CHIMERE-2017 : from urban to hemispheric chemistry-transport modeling

by S. Mailler et al.

Answer to Anonymous Reviewer 2

Please note that the title of the paper has been updated to CHIMERE-2017 instead of CHIMERE-2016 since a new model version has been issued, with only bugfixes from the 2016 version. All the simulations have been redone with this corrected version, which does not bring any change in the discussion since the changes are only small bugfixes.

We would like to thank Reviewer 1 for accepting to review this paper, and for his/her useful remarks.

Below are, in blue, the comments and requests by Reviewer 1, in black our answers, and in green the description of the corresponding changes that have been brought to the Manuscript, when relevant.

General Comments.

The manuscript introduces the new version of the CHIMERE chemical transport model. The text is rather long and requires an English proofreading.

OK, we have performed a proof-reading of the article to try improving the language level and smooth out the differences between the style of the different coauthors. Also, reviewer 1 provided numerous improvements in the quality of language, which were very useful.

Also, providing examples and evaluations with observational data of several new model features will make the paper further compelling.

In our view, this manuscript is a model description manuscript more than model evaluation, since a number of studies already use the CHIMERE model and compare it to observations and to other comparable models, giving to the interested users a detailes view of the performance of the model depending on the species, the resolution, etc. We added some information in this sense in the revised version, including more references to detailed evaluation papers such as Terrenoire (2015) or Bessagnet (2016) . Even though these papers use earlier versions of the model, the model performance in its "classical" regional configuration only evolves smoothly with time even when lots of new developments are included, this is also the case between the described version and earlier versions that have been thoroughly evaluated. Therefore, the focus in this paper is not put on evaluating a strong increase in model performance, which is not the case (the evolution of modelling scores from one version to the next is slow and smooth), but a change in the scope of the model, including more processes, and extending the capabilities in terms of domain size to the hemispheric scale. This precision of the scope of the manuscript can be found in the introduction of the revised paper, p. 2, l. 29-46.

Besides the questions listed below, I recommend to be added to text:
1) A table of variables presented in text,
2) A table describing all physical input variables that are needed from a meteorological model (as WRF or IFS/ECMWF) to drive a simulation with this version of CHIMERE.

For the CHIMERE model, all variables are already cited and described in [Menut et al., 2013].
A table of all the variables that must/can be read from the Meteorological model is now provided in the

revised version (Table 1).

Questions/Comments

Pag 2, abstract, lines 4-10 It seems that there is a mix-up be-tween the words ‘scales’ and ‘domain sizes’ . The authors should refer to scale as the smallest eddy resolved by the model and not mix with the size of the computational grid used to simulated certain phenomena. In this sense, stating that CHIMERE-2016 can be applied at any scale seems to be unsuitable. I invite the authors to rephrase those sentences.

There is maybe a problem of vocabulary in different communities here. For the word “scale” as understood by the Reviewer, we would tend to use “resolution” or “grid spacing”. Due to this remark, we have looked for the use of “scale” as we mean it in the article, finding many example that seem to comfort the use of “scale” to actually mean “domain extension”, as we understand it:
“Hemispheric-scale modelling of Sulphate and Black Carbon and their Direct Radiative Effects” (1998, Book chapter by Alf Kirkevåg and Øyvind Seland)
“Around the world in 17 days - hemispheric-scale transport of forest fire smoke from Russia in May 2003” (Damoah et al., Atmos. Chem. Phys, 2004)
This, and the very widespread use of “regional scale”, “urban scale”, not to mean that the smallest eddy resolved by the model has the scale of a urban area, or a region, but that the whole simulation domain has this size, seems to us the most common way to understand “scale” in this context. See, e.g., “Impact of model grid spacing on regional- and urban- scale air quality predictions of organic aerosol.”, Stroud et al., 2011, Atmos. Chem. Phys., who clearly use “scale” to specify the domain extension, and another notion, “grid spacing”, which is actually equivalent to the smallest resolved eddy - speaking of a chemistry-transport model, whether eddies at this scale are resolved or not depends not on the model itself but on the meteorological data used to force the model. Therefore, as the use of “scale” the way we understand it seems not to be uncommon in our community, and replacing it by “domain size” or an other similar formulation would make many formulations more tedious, we wish to maintain this use of the world scale.

However, to avoid any possible misunderstanding by the readers due to the various possible meaning of the world “scale”, we included the following sentence in the Introduction of the paper in order to (hopefully) lift any ambiguity, and also to bring useful information to the readers of this study:
“The typical resolution (grid-spacing) of the simulation domains range from about 4~km for urban-scale domains to about 50km for regional-scale domains (Markakis et al., 2015, Valari et al., 2008).” (p. 1, l. 49-51)

Pag 2, Introduction State clearly the class of atmospheric-chemistry models which CHIMERE-2016 fits. Is it a coupled online atmospheric-meteorological model? If yes, does it include feedbacks between atmospheric composition and the model dynamics?
Offline model. The following statement has been added :
“CHIMERE-2016 is an offline chemistry-transport model, meaning that it needs to be provided with input meteorological fields, and does not implement any feedback of atmospheric chemistry on atmospheric dynamics.” (p. 2, l. 76-80)

How does it compare with other state-of-the-art models like WRF-Chem and COSMO-ART?

