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*Supplement of*

# Evaluation of European air quality modelled by CAMx including the volatility basis set scheme

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## Supplement

Table S1*. Properties of the VBS space (adapted from Koo et al., 2014). Carbon numbers for each volatility bin are calculated using the group-contribution of Donahue et al. (2011).

| Basis sets | C* ($\mu g\ m^{-3}$) | Carbon oxidation state | Carbon Number | Oxygen Number | Hydrogen number | Molecular weight | OA/OC |
|---|---|---|---|---|---|---|---|
| | 0 | 0.102 | 7 | 4.90 | 9.10 | 172 | 2.05 |
| | 1 | −0.188 | 7.25 | 4.38 | 10.1 | 167 | 1.92 |
| SV-OOA | 10 | −0.463 | 7.5 | 3.84 | 11.2 | 163 | 1.81 |
| | 100 | −0.724 | 7.75 | 3.30 | 12.2 | 158 | 1.70 |
| | 1000 | −0.973 | 8 | 2.74 | 13.3 | 153 | 1.59 |
| | 0 | −1.52 | 17 | 2.69 | 31.3 | 278 | 1.36 |
| | 1 | −1.65 | 17.5 | 2.02 | 33.0 | 275 | 1.31 |
| HOA-like | 10 | −1.78 | 18 | 1.34 | 34.7 | 272 | 1.26 |
| | 100 | −1.90 | 18.5 | 0.632 | 36.4 | 268 | 1.21 |
| | 1000 | −2.00 | 19 | 0.0 | 38.0 | 266 | 1.17 |
| | 0 | −0.704 | 10 | 4.32 | 15.7 | 205 | 1.71 |
| | 1 | −1.02 | 11 | 3.60 | 18.4 | 208 | 1.58 |
| BBOA-like | 10 | −1.29 | 12 | 2.85 | 21.1 | 211 | 1.47 |
| | 100 | −1.52 | 13 | 2.08 | 23.9 | 213 | 1.37 |
| | 1000 | −1.73 | 14 | 1.27 | 26.7 | 215 | 1.28 |

* Properties of the lowest volatility bins refer to all OA with $C^* \leq 0.1\ \mu g\ m^{-3}$ (non-volatile OA).

Table S2. Statistical analysis for nitrate for February-March 2009 at different AMS sites with 50% reduction of ammonia scenario.

| Site | Mean observed $NO_3^-$ (μg $m^{-3}$) | Mean modelled $NO_3^-$ Base case (VBS_BC) (μg $m^{-3}$) | Mean modelled $NO_3^-$ 50% red. $NH_3$ (μg $m^{-3}$) | MB Base case (VBS_BC) (μg $m^{-3}$) | MB 50% red. $NH_3$ (μg $m^{-3}$) |
|---|---|---|---|---|---|
| Barcelona | 3.6 | 5.8 | 3.6 | 2.19 | < 0.1 |
| Cabauw | 2.2 | 6.7 | 5.3 | 4.49 | 3.08 |
| Chilbolton | 2.7 | 4.0 | 2.7 | 1.33 | < 0.1 |
| Helsinki | 1.0 | 1.9 | 0.7 | 0.93 | -0.28 |
| Hyytiälä | 0.2 | 1.0 | 0.3 | 0.75 | < 0.1 |
| Mace Head | 0.6 | 1.7 | 0.8 | 1.11 | 0.17 |
| Melpitz | 3.1 | 4.3 | 3.1 | 1.25 | < 0.1 |
| Montseny | 3.1 | 5.9 | 3.2 | 2.83 | < 0.1 |
| Payerne | 3.9 | 5.7 | 5.0 | 1.81 | 1.11 |
| Puy de Dôme | 0.9 | 2.7 | 2.0 | 1.81 | 1.15 |
| Vavihill | 2.8 | 3.7 | 2.3 | 0.89 | -0.56 |

Table S3. Statistical analysis for the OA concentration and different sensitivity scenarios for February-March 2009 periods at 11 AMS sites.

