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Supplement of

Implementation of the sectional aerosol module SALSA2.0 into the PALM model system 6.0: model development and first evaluation

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S1 Dry deposition scheme by Petroff and Zhang (2010)

Deposition velocity $v_{d,i}$ for aerosol size bin i is calculated by Petroff and Zhang (2010) as follows:

$$v_{d,i} = v_{c,i} + U \left[\underbrace{C_B Sc_i^{-2/3} \left(\frac{UL}{\nu_a} \right)^{-1/2}}_{\text{Brownian diffusion}} + \underbrace{C_{IN} \frac{\overline{D}_i}{L} \left(2 + \ln \frac{4L}{\overline{D}_i} \right)}_{\text{interception}} + \underbrace{C_{IM} \left(\frac{St_i}{St_i + \beta_{IM}} \right)^2}_{\text{impaction}} \right] + \underbrace{C_{IT} \Upsilon}_{\text{turbulent impaction}} \tag{1}$$

where

$$\Upsilon = \begin{cases} 2.5 \times 10^{-3} \tau_{\text{ph}}^{+2} & \text{if } \tau_{\text{ph}}^{+} < 20 \\ 1.0 & \text{if } \tau_{\text{ph}}^{+} \geq 20 \end{cases}$$

and

$$\tau_{\text{ph},i}^{+} = \frac{G_i \rho_p \overline{D}_i^2 u_*^2}{18 \mu_a \nu_a} \,. \tag{2}$$

Here $v_{c,i}$ ($\mathrm{m\,s^{-1}}$) is the settling velocity, U ($\mathrm{m\,s^{-1}}$) is the wind speed, Sc_i is the particle Schmidt number, L (m) is the obstacle characteristic dimension for different surface types, ν_a ($\mathrm{m^2\,s}$) is the kinematic viscosity of air, $\overline{D}_i$ (m) is the particle diameter, St_i is the Stokes number, ρ_p ($\mathrm{kg\,m^{-3}}$) is the particle density, u_* ($\mathrm{m\,s^{-1}}$) is the friction velocity of above a surface and μ_a ($\mathrm{kg\,m^{-1}\,s^{-1}}$) the dynamic viscosity of air. Furthermore, C_B, C_{IN}, C_{IM}, β_{IM} and C_{IT} are empirical constants.

S2 Simple test set-up

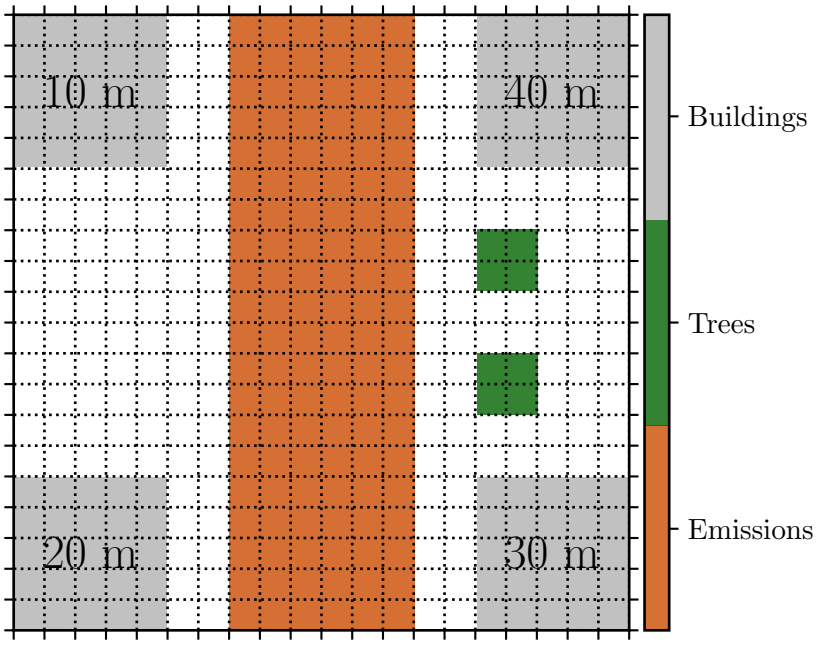

Figure S1. Visualisation of the simple test domain. Grid shows the horizontal model grid.

