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Modeling organic aerosol over Central Europe: uncertainties linked to different chemical mechanisms, parameterizations, and boundary conditions

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S1 Statistical measures used in the validation of model experiments

The mean bias (MB), root mean square error (RMSE), normalized mean square error (NMSE), and index of agreement (IOA) are defined as:

$$\mathrm{MB} = \frac{1}{N}\sum_{i=1}^{N}(m_i - o_i), \tag{S1}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(m_i - o_i)^2}, \tag{S2}$$

$$\mathrm{NMSE} = \frac{\frac{1}{N}\sum_{i=1}^{N}(m_i - o_i)^2}{\overline{m}\,\overline{o}}, \tag{S3}$$

$$\mathrm{IOA} = 1 - \frac{\sum_{i=1}^{N}(m_i - o_i)^2}{\sum_{i=1}^{N}(|m_i - \overline{o}| + |o_i - \overline{o}|)^2}, \tag{S4}$$

where m_i and o_i denote the corresponding modeled and observed values in a compared sample, respectively, N is the total number of pairs m_i vs. o_i in the sample, and $\overline{m}$ and $\overline{o}$ stand for the mean of the modeled and observed values in the sample.

We will construct the ratios of the corresponding modeled (m_i) and observed (o_i) values in the sample, denoting these ratios as r_i. The fraction of predictions within a factor of two of observations (FAC2) is defined as the proportion of the r_i ratios in the sample that meet the following criteria:

$$0.5 \leq r_i \leq 2. \tag{S5}$$

S2 Tables and figures

Table S1. Chemical species included in the default chemical boundary conditions (CBCs) depending on the applied gas-phase chemistry mechanism.

Gas-phase chemistry mechanism (GPCM) applied	Chemical species included in the default CBCs
Independent on GPCM	Nitrogen monoxide, nitrogen dioxide, ozone, carbon monoxide, nitric acid, nitrous acid, hydrogen peroxide, ethen, isoprene, toluene, methanol, ethanol, formaldehyde, acetaldehyde, peroxyacetyl nitrate
CB6r5	Xylene, PAR* (paraffin carbon bond), OLE* (terminal olefin carbon bond)
SAPRC07TC	o-Xylene, m-xylene, p-xylene, OLE1* (alkenes other than ethene with $k_{\mathrm{OH}}{}^{\dagger} < 7 \times 10^4$ ppm^{-1} min^{-1}), OLE2* (alkenes with $k_{\mathrm{OH}} > 7 \times 10^4$ ppm^{-1} min^{-1})

* A lumped chemical species defined in the gas-phase chemistry mechanism.

† k_{OH} – rate constant for the reaction with OH radical.

Table S2. Gas-phase chemical species and aerosol species included in the EAC4 CBCs. The mapping of the aerosol species from the EAC4 dataset to the aerosol species recognized by the CF scheme is also depicted.

Gas-phase chemical species included in the EAC4 CBCs
Ozone, nitrogen monoxide, nitrogen dioxide, nitric acid, carbon monoxide, sulphur dioxide, hydroxyl radical, methane, ethane, propane, formaldehyde, isoprene, peroxyacetyl nitrate

Aerosol species in the EAC4 dataset	Mapping to the aerosol species in the CF scheme*
Sea salt (0.03–0.5 μm) Sea salt (0.5–5 μm)	NA (sodium) + PCL (particulate chloride) + PSO4 (sulfate)
Sea salt (5–20 μm)	CPRM (coarse other primary)
Dust (0.03–0.55 μm) Dust (0.55–0.9 μm)	FCRS (fine crustal)
Dust (0.9–20 μm)	CCRS (coarse crustal)
Hydrophilic organic matter Hydrophobic organic matter	POA surrogate species + SOA surrogate species
Hydrophilic black carbon Hydrophobic black carbon	PEC (primary elemental carbon)
Sulfate	PSO4

* The EAC4 CBSs include these aerosol species recognized by the CF scheme. They were obtained by remapping the corresponding aerosol species from the EAC4 dataset.

Table S3. Volatility distribution factors for allocating POM_{SV} emissions to one of three volatility basis sets by source category in the CVb and CVa experiments. The volatility distribution factors were proposed by: [1]Zhao et al. (2016), [2]Zhao et al. (2015), [3]May et al. (2013), and [4]Robinson et al. (2007).

	Emission fraction for volatility bin with C° (in $\mu g\, m^{-3}$) of				
Source of POM_{SV}	10^{-1}	10^{0}	10^{1}	10^{2}	10^{3}
Gasoline vehicles[1]	0.11	0.07	0.36	0.25	0.21
Diesel vehicles[2]	0.23	0.05	0.14	0.14	0.44
Biomass burning[3]	0.2	0.1	0.1	0.2	0.4
Other sources[4]	0.09	0.09	0.14	0.18	0.5

Table S4. Seasonal factors used to allocate the total SOA concentration at the boundary of the model domain to the six surrogate SOA species* (SOA1, SOA2, SOA3, SOA4, SOPA, and SOPB) used in SOAP. Seasons used: winter (DJF: December–January–February), spring (MAM: March–April–May), summer (JJA: June–July–August), and autumn (SON: September–October–November).

	Seasonal fraction of the total SOA concentration in					
Season	SOA1	SOA2	SOA3	SOA4	SOPA	SOPB
DJF	0.1064	0.4174	0.0513	0.0488	0.2206	0.1555
MAM	0.0605	0.2938	0.0776	0.1369	0.1644	0.2668
JJA	0.0159	0.1328	0.0861	0.2632	0.0957	0.4063
SON	0.0470	0.2868	0.0869	0.1578	0.1646	0.2569

* SOA1 and SOA2 are surrogate SOA species that partition with the condensable gases (CGs) formed from the oxidation of the anthropogenic gaseous species, with SOA1 associated with the more-volatile CG and SOA2 with the less-volatile one. SOPA is a non-volatile surrogate SOA species formed from the oxidation of the anthropogenic gaseous species. Similarly, SOA3 and SOA4 represent surrogate SOA species that partition with the CGs formed from the oxidation of the biogenic volatile organic compounds (BVOCs), with SOA3 linked to the more-volatile CG and SOA4 to the less-volatile one. SOPB is a non-volatile SOA species formed from the oxidation of BVOCs.

Table S5. Seasonal factors used to allocate the total SOA concentration at the boundary of the model domain to the ten surrogate SOA species* (PAS0, PAS1, PAS2, PAS3, PAS4, PBS0, PBS1, PBS2, PBS3, and PBS4) used in 1.5D-VBS.

	Seasonal fraction of the total SOA concentration in									
Season	PAS0	PAS1	PAS2	PAS3	PAS4	PBS0	PBS1	PBS2	PBS3	PBS4
DJF	0.0534	0.1091	0.1004	0.0144	0.0009	0.2556	0.1200	0.2908	0.0551	0.0003
MAM	0.2284	0.1572	0.0429	0.0040	0.0002	0.3647	0.0825	0.0930	0.0265	0.0006
JJA	0.2841	0.0954	0.0162	0.0014	0.0001	0.4595	0.0828	0.0373	0.0221	0.0011
SON	0.1779	0.1334	0.0432	0.0045	0.0002	0.4284	0.0888	0.0903	0.0326	0.0007

* PAS0–PAS4 represent surrogate SOA species included in the basis set for chemically aged, oxygenated OA originating from other anthropogenic sources. PBS0–PBS4 represent surrogate SOA species included in the basis set for chemically aged, oxygenated OA originating from biomass burning, BVOCs, and meat cooking (although the latter was not considered in this study). In both groups, the numbers from 0 to 4 refer to the five volatility bins defined by the saturation concentrations ranging from 10^{-1} to 10^{3} $\mu g\,m^{-3}$ at 298 K.

Table S6. Seasonal factors used to allocate the total POA concentration at the boundary of the model domain to the ten surrogate POA species* (PAP0, PAP1, PAP2, PAP3, PAP4, PFP0, PFP1, PFP2, PFP3, and PFP4) used in 1.5D-VBS.