| Site | Mean observed OA (μg/m$^3$) | Mean modelled OA (μg/m$^3$) | MB (μg/m$^3$) | ME (μg/m$^3$) | MFB [-] | MFE [-] |
|---|---|---|---|---|---|---|
| NOVBS | | | | | | |
| Barcelona | 8.2 | 2.0 | -6.25 | 6.27 | -1.08 | 1.10 |
| Cabauw | 1.2 | 1.0 | -0.27 | 0.52 | -0.18 | 0.49 |
| Chilbolton | 2.4 | 0.6 | -1.82 | 1.82 | -1.14 | 1.15 |
| Helsinki | 2.7 | 2.0 | -0.64 | 1.46 | -0.21 | 0.64 |
| Hyytiälä | 1.3 | 0.6 | -0.67 | 0.69 | -0.69 | 0.72 |
| Mace Head | 0.8 | 0.2 | -0.61 | 0.62 | -0.71 | 0.90 |
| Melpitz | 1.5 | 0.5 | -0.98 | 0.99 | -0.86 | 0.88 |
| Montseny | 3.1 | 2.5 | -0.53 | 1.69 | -0.05 | 0.62 |
| Payerne | 4.1 | 1.1 | -2.97 | 2.99 | -1.03 | 1.07 |
| Puy de Dôme | 0.6 | 1.0 | 0.36 | 0.68 | 0.56 | 0.92 |
| Vavihill | 3.9 | 1.1 | -2.79 | 2.79 | -1.06 | 1.07 |
| VBS_ROB | | | | | | |
| Barcelona | 8.2 | 1.3 | -6.96 | 6.96 | -1.39 | 1.39 |
| Cabauw | 1.2 | 0.4 | -0.85 | 0.87 | -0.96 | 1.01 |
| Chilbolton | 2.4 | 0.3 | -2.10 | 2.10 | -1.50 | 1.50 |
| Helsinki | 2.7 | 0.9 | -1.73 | 1.76 | -0.88 | 0.92 |
| Hyytiälä | 1.3 | 0.4 | -0.90 | 0.90 | -1.18 | 1.18 |
| Mace Head | 0.8 | 0.2 | -0.54 | 0.57 | -0.43 | 0.77 |
| Melpitz | 1.5 | 0.2 | -1.26 | 1.26 | -1.48 | 1.48 |
| Montseny | 3.1 | 1.6 | -1.51 | 1.87 | -0.51 | 0.78 |
| Payerne | 4.1 | 0.7 | -3.44 | 3.44 | -1.45 | 1.46 |
| Puy de Dôme | 0.6 | 0.5 | -0.15 | 0.46 | -0.14 | 0.81 |
| Vavihill | 3.9 | 0.4 | -3.44 | 3.44 | -1.61 | 1.61 |
| VBS_BC | | | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| Barcelona | 8.2 | 3.1 | -5.11 | 5.15 | -0.80 | 0.82 |
| Cabauw | 1.2 | 1.1 | -0.14 | 0.53 | -0.13 | 0.50 |
| Chilbolton | 2.4 | 0.7 | -1.70 | 1.70 | -1.09 | 1.10 |
| Helsinki | 2.7 | 2.9 | 0.26 | 1.64 | 0.08 | 0.62 |
| Hyytiälä | 1.3 | 1.0 | -0.28 | 0.52 | -0.48 | 0.60 |
| Mace Head | 0.8 | 0.4 | -0.38 | 0.43 | -0.29 | 0.70 |
| Melpitz | 1.5 | 0.5 | -0.95 | 0.98 | -0.94 | 0.97 |
| Montseny | 3.1 | 3.9 | 0.88 | 1.88 | 0.31 | 0.57 |
| Payerne | 4.1 | 1.8 | -2.33 | 2.43 | -0.85 | 0.90 |
| Puy de Dôme | 0.6 | 1.4 | 0.78 | 0.96 | 0.68 | 0.91 |
| Vavihill | 3.9 | 1.4 | -2.53 | 2.53 | -1.04 | 1.04 |
| | | VBS_BC_2xBVOC | | | | |
| Barcelona | 8.2 | 3.3 | -4.98 | 5.03 | -0.77 | 0.80 |
| Cabauw | 1.2 | 1.1 | -0.11 | 0.54 | -0.12 | 0.50 |
| Chilbolton | 2.4 | 0.7 | -1.67 | 1.68 | -1.08 | 1.09 |
| Helsinki | 2.7 | 2.9 | 0.26 | 1.64 | 0.08 | 0.62 |
| Hyytiälä | 1.3 | 1.0 | -0.28 | 0.52 | -0.48 | 0.60 |
| Mace Head | 0.8 | 0.4 | -0.37 | 0.42 | -0.29 | 0.70 |
| Melpitz | 1.5 | 0.5 | -0.92 | 0.97 | -0.92 | 0.96 |
| Montseny | 3.1 | 4.1 | 1.02 | 1.96 | 0.33 | 0.58 |
| Payerne | 4.1 | 1.8 | -2.27 | 2.39 | -0.83 | 0.88 |
| Puy de Dôme | 0.6 | 1.5 | 0.86 | 1.04 | 0.70 | 0.93 |
| Vavihill | 3.9 | 1.4 | -2.51 | 2.51 | -1.03 | 1.03 |
| | | VBS_BC_2xBBOA | | | | |
| Barcelona | 8.2 | 4.8 | -3.43 | 3.91 | -0.45 | 0.56 |
| Cabauw | 1.2 | 1.7 | 0.45 | 0.81 | 0.20 | 0.55 |
| Chilbolton | 2.4 | 1.0 | -1.40 | 1.42 | -0.87 | 0.89 |
| Helsinki | 2.7 | 5.0 | 2.32 | 2.93 | 0.50 | 0.75 |
| Hyytiälä | 1.3 | 1.9 | 0.59 | 0.96 | 0.07 | 0.54 |
| Mace Head | 0.8 | 0.5 | -0.26 | 0.36 | -0.23 | 0.68 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Melpitz | 1.5 | 0.9 | -0.59 | 0.85 | -0.55 | 0.70 |
| Montseny | 3.1 | 6.2 | 3.11 | 3.37 | 0.67 | 0.73 |
| Payerne | 4.1 | 3.2 | -0.94 | 1.90 | -0.37 | 0.57 |
| Puy de Dôme | 0.6 | 2.8 | 2.16 | 2.24 | 1.11 | 1.18 |
| Vavihill | 3.9 | 2.6 | -1.31 | 1.93 | -0.60 | 0.72 |

Table S4. Statistical analysis for the OA concentration and different sensitivity scenarios for June 2006 period at Payerne site.

| Scenario | Mean observed OA ($\mu g/m^3$) | Mean modelled OA ($\mu g/m^3$) | MB ($\mu g/m^3$) | ME ($\mu g/m^3$) | MFB [-] | MFE [-] |
|---|---|---|---|---|---|---|
| NOVBS | 6.0 | 2.6 | -3.5 | 3.5 | -0.91 | 0.93 |
| VBS_ROB | 6.0 | 1.7 | -4.3 | 4.3 | -1.11 | 1.11 |
| VBS_BC | 6.0 | 2.4 | -3.6 | 3.6 | -0.85 | 0.86 |
| VBS_BC_2xBVOC | 6.0 | 3.4 | -2.6 | 2.8 | -0.63 | 0.66 |
| VBS_BC_2xBBOA | 6.0 | 2.8 | -3.3 | 3.3 | -0.75 | 0.76 |

