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Supplement of

Modeling organic aerosol composition at the puy de Dôme mountain (France) for two contrasted air masses with the WRF-Chem model

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Supplementary Material

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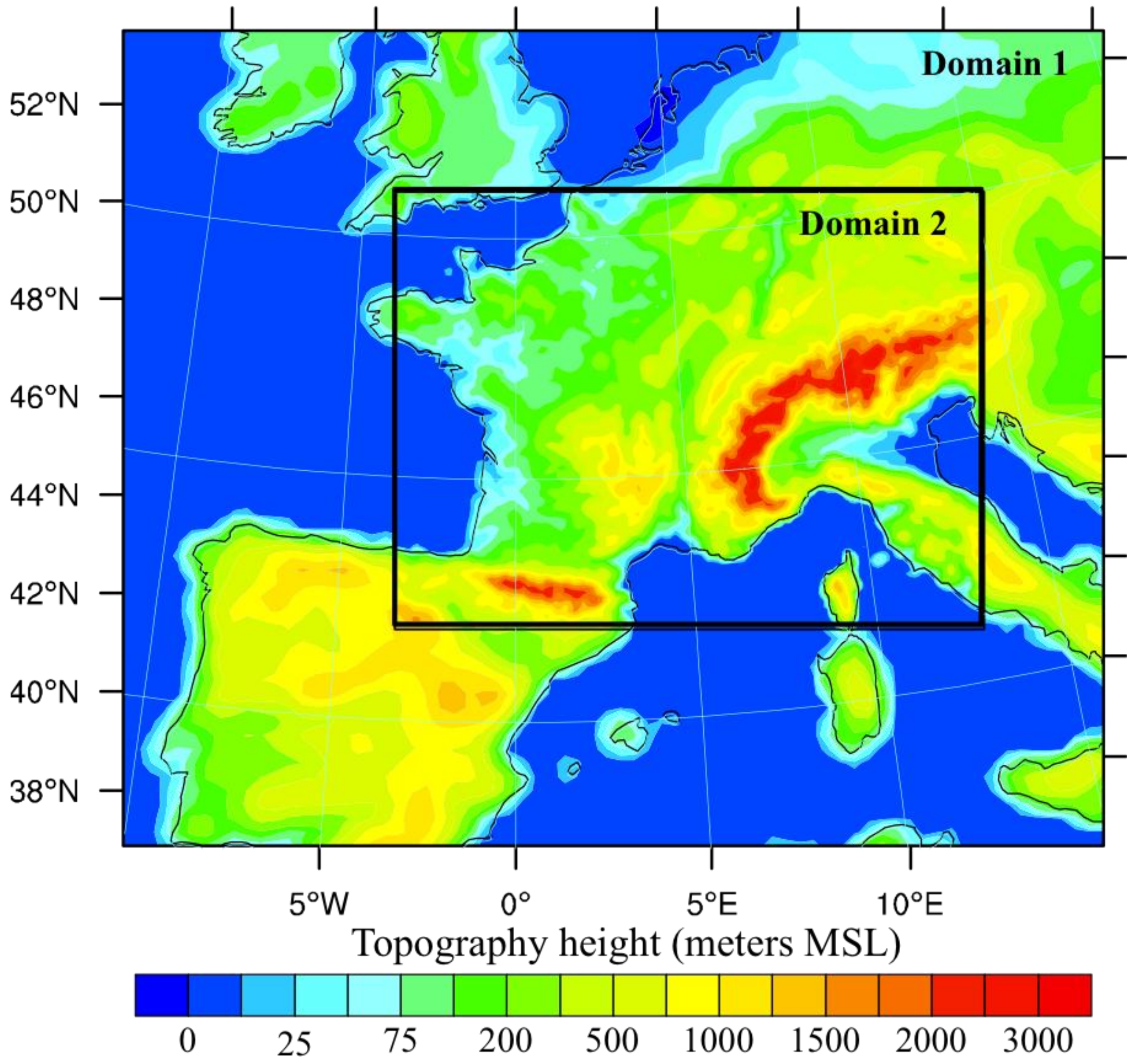

Figure S1: WRF-Chem nested domains used for the simulations.

Figure S2: Sector definitions for different air masses reaching the PUY site.

Table S1: Partitioning ratios used to redistribute emitted species into emission categories and aggregation factors used to allocate MACCity inventory species to the species of the RACM chemical mechanism.

