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Application of the CAPRAM Halogen Module 2.0 in mixed urban and maritime coastal areas

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Approximately 20% of the earth's surface is covered with coastal regions. About one half of the world's population live in these areas (Gelpke and Visbeck, 2010). Therefore, there is a great interest to understand interactions of marine and continental air masses in coastal areas.
A comprehensive halogen multiphase chemical mechanism, the CAPRAM Halogen Module 2.0 (HM2), together with the multiphase chemical mechanism RACM-MIM2ext/CAPRAM 3.0n has been used to investigate the tropospheric multiphase chemistry in coastal areas, where clean marine air masses mix with urban air masses. While marine air masses are strongly influenced by halogen chemistry expressed in the HM2, urban air masses are affected by organic chemistry (implemented in CAPRAM 3.0). An innovation of the HM2 is the linkage of organic and halogen chemistry in an explicit chemical mechanism.
Two different scenarios have been used to investigate the interactions of halogens with organic and inorganic systems. In the first scenario, a maritime air mass moves over an urban area while in the second scenario, a polluted air mass passes the coastal ocean. Both scenarios include non-permanent clouds with 8 cloud passages of the air parcel, which allows the investigation of the influence of clouds on the halogen multiphase chemistry. As an advantage of this scenario not only the chemistry under non- and in-cloud conditions can be investigated, but under cloud formation and evaporation conditions as well. Furthermore, modifications of the air parcel after cloud passages are noticeable.
Besides investigations of the concentration-time profiles of important halogen and non-halogen species, detailed time-resolved flux analyses have been performed to determine the most important chemical cycles and to understand the time evolution of the concentration profiles. The simulations have shown that the influence of the origin of the air mass is significant only on the first day. Thereafter, the emissions of the new environment dictate the multiphase chemistry. Time-resolved flux analyses have been used to determine the most important sinks and sources for halogen atoms in the troposphere, investigate halide activation and the destruction of ozone in both regimes. The analysis includes a distinction between non-cloud and in-cloud periods. Furthermore, interactions with organic compounds are investigated in both the gas and the aqueous phase. Interactions with inorganic species such as NO_x are investigated as well. However, a significant importance of NO_x is restricted to the polluted regimes. Results are also compared to previous model studies in pristine open ocean regions.

References

Gelpke, N., Visbeck, M. (eds.): World Ocean Review 2010 - Living with the Oceans, Mare, Bremen (2010)