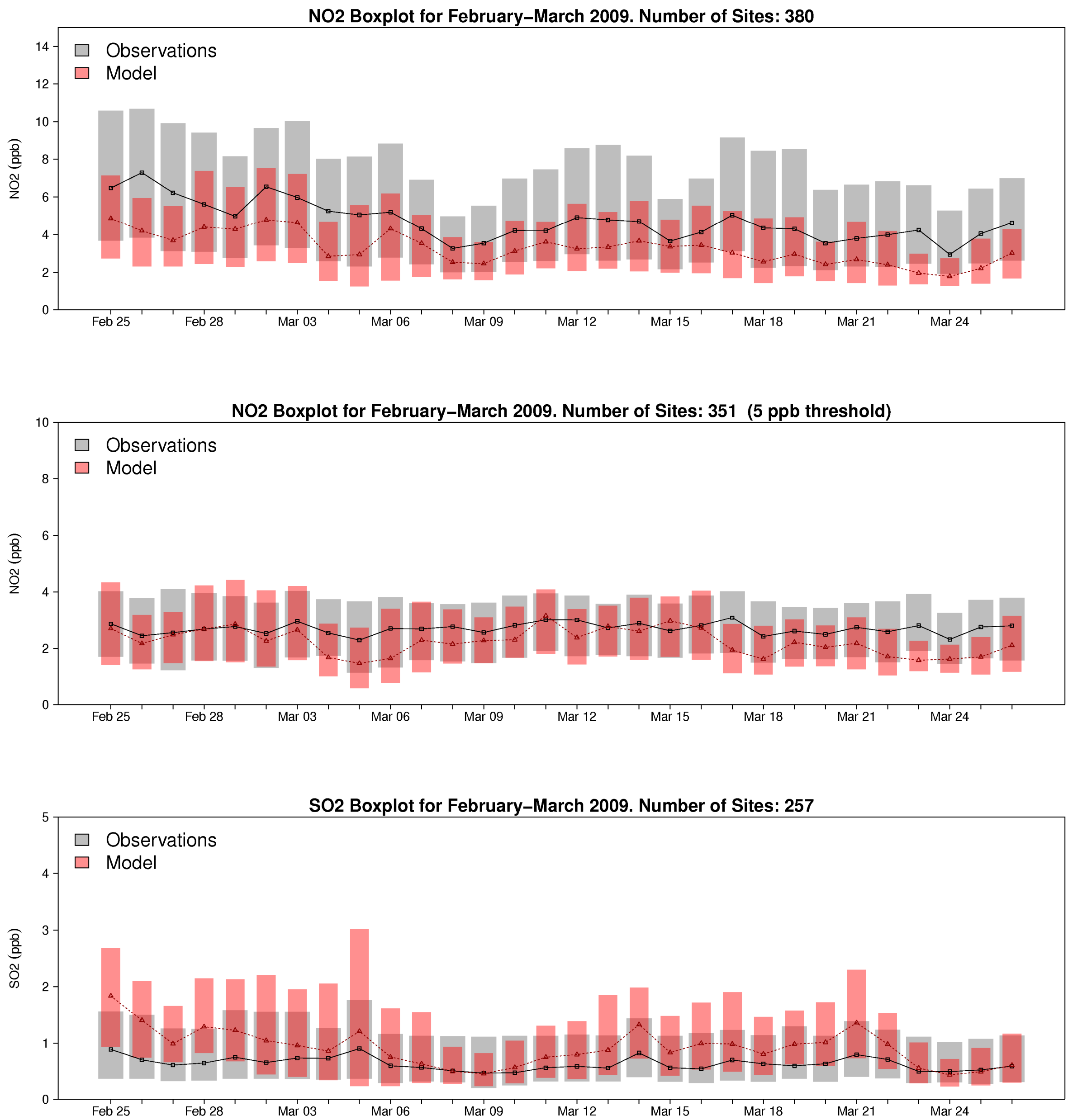



Figure S1. Comparison of modelled (VBS_BC) (red) and measured (grey) $NO_2$ (upper panel) and $SO_2$ (lower panel) concentrations at AirBase rural background sites (as in Table 2). The middle panel shows the comparison at stations where $NO_2$ concentrations do not exceed 5ppb. The extent of the bars indicates the 25$^{th}$ and 75$^{th}$ percentiles. The black and red lines represent measured and modelled medians, respectively.