	Seasonal fraction of the total POA concentration in									
Season	PAP0	PAP1	PAP2	PAP3	PAP4	PFP0	PFP1	PFP2	PFP3	PFP4
DJF	0.0827	0.0679	0.1160	0.0399	0.0159	0.2654	0.1385	0.1321	0.1004	0.0412
MAM	0.1455	0.1308	0.1076	0.0265	0.0172	0.2654	0.1418	0.0906	0.0482	0.0264
JJA	0.3881	0.2074	0.1008	0.0230	0.0244	0.1603	0.0582	0.0197	0.0088	0.0093
SON	0.1578	0.1244	0.1183	0.0276	0.0156	0.2709	0.1379	0.0832	0.0424	0.0219

* PAP0–PAP4 represent surrogate POA species included in the basis set for freshly emitted OA originating from other anthropogenic sources. PFP0–PFP4 represent surrogate POA species included in the basis set for freshly emitted OA originating from biomass burning. In both groups, the numbers from 0 to 4 refer to the five volatility bins defined by the saturation concentrations ranging from 10^{-1} to 10^{3} $\mu g\,m^{-3}$ at 298 K.

Table S7. Coordinates and station types of the stations used for the validation. The number of daily OC measurements at individual stations used in the validation is also displayed.

Campaign	Station name	Station type[1]	Longitude	Latitude	Number of daily OC measurements[2] winter	summer
Třinecko[3]						
	Kosmos	UB	18.6778	49.6681	35	29
	Ropice	I	18.6245	49.7153	35	29
	Vrchy	RB	18.6102	49.6668	35	29
Kladensko[4]						
	Švermov	UB	14.1062	50.1674	31	30
	Libušín	UB	14.0567	50.1684	31	30
	Zbečno	RB	13.9199	50.0418	31	30

Station name	Station type[1]	Longitude	Latitude	Number of daily OC measurements DJF	MAM	JJA	SON
Košetice	RB	15.0803	49.5735	171	53	104	117
Prague–Suchdol[6]	UB	14.3849	50.1268	15[5]	23	–	–
Prague–Kbely[7]	–	14.5380	50.1232	–	–	–	–

[1] Station types used: UB – urban background, RB – rural background, I – industrial.
[2] Mean daily OC concentrations were derived from mean 12-hour OC measurements, which consistently commenced at 06:00 and 18:00 UTC. Therefore, for each day, the mean daily OC concentration is defined as the 24-hour average spanning from 06:00 UTC on the current day to 06:00 UTC on the following day.
[3] The campaign in the Třinecko area was divided into two phases. The summer sampling commenced on 5 June 2018, 06:00 UTC and concluded on 4 July 2018, 18:00 UTC. The winter sampling started on 14 December 2018, 06:00 UTC and ended on 21 January 2019, 18:00 UTC.
[4] The campaign in the Kladensko area campaign was also divided into two phases. The summer sampling started on 28 June 2019, 06:00 UTC and ended on 28 July 2019, 18:00 UTC. The winter sampling started on 14 November 2019, 06:00 UTC and finished on 15 December 2019, 18:00 UTC.
[5] These measurements encompass only the period from January to February 2018.
[6] Measurements at the Prague–Suchdol station represent OC within the PM_{10} fraction, while measurements at all other stations represent OC within the $PM_{2.5}$ fraction.
[7] The Prague–Kbely station is a professional meteorological station closest to the Prague–Suchdol station. It was chosen to validate meteorological conditions near the Prague–Suchdol station, as meteorological data from that site were not available to us.

Table S8. Statistical analysis of the mean daily air temperature (in K), wind speed (in $m\,s^{-1}$), and relative humidity (in %) predicted in the WRF simulation at (1) the Prague–Kbely and Košetice stations during the individual seasons and (2) six stations included in the Třinecko and Kladensko campaigns during their winter and summer phases. Statistical measures used: mean bias (MB), root mean square error (RMSE), normalized mean square error (NMSE), and index of agreement (IOA).

Station	Season	Mean daily air temperature MB (K)	RMSE (K)	NMSE (%)	IOA	Mean daily wind speed MB ($m\,s^{-1}$)	RMSE ($m\,s^{-1}$)	NMSE (%)	IOA	Mean daily relative humidity MB (%)	RMSE (%)	NMSE (%)	IOA
Prague–Kbely													
	JF	0.5	1.1	1.6×10^{-3}	0.98	-0.2	0.7	4.4	0.96	-7.4	10.0	1.8	0.78
	MAM	0.2	0.9	1.0×10^{-3}	1.0	-0.6	0.8	6.8	0.89	-1.3	5.8	0.8	0.90
Košetice													
	DJF	-0.3	1.0	1.3×10^{-3}	0.98	0.9	1.3	8.6	0.91	-5.2	8.3	1.1	0.83
	MAM	-0.1	0.9	1.1×10^{-3}	1.00	1.3	1.7	12.9	0.85	-1.2	6.1	0.8	0.91
	JJA	-0.3	1.1	1.3×10^{-3}	0.97	-0.2	0.6	4.2	0.86	-1.8	7.7	1.4	0.80
	SON	0.1	0.8	0.9×10^{-3}	0.99	0.7	1.2	9.5	0.91	-7.9	9.3	1.5	0.85

Campaign	Station	Mean daily air temperature MB (K)	RMSE (K)	NMSE (%)	IOA	Mean daily wind speed MB ($m\,s^{-1}$)	RMSE ($m\,s^{-1}$)	NMSE (%)	IOA	Mean daily relative humidity MB (%)	RMSE (%)	NMSE (%)	IOA
Třinecko–winter													
	Kosmos	-0.8	1.4	2.5×10^{-3}	0.95	4.3	4.9	200	0.20	0.3	6.0	0.5	0.84
	Ropice	-0.8	1.3	2.3×10^{-3}	0.96	3.7	4.1	188	0.26	-6.8	8.9	1.2	0.75
	Vrchy	-1.5	1.8	4.6×10^{-3}	0.92	3.2	3.6	47	0.54	-1.3	6.6	0.6	0.83
Kladensko–winter													
	Švermov	-1.4	2.1	5.5×10^{-3}	0.88	3.6	4.1	512	0.29	–	–	–	–
	Libušín	-0.3	1.6	3.5×10^{-3}	0.92	3.4	3.8	266	0.42	-9.5	12.5	2.5	0.56
	Zbečno	-0.6	1.9	4.6×10^{-3}	0.91	3.9	4.4	1320	0.11	-11.9	15.1	3.6	0.45
Třinecko–summer													
	Kosmos	-0.6	1.0	1.1×10^{-3}	0.98	1.6	1.8	86	0.28	-0.8	6.7	0.9	0.85
	Ropice	-0.4	0.8	0.8×10^{-3}	0.98	1.9	2.1	146	0.26	-7.7	9.3	1.8	0.76
	Vrchy	0.1	0.8	0.7×10^{-3}	0.99	1.1	1.3	29	0.54	6.3	8.8	1.7	0.77
Kladensko–summer													
	Švermov	-3.2	3.4	1.4×10^{-2}	0.82	2.2	2.4	421	0.17	5.3	9.7	3.0	0.72
	Libušín	-1.8	2.2	5.7×10^{-3}	0.92	2.2	2.4	361	0.21	4.7	9.5	2.8	0.72
	Zbečno	-1.7	2.0	4.6×10^{-3}	0.93	2.0	2.2	522	0.10	-1.5	9.1	2.2	0.71

Table S9. Domain-averaged difference of the mean seasonal POA concentration in a specific model experiment and its counterpart in the reference experiment (Δ POA) (in $\mu g\,m^{-3}$) during the winter (DJF) and summer (JJA) 2018–2019. Δ SOA (in $\mu g\,m^{-3}$) represents the analogous domain-averaged difference for the mean seasonal SOA concentration. Note that the reference experiment for CSwI, SSnI, SSwI, CVb, and CVa is CSnI. At the same time, the reference experiment for Sp0s100, Sp50s50, and Sp100s0 is CSwI, while for Vp0s100, Vp50s50, and Vp100s0, it is CVb.

