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Modelling of the tropospheric halogen multiphase chemistry with CAPRAM

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Halogens play a key role in marine chemistry. There has been a great effort to understand halogen chemistry in the atmosphere, either by field experiments (e.g. Pszenny et al., 2007), laboratory studies (e.g. Burkholder et al., 2004) or modelling studies (e.g. Pechtl et al., 2007).
In the present study a comprehensive reaction mechanism – the halogen module 2.0 (HM2) – was developed for the use with the multiphase chemical mechanism RACM-MIM2ext/CAPRAM 3.0i (Tilgner and Herrmann, 2010). The module is an update of its former version 1.0 (Herrmann et al., 2003) to allow for near-explicit modelling of marine environments. The HM2 totals to 204 halogen (i.e. chlorine, bromine, and iodine) species and 597 reactions. Besides a detailed description of the inorganic halogen chemistry in the gas and the aqueous phase, interactions with organic compounds and nitrogen species in either phase and with sulphur species in the aqueous phase are included. As a gas phase source for halogens the emission of alkyl halides is implemented in the HM2, whose oxidation is described explicitly in contrast to other modelling studies. The mechanism module was designed in a way that it can be used for a great variety of different scenarios including remote and polluted regimes.
Simulations have been carried out with the air parcel model SPACCIM (Wolke et al., 2005) under remote marine conditions using a meteorological scenario with 8 cloud passages. For a more detailed understanding of the tropospheric halogen multiphase chemistry (e.g. the recycling of the halogen species or their influence on organic compounds and other important key species) a detailed time-resolved analysis of the source and sink fluxes was done. Sensitivity runs investigate the importance of the different halogens by omitting iodine, both bromine and iodine species, and halogen species at all in the mechanism. The influence of the aqueous phase was researched with a sensitivity run treating only gas phase species.
With the HM2 it is possible to explain the tropospheric halogen multiphase chemistry in more detail than before. Typical concentrations of key halogen species and important trace gases such as ozone or HO_x species could be reproduced. The time-resolved analysis of sink and source fluxes revealed new reaction cycles that might have a major influence under cloudy conditions. Further investigations concern the influence of cloud phases regarding the enhancement or suppression of halogen chemistry or the relative contributions of alkyl iodides to the inorganic iodine budget.

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