As stated above, CHIMERE-2016 is an offline model, so comparison with WRF-CHEM and COSMO-ART is not relevant. This being said, the question of how CHIMERE compares with similar models is

of interest. For that, the reader is now referred to publications from recent intercomparison exercises in which CHIMERE has participated: AQMEII, Eurodelta I and III, CityDelta etc.. This paragraph is in the introduction of the revised manuscript (p. 2, l. 24-49). The interested reader is referred to these publication who detail the characteristics of each of the participating models for many atmospheric trace components.

Pag 3, line 5 State clearly the means of 'CHIMERE core' . Did you say 'dynamic core'?

The notion of "core" for a Chemistry-transport model is actually not clearly defined, and we suppressed it from the manuscript. We initially meant it as the parallelized part of the model (contrary to preprocessors and I/O which was not parallelized), but this is more internal jargon than a recognized notion. In some other parts of the paper, we also removed this ambiguous notion of "core". This statement has been changed as follows (p. 3, l. 11-16):

"Several technical changes were made in the CHIMERE code to improve code scalability: these changes regard the parallelization of many preprocessors into the parallelized section of the model, along with improvement of the parallelization strategy for some parts of the model that were already parallelized in order to improve code scalability."

Page 3, line 20. The expression master/slaves are more common in this context.

OK, we performed this change throughout the paper.

Page 4, lines 1 – 3. In the new version, clarify if the model output is split into several files (each slave writes its model solution in a particular file) or if each slave writes its own sub-domain but in a single file, which comprises the entire domain.

This precision has been added :

Each slave process writes its own sub-domain into a single output netcdf file common to all slaves (p. 3, l. 67-71).

Page 7, Line 20 Include a brief description of the numerical properties of the advection scheme applied in this chimere version to transport scalars.
These precisions have been added a bit earlier than suggested by the Reviewer, because they did not need to be changed for the new model version. The precisions are brought as follows:

In CHIMERE-2017 as in earlier versions, the user can choose between three different options for horizontal transport schemes, namely the basic upwind scheme, the slope-limited Van Leer scheme (Van Leer 1979), and the Piecewise-parabolic method (Collella and Woodward 1984), all of which are examined in the CHIMERE model in lo2009}. Thes three schemes are designed to estimate the trace species concentration at grid cell interfaces in order to convert the mass flux of total air through cell boundaries into mass fluxes for each of the model species through these boundaries. While the implementation of these schemes has needed no change in building the present model version, the estimate of the atmospheric mass flux between neighbouring model grid cells has been revised by switching to a new coordinate system in order to lift model limitations concerning the geographic poles and the date-change lines. These three schemes are designed to be monotonous (because they include the use of slope-limiting algorithms, except the Upwind scheme which does not need the use of such

algorithm), and mass-conservative because of their flux formulation. (from p. 3, l. 87)

Page 8, section 3.1 The new version aims to simulate tracer transport on continental/hemispheric scales with the model top at 200hPa. How the organized vertical transport of pollutants associated with convective and moist plumes are handled in this configuration?

Vertical transport due to deep convection can be activated by the user. If so, the mass fluxes associated to deep convection are estimated using the Tiedke (1989) scheme, and taking into account the fluxes for each model species in the vertical transport and mixing scheme. This is now mentioned in the revised version.

The following sentence has been added :
"Vertical transport on this mesh can be calculated using either a slope-limited Van Leer scheme (Van Leer 1979) or a upwind scheme, depending on user's choice, also taking into account turbulent mixing and, optionally, deep-convection fluxes, following the Tiedke (1989) formulation as described in Menut et al. (2013)."

Page 16, section 5. Describe the numerical solver of the chemical mechanism applied in this model version.

This was not described in the first version of the Manuscript because the solver is the same as in earlier model version. In the revised version of the manuscript, we added the following text :
"As for earlier model versions, the stiff system of partial differential equations resulting from the chemical mechanism is based on the application of a Gauss–Seidel iteration scheme to the 2-step implicit backward differentiation formula, adapted from the algorithm proposed by [Verwer, 1994] More details on this method can be found in Menut (2013)." (p. 6, l. 74-79)

Page 28, line 12 The emission configuration does not agree with the general observed 'umbrela' shape of the volcanic plume. Page 29, Section 7.4

We agree that the volume and distribution of the volcanic emissions is highly uncertain, in terms of emitted mass, vertical profile and deduced optical properties. But the goal of this new experiment was mainly to evaluate the model ability to correctly reproduce long-range transport with the new configuration of the hemispheric model grid.

The simulation outputs discussion lack comparison with observational data. It would be very instructive for the readers to perceive the fidelity of the model transport and AOD simulations.

It is true that comparison to observational data is missing. However, making a comparison with observational data would require a better input regarding volcanic emissions, which we are not able to do at this point. As an example, the parameter m_{63} quantifying the proportion of fine ash / total ash, is highly uncertain, as well as the total ash quantities emitted, etc.

Page 32, Conclusions. Line 16: Is it true that this version 'has the ability to include all types of emissions'

We agree with the Reviewer that this statement is of course exagerated since some kinds of emissions will always be missing in any model. In the case of CHIMERE, one could mention, for example, the

lightning emission, oceanic DMS emissions, among others. So, we just removed this statement, since the next sentences describe objectively which kinds of emissions have been added since previous model version, which gives more objective and useful information.