Article gmd-2024-20: The CHIMERE chemistry-transport model v2023r1 L.Menut et al.

1 Answer to the Editor

Dear Editor and Reviewers,

Thanks for your interesting comments. We have responded to all the comments made by the three reviewers. Most of the requests resulted in changes in the manuscript. Many of the reviewers' comments concern details of added processes and associated results. These results and discussions are generally contained in the publications dedicated to these processes. This article is rather a concatenation of the changes made in the CHIMERE model to synthesize all that is new between two versions. For details and scientific results, please refer to the individual publications (often in ACP and GMD).

Following the rules of Copernicus, the repository of the model was changed and is now on Zenodo.

Best regards, Laurent Menut April 17, 2024

2 Answers to the Reviewer 1

This paper describes the updated version of the regional chemical transport model CHIMERE. Details of various improvements are introduced. It is shown that the new version has better model performance and lesser computational demand.

This manuscript seems to me as a technical document of the model. I think following information is important as a scientific paper describing the new model.

 \rightarrow We acknowledge the Reviewer #1 for the positive comments. In the revised version, we added several explanations to be more scientific than technical in the model decription.

• What were the problems in the previous version?

 \rightarrow The main problem was numerical and was the management of the input/output. It is why the change to the new XIOS code helps a lot for the output management and calculation time.

• How were the problems in the previous version solved in the new version?

 \rightarrow Computation time is not really a problem. It is a constraint, especially for operational users. The problems that have been solved are mainly parameterizations improvements and updates, such as the new formulation of turbulent diagnostics, consideration of interactions between emissions, such as fires on dust and biogenic emissions. It improves the results even though the previous version didn't really have any problems. An improvement for the code stability was the change of the Isorropia code version (an external model embedded in CHIMERE and written in an old Fortran).

• How did the improvements in the new version contributed to better performance?

 \rightarrow There are two types of performance. Firstly, computation time, which has been reduced mainly by the use of XIOS. Secondly, the results of comparisons with observations, to which the improved parameterizations described in the manuscript have contributed.

• We hope to know which improvements contributed the most to the better model performance shown in Section 8.

 \rightarrow Improvements are a whole. There is no single improvement that has really changed the scores. Improvements also vary according to species, region and time of year. There can not be a single answer.

• I think the pollen modeling is one of new important improvements. How about the performance of this pollen modeling?

 \rightarrow The pollen modeling in this model version is not only an improvement but also a novelty. The pollen model is daily used in the framework of the CAMS daily forecast and scores are calculated every day. In addition, and for the development of the release scheme, performances are already published in (Menut et al., 2021). We don't repeat these scores as the goal in this paper is to present all novelties in the distributed CHIMERE model version. Note that until 2023, the pollen modelling was implemented in a specific model version, not distributed, and only used for forecast.

Specific comments:

• Figure 1

I think this figure needs to be improved. Everything is not written by English words. I cannot understand some (computational?) words. The boxes are connected by allows. Some boxes just show the name of the routine, and others describe their roles (?). I do not understand why they are separated by boxes and connected by allows, and what their colors represent. And I do not understand what the allows within the two of the three boxes represent. I think the data transfer between CHIMERE and WRF is not well shown in this figure. I cannot imagine "the XIOS routine is called to write the results on disc" in this figure.

 \rightarrow All words corresponded to the routines names of the code, but we changed that to have real words. In addition, the caption was changed and now explain the colors, the boxes and the arrows. Note: we assume "arrows" in place of "allows".

• P3L13-15

What does "at least two are recommended (not recommanded)" mean? These three levels should be well represented in Figure 1.

 \rightarrow The complete sentence is "Gauss-Seidel iterations (at least two are recommended)" means that at least two iterations of the Gauss-Seidel algorithm are recommended. The three levels are clearly identified in the Figure 1 with "physical time-step", "chemical time-step" and "loop over Gaudd Seidel".

• Figure 2

Uppercase and lowercase letters (e.g. XIOS and xios) should be consistent among the figure, its title, and the main text.

\rightarrow Yes, OK, corrected.

• P5L5-6

Does "v2020r3" include full outputs with nc4? What else contributed to the faster computation?

 \rightarrow Yes, the full output with nc4 was the default way to write results in all CHIMERE version before this one, the v2023r1. The faster compitation is mainly due to this management of input/output. Other improvements have been achieved by modularizing the code and optimizing modules.

