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Atmospheric Chemistry and Physics Discussions

*Supplement of*

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

**G. Ciarelli et al.**

*Correspondence to:* S. Aksoyoglu (sebnem.aksoyoglu@psi.ch)

# 6 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 |
|---|---|---|---|---|---|---|---|
| SV-OOA | 0 | 0.102 | 7 | 4.90 | 9.10 | 172 | 2.05 |
| | 1 | −0.188 | 7.25 | 4.38 | 10.1 | 167 | 1.92 |
| | 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 |
| HOA-like | 0 | −1.52 | 17 | 2.69 | 31.3 | 278 | 1.36 |
| | 1 | −1.65 | 17.5 | 2.02 | 33.0 | 275 | 1.31 |
| | 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 |
| BBOA-like | 0 | −0.704 | 10 | 4.32 | 15.7 | 205 | 1.71 |
| | 1 | −1.02 | 11 | 3.60 | 18.4 | 208 | 1.58 |
| | 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 |

Table S2. Measured and modelled $NH_3$ monthly average concentrations at Payerne for June 2006 and February-March 2009. Measurement data "Ammoniak Immisionsmessungen in der Schweiz" available on http://www.bafu.admin.ch/luft/00585/10770/index.html?lang=de.

| Period | $NH_3$ Model ($\mu g\ m^{-3}$) | $NH_3$ Observation ($\mu g\ m^{-3}$) | MB [-] |
|---|---|---|---|
| June 2006 | 4.7 | 5.0 | -6% |
| March 2009 | 6.1 | 5.1 | +20% |

Table S3. Statistical analysis for nitrate for February-March 2009 at different AMS sites with 50% reduction of ammonia scenario.

| Site | Mean observed $NO_3^-$ ($\mu g\ m^{-3}$) | Mean modelled $NO_3^-$ Base case (S3) ($\mu g\ m^{-3}$) | Mean modelled $NO_3^-$ 50% red. $NH_3$ ($\mu g\ m^{-3}$) | MB Base case (S3) ($\mu g\ m^{-3}$) | MB 50% red. $NH_3$ ($\mu g\ m^{-3}$) |
|---|---|---|---|---|---|
| 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 S4. Statistical analysis for the OA concentration and different sensitivity scenarios for February-March 2009 periods at 11 AMS sites.

| Site | Mean observed OA (μg/m3) | Mean modelled OA (μg/m$^3$) | MB (μg/m$^3$) | ME (μg/m$^3$) | MFB [-] | MFE [-] |
|---|---|---|---|---|---|---|
| | | Scenario S1 | | | | |
| 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 |
| | | Scenario S2 | | | | |
| 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 |
| | | Scenario S3 | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| 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 |
| Scenario S4 | | | | | | |
| 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 |
| Scenario S5 | | | | | | |
| 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 S5. Statistical analysis for the OA concentration and different sensitivity scenarios for June 2006 period at Payerne site.

| Scenario | Mean observed OA (µg/m3) | Mean modelled OA (µg/m$^3$) | MB (µg/m$^3$) | ME (µg/m$^3$) | MFB [-] | MFE [-] |
|---|---|---|---|---|---|---|
| S1 | 6.03 | 2.56 | -3.47 | 3.54 | -0.91 | 0.93 |
| S2 | 6.03 | 1.74 | -4.29 | 4.29 | -1.11 | 1.11 |
| S3 | 6.03 | 2.43 | -3.6 | 3.62 | -0.85 | 0.86 |
| S4 | 6.03 | 3.4 | -2.63 | 2.78 | -0.63 | 0.66 |
| S5 | 6.03 | 2.75 | -3.28 | 3.32 | -0.75 | 0.76 |