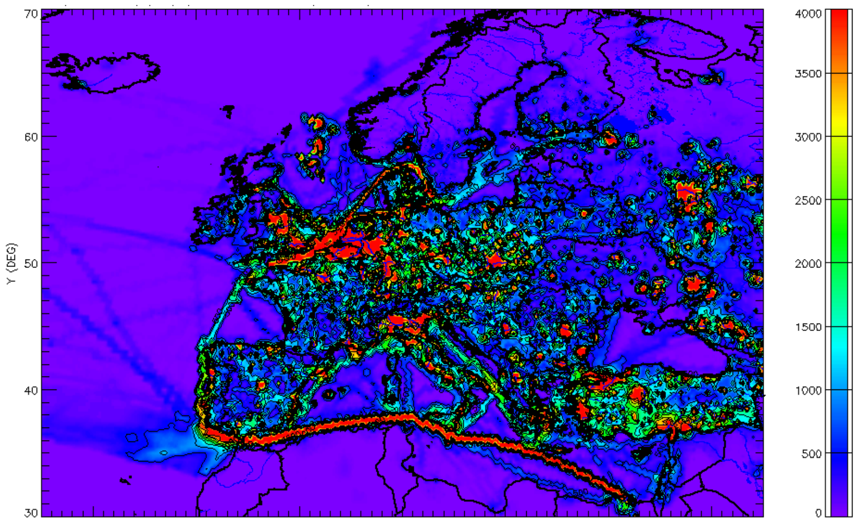
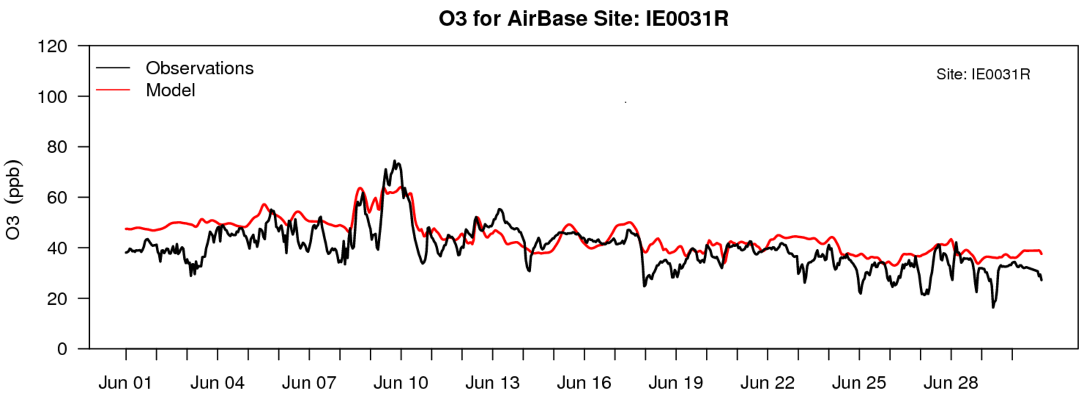
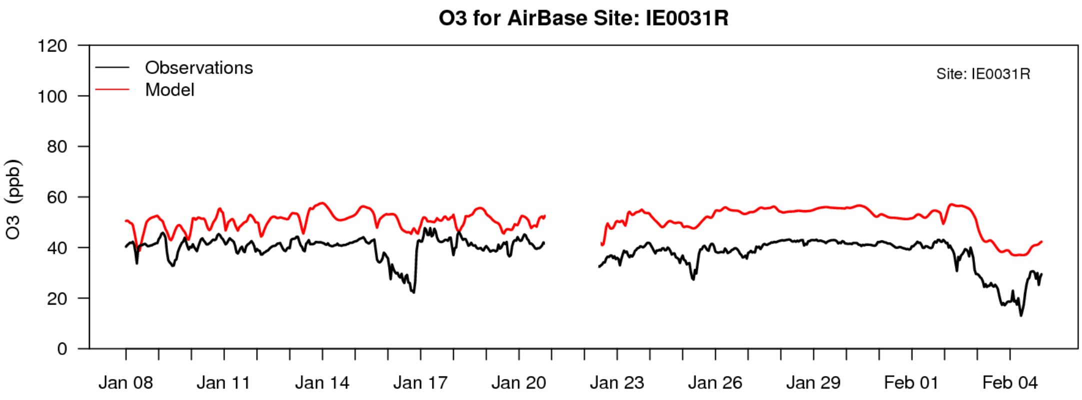
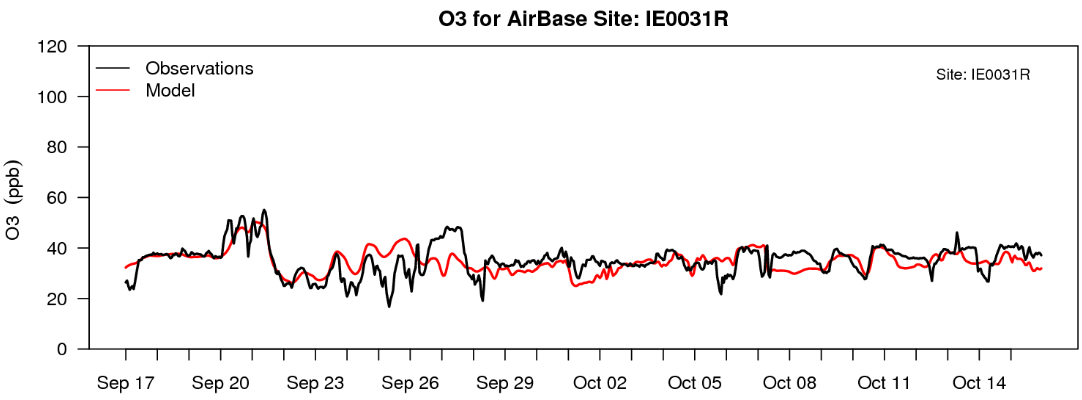



Figure S2. NO emissions in [mol / (h cell)] for 1 March 2009, at 6:00 AM


O3 for AirBase Site: IE0031R
Observations
Model
Site: IE0031R
O3 (ppb)
120
100
80
60
40
20
0
Jun 01
Jun 04
Jun 07
Jun 10
Jun 13
Jun 16
Jun 19
Jun 22
Jun 25
Jun 28


O3 for AirBase Site: IE0031R
Observations
Model
Site: IE0031R
O3 (ppb)
120
100
80
60
40
20
0
Jan 08
Jan 11
Jan 14
Jan 17
Jan 20
Jan 23
Jan 26
Jan 29
Feb 01
Feb 04


O3 for AirBase Site: IE0031R
Observations
Model
Site: IE0031R
O3 (ppb)
120
100
80
60
40
20
0
Sep 17
Sep 20
Sep 23
Sep 26
Sep 29
Oct 02
Oct 05
Oct 08
Oct 11
Oct 14

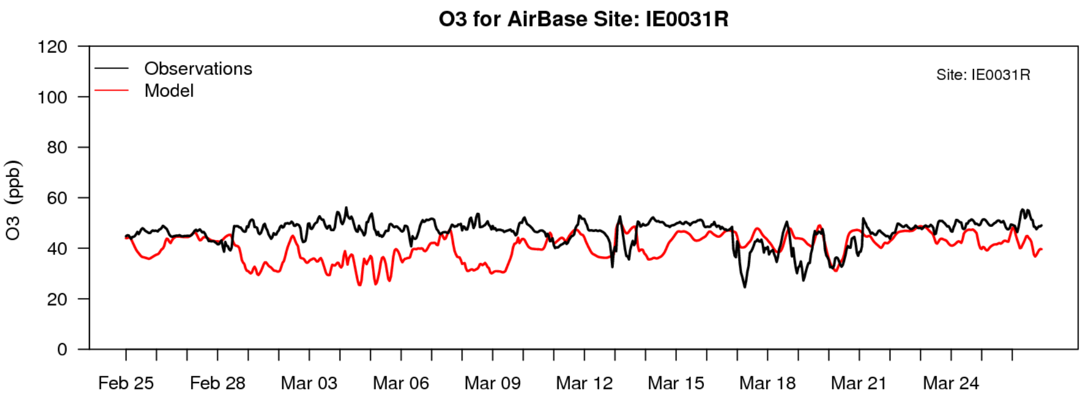

O3 for AirBase Site: IE0031R
Observations
Model
Site: IE0031R
O3 (ppb)
120
100
80
60
40
20
0
Feb 25
Feb 28
Mar 03
Mar 06
Mar 09
Mar 12
Mar 15
Mar 18
Mar 21
Mar 24

Figure S3. Comparison of modelled (base case, VBS_BC) and measured $O_3$ mixing ratios at Mace Head (IE0031R) for the four simulated periods: from top to bottom: June 2006, January-February 2007, September-October 2008, February-March 2009.