S3 Emission number size distributions

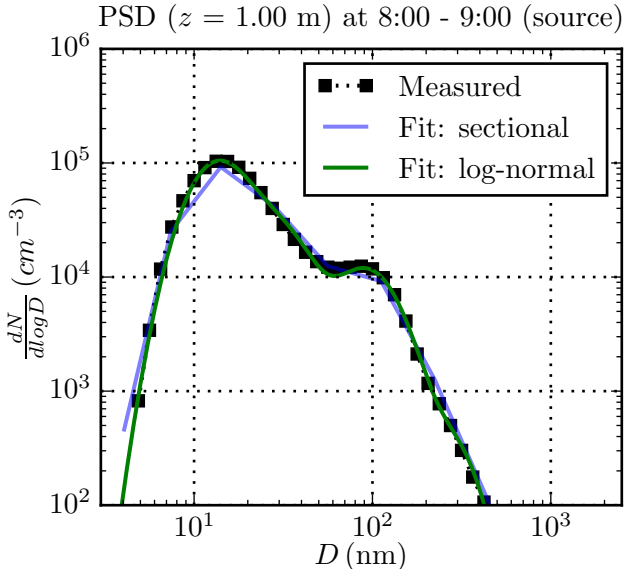

Figure S2. Measured aerosol size distribution (PSD) as a function of particle diameter D (nm) at the lowest measurement level $z = 1.0$ m for the morning simulation. Measurements are shown with a black dotted line with squares, sectional fitting with a blue line and log-normal fitting with a green line.

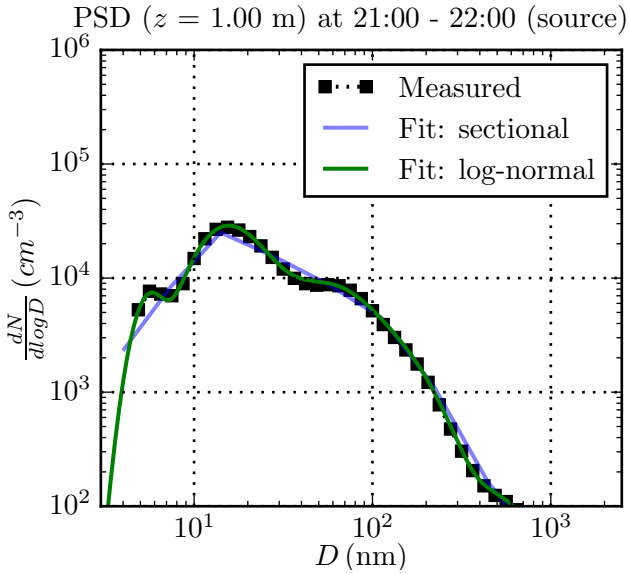

Figure S3. Measured aerosol size distribution (PSD) as a function of particle diameter D (nm) at the lowest measurement level $z = 1.0$ m for the evening simulation. Measurements are shown with a black dotted line with squares, sectional fitting with a blue line and log-normal fitting with a green line.