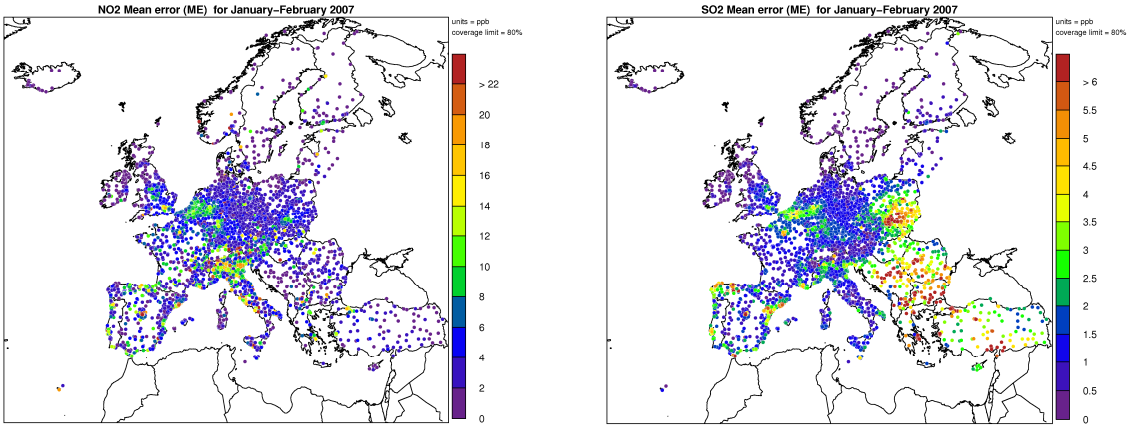



Figure S1: Spatial distribution of mean error for $NO_2$ (left) and $SO_2$ (right) for the January-February 2007 episode for all Airbase stations with 80% of daily measurement available. Units are in ppb.