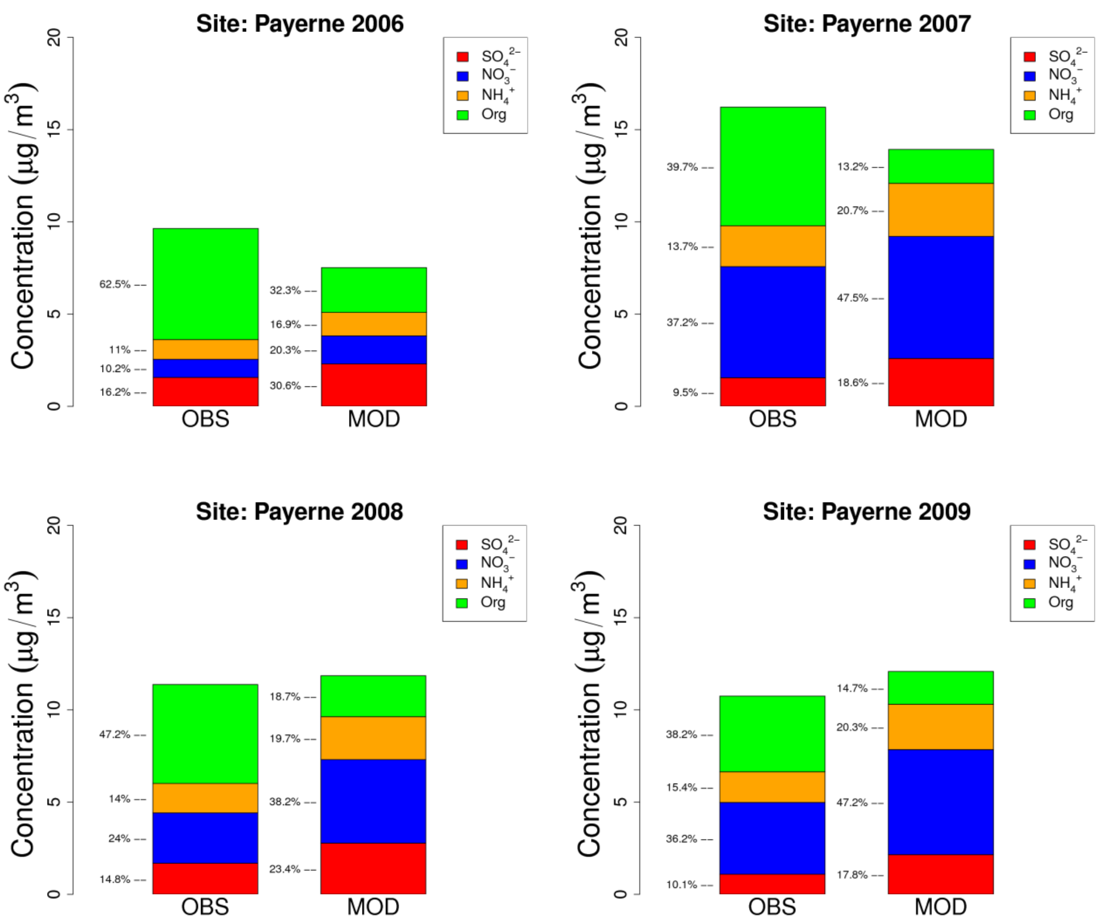



Figure S4. Comparison of observed (OBS) non-refractory $PM_1$ and modelled (MOD) $PM_{2.5}$ components at Payerne for all the investigated periods.

