Supplementary information to

Formation of organic aerosol in the Paris region during the MEGAPOLI summer campaign: evaluation of the Volatility-Basis-Set approach within the CHIMERE model

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Table S1. Parameters used to simulate the partitioning of POA emissions into different volatility bins; the mass weight of each lumped species is 250 g mol^{-1}. The enthalpies are derived from measurements and theoretical estimation for specific low-volatile species in POA emissions by Dohanue et al., (2006).

	Lumped species								
C* (µg m^{-3}) at 298K	10^{-2}	10^{-1}	10^{0}	10^{1}	10^{2}	10^{3}	10^{4}	10^{5}	10^{6}
ΔHv (kJ mol^{-1})	112	106	100	94	88	82	76	70	64
Emission factors	0.03	0.06	0.09	0.14	0.18	0.3	0.4	0.5	0.8

Table S2. Lumped anthropogenic and biogenic VOCs and their major components for the 4 bins VBS approach for SOA formation.

Anthropogenic origin		Biogenic origin	
Lumped species	Major components	Lumped species	Major components
ALK4	n-pentane, n-hexane, Branched C5-C6 Alkanes, Cyclopetane, Trimethyl Butane, Trimethyl Pentane, Isopropyl alcool, n-Propyl Alcool	Terp	α-pinene and sabinene; β-pinene and δ^3-carene; limonene; ocimene and myrcene
ALK5	C7-C22 n-Alkanes, C6-C16 Cycloalkanes, branched/Unspeciated C8-C18 Alkanes		
OLE1	Propene, C4-C15 terminal Alkanes		
OLE2	Isobutene, C4-C15 Internal Alkenes, C6-C15 Cyclic or di-olefins, Styrenes	ISO	Isoprene
ARO1	Toluene, benzene, Ethyl benzene, C9-C13 Monosubstituted Benzenes		
ARO2	Xylenes, Ethyl Toluenes, Dimethyl and Trimethyl Benzenes, Ethylbezenes, naphthalene, C8-C13 Di-, Tri-, Tetra-, Penta-, Hexa-substituted Benzenes, Unspeciated C10-C12 Aromatics		

Table S3. Normalized SOA yields α_i in the 4 bins VBS approach with saturation concentrations from 1 to 10^3 µg m^{-3}; ΔH: enthalpy of products; Molar mass (MW) of products; the density of OA is assumed as 1.5 g cm^{-3} (Murphy and Pandis, 2009).

VOC precursors	Yields of each bin				ΔH	MW
C* (µg m^{-3})	1	10	100	1000	(kJ mol^{-1})	(g mol^{-1})
ALK4	0.0	0.075	0.0	0.0	30	120
ALK5	0.0	0.300	0.0	0.0	30	150
OLE1	0.0045	0.009	0.060	0.225	30	120
OLE2	0.0225	0.435	0.129	0.375	30	120
ARO1	0.075	0.225	0.375	0.525	30	150
ARO2	0.075	0.300	0.375	0.525	30	150
TERP	0.1073	0.0918	0.3587	0.6075	30	180
ISOP	0.009	0.03	0.015	0.000	30	180

Table S4. Statistics for comparisons between MM5 results and meteorological measurements at SIRTA

Statistics at SIRTA	Wind speed (m s^{-1})	Temperature (K)	PBL height (m)
Bias (relative)	+1.07 (+42%)	-0.86	-268 (-28%)
RMSE (relative RMSE)	1.64 (+64%)	1.93	764 (+79%)
R	0.73	0.92	0.37

Table S5. Statistics for comparison of modelled and measured NOx, BC, O₃, inorganic aerosol, and organic aerosol from three configurations (CSS, VBS-T1 and VBS-T2) by using the LA emission inventory at GOLF, LHVP and SIRTA.