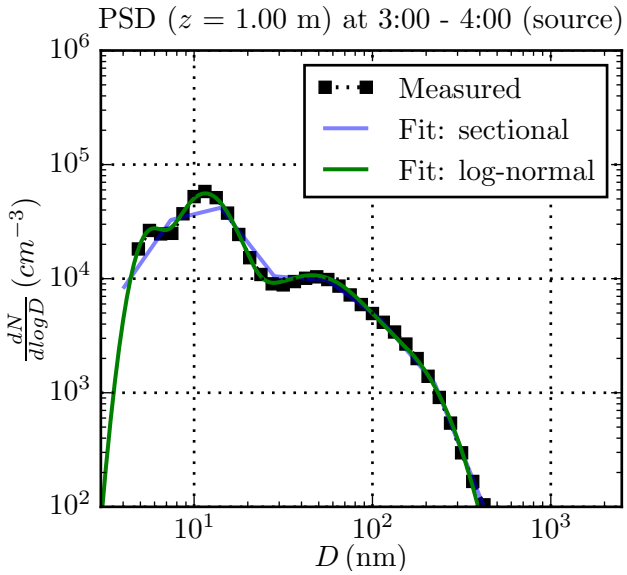

Figure S4. Measured aerosol size distribution (PSD) as a function of particle diameter D (nm)at the lowest measurement level $z = 1.0$ m for the night-time simulation. Measurements are shown with a black dotted line with squares, sectional fitting with a blue line and log-normal fitting with a green line.

S4 HYSPLIT air mass trajectories

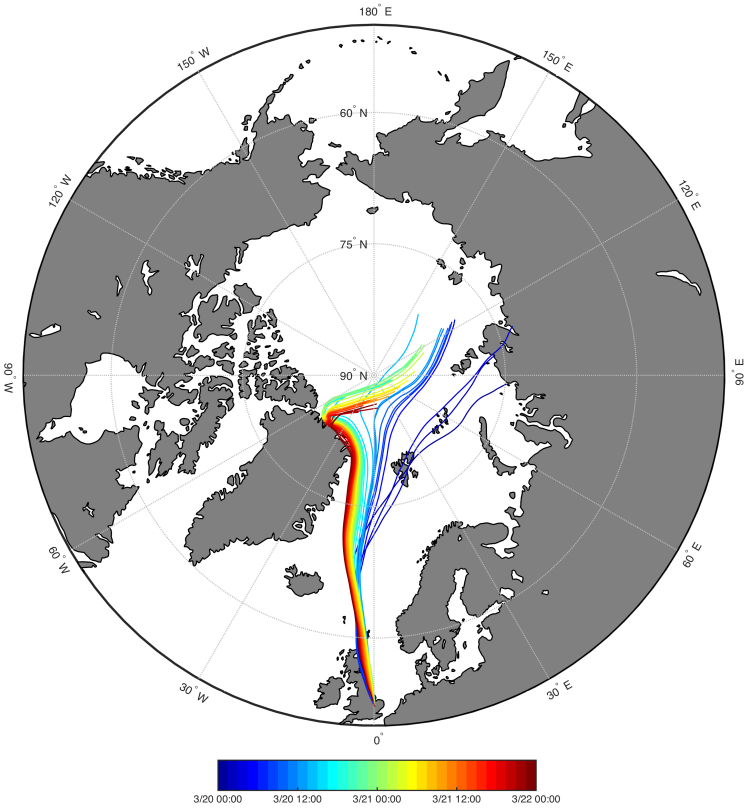

Figure S5. The HYSPLIT air mass trajectories along which ADCHEM was run from 20 March 00:00 UTC to 22 March 00:00 UTC.

S5 Background concentration profiles from ADCHEM

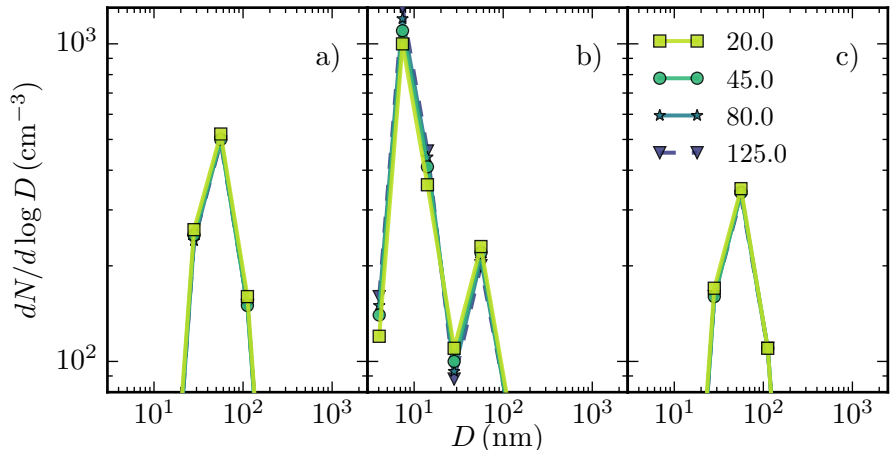

Figure S6. Background aerosol size distributions at 20.0, 45.0, 80.0 and 125.0 m AGL for the a) morning, b) evening and c) night-time simulations.