	Δ POA ($\mu g\,m^{-3}$)		Δ SOA ($\mu g\,m^{-3}$)	
Experiment	DJF	JJA	DJF	JJA
CSwI	0.00	0.00	0.17	0.09
SSnI	0.00	0.00	0.00	-0.07
SSwI	0.00	0.00	0.12	-0.01
CVb	0.76	0.15	0.49	0.58
CVa	0.78	0.17	0.62	1.17
Sp0s100	0.01	0.00	1.15	2.27
Sp50s50	0.69	1.71	0.55	1.22
Sp100s0	1.37	3.45	-0.04	0.12
Vp0s100	0.08	0.03	0.83	2.03
Vp50s50	0.63	1.29	0.41	1.15
Vp100s0	1.17	3.10	-0.01	0.05

Table S10. Statistical analysis of the mean daily OC concentrations (in $\mu g\,m^{-3}$) predicted in the individual experiments of the first sensitivity analysis at the Prague–Suchdol and Košetice stations during the individual seasons. The last three columns show analogous statistical analysis at the Košetice station corresponding to the time periods of the winter campaign phases in the Třinecko (Tř-w) and Kladensko (Kl-w) areas, and the summer campaign phase in the Kladensko (Kl-s) area, respectively. Statistical measures used: mean bias (MB), root mean square error (RMSE), normalized mean square error (NMSE), index of agreement (IOA), and the fraction of predictions within a factor of two of observations (FAC2).

Statistical measure	Prague–Suchdol		Košetice						
Experiment	JF*	MAM	DJF	MAM	JJA	SON	Tř-w	Kl-w	Kl-s
MB ($\mu g\,m^{-3}$)									
CSnI	-2.32	-2.56	-1.60	-2.30	-2.21	-1.88	-0.83	-1.36	-2.21
CSwI	-2.15	-2.41	-1.47	-2.17	-2.14	-1.75	-0.78	-1.26	-2.16
SSnI	-2.32	-2.59	-1.61	-2.31	-2.28	-1.90	-0.84	-1.37	-2.28
SSwI	-2.20	-2.46	-1.51	-2.20	-2.25	-1.79	-0.80	-1.29	-2.25
CVb	0.06	-1.53	-0.33	-1.61	-1.83	-1.30	-0.23	-0.65	-1.84
CVa	0.17	-1.22	-0.24	-1.39	-1.37	-1.04	-0.21	-0.58	-1.44
RMSE ($\mu g\,m^{-3}$)									
CSnI	4.10	3.65	2.25	2.98	2.31	2.35	1.09	1.67	2.32
CSwI	3.97	3.51	2.11	2.84	2.24	2.23	1.03	1.57	2.26
SSnI	4.10	3.66	2.25	2.99	2.38	2.37	1.09	1.67	2.39
SSwI	4.00	3.55	2.15	2.87	2.35	2.27	1.05	1.60	2.36
CVb	4.29	2.92	1.70	2.22	1.96	1.95	1.01	0.98	1.97
CVa	4.30	2.73	1.71	2.09	1.51	1.77	1.01	0.93	1.54
NMSE (%)									
CSnI	67.1	126.1	57.8	197.1	243.6	169.6	29.7	51.4	252.4
CSwI	60.3	109.2	48.2	161.7	213.0	135.5	26.1	43.1	224.5
SSnI	67.1	128.6	58.2	200.0	291.0	174.3	29.9	51.8	296.6
SSwI	61.8	114.5	50.6	169.2	267.0	145.4	27.2	45.2	277.6
CVb	46.0	55.0	21.2	70.3	116.9	76.2	18.6	12.5	120.0
CVa	45.4	43.8	21.0	56.5	49.2	54.5	18.7	11.1	54.0
IOA									
CSnI	0.68	0.44	0.64	0.43	0.37	0.52	0.73	0.66	0.37
CSwI	0.69	0.46	0.68	0.46	0.38	0.54	0.75	0.69	0.38
SSnI	0.68	0.44	0.64	0.43	0.36	0.51	0.73	0.66	0.37
SSwI	0.69	0.45	0.67	0.46	0.37	0.53	0.74	0.68	0.37
CVb	0.73	0.62	0.85	0.68	0.42	0.61	0.85	0.88	0.42
CVa	0.73	0.66	0.85	0.71	0.52	0.65	0.85	0.89	0.52
FAC2 (%)									
CSnI	66.7	47.8	66.1	32.1	0.0	21.4	74.3	78.6	0.0
CSwI	73.3	47.8	69.6	34.0	0.0	22.2	77.1	85.7	0.0
SSnI	66.7	47.8	65.5	30.2	0.0	20.5	74.3	78.6	0.0
SSwI	73.3	47.8	67.8	34.0	0.0	22.2	74.3	85.7	0.0
CVb	80.0	56.5	81.9	56.6	16.4	50.4	82.9	100.0	11.5
CVa	80.0	69.6	81.9	60.4	56.7	60.7	82.9	100.0	57.7

* Period from January to February 2018.

Table S11. Statistical analysis of the mean daily OC concentration (in $\mu g\,m^{-3}$) predicted in the individual experiments of the first sensitivity analysis at six stations included in the Třinecko and Kladensko campaigns during during their winter and summer phases. Statistical measures used: mean bias (MB), root mean square error (RMSE), normalized mean square error (NMSE), index of agreement (IOA), and the fraction of predictions within a factor of two of observations (FAC2).

Statistical measure	Experiment	Třinecko–winter			Kladensko–winter			Třinecko–summer			Kladensko–summer		
		Kosmos	Ropice	Vrchy	Švermov	Libušín	Zbečno	Kosmos	Ropice	Vrchy	Švermov	Libušín	Zbečno
MB ($\mu g\,m^{-3}$)													
	CSnI	-7.21	-6.99	-5.98	-5.76	-5.28	-6.24	-3.84	-3.51	-3.25	-3.98	-3.60	-3.46
	CSwI	-7.14	-6.91	-5.91	-5.67	-5.19	-6.15	-3.77	-3.44	-3.18	-3.92	-3.55	-3.41
	SSnI	-7.21	-6.99	-5.98	-5.76	-5.28	-6.24	-3.91	-3.58	-3.32	-4.02	-3.64	-3.51
	SSwI	-7.16	-6.93	-5.93	-5.69	-5.21	-6.18	-3.87	-3.54	-3.28	-3.99	-3.61	-3.48
	CVb	-5.93	-4.82	-4.70	-4.18	-3.93	-5.34	-3.47	-3.00	-2.89	-3.57	-3.21	-3.08
	CVa	-5.90	-4.78	-4.67	-4.12	-3.86	-5.28	-3.17	-2.68	-2.58	-3.25	-2.90	-2.76
RMSE ($\mu g\,m^{-3}$)													
	CSnI	10.12	9.80	8.29	7.49	7.19	7.48	4.06	3.77	3.52	4.19	3.81	3.65
	CSwI	10.06	9.72	8.22	7.43	7.13	7.42	3.99	3.70	3.45	4.13	3.76	3.59
	SSnI	10.13	9.80	8.29	7.49	7.19	7.49	4.13	3.84	3.59	4.23	3.86	3.69
	SSwI	10.08	9.75	8.24	7.44	7.14	7.43	4.09	3.80	3.55	4.20	3.83	3.67
	CVb	8.78	7.79	7.01	6.36	6.24	6.76	3.71	3.30	3.17	3.78	3.44	3.27
	CVa	8.76	7.77	6.98	6.34	6.22	6.72	3.39	2.99	2.86	3.42	3.10	2.92
NMSE (%)													
	CSnI	460.0	260.8	354.0	172.8	204.9	258.2	498.3	344.9	429.5	600.5	584.4	506.4
	CSwI	441.1	251.2	338.5	165.2	195.4	245.0	436.7	306.6	374.4	538.3	521.9	454.8
	SSnI	460.9	261.0	354.8	172.8	205.1	259.0	570.7	383.6	494.4	653.8	642.1	560.6
	SSwI	447.2	254.2	343.4	167.3	198.0	249.0	527.9	358.4	456.0	614.4	603.1	527.7
	CVb	223.8	102.0	163.6	85.8	106.8	154.7	275.6	170.0	231.6	298.7	288.6	253.4
	CVa	220.3	100.8	160.7	84.2	104.5	150.4	180.4	114.2	147.5	186.6	177.5	154.7
IOA													
	CSnI	0.46	0.47	0.47	0.52	0.50	0.50	0.37	0.40	0.41	0.39	0.40	0.39
	CSwI	0.46	0.47	0.48	0.52	0.50	0.50	0.37	0.40	0.42	0.39	0.41	0.39
	SSnI	0.46	0.47	0.47	0.52	0.50	0.50	0.36	0.39	0.40	0.38	0.40	0.38
	SSwI	0.46	0.47	0.47	0.52	0.50	0.50	0.36	0.39	0.41	0.38	0.40	0.38
	CVb	0.50	0.57	0.53	0.58	0.56	0.53	0.39	0.44	0.45	0.41	0.43	0.42
	CVa	0.50	0.57	0.53	0.58	0.56	0.53	0.43	0.48	0.49	0.46	0.48	0.46
FAC2 (%)													
	CSnI	25.7	37.1	28.6	25.8	25.8	12.9	0.0	3.5	0.0	0.0	0.0	0.0
	CSwI	25.7	37.1	28.6	25.8	29.0	12.9	0.0	3.5	0.0	0.0	0.0	0.0
	SSnI	25.7	37.1	28.6	25.8	25.8	12.9	0.0	3.5	0.0	0.0	0.0	0.0
	SSwI	25.7	37.1	28.6	25.8	29.0	12.9	0.0	3.5	0.0	0.0	0.0	0.0
	CVb	37.1	65.7	40.0	48.4	41.9	22.6	0.0	17.2	3.5	0.0	0.0	3.3
	CVa	37.1	68.6	40.0	48.4	41.9	22.6	6.9	31.0	17.2	0.0	3.3	6.7