• P5L15-16

Is it impossible to share processors between CHIMERE and WRF?

 $\rightarrow\,$ Absolutly not, there are two different models.



Figure 1: Organization chart of the CHIMERE v2023r1 version. The first yellow boxes present the initialization phase: static namelist and initial values are selected only on one processor (inichimere). Second, on all processors, the main fields are initialized for the first hour: boundary conditions, meteorology and concentrations of all chemical species (iniworker). Finally, the main temporal loop is performed (worker). It includes an hourly time-step (in offline mode), then a physical, then a chemical time-step. Depending on the 'offline' or 'online' mode, some exchanges are performed between the WRF model and the CHIMERE model.

• P6L22-25

I think the size here means the aerosol size. It should be shown.

 $\rightarrow\,$ Yes, that is right. In place of a figure (just a special case), more explanations are provided in the text.

<u>dmin</u> and <u>dmax</u> enable the definition of the limits of the aerosol size distribution. <u>dmin</u> and <u>dmax</u> are the size of the first interval of the first bin and the last interval of the last bin respectively. These limits are the same for all aerosols. Values of 0.01 μ m and 40 μ m are recommended.

• P7L6-8

Readers may not understand these sentences if they do not know "operator splitting", "twostep", and "Melchior 2".

 $\rightarrow~$ Yes, OK. The following explanations and references are added.

Note that, in this version, the SSH-aerosol package is currently compatible only with the *operator* splitting option and not with the *twostep* option. *operator splitting* and *twostep* are two different ways to integrate the processes impact on chemical concentrations and are explained in (Menut et al., 2013). For consistency between the SOA compounds in gas and particle phases, the Melchior 2 chemical mechanism is recommended. In this model version, three different chemical mechanisms for gases are available: Melchior 1, Melchior 2 (the simplified version of Melchior 1) and SAPRC, as described in (Mailler et al., 2017)

• P7L22

I do not understand a relationship between these four modifications and the Després and Lagoutière

scheme described in the previous paragraph. In addition, these four schemes are relatively old. What is a motivation of these four modifications?

 \rightarrow There is no link between the four modifications. It is just four possible transport schemes. The paragraph was reformulated to be more clear such as:

The advection schemes have been corrected, updated and new schemes were added as a user's choice. The user can select different schemes for the horizontal and the vertical transport, the two being calculated separately.

In the vertical direction, the Després and Lagoutière (1999) has been implemented. As described in Lachatre et al. (2020), two options are now available for the representation of vertical velocity: either diagnose it from the horizontal wind components, as it was historically done in CHIMERE, or use the vertical wind speed provided by the meteorological model. Lachatre et al. (2022) has shown that reducing numerical diffusion by using the Després and Lagoutière (1999) advection scheme and using the vertical wind speed w from the meteorological model ($is_diagwinw = .false.$ in chimere.par) also modifies the chemical processes in thin plumes: due to the nonlinearity of tropospheric chemistry, diluting a plume over a larger volume changes not only its distribution, but also the kinetics and relative importance of the chemical processes.

For horizontal advection, five different schemes are available. First, the simple first-order advection scheme of Godunov and Bohachevsky (1959). It is the faster scheme and may be used in case of low resolution. But it is also diffusive and is not recommended in case of thin plumes studies. Second, the Van Leer scheme Van Leer (1977). Third, the PPM scheme (Colella and Woodward (1984)) has been revised and is now faster than the previous implementation. Fourth, the Walcek (2000) advection scheme has been implemented. Finally, the PPM+W advection scheme has been implemented (Mailler et al., 2023). In an academic framework, Mailler et al. (2023) have shown that the PPM+W performs best among these schemes in terms of accuracy, while the Van Leer and Walcek schemes are computationnally cheaper. The PPM+W scheme has a computational cost similar to PPM.

• P7L23 and L26

Implementation of the Walcek (2000) advection scheme is duplicated.

 \rightarrow Yes, it is corrected with the new paragraph.

• P8L11

How are products from tracers due to chemical reactions treated in the model?

 \rightarrow In this case, the word "tracer" is applied due to the emissions type but not the chemical type of the pollutant. It means that a chemical species included in the chemical mechanism is calculated as all other chemical species. The term tracer is used only because this species is emitted at a given point and for a limited time.

