Comparison of the atmospheric Chemistry Transport Model COSMO-MUSCAT with experimentally determined aerosol parameters

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The chemistry-transport model system COSMO-MUSCAT was used for a detailed observation-model comparison. The model system consist of the online coupled code of the operational forecast model COSMO (Schättler et al., 2009) and the chemistry-transport model MUSCAT (Wolke et al., 2012). For the description of the particle size distributions, an extended version of the modal aerosol model M7 (Vignati at al., 2004) was used.

Experimentally determined particle number size distributions from the GUAN-Network in Germany (Birmili et al., 2009) were used for the comparison of a spring episode in 2009. In the beginning, very low pollutant concentrations were observed due to north-westerly advection. Afterwards a stable high pressure system leaded to accumulation and thus high pollutant concentrations. The flow changed to westerly and back to a stable high pressure system above the considered area resulting in dilution and again accumulation of pollutants. In the end of the episode, very low pollutant concentrations due to zonal advection of maritime air.

The total mass and chemical composition of PM_{10} and PM_1 (regarded as representative for the accumulation mode) was compared at one location. The mass of PM_{10} was significantly underestimated; the mass of PM_1 was in better agreement with the observed data. The sulphate concentration was in good agreement for both, PM_{10} and PM_1. Nitrate was underestimated in PM_{10} and overestimated in PM_1. Ammonium was slightly underestimated in PM_{10}, but rather overestimated in PM_1. The sea salt concentration was significantly too high, whereas the dust concentration was significantly too low for both, PM_{10} and PM_1. Table 1 shows the correlation coefficients and the relative deviation between the model and the experimental data for a subset of parameters.

Parameter	R^2	Mean deviation (relative)
N_{accu}	0.13	2.7
$D_{p,accu}$	0.07	1.2
PM_{10} (24h)	0.75	0.44
sulfate (PM_{10})	0.61	0.77
nitrate (PM_{10})	0.82	0.74
ammonium (PM_{10})	0.69	0.58

Table 1. Comparison between model simulations and experimental data in Melpitz, Germany.

The physical aerosol parameters were compared for the accumulation mode, since there were only scarce observations of the coarse mode available and modeling of the Aitken mode appeared difficult. The comparison included three stations, which showed more or less the same features. The particle volume was underestimated in the model, but temporal trends were represented well. The simulated number concentration was in the correct order of magnitude but decreased over the period of concern. This is probably due to too large deposition processes or because of too less emissions. This has to be investigated further.

In order to compare the particle diameter, the measured particle number size distributions were fitted with mostly three log-normal modes with the same sigma as used in the model. The comparison resulted in the particle diameter being also in the right order of magnitude but more or less uniform, in contrast to the observations. It tended to be overestimated. Figure 1 shows an example of the comparison of the accumulation mode particle diameter at one out of three stations.

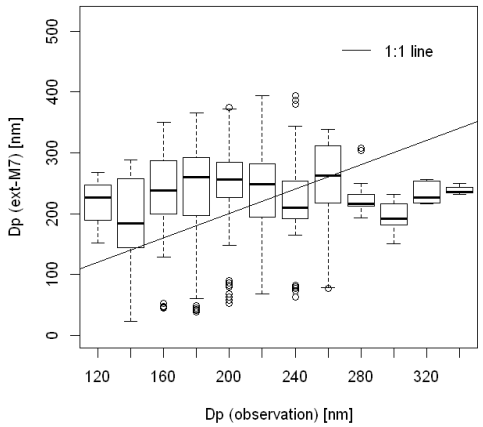

Figure 1. Comparison of experimentally determined and simulated particle diameter in the accumulation mode in Melpitz, Germany.

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