S1 Evaluation criteria equations

The normalized mean bias (NMB), the normalized mean error (NME), the mean bias (MB), the mean absolute gross error (MAGE), the fractional bias (FBIAS), and the fractional error (FERROR) were calculated for the results of all eight simulations.

$$\mathrm{NMB} = \frac{\sum_{i=1}^{n}(P_i - O_i)}{\sum_{i=1}^{n} O_i} \quad (1)$$

$$\mathrm{NME} = \frac{\sum_{i=1}^{n}|P_i - O_i|}{\sum_{i=1}^{n} O_i} \quad (2)$$

$$\mathrm{MB} = \frac{1}{n}\sum_{i=1}^{n}(P_i - O_i) \quad (3)$$

$$\mathrm{MAGE} = \frac{1}{n}\sum_{i=1}^{n}|P_i - O_i| \quad (4)$$

$$FBIAS = \frac{2}{n}\sum_{i=1}^{n}(P_i - O_i)/(P_i + O_i) \quad (5)$$

$$FERROR = \frac{2}{n}\sum_{i=1}^{n}|P_i - O_i|/(P_i + O_i) \quad (6)$$

Table S1: Average percent contributions of IVOCs emitted from on-road diesel and gasoline vehicles to the formation of $PM_{2.5}$ OA and SOA over 44 European capital cities for May 2008. The mean ground-level concentrations of SOA and OA in μg m^{-3} are included in the parenthesis.

European Capital	PMCAMx-iv	
	SOA (%)	OA (%)
Tirana	3.9 (2.27)	2.6 (3.45)
Yerevan	7.5 (0.28)	1.6 (1.33)
Vienna	4.7 (2.08)	2.7 (3.55)
Baku	6.4 (0.32)	1.5 (1.35)
Minsk	3.7 (2.92)	2.3 (4.65)
City of Brussels	3.9 (1.26)	2.2 (2.27)
Sarajevo	3.8 (1.32)	2.2 (2.33)
Sofia	7.2 (1.42)	4.2 (2.44)
Zagreb	4.2 (1.62)	2.4 (2.8)
Nicosia	7.0 (1.24)	3.3 (2.64)
Prague	4.3 (2.37)	2.7 (3.72)
Copenhagen	3.4 (2.78)	2.2 (4.26)
Tallinn	3.3 (2.03)	1.6 (4.32)
Helsinki	5.5 (0.54)	2.0 (1.48)
Paris	2.9 (1.44)	1.2 (3.38)
Tbilisi	3.3 (1.18)	1.5 (2.67)
Berlin	4.5 (2.93)	1.8 (7.16)
Athens	3.9 (2.8)	2.4 (4.48)
Budapest	7.0 (0.42)	2.2 (1.38)
Dublin	7.2 (1.84)	3.6 (3.72)
Rome	4.0 (1.91)	2.6 (2.99)
Prizren	5.3 (2.02)	3.3 (3.24)
Riga	4.0 (1.77)	2.5 (2.9)
Vilnius	5.0 (1.97)	3.0 (3.28)
Luxembourg	3.8 (1.18)	2.1 (2.15)
Valletta	4.4 (1.45)	2.6 (2.48)
Chisinau	3.5 (2.41)	2.1 (4.05)
Podgorica	3.3 (1.41)	1.6 (2.95)
Amsterdam	5.8 (1.48)	3.4 (2.57)
Oslo	3.8 (1.21)	2.1 (2.24)
Warsaw	3.9 (1.05)	1.8 (2.26)
Lisbon	3.7 (1.28)	2.1 (2.3)
Skopje	3.5 (2.9)	2.0 (5.14)
Bucharest	2.6 (1.21)	1.1 (2.9)
Moscow	4.7 (1.63)	2.7 (2.82)
Belgrade	4.0 (0.59)	1.6 (1.51)
Bratislava	4.8 (1.39)	2.8 (2.38)
Ljubljana	8.8 (1.91)	4.0 (4.23)
Madrid	3.8 (1.63)	2.4 (2.61)
Stockholm	4.7 (2.11)	3.0 (3.28)

Bern	3.8 (1.83)	2.4 (2.85)
Ankara	2.7 (1.19)	1.3 (2.47)
Kyiv	7.3 (0.82)	3.0 (1.96)
London	6.6 (1.56)	3.5 (2.93)

Table S2: Prediction skill metrics of PMCAMx, PMCAMx-iv and the six sensitivity tests against AMS hourly ground measurements of PM_1 OA concentration from the four measuring stations that were part of the EUCAARI campaign in May 2008.