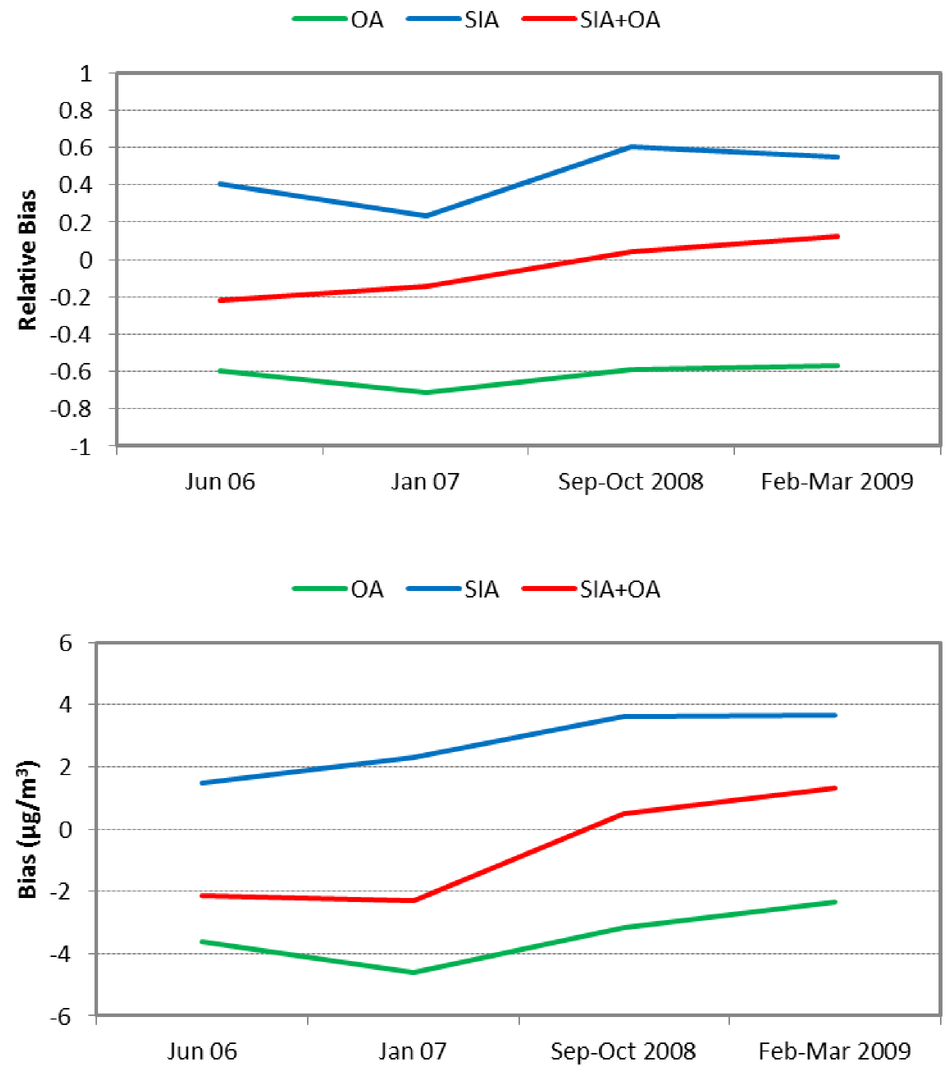
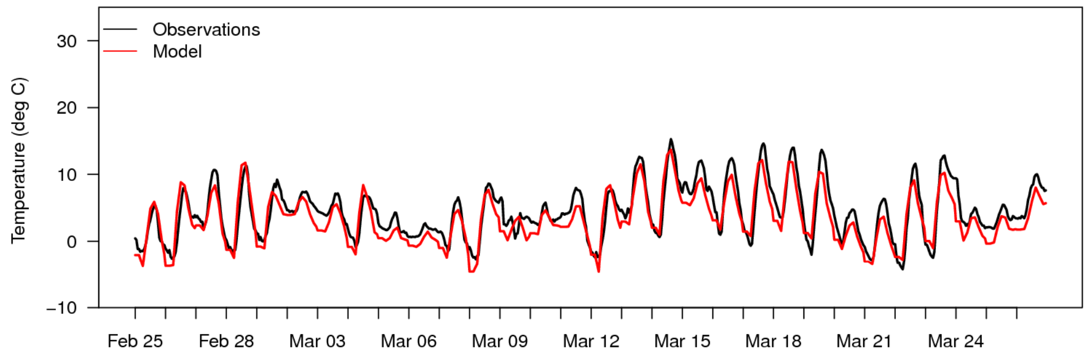
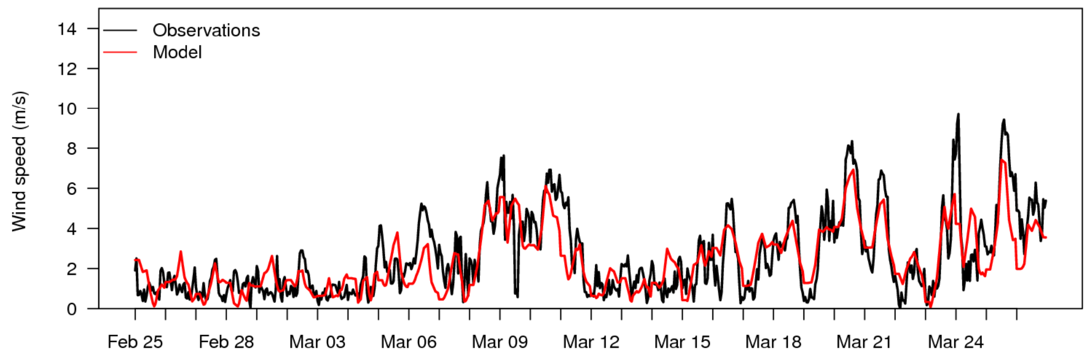
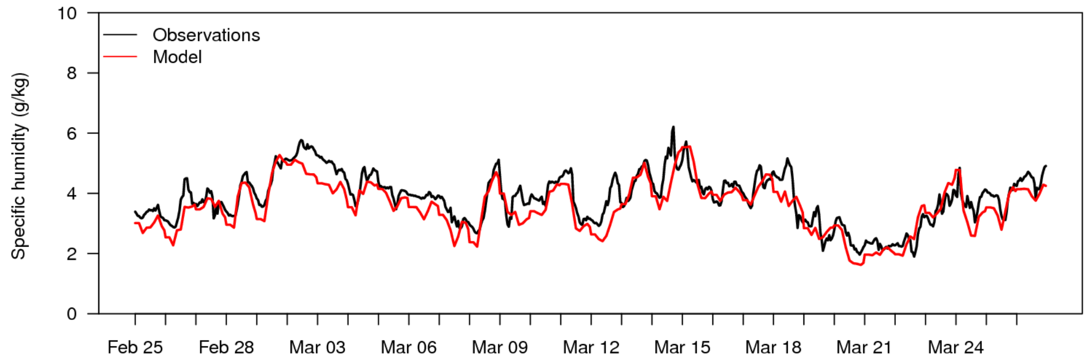



Figure S5. Absolute and relative biases for organic aerosol (OA), secondary organic aerosol (SIA) and OA+SIA in Payerne for all the investigated periods.