• P9L3

"between" is duplicated.

 \rightarrow OK corrected.

• P9L18-26

Is new CHIMERE compatible only with the USGS landuse? How about MODIS or other landuses which can be selected in WRF?

 \rightarrow It is possible to use also these landuses since CHIMERE only needs WRF tables such as "green-frac". In case of other landuses, it is necessary to update the Table descried in section 4 and Appendix.

• P10L6 What is Q0? \rightarrow The surface sensible heat flux. It was added in the manuscript.

• P10L10-11

"10m wind speed, the one of WRF being dependent on the boundary layer height scheme and not always satisfying". What does this mean?

 \rightarrow It means that depending on the boundary layer scheme used in WRF (several are available), the diagnostic of the 10m wind speed may be different. It is a typical problem of WRF, not CHIMERE. But to avoid an uncontrolled variability due to this choice, we can diagnose this variable directly in CHIMERE, ensuring to the user to always calculate it with the same method.

• P12L7

Is P0=10000 Pa correct?

 \rightarrow Yes, correct. It is the standard way in meteorological model to estimate vertical pressure.

• P13L7-8

"the multiplication is replaced in the calculation by its result 7.2868 1022" I cannot understand it.

 $\rightarrow~$ Ok. In place of the "multiplication", this is "this ratio..."

• P13L15

What is "q"?

 $\rightarrow~q$ is the specific humidity. It was added in the text.

• P14L12 and Figure 3

The Charnock constant is set to be 0.018. Why are roughness lengths calculated for three different Charnock constants displayed in Figure 3?

 \rightarrow The Charnock "constant" has different values depending on studies and authors. These values are different depending on the field experiments performed to estimate it. An example and a reference were adde in the text.

... with k=0.41, the Von Karman constant, $\nu=1.5 \ 10^{-5} \ m^2 \ s^{-1}$, the kinematic visocosity, u_n the wind speed at height z (here z=10m), $\alpha_M=0.11$ and $\alpha_{ch}=0.018$, the Charnock constant. But this constant varies following studies and ways to determine it as, for example, explained in (Feng et al., 2021). This roughness length calculated for three different Charnock constants...

• Section 5.4

Has this urban correction been newly implemented in this version of CHIMERE? What is the motivation? Is there any reference showing the default values used in this study?

 \rightarrow No, it is not new. It was implemented in all CHIMERE version. The way to use was changed, is now more easy because parameters are in the namelist and not in the code. It is why it is presented here.

• P16L15-17

Which equation was finally used to calculate z0h?

 $\rightarrow~$ Yes, the sentence was not clear and is reworded as:

 z_{0m} is the momentum roughness length and is tabulated. For the heat roughness length, several formulations and uses exist. For example, Beljaars and Holtslag (1991) use $z_{0h} = z_{0m}/10$. In Jiménez et al. (2012), all equations are using only " z_0 " without distinction between momentum and heat. We thus apply here the relation $z_{0h} = z_{0m}$, because the use of a lower z_{0h} gives too low surface sensible heat flux. The stability functions $\psi_m(z/L)$ (for momentum) and $\psi_h(z/L)$ (for heat) are calculated using the modified formulation of Jiménez et al. (2012) such as:

• Table 4

These values are also shown in Table 3.

 \rightarrow Yes, correct. The Table 4 was removed and the text uses now the Table 3 as reference.

• Section 6.3.2

What kind of input information is necessary to consider influences of fire? I suppose influences of fire become evident only after fires. That means information of dates when fires occur is required. In addition, burned vegetation may recover after a certain period. How is such recover of vegetation modeled? I am curious how much this modeling on impacts of fires realizes improvements in performance.

 \rightarrow This is an interesting question, but already extensively discussed in (Menut et al., 2022). Trying not to repeat what is already in the article, we have added a few details to best answer this question.

\rightarrow In place of:

A link is added between the vegetation fires emission and the mineral dust emission (Menut et al., 2022) depending if ifire2lai flag is activated or not. This link is only valid using the CAMS vegetation fires emissions, because some specific information (such as the burnt area surface) are needed and only the CAMSfires program, distributed with CHIMERE, has received this development.