Test name	Mean Observed (μg m^{-3})	Mean Predicted (μg m^{-3})	MB (μg m^{-3})	MAGE (μg m^{-3})	NMB	NME	FBIAS	FERROR
Cabauw								
VBS-scheme (PMCAMx)	4.1	4.6	0.7	1.6	16.5	37.9	0.2	0.4
Base case (PMCAMx-iv)	4.1	4.7	0.7	1.6	17.9	38.4	0.2	0.4
Lumped IVOC emissions × 2	4.1	4.8	0.9	1.6	21.3	39.8	0.2	0.4
No gas-phase chemistry	4.1	4.7	0.7	1.6	17.7	38.2	0.2	0.4
Multigenerational aging	4.1	4.8	0.9	1.6	21.3	39.8	0.2	0.4
MW effect	4.1	4.8	0.9	1.6	20.7	39.6	0.2	0.4
ΔH effect	4.1	4.7	0.8	1.6	19.5	39.1	0.2	0.4
Different yields	4.1	4.7	0.7	1.6	18.1	38.5	0.2	0.4
Finokalia								
VBS-scheme (PMCAMx)	2.5	2.4	0.1	0.8	2.7	31.4	0.1	0.3
Base case (PMCAMx-iv)	2.5	2.4	0.1	0.8	4.0	31.4	0.1	0.3
Lumped IVOC emissions × 2	2.5	2.5	0.2	0.8	7.5	32.1	0.1	0.3
No gas-phase chemistry	2.5	2.4	0.1	0.8	4.0	31.4	0.1	0.3
Multigenerational aging	2.5	2.6	0.3	0.9	13.4	34.5	0.1	0.4
MW effect	2.5	2.5	0.2	0.8	7.5	32.1	0.1	0.3

ΔH effect	2.5	2.4	0.1	0.8	5.4	31.5	0.1	0.3
Different yields	2.5	2.4	0.1	0.8	4.5	31.5	0.1	0.3
Mace Head								
VBS-scheme (PMCAMx)	2.3	2.5	-0.1	1.0	-3.9	41.1	-0.2	0.5
Base case (PMCAMx-iv)	2.3	2.5	-0.1	1.0	-3.8	41.3	-0.2	0.5
Lumped IVOC emissions × 2	2.3	2.5	0.0	1.0	-1.9	41.7	-0.2	0.5
No gas-phase chemistry	2.3	2.5	-0.1	1.0	-3.9	41.3	-0.2	0.5
Multigenerational aging	2.3	2.6	0.0	1.0	0.2	42.1	-0.2	0.5
MW effect	2.3	2.5	0.0	1.0	-1.9	41.7	-0.2	0.5
ΔH effect	2.3	2.5	-0.1	1.0	-2.3	41.6	-0.2	0.5
Different yields	2.3	2.5	-0.1	1.0	-3.7	41.3	-0.2	0.5
Melpitz								
VBS-scheme (PMCAMx)	5.1	3.8	-1.2	1.8	-23.3	34.2	-0.3	0.4
Base case (PMCAMx-iv)	5.1	3.8	-1.1	1.7	-21.8	33.8	-0.2	0.4
Lumped IVOC emissions × 2	5.1	3.9	-1.0	1.7	-18.7	33.4	-0.2	0.4
No gas-phase chemistry	5.1	3.8	-1.1	1.7	-21.7	33.7	-0.2	0.4
Multigenerational aging	5.1	4.0	-0.9	1.7	-17.4	33.5	-0.2	0.4
MW effect	5.1	3.9	-1.0	1.7	-19.0	33.4	-0.2	0.4
ΔH effect	5.1	3.9	-1.1	1.7	-20.7	33.3	-0.2	0.4
Different yields	5.1	3.8	-1.1	1.7	-21.4	33.7	-0.2	0.4

Table S3: Average percent contributions of on-road IVOCs to the formation of PM_1 OA concentrations over the four measuring stations were part of the EUCAARI campaign in May 2008. The contributions are calculated for all eight simulation cases.

