

We thank Reviewer #2 for their positive evaluation of our manuscript, and numerous remarks that are very useful to improve the paper. R2's comments are reproduced below in black fonts, our answers are displayed in blue fonts.

## Remarks

Title: I find the term "chemistry" in the title a bit reductive, as the model can also represent some aerosol processes, like particle nucleation. You might consider extending the title.

Thank you for your suggestion to extend the paper's title to also mention the aerosol processing aspects. However, the title is already long, all the more so since we extended it following the comments by Rolf Sander and Linda Smoydzin, to clarify that MISTRA is both 0D and 1D, and that it focuses on the 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*

L13: you might cite also Bellouin et al. (Rev. Geophys. 2020, doi:10.1029/2019rg000660), for a more recent assessment.

We added this reference, the sentence now reads:

*They significantly affect the radiative balance of the atmosphere, through direct (scattering and absorption) and indirect effects (cloud properties modification) (Carslaw et al., 2010; Boucher et al., 2014; Bellouin et al., 2020).*

L17: please add some references for these two other effects you mention.

We added references for these two effects, the sentence now reads:

*Other impacts include the reduction of visibility (see for instance Seinfeld and Pandis (2016, Chap. 15); Zhang et al. (2020) and ref. therein) and health effects of pollution (e.g. Pöschl (2005), Molina et al. (2020) and ref. therein).*

L46: *In this work*, do you mean Bott (1997)? I would be more specific, since "this work" could mean the present manuscript.

"this work" indeed referred to the study of Bott (1997). We merged both sentences to clarify, it now reads:

*Based on this first version of MISTRA, Bott (1997) further included typical particle distributions of urban and rural aerosols for the study of MBLs influenced by continental air masses, and assessed the radiative forcing of stratiform cloud.*

L76: can you provide some example of the strict coding rules mentioned here?

The most prevalent change in the model code is the explicit declaration of all variables, to replace `implicit double precision (a-h,o-z)` that was used so far. Other examples include the rewriting of obsolete features such as arithmetic `if`, and `go to` statements, which are strongly discouraged in modern code.

We believe that these technical examples do not need to be provided in the manuscript. Instead, we added two references to practical guidelines for Fortran coding, which include the aforementioned examples. Though these guidelines are only published online, they are often referred to in the atmospheric sciences modelling community, and we think they deserve to be cited in the manuscript.

The sentence now reads:

*To improve robustness and portability of the code, intensive controls throughout the code have been performed to track issues, fix bugs, and conform to strict coding rules (Metcalf et al., 2004) and coding standards (see for instance <http://www.umr-cnrm.fr/gmapdoc/IMG/pdf/coding-rules.pdf> and <http://www.reading.ac.uk/physicsnet/units/3/3phss/F90Style.pdf>, last accessed 26/10/2021)*

L77: how would you ensure future maintainability if the Forcheck tool is no longer distributed?

Forcheck is no longer distributed, but any current user with a valid licence can still use it. Furthermore, using such a tool (other might exist as well, and regular Fortran compilers also perform lexical analysis) is not mandatory to maintain the model code.

L79: please provide a reference to KPP (I think this is Sandu and Sanders, 2006, doi:10.5194/acp-6-187-2006).

The reference to KPP papers was indeed missing, thank you for noticing this. We added the reference you suggested, plus the paper describing the first version that was used in MISTRA before we updated it. In the same sentence, we also clarified that a version of KPP specifically tuned for MISTRA is provided along with the model code. The sentence 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) with minor tuning for use in MISTRA (see the Code availability section at the end of the paper).*

L92: all model layers: how many? Is this configurable? Please clarify.

We added the following text in Sect. 2.1:

*The vertical grid is separated into three regions: the lowest part is made of 100 layers with a constant thickness of 10 m, followed by 50 layers with logarithmically equidistant layers up to 2000 m height. The third region is a constant atmosphere whose characteristics are based on the standard atmosphere. It extends up to 50 km height and is only used for radiation calculations. These vertical grid settings (number and thickness of layers) can be easily configured as required.*

L94: *Fluxes of seasalt... are included*, I would add "(see Sect. 2.3.6)".

We added this reference to Sect. 2.3.6.

L95: could you elaborate a bit more on the nucleation module? How is this process parametrized?

We added a subsection 2.3.7 to present the nucleation module, with the following description:

*A module computing the nucleation process was implemented in MISTRA by Pechtl et al. (2006). Only a brief overview is given here, while a comprehensive description is given in the model manual (Chapter 4). The nucleation module developed by Pechtl et al. (2006) includes both ternary sulfuric acid-ammonia-*

water ( $H_2SO_4-NH_3-H_2O$ ) nucleation, and homomolecular homogeneous OIO nucleation. The former is explicitly calculated as a function of  $H_2SO_4$  and  $NH_3$  concentrations, relative humidity, and temperature following the work by Napari et al. (2002). The latter is parameterised following Burkholder et al. (2004). Each process can be activated or not independently (see Table 1), and lead to the computation of "real" nucleation rates. In a second step, the "apparent" nucleation rate is computed after the work of Kerminen and Kulmala (2002) and Kerminen et al. (2004).

The nucleated particles computed in this module can then be integrated in the model, with three possible options: (i) no coupling, (ii) coupling with the microphysics without feedback on chemistry, and (iii) coupling with microphysics and chemistry (see Table 1).

L126-127: What about nucleation? Newly nucleated particles can have size below 5 nm, hence outside this range.