 \rightarrow The text is now:

Vegetation fires emission are parameterized using the emifiresCAMS program, reading the CAMS daily data. For each day, the data provide informations on the chemical species flux and on Fire Radiative Power. Based on hypothesis, (Menut et al., 2022), the burnt area is deduced from this FRP value. The burnt area surface is cumulated from a starting date, then considered as surface having lost its vegetation. In this model version, the surface recovery is not taken into account but it is considered that this recovery can take years, whereas we only simulate a few months just during and after the fires. The informations needed are only valid using the CAMS vegetation fires emissions, because the specific information of the burnt area surface was specifically developed developed in the CHIMERE emifiresCAMS program.

3 Answers to the Reviewer 2

This paper provides a technical description of the latest CHIMERE model updates and developments, including a comparison of the new and old model version against a number of observational datasets. The information provided here is useful for both the CHIMERE community and other chemistry-transport modeling groups, making it suited for publication in GMD.

While the general structure of the paper is good, the text should be be expanded in places to add depth and clarity to the described approaches. The below comments follow the chronological order of the manuscript and include both specific and general comments (bold), hopefully avoiding points already raised by the first reviewer. As a general comment, please make sure that acronyms are appropriately defined throughout the text. For the revised manuscript it would also be helpful if the line numbering was not reset for each (sub-)subsection.

 \rightarrow We thank the Reviewer for the helpful comments. They are all taken into account. The way to initialize the line numbers every new page is an internal choice of Copernicus with their Latex package. However, we changed their file by removing the command \setpagewiselinenumbers in the line of the copernicus.cls class file and we hope it is OK now.

• Line 10 page 4: What is meant by "the chimere ranks"?

 \rightarrow The CHIMERE ranks refer to the CHIMERE processes running in parallel using the MPI library. The "rank" is commonly used as an identifier of the process within the MPI communicator.

• Line 13 page 4: Please define "xml files".

 \rightarrow XML is a language. The Wikipedia page (https://en.wikipedia.org/wiki/XML) indicates: "Extensible Markup Language (XML) is a markup language and file format for storing, transmitting, and reconstructing arbitrary data. It defines a set of rules for encoding documents in a format that is both human-readable and machine-readable. The World Wide Web Consortium's XML 1.0 Specification of 1998 and several other related specifications all of them free open standards-define XML." We are not sure it is necessary to add this in the article.

• Section 2.2 general comments: The increase in run-time of 69.4 % when using the nc4 system seems very high, considering that then around 1/3rd of the total CPU time is spent on writing outputs. Did the old system somehow always include all possible outputs? It would be useful to mention in the text to what extent the XIOS_full scenario corresponds to the outputs that users would have typically requested using the old system. If the old system was also configurable, a "nc4_slim" experiment should probably be added to Figure 2.

 \rightarrow About the possibility of a "nc4_slim": no, it is not possible since the change in this version is to add this flexibility and it was not existing in the previous version. About the definition of XIOS_full, it is already written in the manuscript: "the standard configurations that replicates the "nc4" output files to the letter (called "XIOS_full")..."

• Figure 2 also shows that v2020r3 was slower by ≈35 % due to things unrelated to I/O. Since this seems to be valid as a general conclusion, I think this should be mentioned/discussed in the text. Have there also been any experiments investigating the impact of model resolution on the performance gains, considering that, e.g., the time-step depends on the grid-size of the meteorology? The conclusion (Section 9) mentions that the computational cost of the model is 40 % less than previous versions, also for forecast runs. To my knowledge, the CHIMERE forecasts use a 10 km x 10 km horizontal grid, for which the I/O performance gains might have a different impact?

 \rightarrow It is not a problem of model resolution: to properly compare the model versions, we use the same configuration: domain, resolution and period. The knowledge of a forecast with 10 km resolution is related to CAMS? It is a particular case and CHIMERE is used with resolutions from 1km to 100km depending on the project, the region, the institute, including in forecast mode where tens of institutes are using the model with various configurations.

- Lastly, it would be helpful if a short description was added about why one would want to output maximum or minimum sub-hourly concentrations. Is it somehow relevant for comparisons to observations, or to how certain health metrics are defined?
 - \rightarrow The following text was added:

Adding the possibility of sub-hourly values is an advantage that can be used in a variety of situations. If the temporal gradients are very strong, it provides additional information on the temporal variability of a chemical species. This is important in terms of pollution, where the aim is to calculate whether thresholds have been exceeded. A high observed value will exceed a threshold, and only the model's sub-hourly variability can give a closer result.