Test name	Contribution to PM_1 OA (%)
Cabauw	
VBS-scheme (PMCAMx)	1.3
Base case (PMCAMx-iv)	2.2
Lumped IVOC emissions × 2	4.4
No gas-phase chemistry	2.2
Multigenerational aging	4.4
MW effect	4.3
ΔH effect	3.2
Different yields	2.3
Finokalia	
VBS-scheme (PMCAMx)	1.7
Base case (PMCAMx-iv)	2.9
Lumped IVOC emissions × 2	5.7
No gas-phase chemistry	2.9
Multigenerational aging	9.5
MW effect	5.8
ΔH effect	4.1
Different yields	3.2
Mace Head	
VBS-scheme (PMCAMx)	1.8
Base case (PMCAMx-iv)	2.0
Lumped IVOC emissions × 2	4.0
No gas-phase chemistry	2.0
Multigenerational aging	5.2
MW effect	4.1
ΔH effect	3.3
Different yields	2.2
Melpitz	

VBS-scheme (PMCAMx)	1.4
Base case (PMCAMx-iv)	2.4
Lumped IVOC emissions × 2	4.8
No gas-phase chemistry	2.4
Multigenerational aging	5.4
MW effect	4.7
ΔH effect	3.3
Different yields	2.6

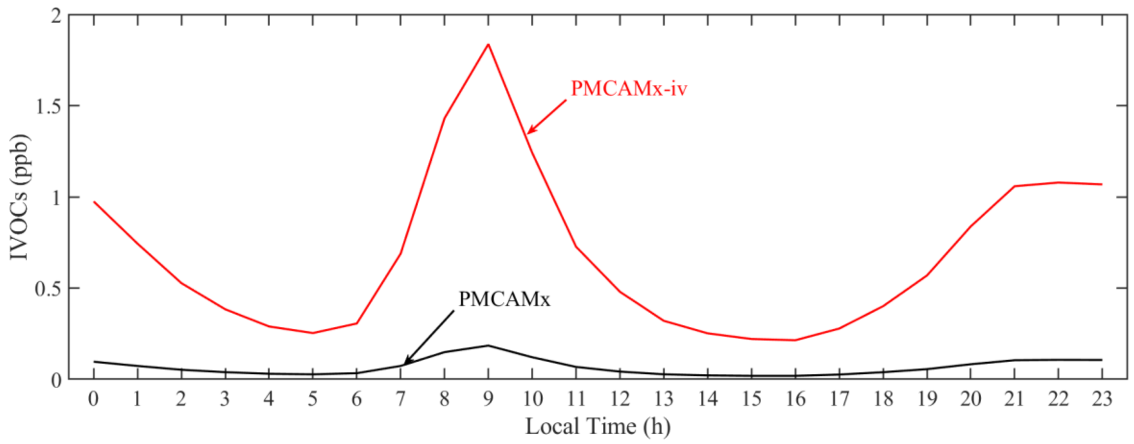

Figure S1: Average diurnal profiles for the ground-level concentrations of IVOCs over Paris as predicted by PMCAMx and PMCAMx-iv for May 2008.

