Concentration Profiles Using a Lognormal Distribution Regarding Aerosols with CAPRAM 2.4 (MODAC Mechanism)

A contribution to the subproject CMD-MPM

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In this study a detailed chemical mechanism (147 species and 438 reactions) describing tropospheric aqueous phase chemistry by CAPRAM2.4 (Chemical Aqueous Phase Radical Mechanism) (Herrmann et al., 2002) was used in order to understand different chemical reaction systems and to determine diurnal concentration profiles for different species in the troposphere (Table 1). The aqueous chemistry is coupled to the gas phase mechanism RACM (Stockwell et al., 1997) and the phase exchange is accounted by using a resistance model (Schwartz, 1986).

The latest development is the application of a size-resolved model system. In the present work different size bins (1, 2, 3, 4, 5, 10, 20, 30, 50) are considered in order to evaluate the effect of the size resolution on the diurnal concentration profiles.

The mechanism was applied for three different scenarios: (i) urban, (ii) remote and (iii) marine varying the atmospheric initial conditions. The obtained results show for all of the considered species in this study an agreement in the diurnal trend but was observed a relevant effect on the daily maximal concentration due to size resolution of the system. In the aqueous phase a lower OH concentration ($6 \cdot 10^{-14}$ M) compared to the non size-resolved system ($1 \cdot 10^{-13}$ M) for the urban scenario was found.

Table 1: List of the species of interest included in the present work.

Species	
Gas phase	**Aqueous phase**
O_3	OH
NO_2	NO_2
NO	Fe^{2+}/Fe^{3+}
NO_3	Cu^{2+}/Cu^{+}
OH	HO_2/O_2^-
HONO	O_3
N_2O_5	$HONO/NO_2^-$
HO_2NO_2	HO_2NO_2
	Oxalate
	HSO_3^-/SO_3^{2-}
	S(IV)

References

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