- Page 5 Bullet point 2: Managing the optimal distribution of CPUs between the three different processes seems like a non-trivial task for users. Could a short description of the default, or recommended, resource splits be included?
 - \rightarrow Yes, examples were added in the text, such as:

For example, for a cluster core of 64 processors (classical configuration), it is recommended to select 15 for WRF, 45 for CHIMERE and 2 for XIOS.

- Page 6 Bullet point 12: Could it be clarified if (and how) these limits impact the number of aerosol bin sizes?
 - \rightarrow The values of the limits of the interval have nothing to do with the number of intervals.
- Page 7 bullet point 2: Please define PPM. Is the PPM+W scheme somehow a combination of the PPM scheme and that of Walcek (2000)?

 $\rightarrow\,$ PPM stands for Parabolic Piecewise Method. The complete paragraph was rewritten because unclear.

• Page 7 bullet point 5: Crudely put, if the simple first-order advection scheme is too diffusive for practical use, why is it included as an option? A short motivation on why one would nevertheless want to use this scheme would be helpful.

 \rightarrow The upwind scheme is diffusive but may be used without damage with a low resolution. It is the case for very large domain. For example this scheme may be useful for forecast and large domains, when you want quickly a realistic result. The following sentence was added:

It is the faster scheme and may be used in case of low resolution or forecast when results are expected soon. But it is also diffusive and is not recommended in case of thin plumes studies.

• Page 9 bullet point 5: Just a suggestion, but rephrasing "multiplicative spread" to "geometric standard deviation" would make sense to me when describing aerosol log-normal distributions.

 \rightarrow Yes, OK, corrected.

• Line 19 page 9: Please define USGS.

 \rightarrow Yes, it is: "... for the United States Geological Survey (USGS) landuse."

• Line 22 page 9: I would suggest adding information about the Charnock (1995) ocean surface roughness calculations Table A1 (e.g., by replacing the 0 entries with "Charnock (1995)", or by adding a footnote). It would also be helpful if the text here refers to Section 5.2, where the Charnock (1995) methodology is discussed in more detail.

 \rightarrow Yes, the calculation is explained in section 5.2 and a reference was added.

• Page 10 bullet point 2: Could the upgrade to a more recent scheme be specified in more detail, or somehow referred to? Currently it reads like a rather vague statement. A short description of how the vertical and horizontal resolution of the CHIMERE grid is treated with respect to that of the input meteorology would also be helpful (here or elsewhere in the text).

 $\rightarrow~$ It is not a vague statement, this paragraph is just a summary of what is detailed below in this section.

• Page 10 bullet point 4: What is meant with the WRF 10-meter wind speed not always being satisfying? How was this diagnosed?

 \rightarrow There is no reference for that. We just read the code and see how it is diagnosed. It depends on the boundary layer scheme used in WRF. And it is often simple and not taking into account the atmospheric stability. But there is no publication about that.

• Table 3: At first glance, it is unclear what the "High cloud option for attenuation" parameter means, even though this is later discussed in Section 5.3. In Table 3 it currently reads as if it is an option that can be turned on or off. Perhaps the wording could be changed to "High cloud attenuation factor"?

 \rightarrow Yes, correct and it was corrected.

• Line 5 page 13: Eq. 9 writes the density in molecules per cubic centimeters, but the equation seems to be for molecules per cubic meter, as is also written in the text above.

 \rightarrow Yes, correct and it was corrected.

• Line 7 page 13: It would be helpful to specify that "the multiplication" refers to the calculation of air density (in molecules per cubic meter) from the atmospheric pressure and temperature fields. Currently it reads as if the resulting 7.2868e22 factor does not include the Ra = 287.04 J K-1 kg-1 term from Eq. 8.

 \rightarrow Yes, the equation was simplified to be more readable.

• Table 3: The relative humidity limit is set to 1.2 (rhmax), even though the table defines the unit to be in the range of 0 to 1. How should this be understood? Does rhmax also apply to the thermodynamic gas-aerosol calculations and the (coupled) WRF cloud microphysics schemes?