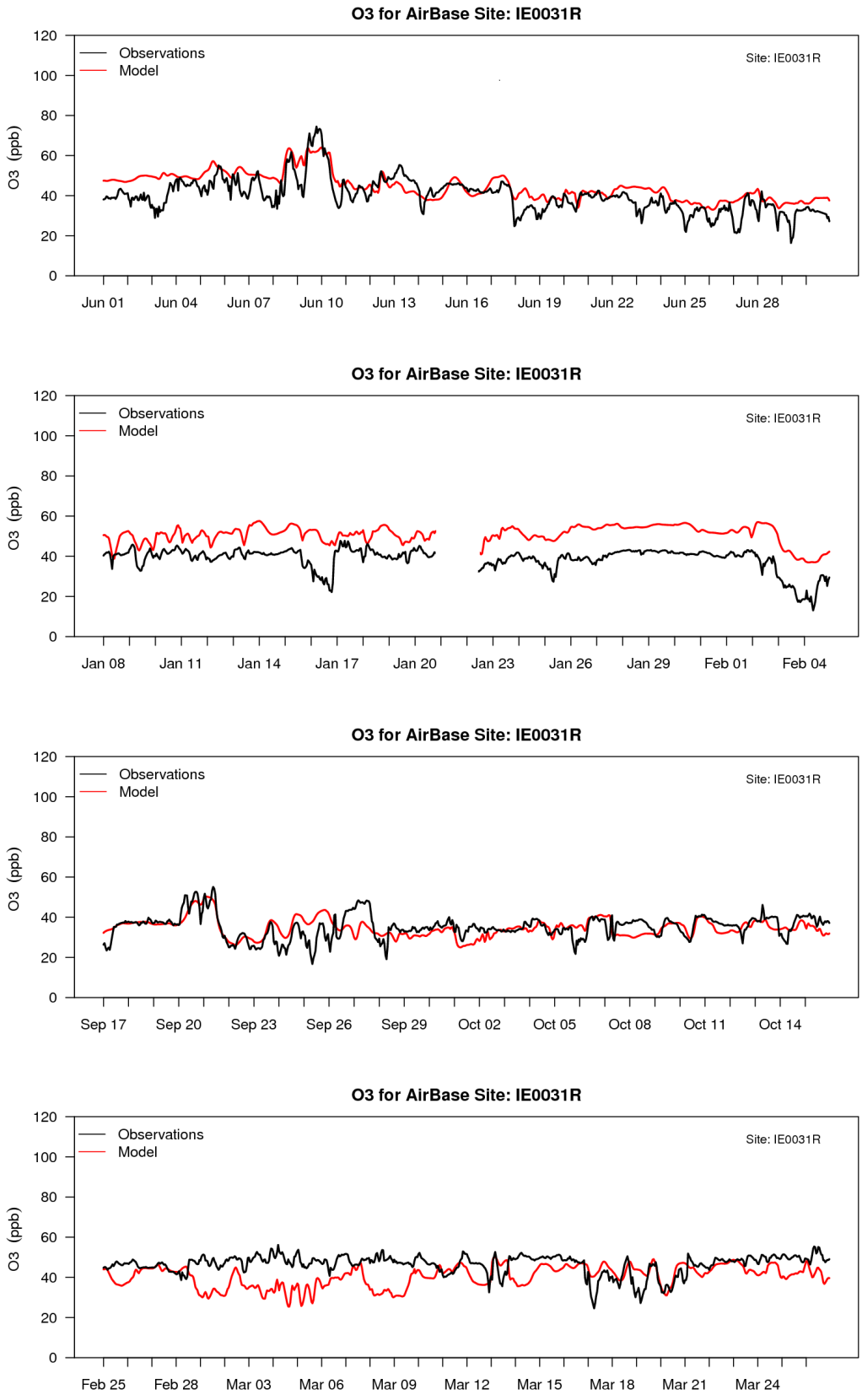



Figure S2. Comparison of modelled (base case, S3) and measured $O_3$ mixing ratios at Mace

Head (IE0031R) for the four simulated periods: from top to bottom: June 2006, January-February 2007, September-October 2008, February-March 2009.

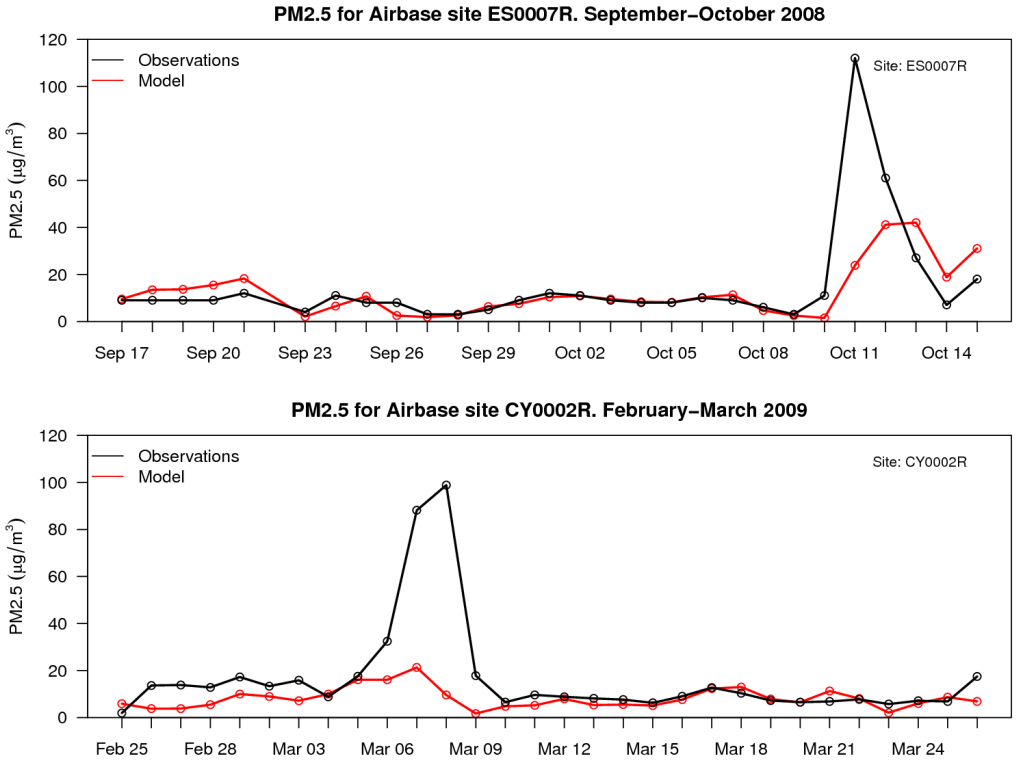



Figure S3. Comparison of modelled (base case, S3) and measured $PM_{2.5}$ concentrations at Viznar (ES0007R) in Southern Spain for September-October 2008 (top) and at Ayia Marina (CY0002R) in Cyprus for February-March 2009 (bottom).