Observations
Model
Temperature (deg C)
30
20
10
0
−10
Feb 25
Feb 28
Mar 03
Mar 06
Mar 09
Mar 12
Mar 15
Mar 18
Mar 21
Mar 24


Observations
Model
Wind speed (m/s)
14
12
10
8
6
4
2
0
Feb 25
Feb 28
Mar 03
Mar 06
Mar 09
Mar 12
Mar 15
Mar 18
Mar 21
Mar 24


Observations
Model
Specific humidity (g/kg)
10
8
6
4
2
0
Feb 25
Feb 28
Mar 03
Mar 06
Mar 09
Mar 12
Mar 15
Mar 18
Mar 21
Mar 24

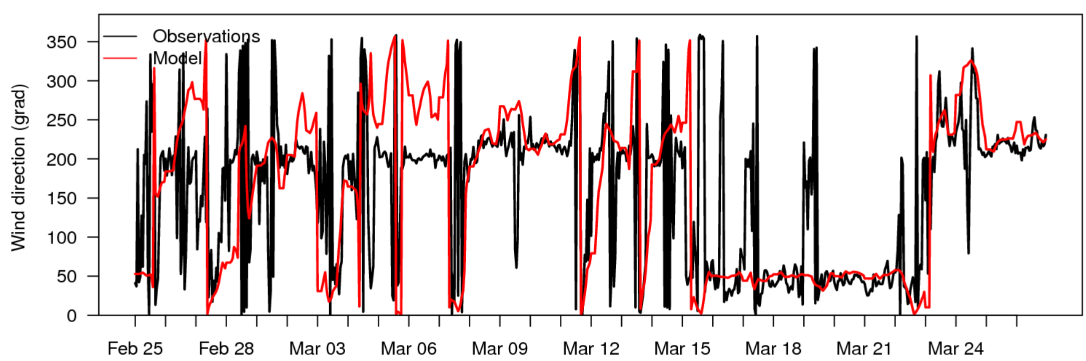
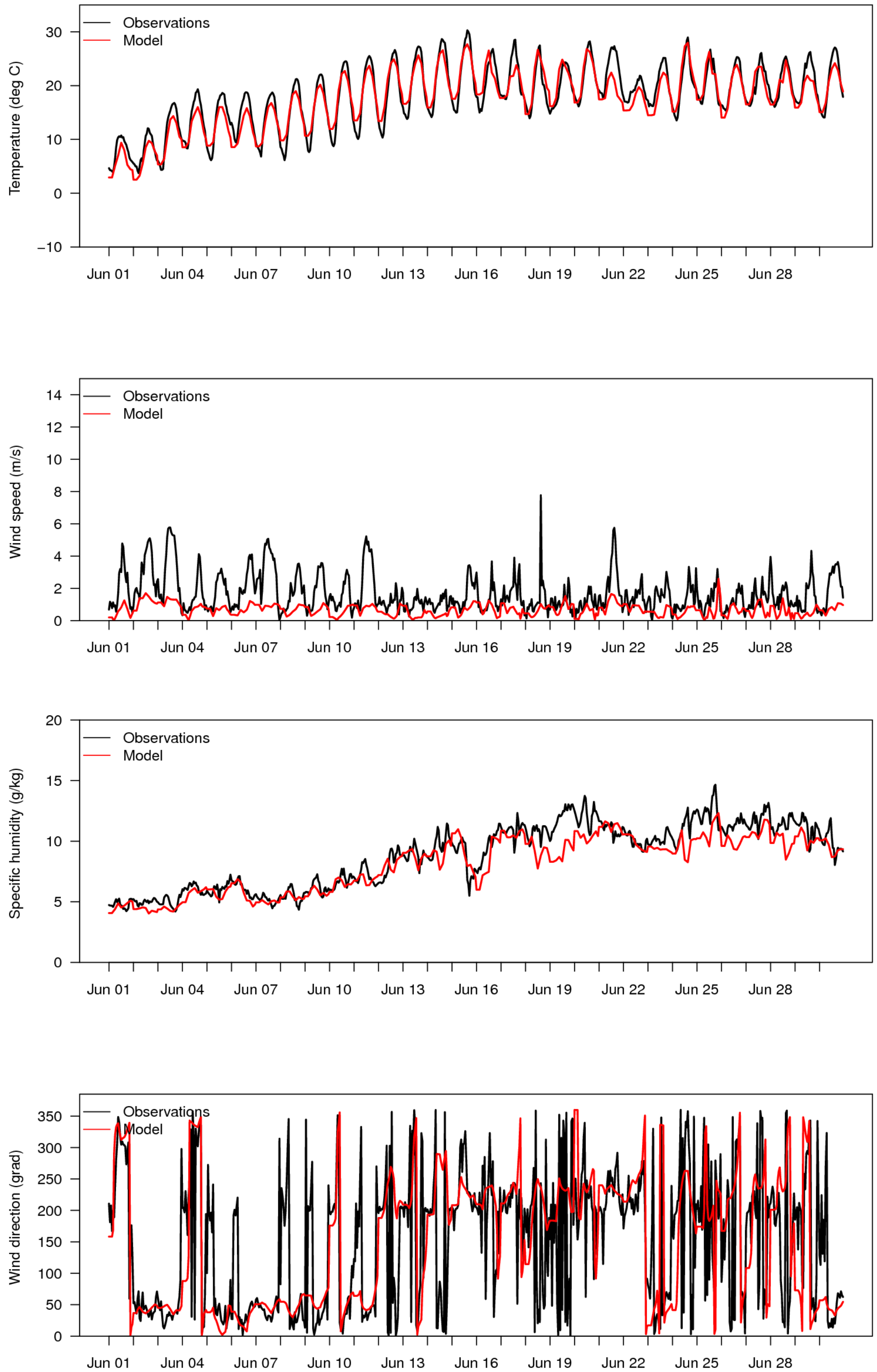

Observations
Model
Wind direction (grad)
350
300
250
200
150
100
50
0
Feb 25
Feb 28
Mar 03
Mar 06
Mar 09
Mar 12
Mar 15
Mar 18
Mar 21
Mar 24

Figure S6. Comparison of observed and modelled temperature (°C), wind speed (m $s^{-1}$), specific humidity (g/kg) and wind direction (°C) comparisons at Payerne in February-March 2009.



