

We thank Linda Smoydzin for her thorough reading, and comments on the manuscript. Her comments are reproduced below in black fonts, our answers are displayed in blue fonts.

License:

I agree with Roberto that a GPL license might be more appropriate. In addition, the authors of this manuscript want to make code publicly available which has however (at least partly) not been written by anyone of them.

GNU General Public License (GPL) and European Union Public Licence (EURL) provide similar rules (authorisations and obligations) regarding the model code (see for instance <https://choosealicense.com/appendix/>). However, the EURL provides wider compatibility with other licences, which means that MISTRA (released under EURL) can be merged with code covered by a compatible license, such that the combined derivative work can be distributed under the compatible licence. We asked developers of legacy parts in the MISTRA-v9.0 code (A. Kerkweg: contribution to netCDF output format; B. Luo: ion activities; S. Pechtl: nucleation; J. Landgraf: photolysis rates) whether they agreed to release of the their contribution under the EURL. The first three confirmed that they were happy with this. Unfortunately, despite repeated attempts via email and phone, we were unsuccessful in making contact with J. Landgraf.

Author contribution:

As the authors themselves emphasise that "the paper develops the branch of MISTRA based on von Glasow (2000)", it should be pointed out clearly and unmistakably (in the manuscript text itself as well as the author contribution section) that development and application of MISTRA took place under the lead of Roland von Glasow.

We modified the sentence cited above as follows:

*Our paper develops the branch of MISTRA of von Glasow (2000), whose development and application until 2015 took place under the lead of Roland von Glasow.* and we added the following sentence in the Author contribution section:

*From the early 2000s to 2015, development and application of the branch of MISTRA presented in this paper took place under the lead of Roland von Glasow.*

Overall, this manuscript appears to me to be half-hearted written. I explain in the following why I come to this conclusion:

Just listing a number of publications written based on simulations using MISTRA (p.2, l.54 - p.3 l.67): (i) is from my point of view not sufficient for publishing the code as the variety of scientific applications is only vaguely mentioned (ii) does not value the work of those people who worked intensely with MISTRA (in Roland von Glasow's working group, first at the university of Heidelberg, later at UEA in Norwich) and all of them contributed to the continuous development and improvement of MISTRA.

We understand the demand to present a thorough review of the capabilities of

MISTRA based on previous applications, and this is what we intended to do, not only by listing all publications based on MISTRA simulations, but also by providing detailed examples of use in a variety of situations (see section 4 of the paper). Since the principal objective of this paper is to present the updated version of MISTRA-v9.0, we believe this presentation is fully suited. Conversely, with over 25 papers published with MISTRA, a more extensive summary of the conclusions of each study would be beyond the scope of our work. Yet, we expanded the conclusion of the paper to give a summary of the model uses and potential.

My own work is cited wrongly (p.3, l.63): One of my publications with Roland deals with organic surface coatings on sea salt aerosols (this is not mentioned at all) but in the manuscript both citations (Smoydzin and von Glasow, 2007 and 2009) refer to chemistry over the Dead Sea. In addition, I did not implement an "ocean model" into MISTRA; I wrote a code making it possible to calculate chemistry in a liquid medium (i.e. the Dead Sea) and to calculate air-sea exchange of gas phase species explicitly!

Thanks you for pointing this out. We have revised the text in the manuscript. The sentences now reads:

*MISTRA was used to investigate the influence of organic coating at the surface of sea salt particles over boundary layer chemistry, and especially on bromine and chlorine chemistry in the aqueous phase (Smoydzin and von Glasow, 2007).* and:

*MISTRA was also used to simulate the boundary layer chemistry over the Dead Sea after implementing a calculation of chemistry in this specific liquid medium and an explicit calculation of sea-air gas exchanges (Smoydzin and von Glasow, 2009).*

Calling Susanne Pechtl's work "an improvement of iodine chemistry" (p.7, l. 167) is - politely spoken - an understatement.

She developed a completely new aqueous phase iodine chemistry mechanism coupled to the gas phase (and the existing chemistry scheme) which was unique and new in atmospheric chemistry research - and which is an essential and outstanding part of MISTRA. In addition, she was the first who investigated the nucleation potential of iodine species and wrote this part of the code in MISTRA which the authors now want to make public.

We agree that the work by Susanne Pechtl is an outstanding part of MISTRA. Please note that her work is also described earlier in the manuscript as follows (p.2-3, l.55-56): "A major improvement was the introduction of a module for aerosol nucleation [...]"