	GOLF			LHVP			SIRTA		
	Bias (relative)	RMSE (relative)	R	Bias (relative)	RMSE (relative)	R	Bias (relative)	RMSE (relative)	R
NOx (ppb)	+6.1 (+58%)	11.6 (111%)	0.56	+2.7 (+16%)	14.8 (86%)	0.56	+1.7 (+23%)	5.6 (77%)	0.65
O₃ (ppb)	+0.3 (+1.0%)	9.6 (32%)	0.80	-1.2 (-4.1%)	9.6 (33%)	0.79	2.6 (8.7%)	10.0 (34%)	0.74
BC (µg m^{-3})	+2.07 (+180%)	3.00 (261%)	0.51	+2.08 (+167%)	2.95 (235%)	0.52	-0.24 (-38%)	0.66 (104%)	0.36
SO₄$^{2-}$ (µg m^{-3})	+0.97 (+84%)	1.40 (122%)	0.74	+0.83 (+65%)	1.36 (108%)	0.70	+0.60 (+50%)	1.0 (84%)	0.73
NO₃$^{-}$ (µg m^{-3})	+0.44 (+137%)	1.11 (347%)	0.78	+0.23 (+59%)	0.82 (203%)	0.85	+0.36 (+138%)	0.88 (342%)	0.85
NH₄$^{+}$ (µg m^{-3})	+0.40 (+73%)	0.62 (112%)	0.81	+0.45 (+97%)	0.62 (136%)	0.82	+0.42 (108%)	0.55 (142%)	0.84
OA-CCS (µg m^{-3})	+1.17 (+33%)	4.02 (114%)	0.22	+1.53 (+46%)	3.58 (108%)	0.43	-1.11 (-49%)	1.96 (86%)	0.66
OA-VBS-T1 (µg m^{-3})	-1.99 (-56%)	3.13 (88%)	0.58	-1.76 (-53%)	2.71 (82%)	0.59	-1.46 (-64%)	2.13 (94%)	0.78
OA-VBS-T2 (µg m^{-3})	-0.47 (-13%)	2.04 (63%)	0.79	-0.27 (-8.2%)	2.14 (65%)	0.76	-0.42 (-18%)	1.46 (64%)	0.84

Table S6. Statistics for comparison of modelled and measured NOx, BC, O$_3$, inorganic aerosol, and organic aerosol from the configuration VBS-MPOLI by using the TNO-MEGAPOLI emission inventory at GOLF, LHVP and SIRTA

VBS-MPOLI	GOLF			LHVP			SIRTA		
	Bias (relative)	RMSE (relative)	R	Bias (relative)	RMSE (relative)	R	Bias (relative)	RMSE (relative)	R
NOx (ppb)	+10.0 (+95%)	15.6 (148%)	0.57	+7.2 (+42%)	17.8 (104%)	0.51	+1.6 (+22%)	6.1 (84%)	0.64
O$_3$ (ppb)	-1.97 (-6.7%)	10.0 (34%)	0.78	-3.7 (-13%)	10.8 (38%)	0.76	+2.65 (8.9%)	10.3 (35%)	0.72
BC (μg m^{-3})	+0.33 (+29%)	0.97 (84%)	0.55	+0.52 (+41%)	1.29 (103%)	0.50	-0.05 (-7.3%)	0.53 (84%)	0.51
SO$_4^{2-}$ (μg m^{-3})	+0.87 (+76%)	1.31 (114%)	0.73	+0.75 (+59%)	1.28 (102%)	0.69	+0.55 (+46%)	0.96 (81%)	0.71
NO$_3^-$ (μg m^{-3})	+0.01 (+2.1%)	0.48 (148%)	0.90	-0.11 (-27%)	0.48 (118%)	0.91	+0.04 (+17%)	0.36 (140%)	0.89
NH$_4^+$ (μg m^{-3})	+0.24 (+43%)	0.45 (80%)	0.82	+0.32 (+69%)	0.49 (107%)	0.81	+0.32 (+81%)	0.43 (111%)	0.82
OA (μg m^{-3})	-1.15 (-32%)	2.16 (61%)	0.80	-0.95 (-29%)	2.10 (64%)	0.77	-0.39 (+17%)	1.36 (60%)	0.84

Table S7. Statistic for comparison of modelled POA and SOA with measured HOA and OOA derived from the 3 factor PMF analysis from the four configurations (CSS, VBS-T1, VBS-T2 and VBS-MPOLI) at LHVP

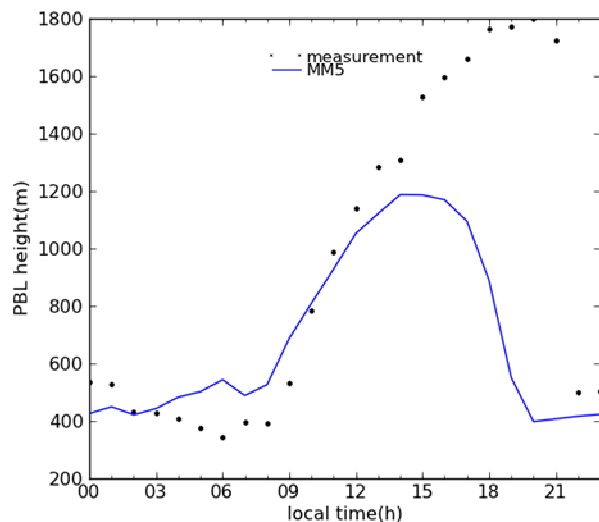| PMF 3 factor at LHVP	POA (μg m^{-3})			SOA (μg m^{-3})		
	Bias (relative)	RMSE (relative)	R	Bias (relative)	RMSE (relative)	R
CCS	+3.42 (+555%)	4.36 (708%)	0.53	-0.73 (-48%)	1.40 (92%)	0.66
VBS-T1	+0.01 (+1.8%)	0.61 (99%)	0.45	-0.61 (-40%)	1.18 (78%)	0.76
VBS-T2	+0.10 (+17%)	0.61 (100%)	0.49	+0.79 (+52%)	2.04 (134%)	0.87
VBS-MPOLI	-0.51 (-75%)	0.67 (99%)	0.55	+0.61 (+37%)	1.80 (108%)	0.91