Observations
Model
Temperature (deg C)
30
20
10
0
−10
Jun 01
Jun 04
Jun 07
Jun 10
Jun 13
Jun 16
Jun 19
Jun 22
Jun 25
Jun 28
Wind speed (m/s)
14
12
10
8
6
4
2
0
Specific humidity (g/kg)
20
15
10
5
0
Wind direction (grad)
350
300
250
200
150
100
50
0

Figure S7. Comparison of observed and modelled temperature (°C), wind speed (m $s^{-1}$), specific humidity (g/kg) and wind direction (°C) comparisons at Payerne in June 2006.

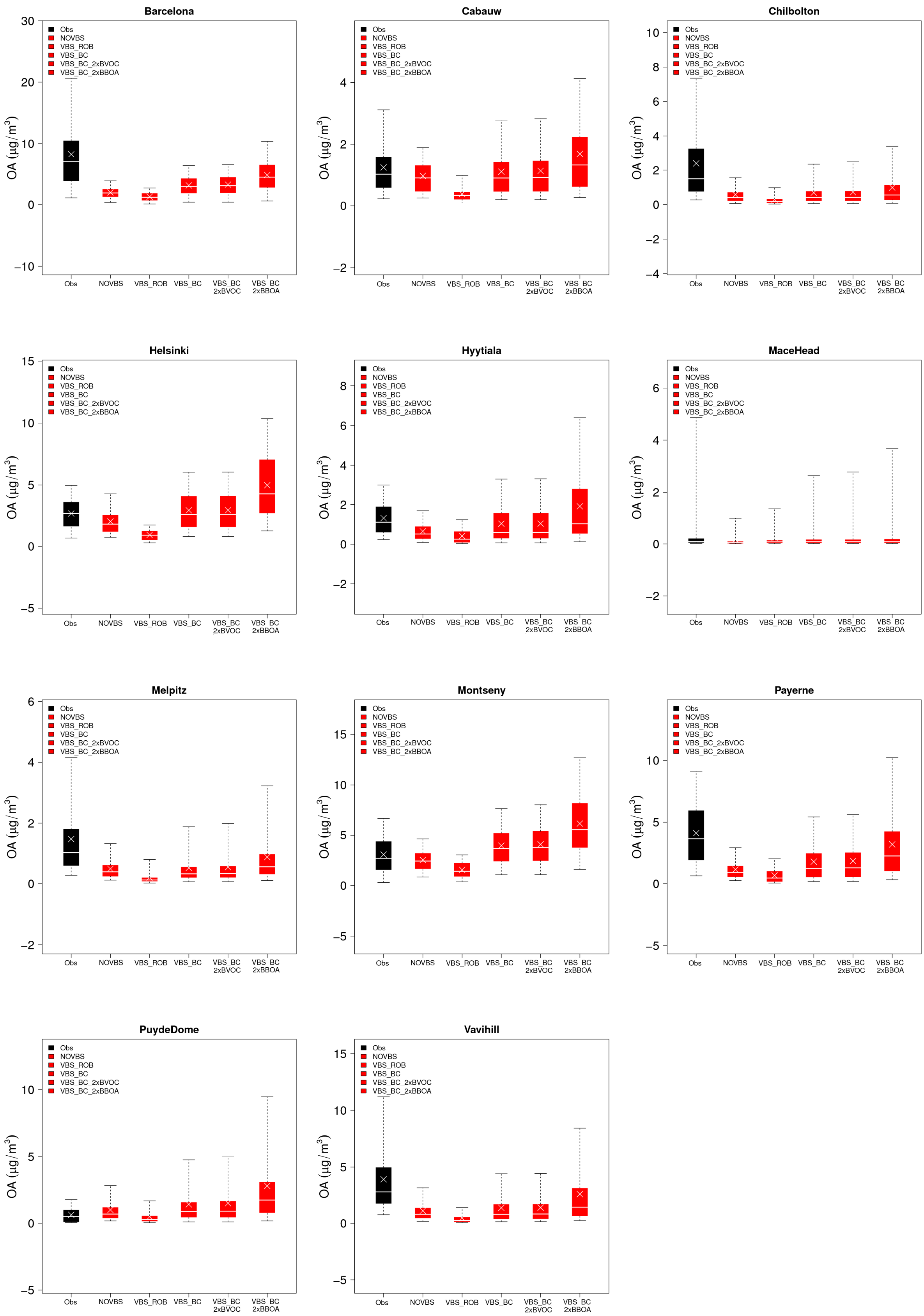

Barcelona
Cabauw
Chilbolton
Helsinki
Hyytiala
MaceHead
Melpitz
Montseny
Payerne
PuydeDome
Vavihill
Obs
NOVBS
VBS_ROB
VBS_BC
VBS_BC_2xBVOC
VBS_BC_2xBBOA
OA (µg/m3)
Obs NOVBS VBS_ROB VBS_BC VBS_BC 2xBVOC VBS_BC 2xBBOA

Figure S8. Observed and modelled OA concentrations using 5 scenarios at AMS sites for the period February-March 2009: Boxplots indicate medians, 5$^{th}$, 25$^{th}$, 75$^{th}$ and 95$^{th}$ quantiles for observations (black) and sensitivity tests (red). The crosses represent the arithmetic means.

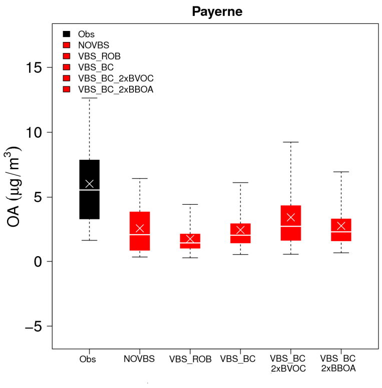



Figure S9. Observed and modelled OA using 5 scenarios at Payerne sites for the period June 2006: Boxplots indicate median, 5$^{th}$, 25$^{th}$, 75$^{th}$ and 95$^{th}$ quantile for observations (black) and sensitivity tests (red). The crosses represent the arithmetic means.