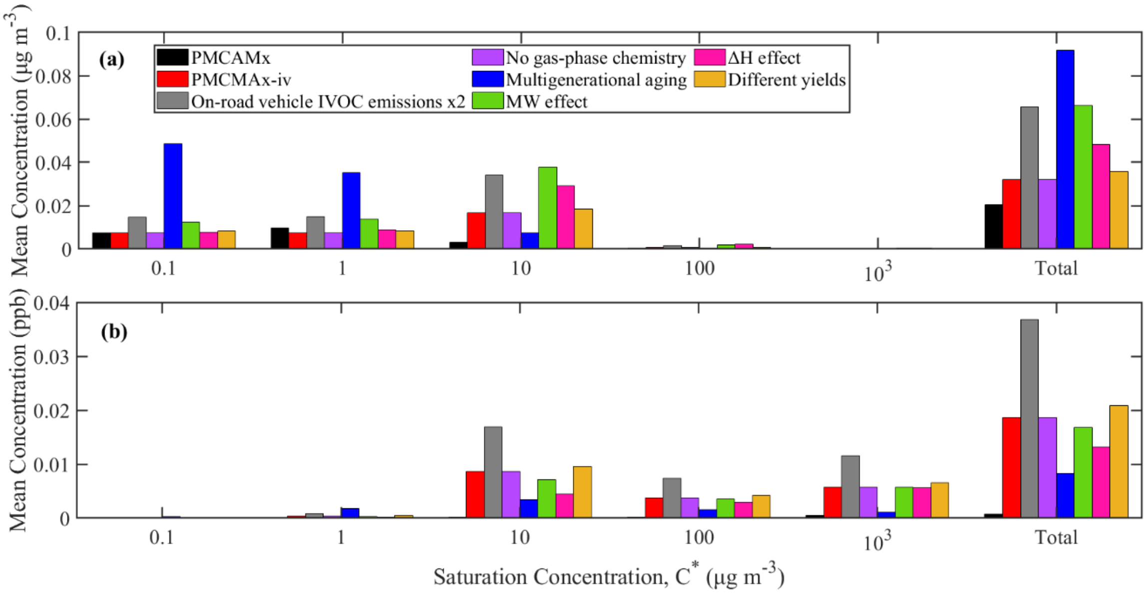

Figure S2: Domain-averaged ground-level concentrations of the SOA-iv products (a) in the aerosol phase and (b) in the gas-phase predicted by PMCAMx, PMCAMx-iv and by the different sensitivity tests for the May 2008 simulations over Europe.