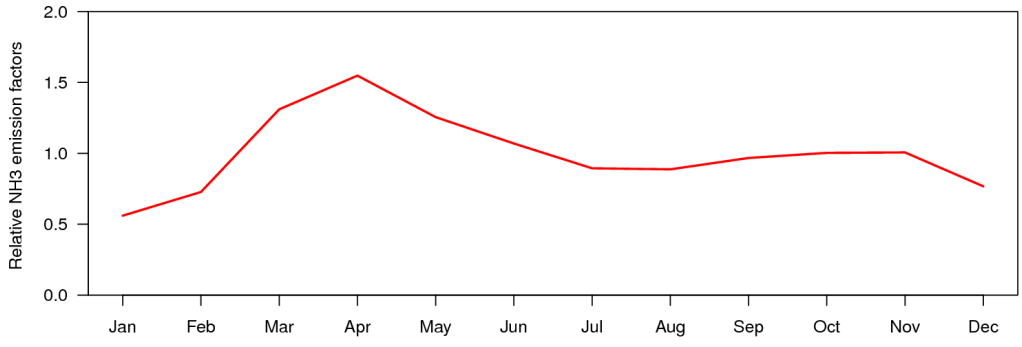
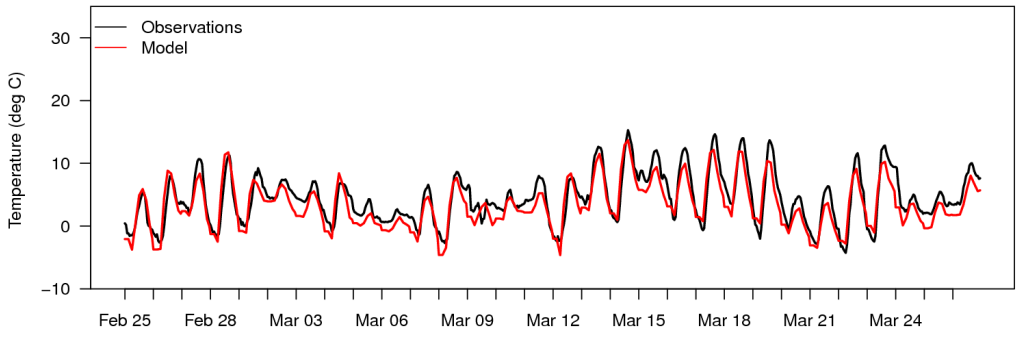
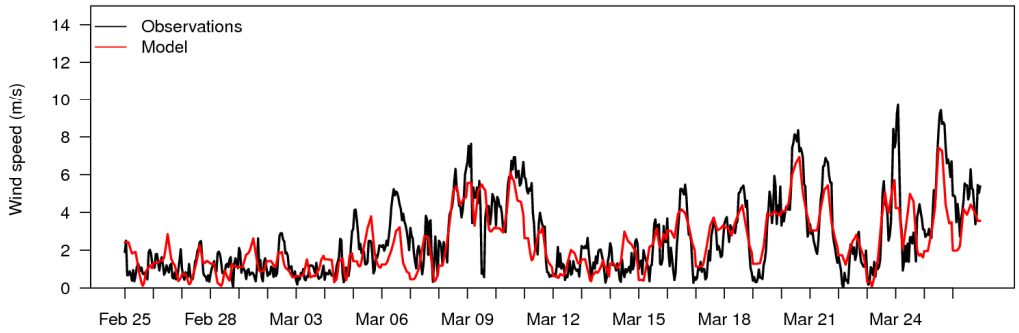
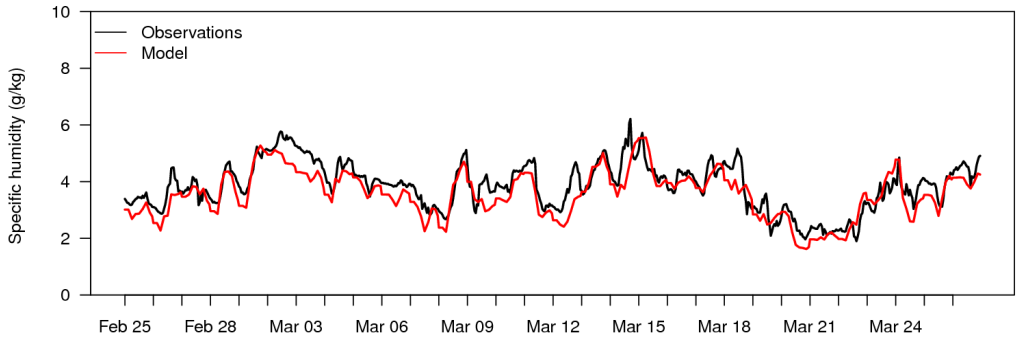