Table S12. Same as in Table S10 but for the individual experiments of the second sensitivity analysis.

Statistical measure / Experiment	Prague–Suchdol JF	Prague–Suchdol MAM	Košetice DJF	Košetice MAM	Košetice JJA	Košetice SON
MB ($\mu g\,m^{-3}$)						
CSwI	-2.15	-2.41	-1.47	-2.17	-2.14	-1.75
Sp0s100	-1.43	-1.57	-1.02	-1.27	-1.22	-1.09
Sp50s50	-1.19	-1.05	-0.87	-0.84	-0.45	-0.77
Sp100s0	-0.95	-0.54	-0.73	-0.41	0.31	-0.46
CVb	0.06	-1.53	-0.33	-1.61	-1.83	-1.30
Vp0s100	0.70	-0.65	0.04	-0.78	-0.94	-0.59
Vp50s50	0.89	-0.37	0.16	-0.52	-0.58	-0.44
Vp100s0	1.08	-0.02	0.27	-0.18	0.09	-0.30
RMSE ($\mu g\,m^{-3}$)						
CSwI	3.97	3.51	2.11	2.84	2.24	2.23
Sp0s100	3.60	3.08	1.83	2.33	1.50	1.66
Sp50s50	3.44	2.86	1.74	2.16	1.11	1.43
Sp100s0	3.29	2.75	1.67	2.09	1.24	1.26
CVb	4.29	2.92	1.70	2.22	1.96	1.95
Vp0s100	4.26	2.68	1.67	1.80	1.27	1.43
Vp50s50	4.26	2.66	1.69	1.74	1.11	1.36
Vp100s0	4.27	2.69	1.72	1.75	1.13	1.31
NMSE (%)						
CSwI	60.3	109.2	48.2	161.7	213.0	135.5
Sp0s100	42.3	61.9	30.4	66.1	44.5	49.0
Sp50s50	36.7	46.1	26.2	47.8	16.9	31.0
Sp100s0	32.1	37.5	23.0	38.8	16.2	21.3
CVb	46.0	55.0	21.2	70.3	116.9	76.3
Vp0s100	41.1	36.6	18.5	32.5	27.4	28.8
Vp50s50	40.0	33.7	18.3	28.0	17.7	24.6
Vp100s0	39.1	31.9	18.4	25.4	14.3	21.5
IOA						
CSwI	0.69	0.46	0.68	0.46	0.38	0.54
Sp0s100	0.71	0.46	0.73	0.48	0.42	0.62
Sp50s50	0.73	0.47	0.75	0.50	0.42	0.67
Sp100s0	0.74	0.51	0.77	0.55	0.44	0.73
CVb	0.73	0.62	0.85	0.68	0.42	0.61
Vp0s100	0.73	0.67	0.85	0.77	0.48	0.72
Vp50s50	0.73	0.68	0.85	0.79	0.47	0.74
Vp100s0	0.72	0.68	0.85	0.78	0.47	0.75
FAC2 (%)						
CSwI	73.3	47.8	69.6	34.0	0.0	22.2
Sp0s100	73.3	69.6	81.9	66.0	57.7	72.7
Sp50s50	66.7	78.3	86.6	75.5	92.3	84.6
Sp100s0	66.7	87.0	88.9	83.0	92.3	90.6
CVb	80.0	56.5	81.9	56.6	16.4	50.4
Vp0s100	80.0	78.3	87.7	69.8	79.8	82.9
Vp50s50	73.3	78.3	89.5	75.5	90.4	84.6
Vp100s0	60.0	78.3	89.5	83.0	93.3	88.9

Table S13. Same as in Table S11 but for the individual experiments of the second sensitivity analysis.

Statistical measure	Třinecko–winter			Kladensko–winter			Třinecko–summer			Kladensko–summer		
Experiment	Kosmos	Ropice	Vrchy	Švermov	Libušín	Zbečno	Kosmos	Ropice	Vrchy	Švermov	Libušín	Zbečno
MB ($\mu g\, m^{-3}$)												
CSwI	-7.14	-6.91	-5.91	-5.67	-5.19	-6.15	-3.77	-3.44	-3.18	-3.92	-3.55	-3.41
Sp0s100	-6.80	-6.55	-5.57	-5.30	-4.82	-5.80	-3.13	-2.77	-2.55	-2.50	-2.12	-2.03
Sp50s50	-6.71	-6.46	-5.48	-5.20	-4.73	-5.70	-2.61	-2.23	-2.02	-1.45	-1.06	-0.99
Sp100s0	-6.63	-6.37	-5.40	-5.10	-4.63	-5.61	-2.09	-1.69	-1.50	-0.42	-0.03	0.03
CVb	-5.93	-4.82	-4.70	-4.18	-3.93	-5.34	-3.47	-3.00	-2.89	-3.57	-3.21	-3.08
Vp0s100	-5.67	-4.55	-4.44	-3.80	-3.56	-4.98	-2.89	-2.38	-2.30	-2.19	-1.83	-1.74
Vp50s50	-5.59	-4.46	-4.36	-3.74	-3.49	-4.92	-2.63	-2.11	-2.04	-1.70	-1.34	-1.25
Vp100s0	-5.50	-4.37	-4.27	-3.67	-3.43	-4.85	-2.13	-1.59	-1.55	-0.75	-0.38	-0.32
RMSE ($\mu g\, m^{-3}$)												
CSwI	10.06	9.72	8.22	7.43	7.13	7.42	3.99	3.70	3.45	4.13	3.76	3.59
Sp0s100	9.78	9.41	7.94	7.19	6.91	7.16	3.44	3.14	2.91	2.91	2.56	2.37
Sp50s50	9.70	9.33	7.87	7.12	6.85	7.09	2.99	2.70	2.49	2.07	1.81	1.57
Sp100s0	9.63	9.26	7.80	7.07	6.80	7.03	2.60	2.34	2.15	1.57	1.53	1.27
CVb	8.78	7.79	7.01	6.36	6.24	6.76	3.71	3.30	3.17	3.78	3.44	3.27
Vp0s100	8.56	7.55	6.78	6.17	6.06	6.53	3.20	2.79	2.69	2.56	2.27	2.08
Vp50s50	8.49	7.48	6.72	6.14	6.03	6.49	2.99	2.59	2.49	2.18	1.92	1.71
Vp100s0	8.43	7.41	6.65	6.11	6.01	6.45	2.62	2.26	2.16	1.64	1.54	1.29
NMSE (%)												
CSwI	441.1	251.2	338.5	165.2	195.4	245.0	436.7	306.6	374.4	538.3	521.9	454.8
Sp0s100	365.4	214.0	276.5	140.5	164.6	200.6	180.7	132.8	148.4	87.3	75.4	66.2
Sp50s50	348.3	205.7	262.8	134.5	157.4	190.7	100.1	74.5	79.5	29.5	25.0	19.3
Sp100s0	333.2	198.1	250.6	129.3	151.1	181.6	59.6	44.8	46.7	12.8	13.5	9.5
CVb	223.8	102.0	163.6	85.8	106.8	154.7	275.6	170.0	231.6	298.7	288.6	253.4
Vp0s100	198.4	91.4	143.1	75.2	93.0	130.4	133.4	85.0	108.0	58.8	52.1	44.4
Vp50s50	190.9	88.4	137.1	73.5	90.8	126.6	100.7	65.0	80.3	35.3	30.9	24.9
Vp100s0	184.1	85.6	131.7	71.9	88.9	123.1	61.7	40.3	48.3	15.1	14.8	10.6

Table S14. Same as in Table S13 but for the index of agreement (IOA) and fraction of predictions within a factor of two of observations (FAC2).