S5.1 Morning

Table S1. Background gas concentrations for the morning simulations. Concentrations in cm^{-3}.

z (m)	$[H_2SO_4]$ ($\times 10^4$)	$[HNO_3]$ ($\times 10^7$)	$[NH_3]$ ($\times 10^10$)	[OCSV] ($\times 10^4$)	[OCNV] ($\times 10^3$)
20.0	7.1	5.9	7.3	5.3	5.5
45.0	7.4	6.1	6.9	5.5	5.8
80.0	7.9	6.4	6.6	5.8	6.3
125.0	8.3	6.2	6.4	6.0	6.7

Table S2. Mass fractions of the background aerosol concentration for the morning simulation.

z (m)	SO_4^{2-}	OC	BC	NH_4^+	NO_3^-
20.0	0.09	0.24	0.64	0.00sac	0.03
45.0	0.09	0.24	0.64	0.00	0.03
80.0	0.09	0.25	0.63	0.00	0.03
125.0	0.09	0.25	0.63	0.00	0.03

S5.2 Evening

Table S3. Background gas concentrations for the evening simulations. Concentrations in cm^{-3}.

z (m)	$[H_2SO_4]$ ($\times 10^4$)	$[HNO_3]$ ($\times 10^8$)	$[NH_3]$ ($\times 10^10$)	[OCSV] ($\times 10^6$)	[OCNV] ($\times 10^4$)
20.0	8.4	5.6	5.1	5.4	3.1
45.0	7.8	5.6	4.9	5.6	3.2
80.0	7.5	5.8	4.8	5.9	3.5
125.0	7.1	5.6	4.7	6.1	3.7

Table S4. Mass fractions of the background aerosol concentration for the evening simulation.

z (m)	SO_4^{2-}	OC	BC	NH_4^+	NO_3^-
20.0	0.12	0.31	0.53	0.01	0.03
45.0	0.13	0.33	0.49	0.02	0.03
80.0	0.13	0.33	0.47	0.04	0.04
125.0	0.13	0.34	0.44	0.05	0.04

S5.3 Night

Table S5. Background gas concentrations for the night-time simulations. Concentrations in cm^{-3}.

z (m)	$[H_2SO_4]$ ($\times 10^4$)	$[HNO_3]$ ($\times 10^7$)	$[NH_3]$ ($\times 10^10$)	[OCSV] ($\times 10^5$)	[OCNV] ($\times 10^4$)
20.0	3.4	9.6	5.1	2.4	1.3
45.0	3.3	9.7	4.9	2.4	1.3
80.0	3.3	9.9	4.8	2.6	1.4
125.0	3.2	9.5	4.7	2.7	1.5

Table S6. Mass fractions of the background aerosol concentration for the night-time simulation.

z (m)	SO_4^{2-}	OC	BC	NH_4^+	NO_3^-
20.0	0.10	0.26	0.61	0.00	0.02
45.0	0.10	0.27	0.60	0.00	0.03
80.0	0.10	0.28	0.59	0.00	0.03
125.0	0.10	0.28	0.59	0.01	0.03