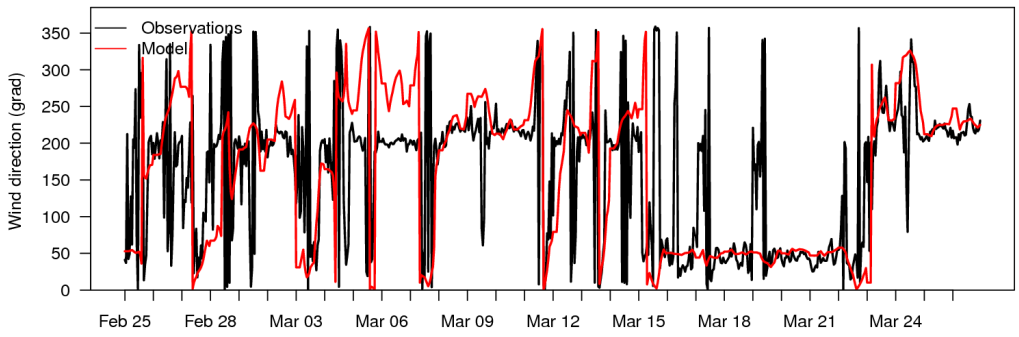

Figure S4. Monthly ammonia emission factor profiles for Switzerland as available in the EDIII exercise.


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

1


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

2

Figure S5. 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.

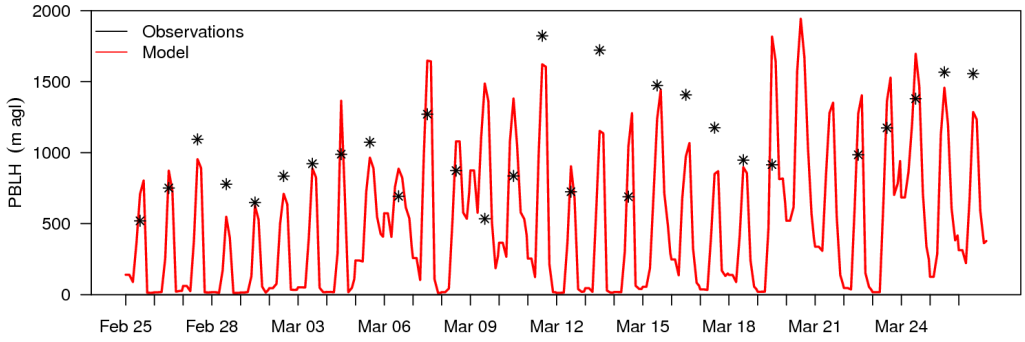
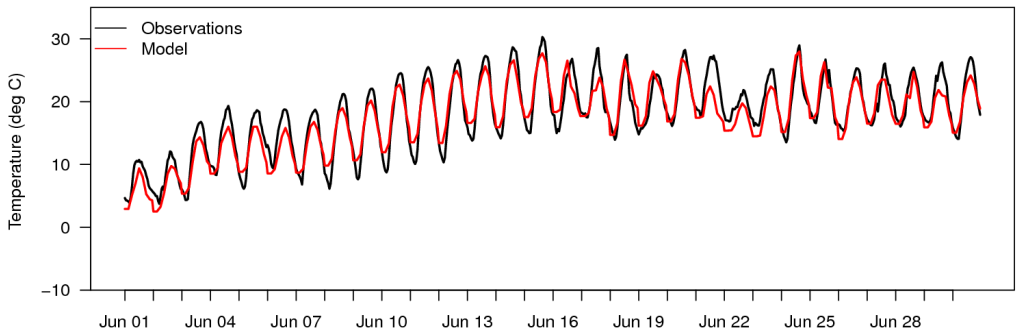
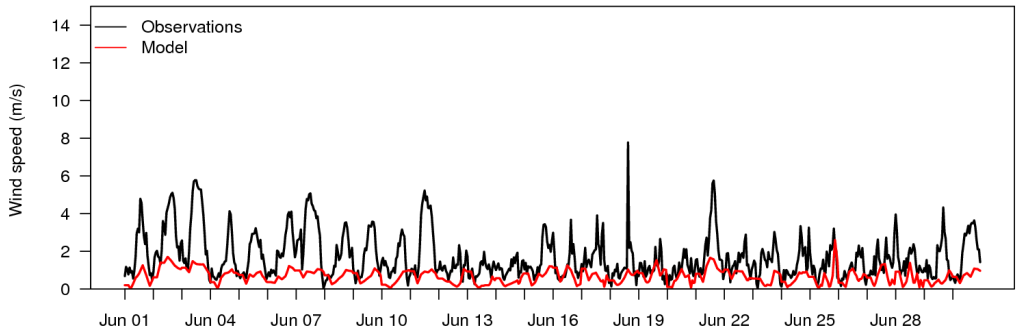
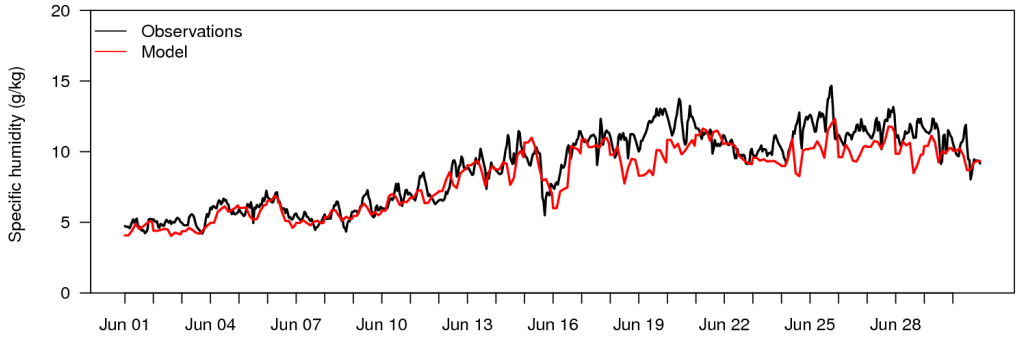