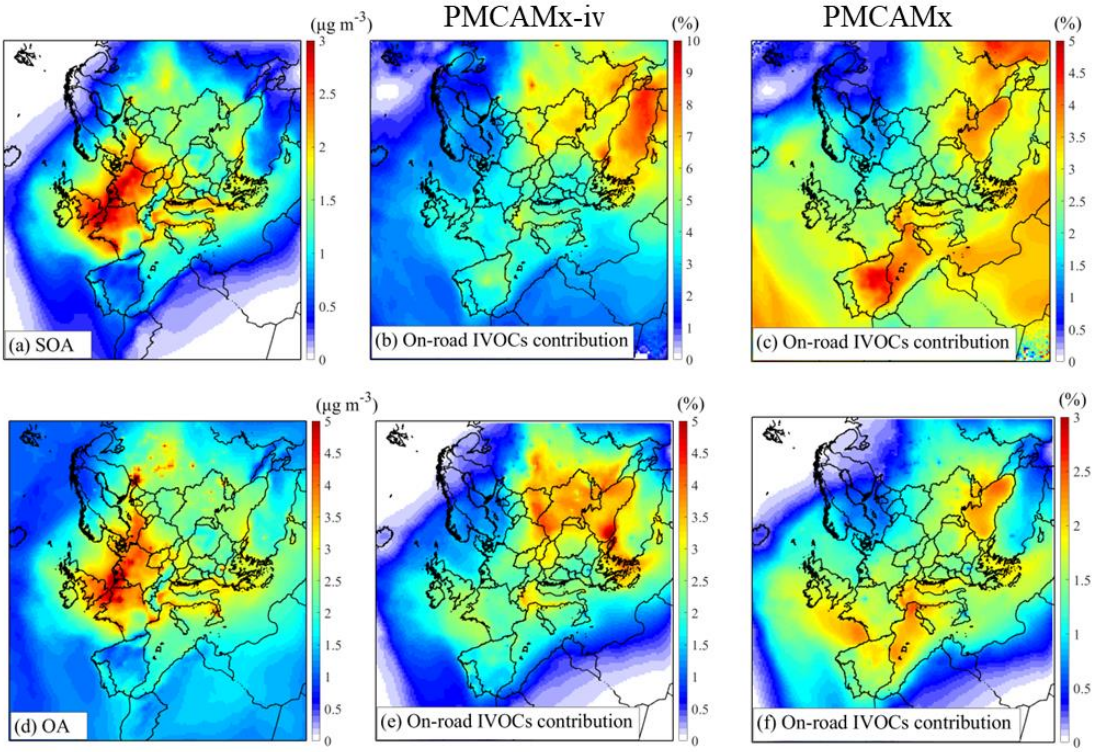

Figure S3: Estimated averaged ground-level $PM_{2.5}$ concentrations of (a) SOA and (d) OA concentrations and the corresponding contributions from on-road diesel and gasoline vehicles IVOCs over Europe for May 2008 using (b,e) PMCAMx-iv and (c,f) PMCAMx-iv.