Fig. S1 Comparison of simulated (blue line) and observed (black dots) July 2009 average daily variation of the PBL height at SIRTA
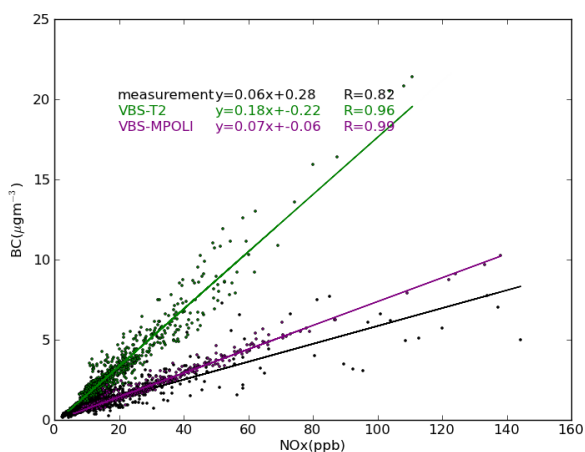

Fig. S2 BC vs. NOx at LHVP from measurements (black), from VBS-T2 for the LA-EMEP inventory (green) and from VBS-MPOLI for the MEGAPOLI inventory (purple).
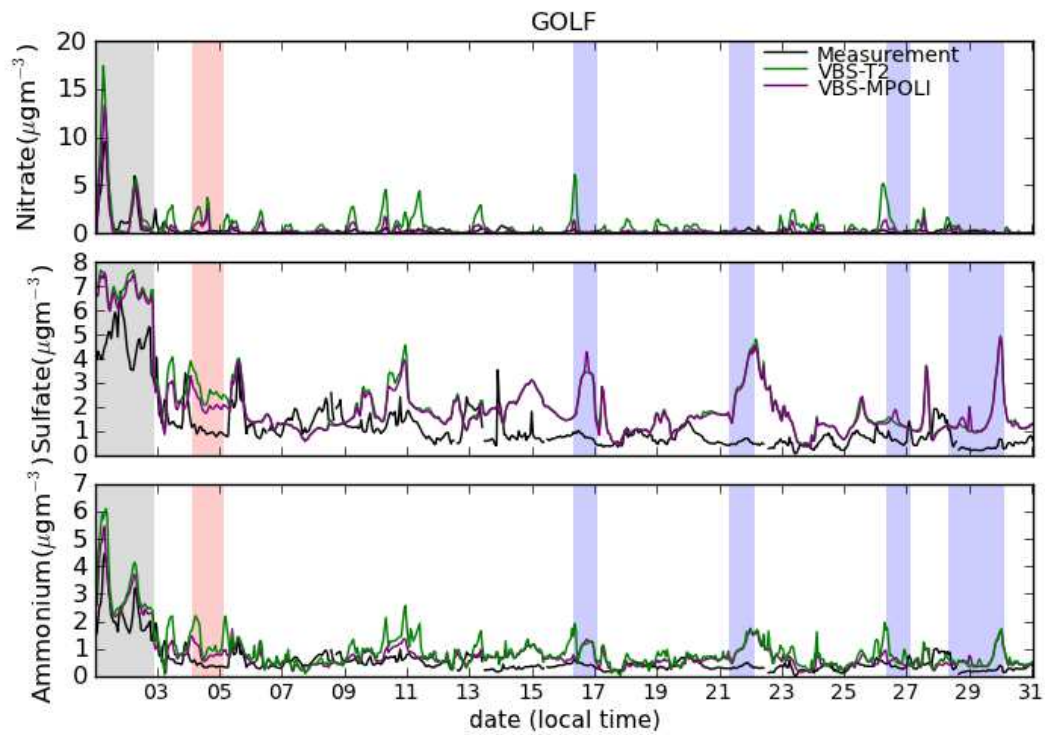
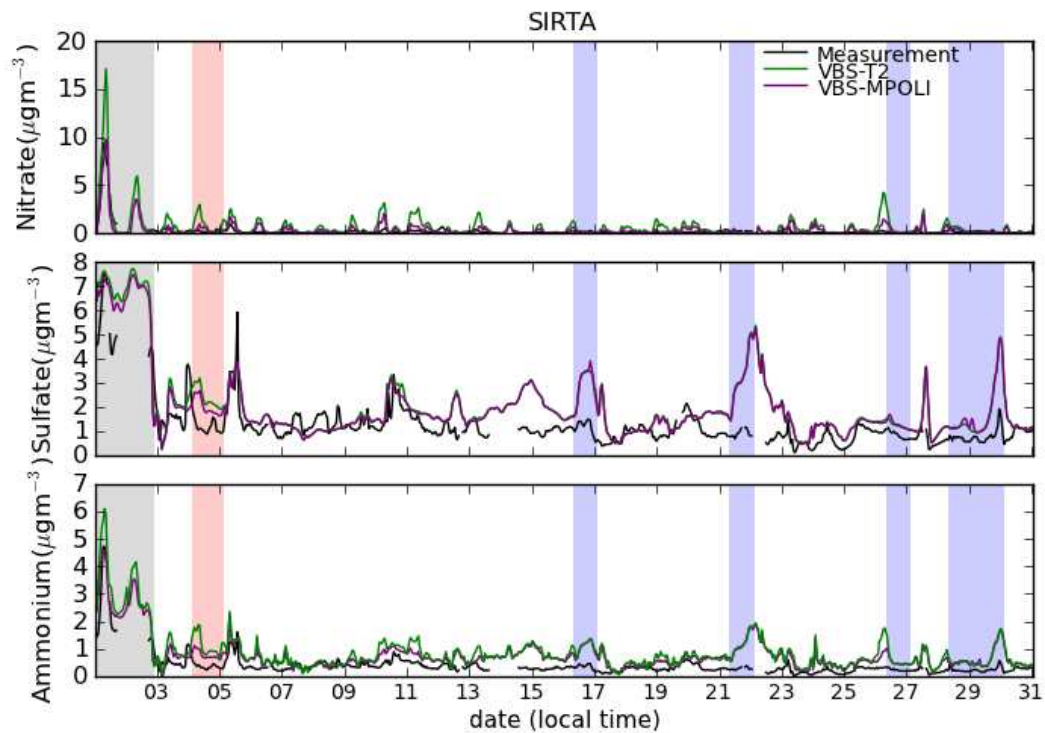Fig. S3 Comparison of simulated and observed inorganic aerosol species at GOLF