S6 Input wind profiles

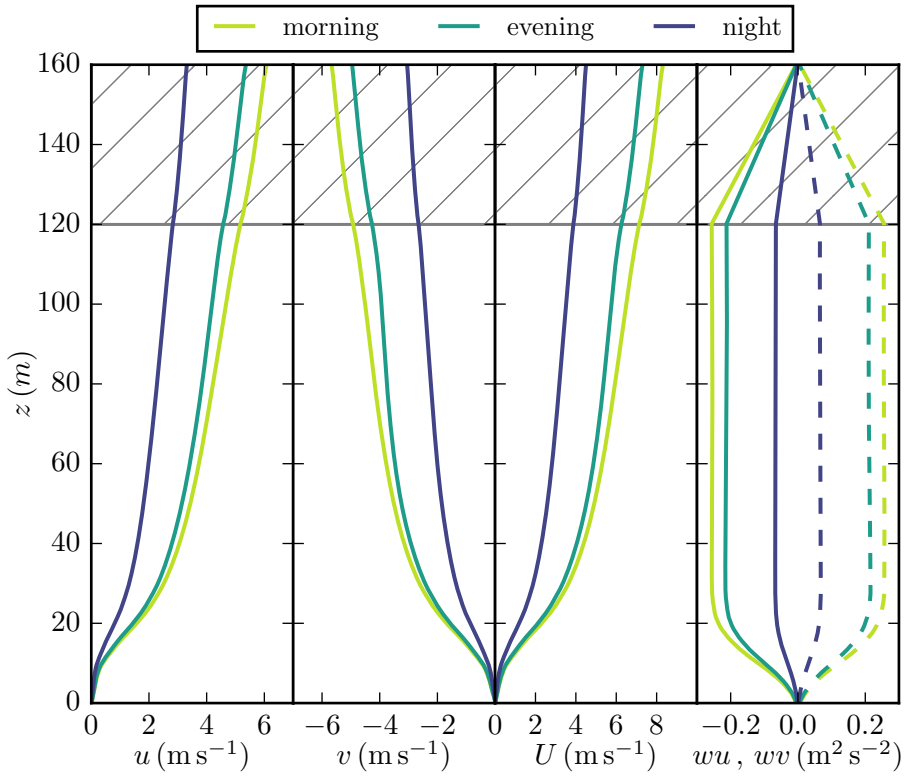

Figure S7. 1-hour mean vertical profiles of the horizontal wind velocities u, v and $U = \sqrt{u^2 + v^2}$ and and the Reynolds stress wu (solid line) and wv (dashed line) for all simulations before switching SALSA on. The area above $z = 120$ m marked with grey lines indicates the height above which a flow-driving pressure gradient is applied.

S7 Results

S7.1 Baseline simulations

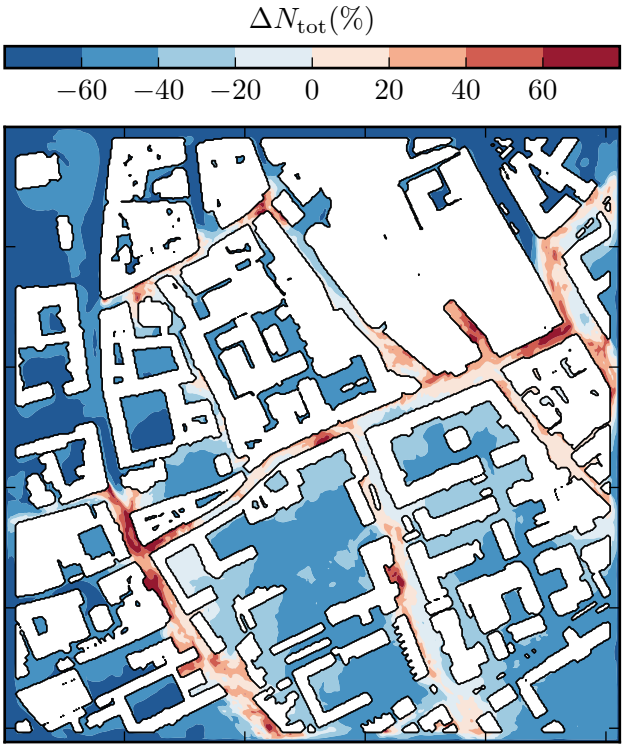

Figure S8. Relative difference in the total aerosol number concentration ΔN_{tot} (%) at $z = 3.5$ m between the evening and night-time simulations. Positive values indicate that N_{tot} is higher at night-time than in the evening, and vice versa.