Statistical measure	Třinecko–winter			Kladensko–winter			Třinecko–summer			Kladensko–summer		
Experiment	Kosmos	Ropice	Vrchy	Švermov	Libušín	Zbečno	Kosmos	Ropice	Vrchy	Švermov	Libušín	Zbečno
IOA												
CSwI	0.46	0.47	0.48	0.52	0.50	0.50	0.37	0.40	0.42	0.39	0.41	0.39
Sp0s100	0.47	0.48	0.48	0.52	0.50	0.50	0.39	0.42	0.45	0.45	0.46	0.47
Sp50s50	0.47	0.48	0.49	0.52	0.50	0.50	0.42	0.45	0.48	0.51	0.49	0.54
Sp100s0	0.47	0.49	0.49	0.52	0.50	0.51	0.45	0.48	0.51	0.52	0.49	0.60
CVb	0.50	0.57	0.53	0.58	0.56	0.53	0.39	0.44	0.45	0.41	0.43	0.42
Vp0s100	0.51	0.58	0.53	0.59	0.56	0.53	0.43	0.47	0.48	0.50	0.51	0.52
Vp50s50	0.51	0.59	0.54	0.59	0.56	0.53	0.44	0.48	0.49	0.53	0.52	0.55
Vp100s0	0.51	0.59	0.54	0.59	0.56	0.53	0.46	0.49	0.52	0.54	0.48	0.59
FAC2 (%)												
CSwI	25.7	37.1	28.6	25.8	29.0	12.9	0.0	3.45	0.0	0.0	0.0	0.0
Sp0s100	25.7	48.6	31.4	25.8	38.7	22.6	10.3	24.1	27.6	50.0	53.3	50.0
Sp50s50	31.4	48.6	31.4	25.8	38.7	22.6	37.9	41.4	48.3	80.0	83.3	90.0
Sp100s0	31.4	48.6	37.1	29.0	38.7	25.8	58.6	69.0	65.5	100.0	93.3	100.0
CVb	37.1	65.7	40.0	48.4	41.9	22.6	0.0	17.2	3.5	0.0	0.0	3.3
Vp0s100	40.0	68.6	48.6	48.4	54.8	25.8	24.1	44.8	44.8	60.0	66.7	70.0
Vp50s50	42.9	68.6	48.6	54.8	61.3	25.8	34.5	58.6	44.8	76.7	80.0	80.0
Vp100s0	45.7	71.4	54.3	54.8	61.3	25.8	58.6	72.4	69.0	93.3	93.3	100.0

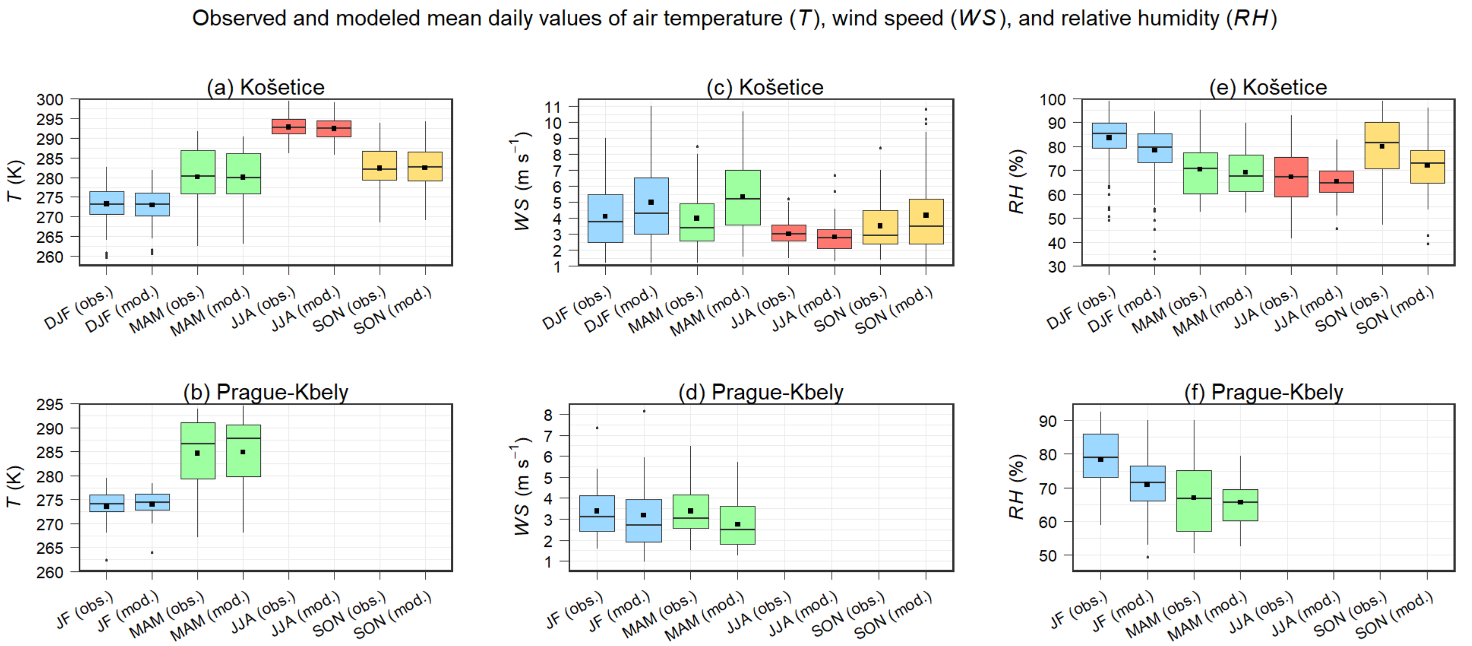

Figure S1. Observed (obs.) and modeled (mod.) mean daily values of air temperature (in K) **(a, b)**, wind speed (in m s^{-1}) **(c, d)**, and relative humiditiy (in %) **(e, f)** at the Košetice station **(a, c, e)** during the winter (DJF), spring (MAM), summer (JJA), and autumn (SON) of 2018 and 2019, and at the Prague–Kbely station **(b, d, f)** during January and February (JF) 2018 and the spring of 2018.