 \rightarrow Yes, corrected. No, this rhmax is only valid for the turbulence calculation.

• Section 5.4 general comment: The urban correction factors for wind speed and surface sensible heat flux seem like an important part of the model, which I think warrants a more detailed discussion and motivation. For example, which observed trends are being referred to, what are the implications for simulations across cities (i.e., how much do the results change), how representative are the parameter choices for other cities, etc. Is this correction factor normally applied only for urban-scale modeling? And if so, is it independent of model resolution?

 \rightarrow Some details were added in the text. This option exists in CHIMERE since the first model version. For the impact of the model resolution, it is zero since "The factor for the wind speed is equal to the proportion of urban surface in the cell multiplied..." The following text was added:

The values correspond to a concatenation of wind and temperature observations found in numerous publications on urban meteorology, such as those since (Oke, 1982), (Calbo et al., 1998), (Arnfield, 2003), among others.

• Section 5.5 general comment: While a detailed overview of the turbulence variable calculations is useful, it is not clear how much of section 5.5 is a more detailed description of the turbulence calculations described in Menut et al. (2013) versus a description of new model updates. Is the iterative process by itself new?

 \rightarrow The complete module was rewritten. Then it is not comparable with the one described in Menut et al. (2013) and it is why it is presented as a whole. Yes, the iterative process is new compared to the previous versions.

• Line 4 page 21: What does the sub-grid variability option refer to? The option to turn on the urban correction described in Section 5.4? If so, does this then imply that the urban correction factors are applied only to certain GNFR activity sectors, as seems to be suggested here?

 \rightarrow No, here it is the "emissions" section. The sub-grid scale variability is for anthropogenic emissions only. The urban correction was for the meteorology and is in another article section.

• Line 4 page 22: It would be useful if the densities and size distributions of each of the 5 pollen species are explicitly mentioned, for example in Table 6 or in Section 6.2.2. In section 6.2.2, it is also unclear if the diameter $Dp = 32 \ \mu m$ and density of 800 kg m-3 refers to grass, ragweed, or both. I agree with RC1 that the pollen updates represent a significant addition to the model, as is also evident from the detail in which the pollen implementation is discussed. Any kind of comparison or validation against observations, or even just a sensitivity comparison to see how the model results are changed, should therefore be included.

 \rightarrow In fact, there is no change in the model results because pollen species are completely different and independent. They thus have no impacts on the other species, gas or aerosols. It was added in the text. For the diameter and the density, the informations were added in Table 6. For examples and validation, it was already documented and the articles are better referenced. The following text was added:

This development comes in addition to the simulation of gases and aerosols: pollens are inert and there are no interactions with other pollutants. Model scores are therefore not modified if pollens are calculated. Additional details about this calculation in CHIMERE are presented in (Sofiev et al., 2015) (for birch) and (Menut et al., 2021) (for ragweed).

• Section 7.1 general comment: In parts of the manuscript, aerosols are described using their lognormal size modes (Section 3.2), whereas in other parts they are described using their size bins (Section 8.1). A brief discussion on the different aerosol treatments in the model would be useful, and how that affects the settling velocity calculations based on the equations for particles with a fixed diameter.

 \rightarrow There is here a confusion between emissions and aerosols representation during transport and chemistry. Aerosols are emitted in three modes but after are redistributed into *nbins* size bins. Details were added in the text to avoid confusion.

These three emitted modes are then distributed into the *nbins* size bins for chemistry and transport, as described in (Menut et al., 2013).

• Section 7.3 general comment: What is meant by the ISORROPIA module being more stable in the Fortran90 implementation? There are other CTMs still using the FORTRAN77 version, and it would be good to know what kind of instabilities were diagnosed using the CHIMERE model. For example, the GEOS-chem community described convergence problems which can lead to extreme non-linearities in the equilibrium solution (http://wiki.seas.harvard.edu/geoschem/index.php/ISORROPIA_II). Did the CHIMERE implementation impact any of this behavior? → Yes and we sent our modified code to GeosChem for an update. The unstability was just a model

crash without any reason.

• Line 4 page 33: On line 3 page 14 the current model top is said to be at 200 hPa, whereas here it is defined as 300 hPa. Was the default value changed from 200 to 300 specifically for the experiments in Section 8?

