Interactive comment on “Consistent simulation of bromine chemistry from the marine boundary layer to the stratosphere, Part I: model description, sea salt aerosols and pH” by A. Kerkweg et al.

A. Kerkweg et al.

Received and published: 4 July 2008

We thank the anonymous referee #2 for the comments, which helped very much to improve the manuscript. In the following we reply to the individual statements:

We fully agree that the aerosol chemistry in the accumulation mode aerosol is important. Nevertheless, even if we were not yet able to include this into our simulations we think a lot can be learned from the simulations even with the known restrictions. We will add a more detailed discussion in the revised manuscript.

i) This is an interesting remark as Section 2.1 to 2.3 can not be shortened any more without information loss and the model setup should be completely described in
a paper showing simulation results. As MESSy is able to handle the same processes by different submodels, we have to name all used submodels to provide a complete model setup description. We see that Section 2.4 and 2.5 are somewhat lengthy. But, as this is the first non-technical publication showing results of M7 and MECCA-AERO we have to describe these submodels in more detail here. We remove Section 2.4.2-2.4.4 and refer to the Technical Note about MECCA-AERO in order to meet the referees suggestions.

ii) The remark is somehow in contradiction to the previous one. Most of these questions are already discussed in the Technical Note about MECCA-AERO. Thus we are reluctant to add these technical details in this article again. Instead we provide the answers here:

Is the liquid water content of the coarse mode aerosol the sole criteria for calculating the aerosol chemistry?
Two criteria are included: The first and most important one is the one with the liquid water content threshold. A second criterion had also to be implemented because of numerical reasons; in grid boxes where the ocean fraction is less than 20% the aerosol chemistry is also switched off.

Is this check performed independently for each grid cell in the whole domain or is the liquid water profile considered?
The check is performed for each individual grid box as the numerical stiffness is different in each individual grid box.

What is the sequence of the processes in the operator splitting approach?
This is discussed in detail in the MECCA-AERO Technical Note (Chap. 2.2). We also included a flowchart (Fig. 1) in that article to clarify the sequence of the process splitting.

How is the KPP solver initialised in the restart case (grid cell with aerosol chemistry calculations in the last coupling time step) and in the new start case (no aerosol chemistry in the last step)?
In all boxes the current mixing ratios of the aerosol tracers are used as input for the (aerosol+gas) chemistry. When no aerosol chemistry is calculated the rate for the aerosol reactions are set to zero. Thus the chemistry leaves the aerosol tracers untouched when no aerosol chemistry is calculated. In the next time step each box starts from the current aerosol mixing ratios, i.e. those mixing ratios from the last chemistry calculation modified by other processes (advection, sedimentation, scavenging etc.). Hence, the chemistry in each grid box is calculated based on the full history of the specific grid box, however a restart issue is not present.

iii) In the simulation the diagnosed marine boundary layer height ranges between 100 and 2000 m above sea level. Annually averaged the MBL reaches between 400 and 800 m high. Therefore, the marine boundary mostly comprises 4 vertical layers. We will add this information and provide a picture showing the annually averaged marine boundary layer height in the supplement.

iv) In general it is not quite clear how to deal with averaging pH values, as the pH is simply the logarithm of the \(H^+\) concentration. Thus it seems to be the most reasonable way to average the \(H^+\) concentrations and then calculate the logarithm of the average \(H^+\) concentration. This method implies the disadvantage that one single box with a very low pH dominates the average, because of the logarithmic scale of the pH value. For this reason we decided to average the pH values, which gives a much more representative average pH for the respective region.

We know about the limitation of averaged pH values. For this reason we show frequency histograms in our further analysis of the pH. These give much more information about the variability of the pH. However, this representation is not applicable to the global scale. To provide somehow a global picture, we had to show averaged pH values.
We will add this explanation as an appendix to the article. We intend to discuss the vertical structure of the aerosol pH in detail in the third part of the article series, which is dedicated to the processing of halogens by the aerosols. This process is strongly pH dependent and also the liquid water content plays an important role. But we realise that the picture given in this article is not complete, if we provide no information about the vertical structure. Therefore, we will add one figure showing the temporal and vertical variability, however, save the major discussion for part III of the article series.

Literature

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 7217, 2008.