Short abstract. 19th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes 3-6 June 2019, Bruges, Belgium

Impact of halogen chemistry on ground-level ozone levels in Europe

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Abstract text

Oceans are the main emission source of halogens (Cl, Br and I). These species modify the oxidation capacity of the atmosphere and have an impact on the formation of secondary compounds, including organic aerosols and tropospheric ozone (O_3). However, chemical-transport models used for regulatory purposes have not considered halogens until very recently. In this study, we apply the multi-scale WRF-SMOKE-CMAQ (v5.2) modelling system to understand the role of halogens on O_3 levels in Europe. We perform a one-month simulation for July 2006 that reflects the typical summer conditions using 12-km horizontal grids and 35 vertical layers. We compare two versions of the Carbon Bond 2015 (CB05) chemical mechanism. One version includes a full description of the halogen gas-phase chemistry through 26, 39 and 53 reactions involving chlorine, bromine and iodine, respectively. The second version, used as a reference, does not include any of these reactions. Both simulations used boundary conditions generated from the corresponding hemispheric CMAQ model results.

We compare O_3 predictions from both model simulations to identify the impacts of including halogens into regulatory simulations. In addition, we compare our modelling results with the observations from more than 450 air quality monitoring stations all over Europe, both inland and in coastal areas. The combined halogen chemistry reduced the concentration of O_3 by as much as 15 $\mu g/m^3$ and improved model performance, especially at those monitoring stations close to the seashore (<24 km). Our results indicate that the index of agreement increases from 0.690 to 0.705 and the average bias decreases from 2.8 to -1.4 $\mu g/m^3$ in these locations. Our results suggest that the inclusion of marine halogens into regional chemical-transport models for regulatory purposes is important, at least in coastal areas since they may play a relevant role in the formation and destruction of O_3 and thus, should be considered when designing air quality plans and measures.

Motivation

Our research identifies a potentially relevant omission in current air quality modelling systems used to simulate the outcomes of air quality plans and strategies. According to our analysis this is more relevant for coastal areas. This implies that O_3 simulations from current chemical-transport models may include biases in coastal areas relative to inland locations. We suggest that incorporating a full description of halogen chemistry will help to harmonize assessment methods and improve the accuracy and comparability of simulations as well as the scientific basis for the development of action plans.