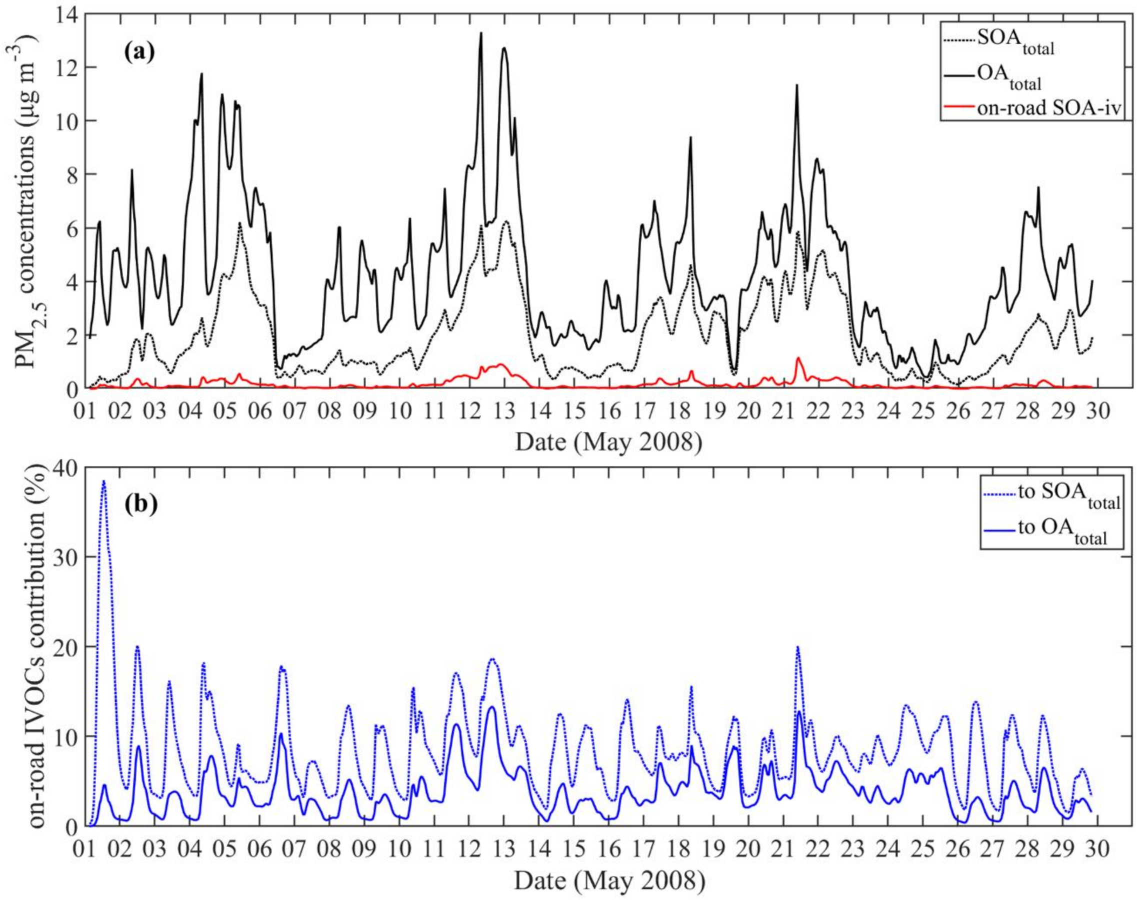

Figure S4: (a) PMCAMx-iv estimated hourly-averaged ground-level concentrations of $PM_{2.5}$ SOA_{total}, OA_{total} and on-road SOA-iv over Moscow and (b) the contributions of on-road IVOCs to the total SOA and OA concentrations for May 2008.

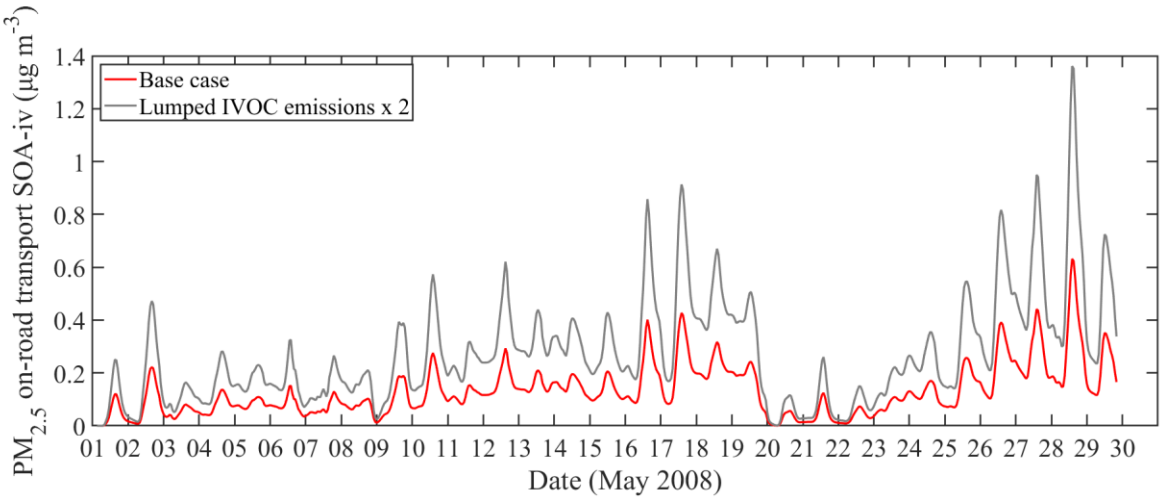

Figure S5: $PM_{2.5}$ hourly-averaged timeseries for the predicted ground-level concentrations of on-road transport SOA-iv by the "VBS scheme", the "base case" and the "lumped IVOC emissions × 2" simulations over the city of Athens for May 2008.

