

We thank Rolf Sander for his positive evaluation of our manuscript, and numerous remarks that are very useful to improve the paper. His comments are reproduced below in black fonts, our answers are displayed in blue fonts.

## 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”.

Thank you for your suggestion. However, we agree with Linda Smoydzin’s comment that ”tropospheric” would not be suited. Instead, we replaced ”atmospheric” by ”atmospheric boundary layer”. The title now reads:  
*A description of the first open source community release of MISTRA-v9.0: a 0D/1D atmospheric boundary layer chemistry 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.

We added the following sentence in Section 1.1:  
*Ultimately, box models (0D) are designed to focus only on a single grid cell processes, further reducing the computing cost as compared to 1D models.*

- 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.

We agree with this suggestion and modified the text accordingly.

- Figure 1: Only DMS emissions are shown here but iodine species can also be emitted in the model.

Indeed MISTRA can account for any gas emission, DMS was just an important example of such emission. We agree that it was too reductive and maybe misleading. We thus replaced ”DMS” in Figure 1 by ”emissions (DMS, iodine, ...)”.

- 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?

In MISTRA, there are aerosols above the clouds, however the aqueous phase chemistry is computed only when a minimum liquid water content threshold is reached, which is never the case above the cloud top, or more generally above the top of the BL. To clarify, we added the following sentence after the one you cited:

*Aqueous chemistry is not computed above the top of the boundary layer (i.e. the top of clouds, if present).*

- 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.

We agree with your suggestion. We reorganised and expanded Section 2.3.1 so that each term of Equation (10) is described in the order it appears 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  $c_g$ ?

The dry deposition is indeed computed with a multiplication by the gas concentration (routine `sedc` in MISTRA). This was implicitly included in the deposition term "D", but we agree this writing was not consistent with the way it was written for the chemical loss. We thus explicitly reformulated the dry deposition term as  $Dc_g$  in Equation (10).

- 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  $kt$  should not be called the "mean" of  $kt$ .

We agree with you. We thus rephrased the sentence presenting Equation (12) as follows:

*The transfer coefficient  $\overline{k_t}$  for a particle population is given by the integral: [...].*

- 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.

We agree the wording was not correct. We rephrased this sentence that now reads:

*The last term in equation (10) describes the transport between the gas phase and the aqueous phases [...]*

- Section 2.3.2: When the unit  $\text{mol}/\text{m}^3$  is used for aqueous-phase concentrations, it would be important to mention if it refers to  $1 \text{ m}^3$  of air or to  $1 \text{ m}^3$  of solution.

We agree this is an important specification. The unit of aqueous-phase concentration is now clarified, the sentence reads:

*In each of these bins the following prognostic equation is solved for each chemical species  $c_{a,i}$  (amount per air volume), [...].*

- Section 2.3.6: It should be explained how the deposition  $D$  in equation (10) is calculated from the dry deposition velocity.

We added the following at the end of Section 2.3.6:

*Finally, the dry deposition term  $D$  is calculated as:*

$$D = \exp(-\Delta t/h \times v_g^{\text{dry}}) \quad (23)$$

*where  $\Delta t$  is the model time step, and  $h$  is the height of the lowermost*

*model layer.*

- 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.

Thank you for clarifying your point of view regarding your own involvement in MISTRA.

During the review process, we contacted several people who contributed to important parts of code in MISTRA, as detailed in our reply to Roberto Sommariva. Those who replied do not claim authorship for this paper and agree with the EUPL licensing.

## Technical Comments

- Section 1.2: The acronyms MBL and PIFM should be explained when they are used for the first time.  
MBL was already explained at line 43.  
We added the meaning of PIFM acronym, plus the reference of the paper (already cited elsewhere in our manuscript) discussing this radiative code (Zdunkowski et al., 1982). The sentence starting at line 47 now reads:  
*The radiation code used in MISTRA, called PIFM1 (Practical Improved Flux Method, developed by Zdunkowski et al., 1982), was updated by Loughlin et al. (1997) and the new radiation code, PIFM2, was evaluated.*
- 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. Thank you, this reference was indeed missing. We added it as suggested, as long as the first paper presenting KPP (Damian et al., 2002). The sentence p. 3, l. 79 now reads:  
*The chemical "Kinetic PreProcessor" (KPP: Damian et al., 2002; Sandu and Sander, 2006) has been updated to the latest version 2.2.3 (<https://people.cs.vt.edu/~asandu/Software/Kpp/> last accessed 23 June 2021).*
- p. 6, ll. 138-139: Something is wrong with the sentence "after Davies (1985) Bott et al. (see also 1996)".

Thank you for noticing this, we corrected the citation command. The end of the sentence now reads:

*after Davies (1985) (see also Bott et al., 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  $L$ . There was indeed an inconsistency, thank you for your careful reading. We now choose to use the symbol  $S$  (as "sink") in both equations (10) and (13) since  $L$  is used elsewhere for the latent heat of condensation.
- 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.  
We agree and modified the symbol accordingly in equation (10).
- Section 2.3.5 and Appendix A:  $J$  is the photolysis rate constant, not the photolysis rate.  
Thank you, we corrected this in Section 2.3.5 and Appendix A.
- 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>.  
We followed your suggestion, and explained the netCDF acronym in Table 1. The added footnote in this Table reads:  
<sup>a</sup> *network Common Data Form, see <https://www.unidata.ucar.edu/software/netcdf/> (last accessed 21/11/2021).*
- Section 3.2.2: Ferret and NCL are mentioned here but not explained. I suggest to add a short explanation or a citation.  
We added the reference for NCL and the link to Ferret webpage. The sentence now reads:  
*Plotting scripts provided as example are written for Ferret (<http://ferret.pmel.noaa.gov/Ferret/>, last accessed 04/11/2021) and NCL (NCAR, 2019), but neither are necessary to run the model.*
- Section 4.2: The term  $NO_x$  should be defined.  
The sentence now reads:  
*An emission scenario of  $NO_x$  ( $NO+NO_2$ ) was 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.  
Thank you for your feedback, we added the units in Appendix A.
- Appendix A: For constants, their values could be shown as well ( $R$ ,  $R_a$ ,  $R_v$ , and maybe more)  
We shown the numerical values for these constants, and for  $c_p$ ,  $g$ ,  $\kappa$ , and  $\rho_w$  in Appendix A.
- Appendix A: Several symbols should be added:

- $g$
- $H^*$  (effective Henry constant)
- $H_s^{cp}$
- $\overline{k_t}$
- $M$  (molar mass)
- $St$  (Stokes number)

Thank you for your careful review, we added these symbols in [Appendix A](#)

- [Appendix B](#): Please add DMS, LWC, MIFOG and PIFM.  
[We have added these four abbreviations in Appendix B.](#)

## References

- Damian, V., Sandu, A., Damian, M., Potra, F., and Carmichael, G. R.: The kinetic preprocessor KPP-a software environment for solving chemical kinetics, *Computers & Chemical Engineering*, 26, 1567–1579, [https://doi.org/10.1016/S0098-1354\(02\)00128-X](https://doi.org/10.1016/S0098-1354(02)00128-X), 2002.
- Zdunkowski, W. G., Panhans, W.-G., Welch, R. M., and Korb, G.: A radiation scheme for circulation and climate models, *Contributions to Atmospheric Physics*, 55, 215–238, 1982.