Indeed, the thermodynamic stable clusters are about 1 nm in diameter. This is why an "apparent" nucleation rate of larger particles is computed from the "real" nucleation rate by means of an analytical formula.

L295-296: Note that default values are for all of them, however they should be systematically redefined by the user to match the simulated atmosphere. I am not sure I understand this sentence, could you be more explicit?

We rephrased this sentence, that now reads:

*All these parameters have default values, even if most of them are expected to be redefined by the user to match the simulated atmosphere.*

L297: still, it would be interesting to know the temporal coverage of a typical run.

We added the following sentence:

*Typical run duration covers a few hours to a few days. Longer run duration is sometimes necessary for model spin up. The restart option of the model allows a single spin up run to initialise the model, and perform a sensitivity analysis from that stage, for instance.*

Sect. 3.1: I would not use subsections here, they are too short anyway.

The text within sections 3.1.x is indeed short, but tables are large and include significant piece of information. We kept the current headers for the sake of clarity of the manuscript, but now used un-numbered subsections to lighten them.

Conclusions: this is quite short. You could extend it, for example, by summarizing again the main capabilities/scope of the model and by adding a few sentences about current plans for model extension/improvement.

We extended the conclusion with the following description:

*MISTRA-v9.0 is a versatile model with a range of capabilities, from the study of status cloud microphysics, radiative forcing and turbulence, to the multiphase atmospheric chemistry of the boundary layer. While its original purpose was*

*only the study of cloud-free and cloudy marine boundary layer, MISTRA was successfully extended in previous studies to model other environments such as polar conditions and volcanic plumes. In this study, we updated the model code to comply with coding standards, [...].*

## Corrections

L15: large area → large surface area.  
Corrected

L23: limited area → limited domain.  
Limited-Area Models (LAMs) is the common wording, see for instance de Elía et al. (2002); Davies (2014) or <https://www.ecmwf.int/en/about/media-centre/news/2017/experts-debate-progress-limited-area-modelling> (last accessed 10/10/2021).

L28: *physic* → *physics*.  
Corrected

L28: *is* → *are*.  
Corrected

L60: *box mode* → *box model*.  
It now reads *box-model mode*

L124: *water is present* → *water were present*.  
Corrected

L125: *minimum aerosol radius* → *minimum aerosol dry radius* (I guess).  
Changed to *minimum dry aerosol radius*.

L137: better "time integration"?  
This is indeed better, thank you.

L138: I think you mean "see also Bott (1996)".  
We corrected the parenthesis for this reference.

L163: it is actually "on aerosol" and "in cloud particles".  
In this context, "aerosol" refers to deliquescent aerosol particles, inside which bulk chemical reactions are accounted for. Surface reactions occurring on aerosol particles are also accounted for in the MISTRA model, as described in the following sentence. We thus rephrased the sentence L163 that now reads:  
*The multiphase chemistry module comprises chemical reactions in the gas phase as well as in deliquescent aerosol and cloud particles.*

L166: DMS acronym not defined.  
It now reads "(...) of the oxidation of dimethylsulfide (DMS).", and we added DMS in Appendix B.

L203: I would use the term "coagulation" instead of "collisions".  
We used coagulation as you suggested.

L315: *mandatory* → *required*.

Changed

L319: please add the references or the links for ferret and NCL.

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.*

L385: please append "(Fig. 6a)" at the end of the sentence.

We added this internal reference at the end of the sentence.

Figure 2 caption: as function → as a function.

Corrected

Figure 3: please use the same contour levels for top and bottom panel (as you do in Fig. 4, for example).

We now increased the maximum contour level to 0.7 instead of 0.6. We added a sentence to clarify the apparent difference regarding the minimum contour level value "*Note the minimum contour level is set to 0.01 in both panels, but was displayed incorrectly in the original figure.*"

Figure 6 caption: please add that the MISTRA-v9.0 is also "without collision-coalescence".

the text now reads "*MISTRA-v9.0 (without collision-coalescence implemented)*" to make clear that this is not an option currently available in MISTRA-v9.0 (even if this was already highlighted in the text).

Figure 8: Scales are identical for both, actually the top right scale goes to 60 instead of 59. Not a big difference, but I would fix it.

Fixed

Eq. (12): the "lg" notation for the logarithm could be ambiguous, please specify the base or use "ln" if natural log.

"lg" is the notation for the decadic logarithm  $\log_{10}$ , as recommended by the IUPAC Green Book ([iupac.org/greenbook](http://iupac.org/greenbook)) and the SI Brochure ([www.bipm.org/en/publications/si-brochure](http://www.bipm.org/en/publications/si-brochure)), both of which GMD authors are asked to follow ([www.geoscientific-model-development.net/submission.html#math](http://www.geoscientific-model-development.net/submission.html#math)).

## References

Davies, T.: Lateral boundary conditions for limited area models, Quarterly Journal of the Royal Meteorological Society, 140, 185–196, <https://doi.org/10.1002/qj.2127>, 2014.

de Elía, R., Laprise, R., and Denis, B.: Forecasting skill limits of nested, limited-area models: a perfect-model approach, Monthly Weather Review, 130, 2006–

2023, [https://doi.org/10.1175/1520-0493\(2002\)130<2006:FSLONL>2.0.CO;2](https://doi.org/10.1175/1520-0493(2002)130<2006:FSLONL>2.0.CO;2),  
place: Boston MA, USA Publisher: American Meteorological Society, 2002.