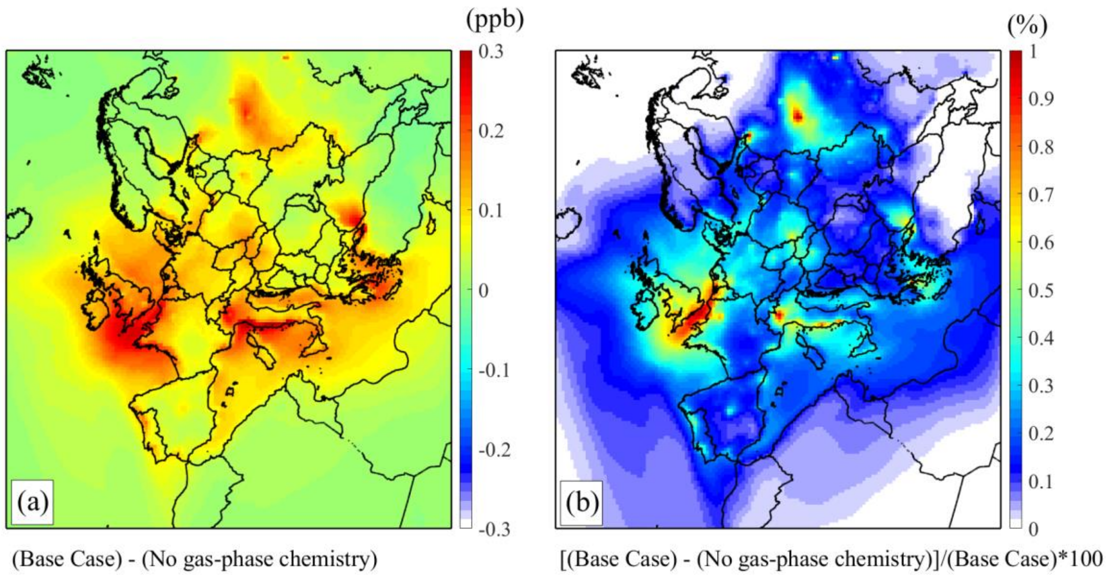

Figure S6: (a) Absolute and (b) percentage differences between the average ground-level concentrations of O_3 predicted in the "base case" and in the "no gas-phase chemistry" simulations.

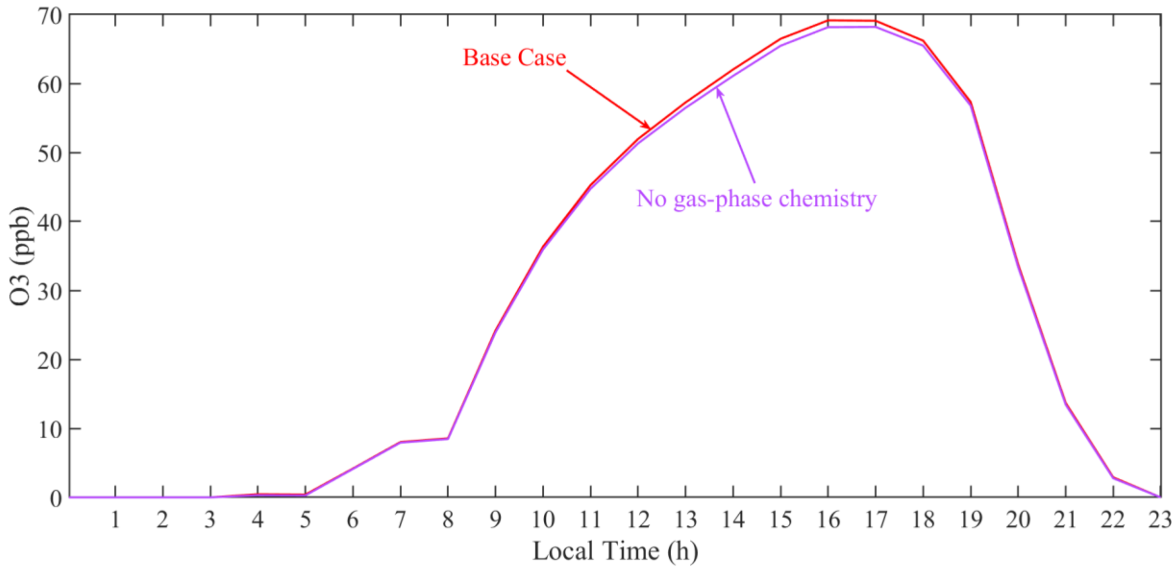

Figure S7: Predicted ground-level ozone concentrations by PMCAMx ("base case" test), PMCAMx-iv ("new IVOC scheme" test) and the "no gas-phase chemistry" sensitivity test over Milan (Italy) on the 8th of May 2008.

