

Review by Rolf Sander

Bock et al. present the 1D tropospheric chemistry model MISTRA-v9.0 as an open-source community release. I strongly support that this previously closed source code is now made available to the research community. I recommend publication of the manuscript in GMD after considering several comments as described below.

Specific comments

- Title: In the title, MISTRA is called an “atmospheric model”. However, as there is apparently no code for the stratosphere or the upper atmosphere, it may be better to call MISTRA a “tropospheric model”.
- Section 1.1: The advantages of a 1D model compared to a 3D model are described in detail. Maybe a short comparison of MISTRA to 0D (box) models could be added as well.
- p. 2, l. 55: I suggest to change “halogen chemistry” to “tropospheric halogen chemistry”. Otherwise, the reader might expect stratospheric ozone hole chemistry as well.
- Figure 1: Only DMS emissions are shown here but iodine species can also be emitted in the model.
- Section 2.3, ll. 168-170: If, outside of clouds, the term “aqueous phase” is used only for sub-cloud aerosol, does this mean that there is no aerosol above the clouds?
- Section 2.3.1, Equation (10): This is the central and most important part of the chemistry code for the gas phase. As such, I think it deserves to be described in more detail. All terms should be explained in the order in which they appear in the equation.
- Section 2.3.1, Equation (10): The chemical loss of a species is proportional to its concentration, therefore the loss term includes c_g as a factor. However, why is the deposition D not multiplied by the concentration c_g ?
- Section 2.3.1: When I calculate the “mean transfer coefficient” for a monodisperse aerosol using equation (11), I get a different value than with equation (12). This is because equation (12) includes the liquid water content and equation (11) does not. Thus, the equations produce different quantities, and $\overline{k_t}$ should not be called the “mean” of k_t .

- Section 2.3.1: “The last term in equation (10) describes the transport from the gas phase into the aqueous phases [...]”
It describes not only the transport *into* the aqueous phases but also the reverse process, i.e., *out of* the aqueous phases.
- Section 2.3.2: When the unit mol/m³ is used for aqueous-phase concentrations, it would be important to mention if it refers to 1 m³ of air or to 1 m³ of solution.
- Section 2.3.6: It should be explained how the deposition D in equation (10) is calculated from the dry deposition velocity.
- As I have been directly mentioned in the Community comment by Roberto Sommariva, I would like to add my view as well: I agree that co-authorship should be offered to all model developers who contributed code which is now converted to open source. However, I think it is necessary to distinguish between model users and model developers. Contributions of other colleagues need to be checked individually and co-authorship should be offered where applicable. As far as I know, Roberto Sommariva and Susanne Pechtl have made substantial code contributions (mechanism update and iodine chemistry, respectively). Roberto Sommariva also mentions my contributions: The first halogen mechanism in MISTRA was taken from Sander and Crutzen (1996), and the KPP code has been presented by Sandu and Sander (2006). It is sufficient for me if these two papers are cited. I do not claim authorship for the current manuscript.

Technical Comments

- Section 1.2: The acronyms MBL and PIFM should be explained when they are used for the first time.
- p. 3, l. 79: When KPP is introduced, I suggest to cite the KPP model description by Sandu & Sander (2006, doi:10.5194/ACP-6-187-2006). Note that I have to declare a COI here because I’m a co-author of that paper.
- p. 6, ll. 138-139: Something is wrong with the sentence “after Davies (1985) Bott et al. (see also 1996)”.
- Section 2.3.1, Equation (10): Why is the symbol S used for the loss term? I suggest to use the same symbol as in equation (13), i.e., the symbol L .

- Section 2.3.1: Both K_h^{cc} and H_s^{cc} are used for the dimensionless Henry constant. I suggest to use only the symbol H_s^{cc} . In the context of equation (10), this also avoids confusion with K_h , the turbulent exchange coefficient for heat.
- Section 2.3.5 and Appendix A: J is the photolysis rate constant, not the photolysis rate.
- Table 1: The term “netCDF” is mentioned in the table but not explained. I suggest to add a link to <https://www.unidata.ucar.edu/software/netcdf/> or <https://en.wikipedia.org/wiki/NetCDF>.
- Section 3.2.2: Ferret and NCL are mentioned here but not explained. I suggest to add a short explanation or a citation.
- Section 4.2: The term NO_x should be defined.
- Appendix A: It is very good to have this list of symbols. It would be even more useful, if you can add the units that are used in MISTRA.
- Appendix A: For constants, their values could be shown as well (R , R_a , R_v , and maybe more)
- Appendix A: Several symbols should be added:
 - g
 - H^* (effective Henry constant)
 - H_s^{cp}
 - $\overline{k_t}$
 - M (molar mass)
 - St (Stokes number)
- Appendix B: Please add DMS, LWC, MIFOG and PIFM.

References

- Sander, R. and Crutzen, P. J.: Model study indicating halogen activation and ozone destruction in polluted air masses transported to the sea, *J. Geophys. Res.*, 101D, 9121–9138, doi:10.1029/95JD03793, 1996.
- Sandu, A. and Sander, R.: Technical note: Simulating chemical systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1, *Atmos. Chem. Phys.*, 6, 187–195, doi:10.5194/ACP-6-187-2006, 2006.