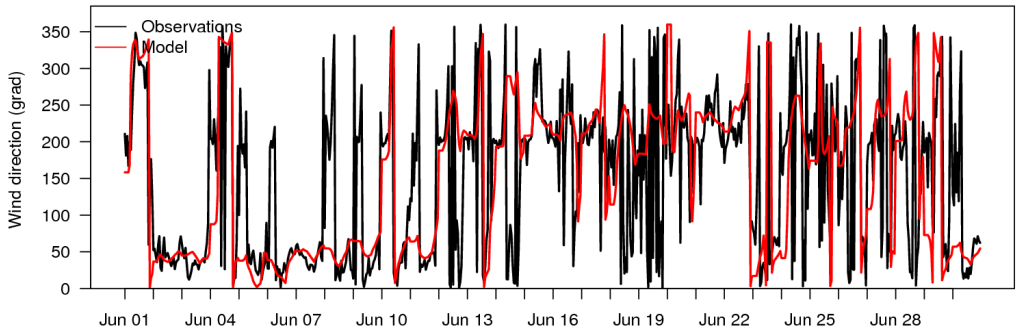

Figure S6. Modelled planetary boundary layer height at Payerne (red) and convective boundary layer height derived from Payerne soundings (stars). Units are meters above ground level.


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


Observations
Model
Wind speed (m/s)
14
12
10
8
6
4
2
0
Jun 01
Jun 04
Jun 07
Jun 10
Jun 13
Jun 16
Jun 19
Jun 22
Jun 25
Jun 28

1


Observations
Model
Specific humidity (g/kg)
20
15
10
5
0
Jun 01
Jun 04
Jun 07
Jun 10
Jun 13
Jun 16
Jun 19
Jun 22
Jun 25
Jun 28


Observations
Model
Wind direction (grad)
350
300
250
200
150
100
50
0
Jun 01
Jun 04
Jun 07
Jun 10
Jun 13
Jun 16
Jun 19
Jun 22
Jun 25
Jun 28

2

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.