MACCIty inventory species	Partitioning ratios	Emissions category*	Aggregation factor*	Model species**
Ethane	100	2	1.00	ETH
Propane	100	3	0.57	HC3
Butanes and higher alkanes	28.3	4	1.11	HC3
	37.2	5	0.97	HC5
	28.4	6	0.94	HC8
	6.1	7	1.14	HC8
Ethene	100	9	1.00	ETE
Propene	100	10	1.00	OLT
Butenes and higher alkenes	26.0	11	1.00	OLT
	59.0	12	1.00	OLI
	15.0	13	0.50	OLT
			0.50	OLI
Aromatics	19.6	14	0.29	TOL
	32.0	15	1.00	TOL
	48.4	16	1.00	XYL
Formaldehyde	100	19	1.00	HCHO
Others aldehydes	100	20	1.00	ALD
Acetone	100	21	0.33	KET
Others ketones	100	22	1.61	KET
Methanol	100	27	0.49	HC3
Others alcohols	95.0	28	1.37	HC3
	5.0	29	1.07	HC5

*Middleton et al. (1990); ** Stockwell et al. (1997)

References

Middleton, P., Stockwell, W. R. and Carter, W. P.: Aggregation and analysis of volatile organic compound emissions for regional modeling, Atmos. Environ., 24(5), 1107–1133, 1990.

Stockwell, W. R., Kirchner, F., Kuhn, M. and Seefeld, S.: A new mechanism for regional atmospheric chemistry modeling, J. Geophys. Res., 102(D22), 25847–25879, doi:199710.1029/97JD00849, 1997.

Table S2: Statistical results and comparison between statistical performance measures and criteria acceptance for meteorological parameters (green cells indicate good model performance).

	Parameters	**NMSE <1.5**	**FB |FB|<0.3**	**FAC >0.5**	**VG <4**	**MG 0.7<MG<1.3**
Autumn 2008	Temperature	0.1	0.2	1.0	1.1	1.2
	Humidity	0.1	0.1	0.9	1.3	1.0
Summer 2010	Temperature	0.1	0.3	1.0	1.1	1.4
	Humidity	0.0	0.0	1.0	1.0	1.0
	Pressure	0.0	0.0	1.0	1.0	1.0

Table S3: Statistical results and comparison between statistical performance measures and criteria acceptance for trace gases concentrations (green cells indicate good model performance).

	Parameters	**NMSE <1.5**	**FB $\lvert FB \rvert<0.3$**	**FAC >0.5**	**VG <4**	**MG 0.7<MG<1.3**
Autumn 2008	O_3	0.0	-0.1	1.0	1.0	0.9
	CO	0.0	-0.1	1.0	1.0	0.9
Summer 2010	O_3	0.0	0.1	1.0	1.0	1.1
	CO	0.0	-0.1	1.0	1.0	0.9

Table S4: Statistical results and comparison between statistical performance measures and criteria acceptance for inorganic aerosol species mass concentrations (green cells indicate good model performance).

	Parameters	**NMSE <1.5**	**FB |FB|<0.3**	**FAC >0.5**	**VG <4**	**MG 0.7<MG<1.3**
Autumn 2008	SO_4^{2-}	0.4	-0.1	0.8	1.7	0.8
	NH_4^+	0.5	0.2	0.7	1.9	1.0
	NO_3^-	1.2	0.4	0.4	37.0	2.1
	BC	4.2	1.2	0.1	10.0	4.1
Summer 2010	SO_4^{2-}	0.1	0.2	1.0	1.1	1.2
	NH_4^+	0.6	0.7	0.5	1.7	2.0
	NO_3^-	1.0	0.8	0.3	3.4	2.4
	BC	0.2	0.4	1.0	1.2	1.5

Table S5: SOA mass yields (Murphy and Pandis, 2009) for the VOCs precursors and volatility bins used in the VBS parameterization* implemented in WRF-Chem by Ahmadov et al. (2012).

VOCs	High NO_x conditions				Low NO_x conditions			
	1	**10**	**100**	**1000**	**1**	**10**	**100**	**1000**
HC5	0.0000	0.0375	0.0000	0.0000	0.0000	0.0750	0.0000	0.0000
HC8	0.0000	0.1500	0.0000	0.0000	0.0000	0.3000	0.0000	0.0000
OLT	0.0008	0.0045	0.0375	0.1500	0.0045	0.0090	0.0600	0.2250
OLI	0.0030	0.0255	0.0825	0.2700	0.0225	0.0435	0.1290	0.3750
TOL	0.0030	0.1650	0.3000	0.4350	0.0750	0.2250	0.3750	0.5250
XYL, CSL	0.0015	0.1950	0.3000	0.4350	0.0750	0.3000	0.3750	0.5250
ISO	0.0003	0.0225	0.0150	0.0000	0.0090	0.0300	0.0150	0.0000
SESQ	0.0750	0.1500	0.7500	0.9000	0.0750	0.1500	0.7500	0.9000
API, LIM	0.0120	0.1215	0.2010	0.5070	0.1073	0.0918	0.3587	0.6075

*Yields are for 4 volatility bins with saturation concentrations of 1, 10, 100 and 1000 μg m^{-3} at 300 K and depend on RO_2/NO_x conditions as described by Ahmadov et al. (2012).