We revised text to emphasise the importance and novelty of the work. It now reads: *A major development was the introduction of a module for aerosol nucleation which significantly improved the iodine chemistry (Pechtl et al., 2006, 2007).*

After the comment of R2, we also added a subsection (2.3.7) to give an overview of the nucleation module.

Regarding the open-source release of the nucleation code, we contacted Susanne

Pechtl and she agreed for this.

Roberto Sommariva wrote a comment himself. He added a substantial part of code to MISTRA and must be offered co-authorship of the manuscript.

As stated in the manuscript, Roberto Sommariva updated the gas phase mechanism in MISTRA. This update of the chemical mechanism was published in Sommariva and von Glasow (2012). This work is already public since the tables of reactions and rate constants are provided in the appendix of Sommariva and von Glasow (2012). We therefore feel citation is an appropriate recognition of that work. We contacted Roberto Sommariva to clarify if he wrote any unattributed part of the code but have to date received no response.

Matthias Piot significantly changed the MISTRA code to apply the model at Arctic conditions. This part of the model development deserves from my point of view more credit than just a citation without any further explanation of this work (neither a co-authorship).

The developments implemented by Matthias Piot in MISTRA are not part of MISTRA-v9.0. Similarly, Linda Smoydzin's developments related to the Dead Sea special case are not part of MISTRA-v9.0. Both their contributions were indeed kept separated in special versions of MISTRA (see the changelog in the model manual).

I am sure, a careful review of the work done by Roland and his co-workers would reveal other code contributors.

In our work, we paid great attention and significant efforts to document the code. We added headers in most (if not all) routines including the author name each time we could get this information. Following this review, we also added a CREDITS file in the Github repository, listing all co-authors of published papers.

A few comments following the review by Rolf Sander:

Rolf suggests to call MISTRA a "tropospheric model" instead of "atmospheric model". Though, this expression is even more wrong. MISTRA (the 1d column version) is a model of the atmospheric boundary layer. It cannot be used for studying chemistry in a column reaching from the surface into the free troposphere or even up to the tropopause as the upper boundary conditions are not suitable for such an application (from a physical/numerical point of view).

We agree that "tropospheric" would not be suited.

After R2 and Rolf Sander's comments, we revised the title to: *"A description of the first open source community release of MISTRA-v9.0: a 0D/1D atmospheric boundary layer chemistry model"*.

This fact answers also one of his questions: "... does it mean that there are not aerosols above clouds?" If (boundary layer!) clouds are simulated, they usually reach to the top of the boundary layer, thus to the top/upper boundary of the column model.

We agree with you, except the column model in MISTRA extends higher than the top of the simulated BL.

Rolf further suggests to compare MISTRA with 0D box models: At first, it should be clearly pointed out, that MISTRA can be used both, as a box model (a comparison with CAABA/MECCA might be obvious) and a column model (which is rather unique).

Actually this was already highlighted in several places:

- p.2 1.34-35: "MISTRA-v9.0 also includes a box-model configuration, which can be adapted for atmospheric simulation chamber applications."
- p.3 1.58-60: "[...] including alternative model configurations where the chemistry was computed in a zero-dimension (0D) atmospheric box mode"
- p.13 Table 1 (code switches to use the box-model mode)
- Section 4.3: comparison with a previous study using the box-model model

We further stressed this by rephrasing the first abstract sentence:

*We present MISTRA-v9.0, a one dimensional (1D) atmospheric chemistry model.*  
which now reads:

*We present MISTRA-v9.0, a one dimensional (1D) and box (0D) atmospheric chemistry model.*

As mentioned above, a more detailed description of the possible scientific applications of MISTRA (marine halogen chemistry in coastal regions, volcanoes, Arctic applications) would also be desirable as well a description of typical model setups (e.g. using the column or box in a pseudo-Lagrangian way as done in many studies discussed in the MISTRA publications).

Following your comment and a comment by R2, we extended the Conclusion to summarise a few applications of MISTRA, developed in previous publications.

A minor comment:

There is a typo in the reference of Joyce et. al (p.31, l.510)

Thank you for your careful reading, we corrected the chemical expression which now displays "NO<sub>x</sub>" instead of " $\text{NO}_x$ ".

## References

Sommariva, R. and von Glasow, R.: Multiphase halogen chemistry in the tropical Atlantic Ocean, *Environmental Science & Technology*, 46, 10 429–10 437, <https://doi.org/10.1021/es300209f>, 2012.