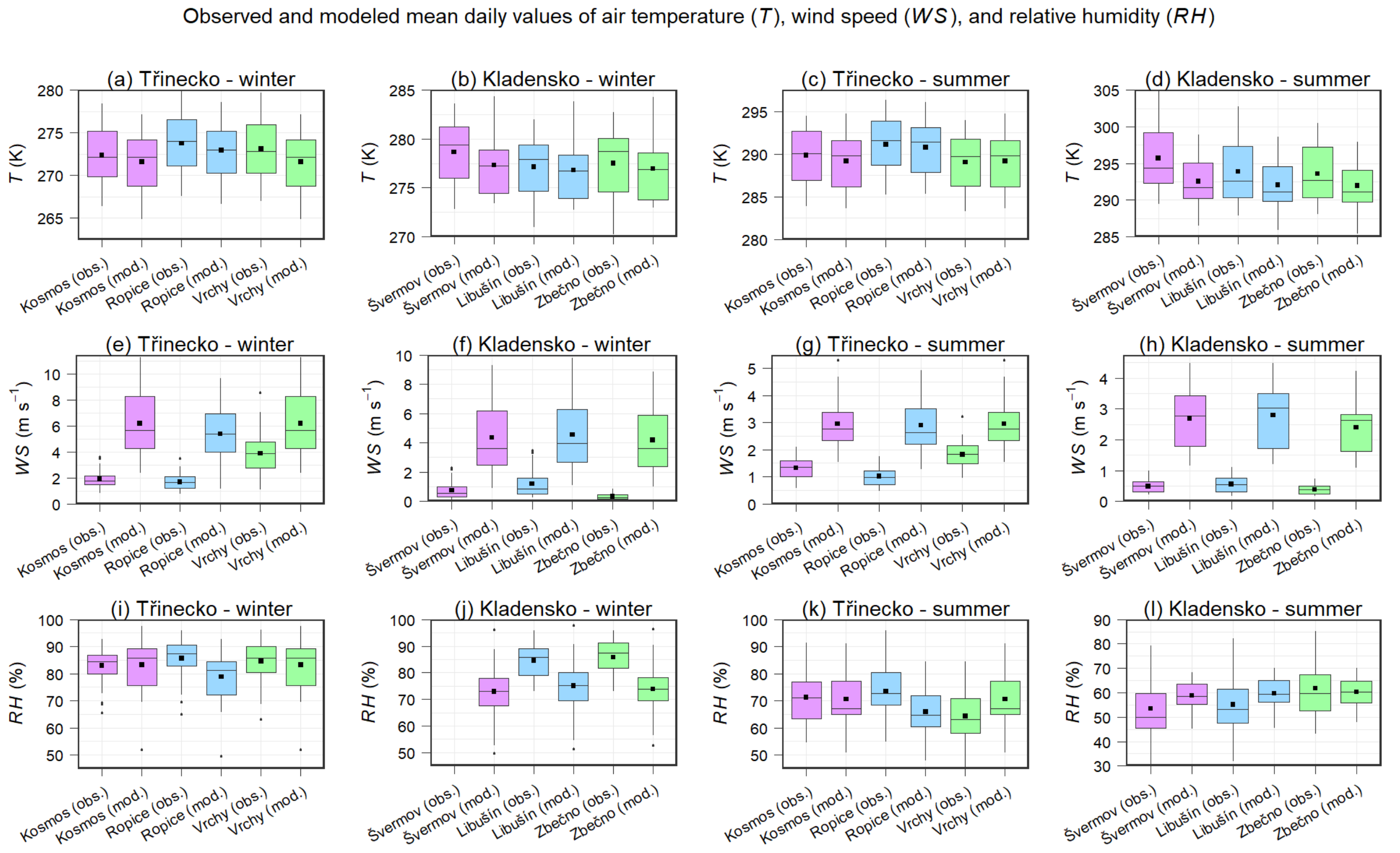

Figure S2. Observed (obs.) and modeled (mod.) mean daily values of air temperature (in K) **(a–d)**, wind speed (in m s^{-1}) **(e–h)**, and relative humidity (in %) **(i–j)** at the Kosmos, Ropice, and Vrchy stations in the Třinecko area during the winter **(a, e, i)** and summer **(c, g, k)** phase of the campaign, and at the Švermov, Libušín, and Zbečno stations in the Kladensko area during the winter **(b, f, j)** and summer **(d, h, l)** phase of the campaign.

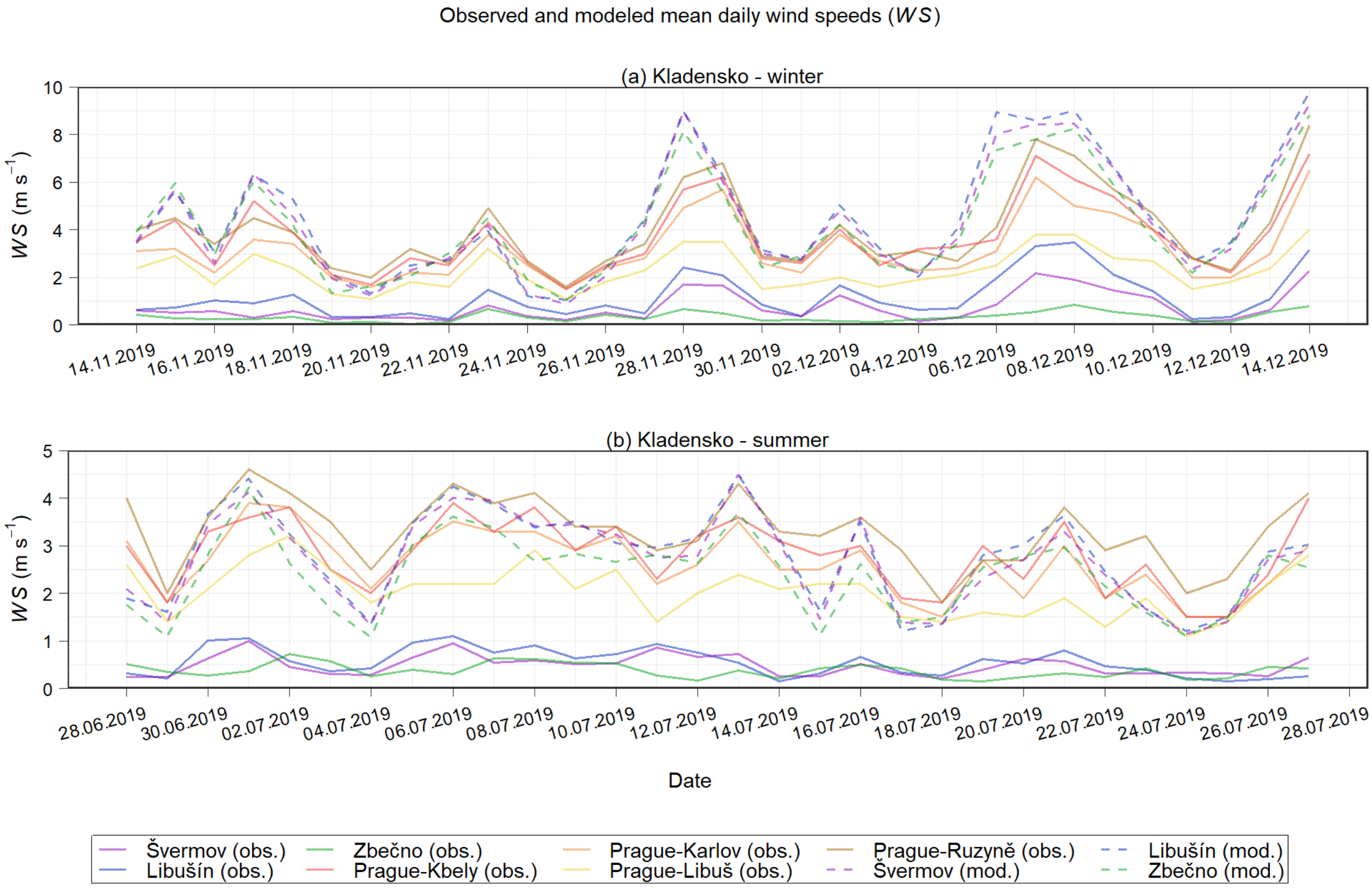

Figure S3. Observed (obs.) and modeled (mod.) mean daily wind speeds (in $\mathrm{m\,s^{-1}}$) at the Švermov, Libušín, and Zbečno stations in the Kladensko area during the winter **(a)** and summer **(b)** phase of the campaign. Mean daily wind speeds measured at four Prague professional meteorological stations (Prague–Ruzyně, Prague–Kbely, Prague–Karlov, and Prague–Libuš) during both phases are also shown. Data from all the stations were provided by the Czech Hydrometeorological Institute.

