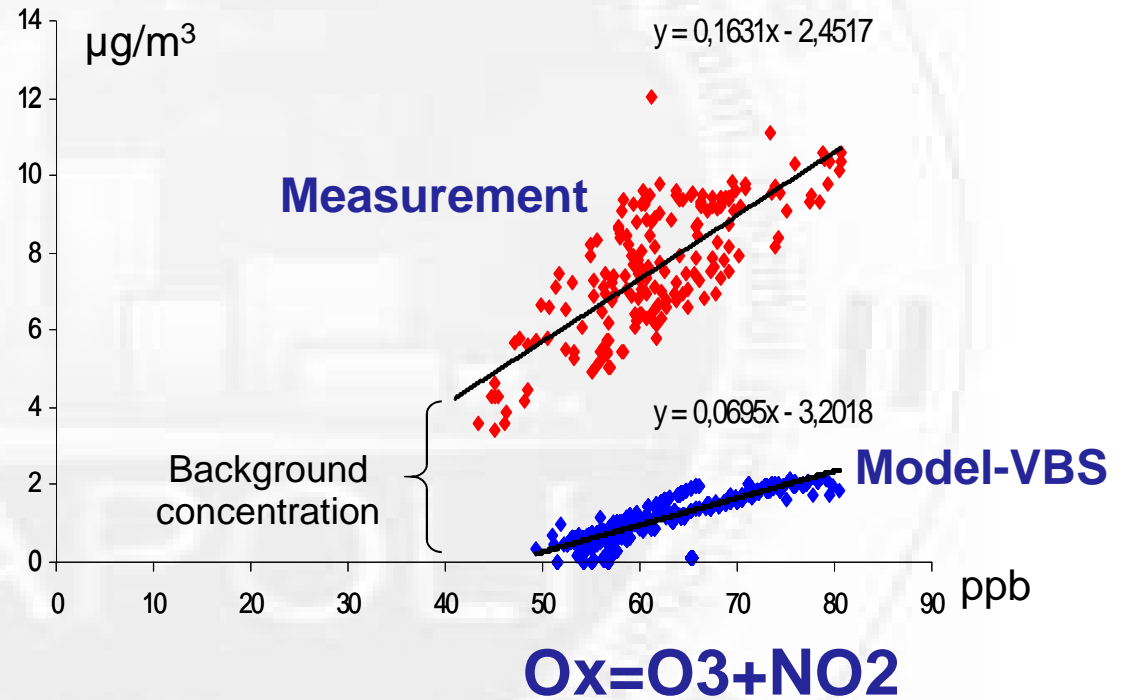
# Local formation of OA vs. measurements on flight

## Flight 32 20090721



100KM

OA



# Conclusion

- The “Volatility Basis Set” VBS approach has been implemented into a regional CTM (CHIMERE) and evaluated with measurements from the MEGAPOLI Paris summer campaign

## Urban / suburban sites

- The VBS approach avoids an overestimation of urban HOA especially in the morning, OOA lacks in the evening
- OOA peaks with strong continental influx, and a local peak with strong simulated anthropogenic aerosol are better simulated by VBS  
=> important contribution from S-SOA vs. ASOA
- Underestimation of OOA peaks with simulated BSOA origin, underestimation of urban background concentrations.
- High yield case overestimates OA peak, but still underestimates local OA background

## Plume evolution (for one flight with strong OA formation in plume):

- VBS under-estimates background OA levels;  
slope of  $\Delta\text{OA} / \Delta\text{Ox}$  plot is OK within a factor of two => OK considering VBS uncertainties

## OUTLOOK :

Sensitivity tests under way (ASOA yield, chemical aging speed, POA emissions and volatility)  
Redo evaluation with full data set , including winter campaign



# Acknowledgement

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IFT, PSI and LaMP teams are thanked for providing AMS measurement data.



Thank you !

# Annexe

**ASOA**

<b>C* (<math>\mu\text{g m}^{-3}</math>) at 300K</b>	<b>1</b>	<b>10</b>	<b>100</b>	<b>1000</b>
<b>Lumped VOC</b>				
<b>ALK4</b>		0.01		
<b>ALK5</b>		0.1		
<b>ARO1</b>	0.01	0.03	0.075	0.25
<b>ARO2</b>	0.02	0.04	0.08	0.25
<b>OLE1</b>	0.001	0.002	0.023	0.045
<b>OLE2</b>	0.003	0.006	0.023	0.076

(SAPRC99)

# Outline

- Context & Objective
- VBS approach in CHIMERE
- CTM configuration
- Simulation results: (from 20090701-20090722)
  1. Comparisons with ground based AMS measurements Organic Aerosol (OA)
    - LHVP (Urban)
    - SIRTA (Suburban)
  2. Regional/local plume of Oxygenated OA (OOA)
- Conclusion