References

Ahmadov, R., McKeen, S. A., Robinson, A. L., Bahreini, R., Middlebrook, A. M., Gouw, J. A. de, Meagher, J., Hsie, E.-Y., Edgerton, E., Shaw, S. and Trainer, M.: A volatility basis set model for summertime secondary organic aerosols over the eastern United States in 2006, J. Geophys. Res., 117, D06301, doi:201210.1029/2011JD016831, 2012.

Table S6: OA mass concentration measured at the PUY site and simulated by the WRF-Chem model for the baseline simulation and sensitivity tests (emission/dry deposition, OA formation processes: oxidation rate of OCVs and SOA yields, and all effects). Percentages represent the variations obtained for each individual tests.

	OA mass concentration ($\mu g\ m^{-3}$)		**OA mass concentration ($\mu g\ m^{-3}$)**	**Variation from baseline to test simulation (%)**	
				ASOA	**BSOA**
Observations	12.55				
Model : baseline	2.02				
Model : dry deposition and emission	3.14	Deposition	2.27	+ 14%	+ 16%
		Emissions of AVOC	2.54	+ 49%	+ 2%
		Emissions of BVOC	2.39	- 8%	+ 67%
Model : oxydation rate of OCVs and SOA yields	8.62	Oxidation rate of anthropogenic OCVs	2.58	+ 51%	+ 5%
		Oxidation rate of biogenic OCVs	2.61	+ 5%	+ 81%
		Yields of AVOC	3.27	+ 116%	+ 10%
		Yields of BVOC	2.85	+ 6%	+ 115%
Model : all effects	10.74				

Statistical performance measures

$$FB = \frac{\left(\overline{C_o} - \overline{C_p}\right)}{0.5\left(\overline{C_o} + \overline{C_p}\right)} \quad (1)$$

$$MG = \exp\left(\overline{\ln C_o} - \overline{\ln C_p}\right) \quad (2)$$

$$NMSE = \frac{\overline{\left(C_o - C_p\right)^2}}{\overline{C_o}\,\overline{C_p}} \quad (3)$$

$$FAC2 = fraction\ of\ data\ that\ satisty\ 0.5 < \frac{C_p}{C_o} < 2.0 \quad (4)$$

where :

- C_p : model predictions
- C_o : observations
- $\bar{C}$: average over the dataset

The fractional bias (FB) is a measure of the systematic bias in the model. Values of FB are symmetrical and bounded: they range between - 2.0 and + 2.0 and are dimensionless numbers. A positive value of FB indicates an underestimation of the observations by the model whereas a negative value of FB corresponds to an overestimation. More particularly, FB = - 0.67 implies overestimation by a factor of two, while FB = + 0.67 is equivalent to underestimation by a factor of two.

The geometric mean bias (MG) corresponds to the ratio of the geometric mean of C_o to the geometric mean of C_p. As it measures a systematic bias, it is similar to FB but based on a logarithmic scale. A value of MG equal to + 0.5 implies overestimation by a factor of two, while MG = + 2.0 corresponds to underestimation by a factor of two.

The normalized mean square error (NMSE) and the geometric variance (VG) represent the scatter of the data set and are representative of both systematic and unsystematic (random) errors.

A value of NMSE at + 0.5 corresponds to an equivalent factor of two mean biases but does not allow us to determine whether the factor of two mean biases is an overestimation or an underestimation of the observations by the model.

VG represents the scatter of a lognormal distribution. A value of VG at +1.6 (+12) implies an equivalent factor of two (five) mean bias, but does not differentiate whether the factor of two (five) mean bias is an overestimation or an underestimation by the model.

According to Chang and Hanna (2004), a perfect model is defined by MG, VG, and FAC2 = 1.0, and FB and MNSE = 0.0. The acceptable model performance, from statistical point of view, estimated by Chang and Hanna (2004) are:

- Criterion 1 (C1): the fraction of model predictions within a factor of two of observations is more than 50% (FAC2 > 0.5);
- Criterion 2 (C2): the mean bias is within ± 30% of the mean ($|FB| < 0.3$ or $0.7 < MG < 1.3$);
- Criterion 3 (C3): the random scatter is about a factor of two to three of the mean (NMSE < 1.5 or VG < 4).

Reference

Chang, J. C. and Hanna, S. R.: Air quality model performance evaluation, Meteorol. Atmos. Phys., 87(1-3), 167–196, doi:10.1007/s00703-003-0070-7, 2004.