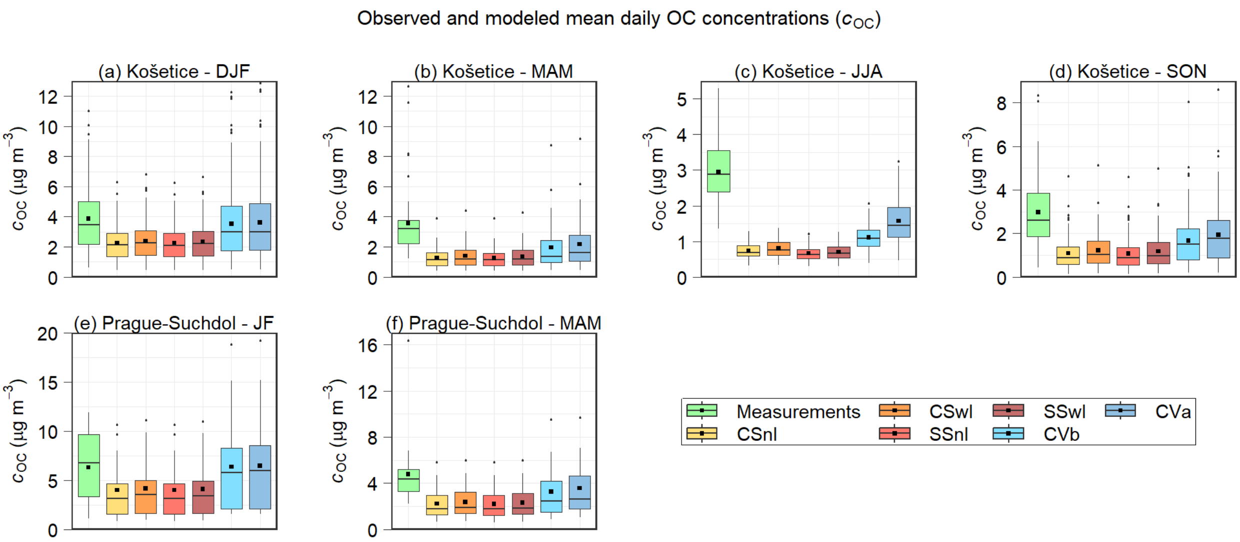

Figure S4. Observed and modeled mean daily OC concentrations (in $\mathrm{\mu g\,m^{-3}}$) at the Košetice station during the winter **(a)**, spring **(b)**, summer **(c)**, and autumn **(d)** of 2018 and 2019, and at the Prague–Suchdol station during January and February 2018 **(e)** and the spring of 2018 **(f)**. The box plots for all the model experiments of the first sensitivity analysis are shown.

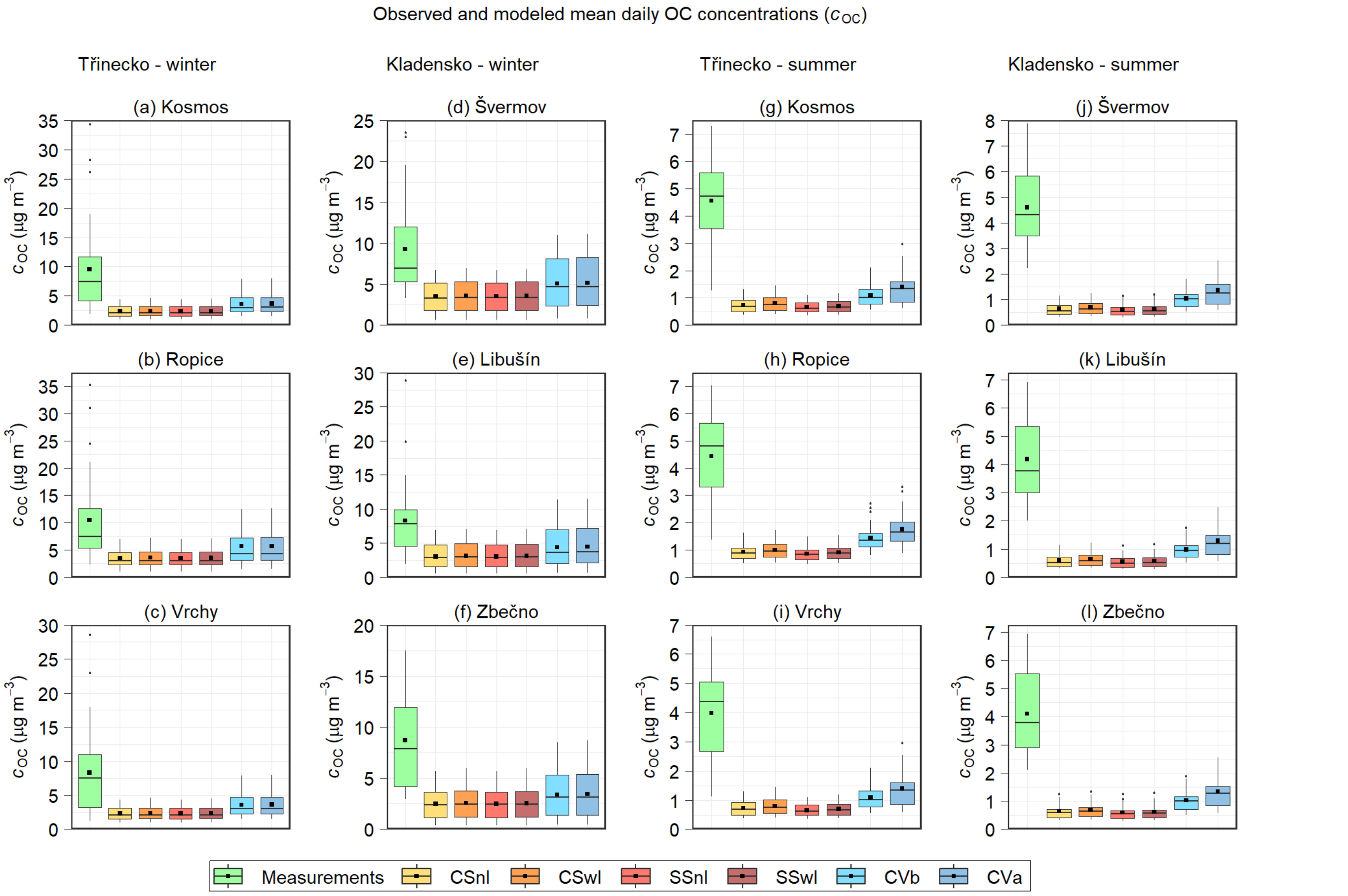

Figure S5. Observed and modeled mean daily OC concentrations (in µg m^{-3}) at the Kosmos, Ropice, and Vrchy stations in the Třinecko area during the winter **(a–c)** and summer **(g–i)** phase of the campaign, and at the Švermov, Libušín, and Zbečno stations in the Kladensko area during the winter **(d–f)** and summer **(j–l)** phase of the campaign. The box plots for all the model experiments of the first sensitivity analysis are shown.

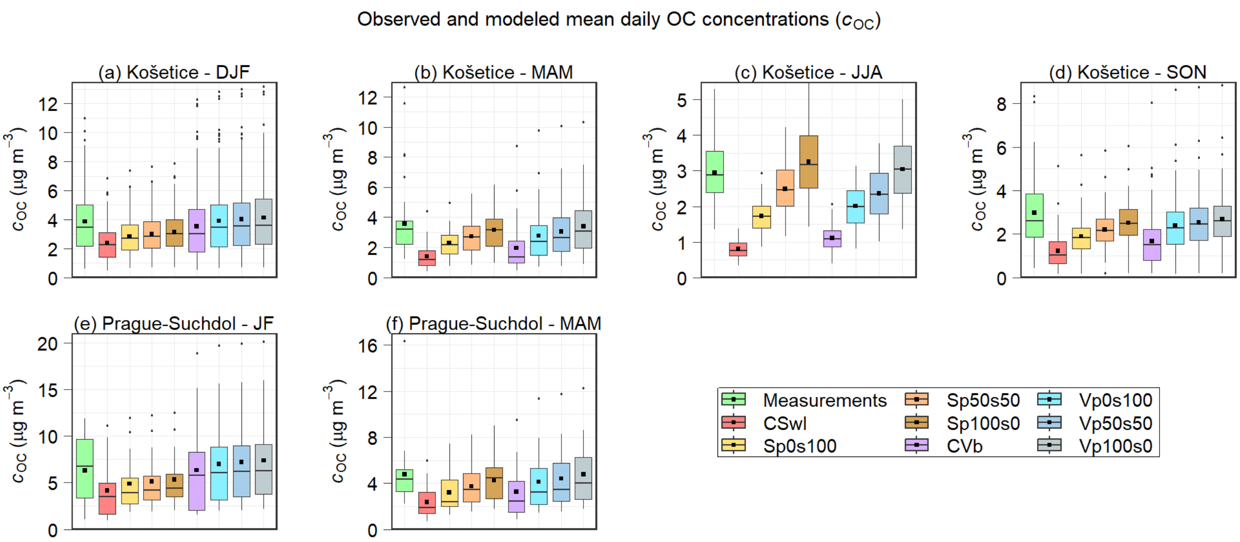

Figure S6. Same as Fig. S4 but for the experiments of the second sensitivity analysis.