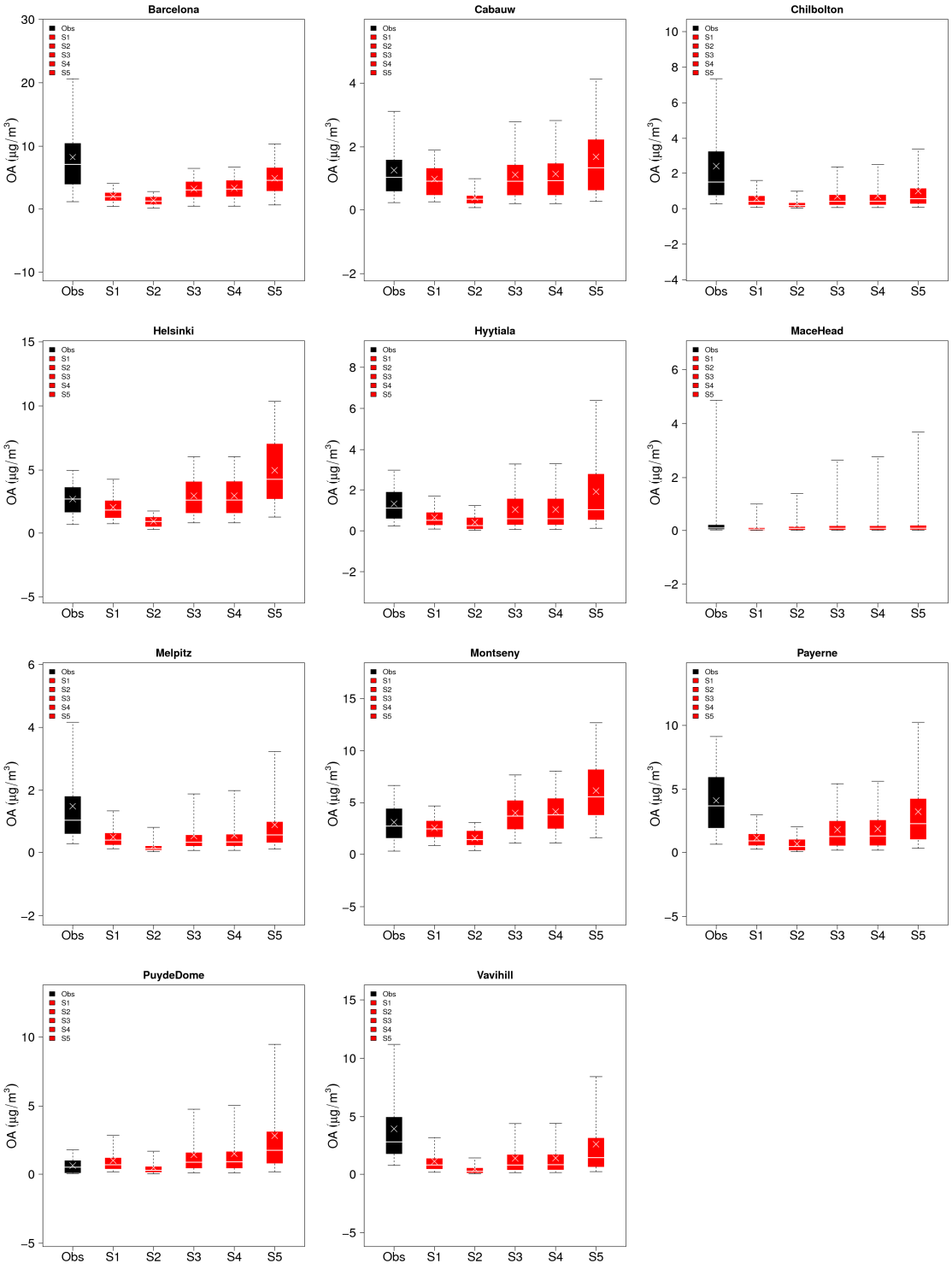



Figure S8. Observed and modelled OA concentrations using 5 scenarios at AMS sites for the period February-March 2009: Boxplots indicate medians, 5th, 25th, 75th and 95th quantiles for observations (black) and sensitivity tests (red). The crosses represent the arithmetic means.

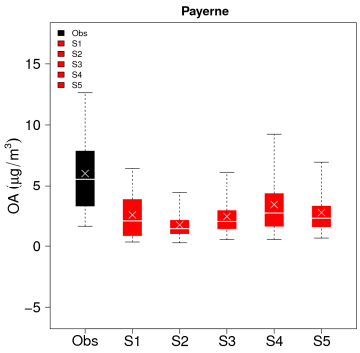



Figure S9. Observed and modelled OA using 5 scenarios at Payerne sites for the period June 2006: Boxplots indicate median, 5$^{th}$, 25$^{th}$, 75$^{th}$ and 95$^{th}$ quantile for observations (black) and sensitivity tests (red). The crosses represent the arithmetic means.