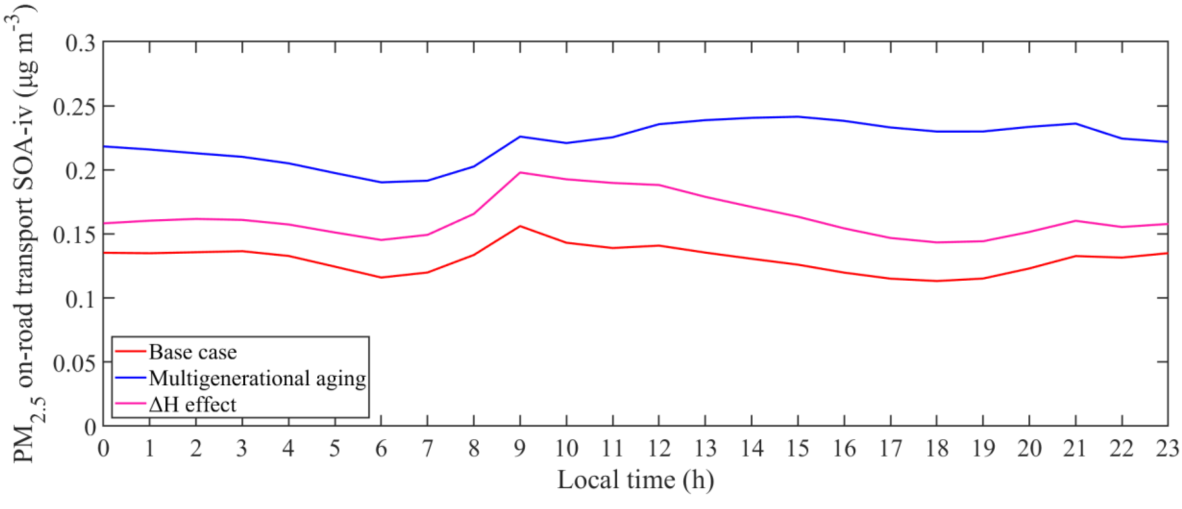

Figure S8: Diurnal profile of the $PM_{2.5}$ ground-level on-road transport SOA-iv concentrations over Paris predicted by the "base case", the "multigenerational aging" test and the "Δ*H* effect" test.

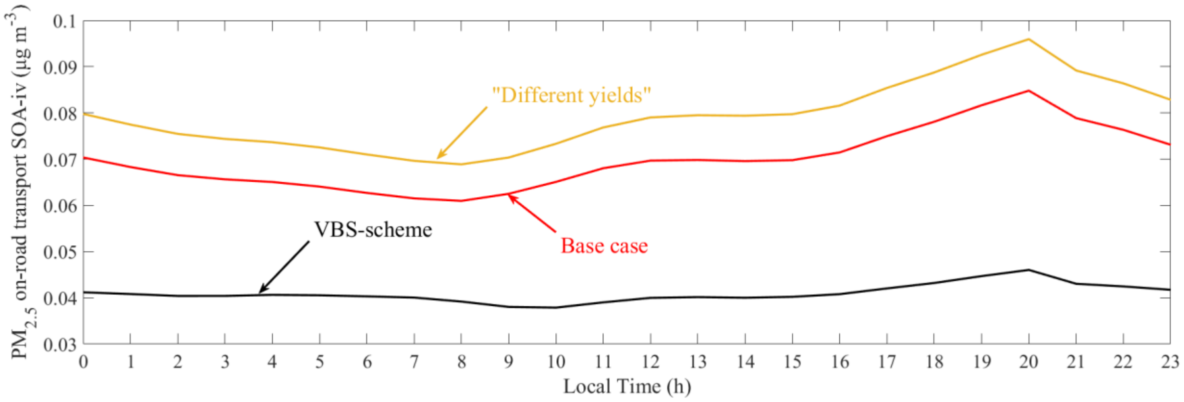

Figure S9: Diurnal profile of the $PM_{2.5}$ ground-level on-road transport SOA-iv concentrations over Finokalia predicted by PMCAMx, PMCAMx-iv and the "different yields" sensitivity test.