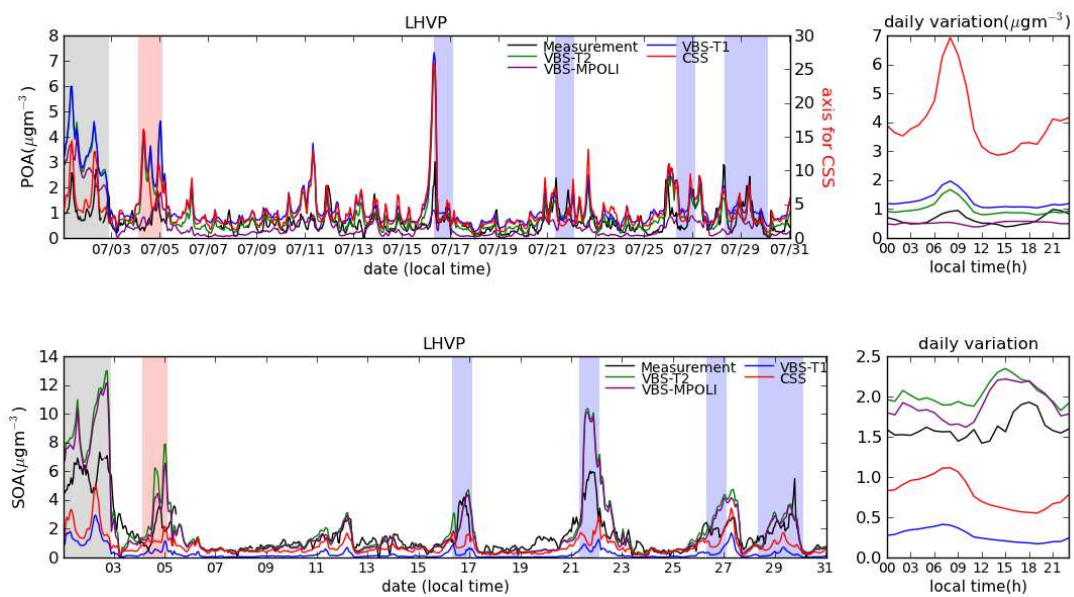Fig. S4 Comparison of simulated and observed inorganic aerosol species at SIRTA.

Fig. S5 Comparison of simulated and observed primary and secondary organic aerosol when simulated OPOA is considered as part of HOA, on the left side time series, on the right side daily average for July 2009. The color code in the diurnal variations (right side) is the same as in the time series (left side).