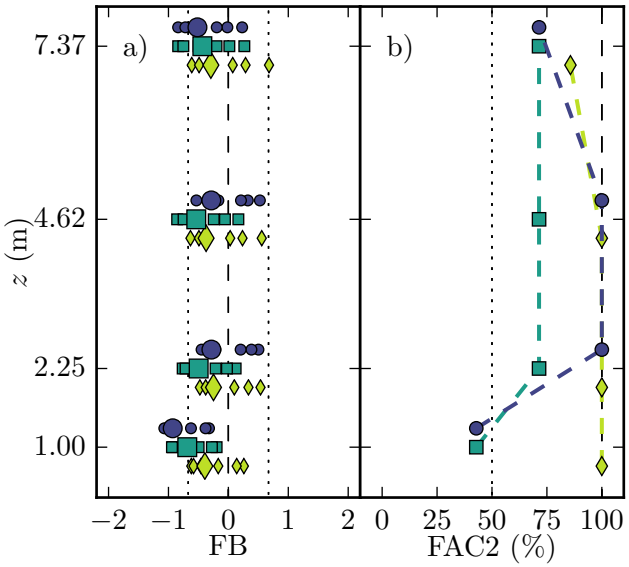

Figure S9. Statistical model performance measures for the total aerosol number concentration N_{tot} in the morning (lime diamonds), evening (greenish squares) and night-time (dark blue circles) at the measurement levels: a) fractional bias (FB) and b) fraction of predictions within a factor of two of observations (FAC2) (Chang and Hanna, 2004). For a perfect model, FB $= 0.0$ and FAC2 $= 100$ % (black dashes lines). Black dotted lines indicate: a) the limit for a factor of two under-/overprediction or b) 50 % fraction limit. The exact measurement location is marked with a larger marker than the additional six evaluation points.

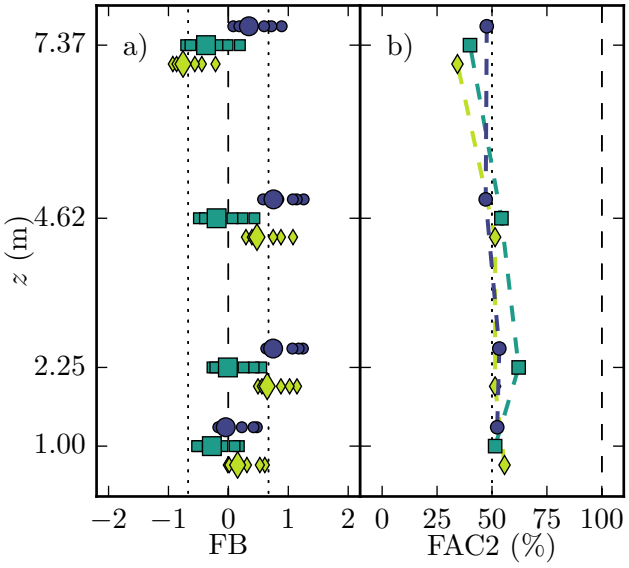

Figure S10. Statistical model performance measures for the aerosol number size distribution in the morning (lime diamonds), evening (greenish squares) and night-time (dark blue circles) at the measurement levels: a) fractional bias (FB) and b) fraction of predictions within a factor of two of observations (FAC2) (Chang and Hanna, 2004). For a perfect model, FB $= 0.0$ and FAC2 $= 100$ % (black dashes lines). Black dotted lines indicate: a) the limit for a factor of two under-/overprediction or b) 50 % fraction limit. The exact measurement location is marked with a larger marker than the additional six evaluation points. Measures are averaged over the whole aerosol size distribution.