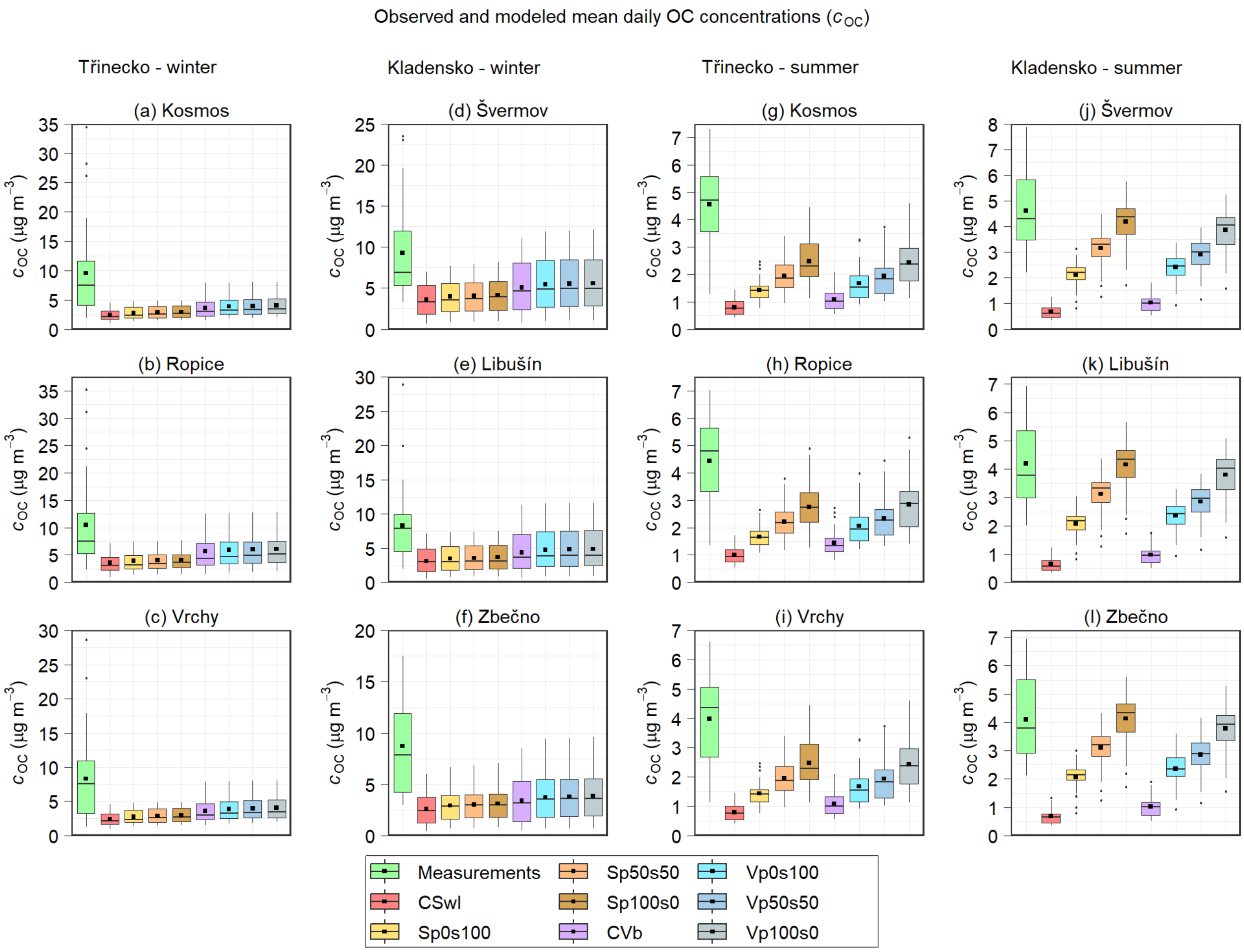

Figure S7. Same as Fig. S5 but for the experiments of the second sensitivity analysis.

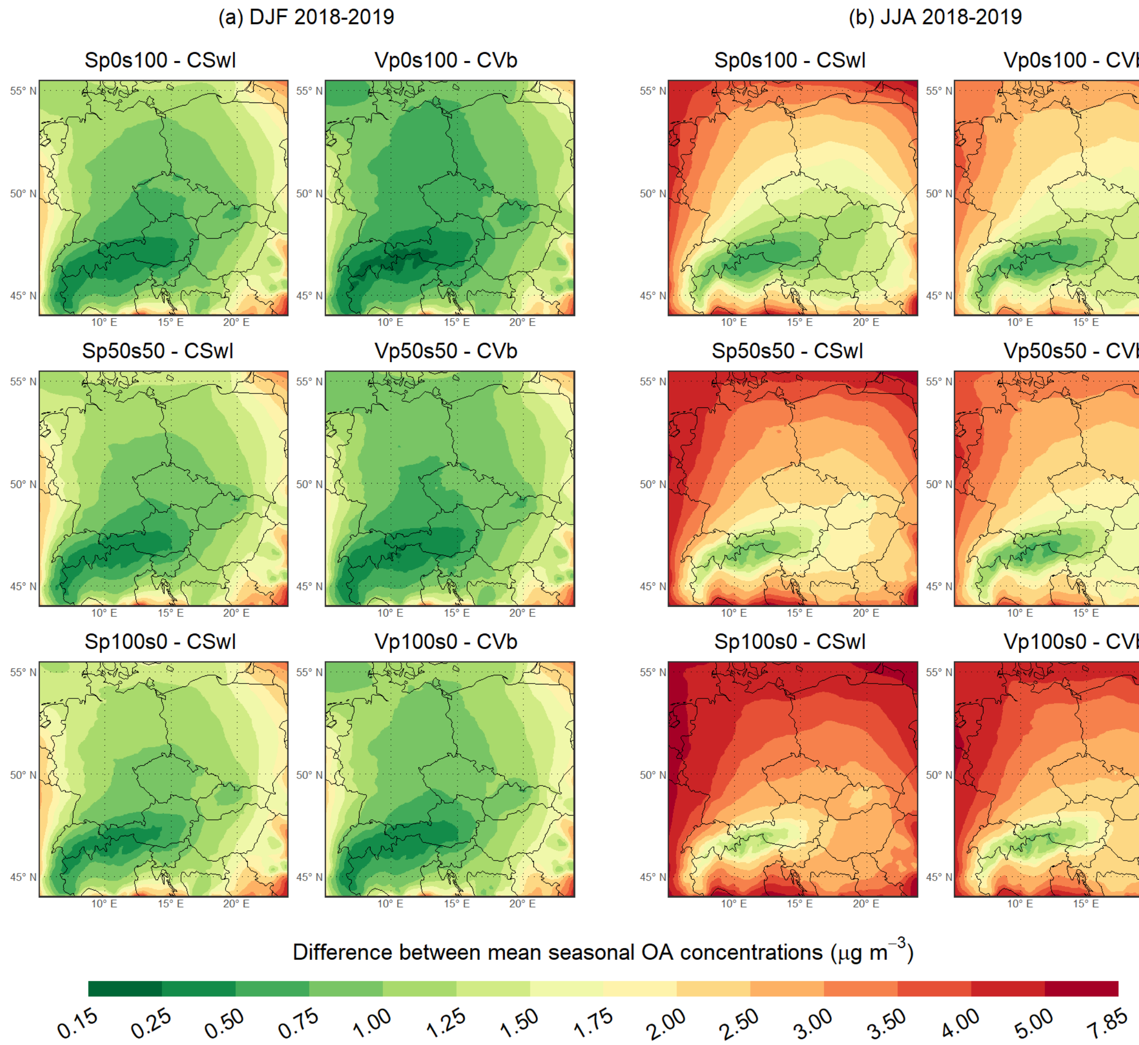

Figure S8. Difference between the mean seasonal OA concentration predicted in each individual experiment of the second sensitivity analysis and that in the corresponding reference experiment (CSwI or CVb) (in $\mu g\,m^{-3}$) during the winter **(a)** and summer **(b)** of 2018 and 2019.

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