S7.2 Sensitivity tests

S7.3 Role of different aerosol processes

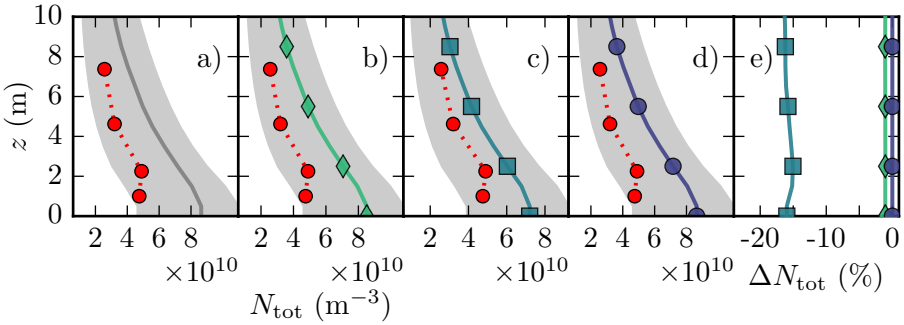

Figure S11. Measured (red dotted line with circles) and simulated vertical profiles of the total aerosol number concentration N_{tot} (m^{-3}) for the a) NOAP (grey solid line), b) COAG (diamonds), c) DEPO (squares) and d) COND (circles) simulation in the morning. Relative difference N_{tot} (%) of b)-d) to a) is shown in e). The line shows the mean vertical profile at the measurement location and the grey shaded area the range of mean vertical profiles at six additional evaluation points within the evaluation domain.

S7.3.1 Number of size bins

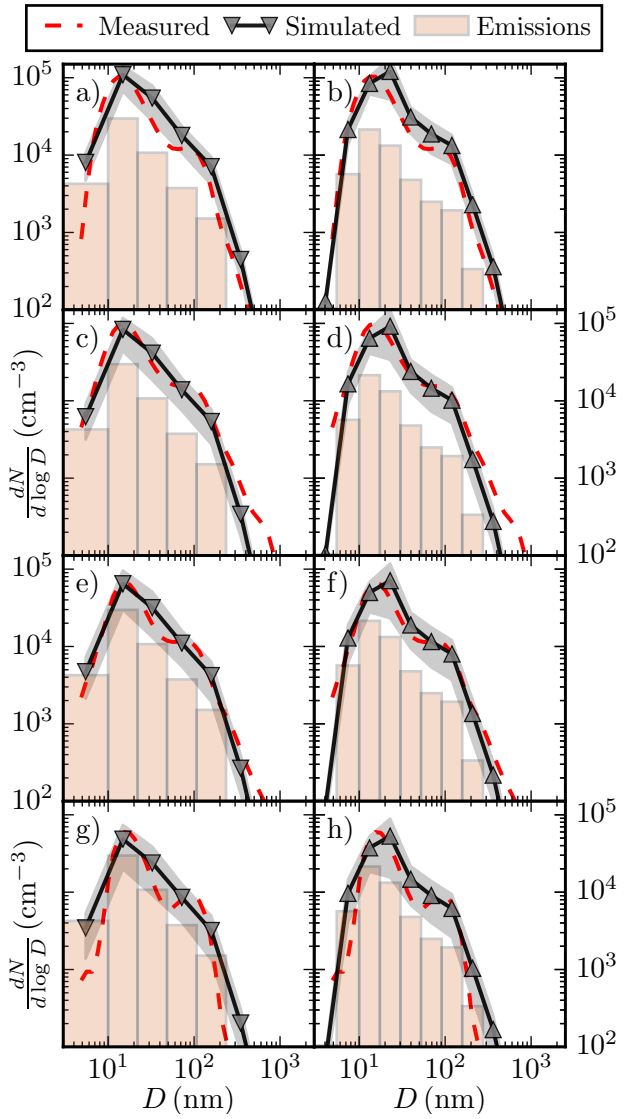

Figure S12. Measured (red dashed line) and simulated (black lines with triangles) aerosol number size distribution $dN/d\log D$ (cm^{-3}) as a function of particle diameter D (nm) in the morning at levels $z = 0.5$, 2.5, 4.5 and 7.5 m (top to bottom). Left column (a, c, e, f): LB and right column (b, d, f, h): MB simulation. The shape of the number size distribution for the emissions is given with bars (not in units cm^{-3}). The grey shaded area shows the span of all horizontal points 1–8 and the line shows their mean value.

References

Chang, J. C. and Hanna, S. R.: Air quality model performance evaluation, Meteorology and Atmospheric Physics, 87, 167–196, https://doi.org/10.1007/s00703-003-0070-7, 2004.

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