 \rightarrow line 3 page 14: "user's choice". Line 4 p. 33: the choice here is 300 hPa. It depends on the simulation the user wants to perform. For example, many operational forecast are using 500 hPa.

• Section 8 general comments: The horizontal resolution of 60 km x 60 km seems quite coarse considering that, for example, 0.25 x 0.25 degree (25 km x 25 km) ECMWF data was available for these simulations. Is the 60 km x 60 km grid representative of what a typical user would use?

 \rightarrow Yes, this is correct that fine resolution meteorological forcings are available. But this is not the main argument for a domain resolution definition. The key point is the cluster power and the running time. For a realistic simulation, knowing the computer and the computing time and over a large horizontal domain, the resolution has to be adapted.

• As another general comment, I think it is important to add at least some form of discussion surrounding the comparisons to observations. For example, for the offline WRF configuration, the ozone bias change from -11.2 % to -1.34 % and correlation coefficient change from 0.56 to 0.66 relative to EBAS surface measurements (Figure 5), strikes me as very large. Which part of the model updates could/would have caused such a big change? Some of these discussion points could then also be added to the conclusion in Section 9 (I think ozone or PM10 bias changes by 5 to 10 percent points should absolutely be mentioned in the conclusion).

 \rightarrow The section 8.2 is completely dedicated to the comparison to the observations. Note that the main goal of this article is to quantify the gain of the new model version. Studies with the model on real test case and analysis of atmospheric composition events are better performed in other publications (JGR, ACP etc.). In addition, it is not possible to disentangle all processes to extract one process for one change: this kind of model is complex and non-linear and all processes act together. The results therefore express the impact of all the improvements, and that's a fact. The good news is that developments are moving in the right direction, since all changes have led to improved results.

4 Answers to the Reviewer 3

The paper has been submitted as model description paper, and describes CHIMERE chemistry-transport model (CTM) v2023r1.

The paper provides an overview of a changelog for last decades, describes technical aspects of running model including the syntax of control files, used libraries, choices of configurable options, details of input data, classical equations used with slight variations in many other atmospheric models, descriptions of various modules and choices for them. At the end results of an evaluation of several 6 configurations (3 pairs of setups before and after the update) are shown. The main conclusion is that the new version is faster, more flexible and more accurate than the previous one.

The paper does not meet the GMD criteria for the model description paper:

"The papers should be detailed, complete, rigorous, and accessible to a wide community of geoscientists."

The paper touches too many aspects to give a description for in each of them that meets these criteria.

 \rightarrow We thank the Reviewer for the rules copy but we already know the Copernicus rules. For the many aspects, it's the principle of an article that generally introduces a new model. This is why we publish an article on a new model when the various parts have been validated and published. This makes it possible to produce a synthesis in which each part has already been evaluated by the scientific community, so all you have to do is read the references. It is not possible to publish a single article describing the development and validation of each part, given that a model like CHIMERE is multi-process.

The paper does not follow the required structure:

"The publication should consist of three parts: the main paper, a user manual, and the source code, ideally supported by some summary outputs from test case simulations"

 \rightarrow This structure is truly amazing, and if you look at the articles currently published, it is impossible to follow. There has never been a publication in GMD that included the documentation in extenso (CHIMERE's is 250 pages long) or the code (CHIMERE's is 100,000 lines long). But the documentation and code are properly referenced and fully accessible to readers.

CHIMERE is one of the leading European offline chemistry-transport models, so a publication on is of a major interest, therefore I suggest a major revision or "encourage to resubmit":

 \rightarrow We are going to answer all the questions below. This can be considered as 'major revision' even though this term usually represents a fundamental problem with a result. That is not what the review below says, which mostly describes problems of form or questions of unfamiliarity with the topic.

• move all the aspects of used formulations and technical implementations for different modules to the model description. Such documents are normally rather long and can accommodate for a necessary level of details. They can also be versioned and distributed together with the model.

 \rightarrow The full article is on the model description. The formulations and technical implementations are contained in the PDF documentation, freely available on the CHIMERE web site.

• ways to run the simulation, details of configuration namelists and guidelines to chose specific options, belong to the user manual

 \rightarrow Yes, and it is the case in our documentation. But here the configurations and example cases are given only to support the details given on model running time. Without specifying this, discussions of model running time are meaningless.

• the paper should give a concise and accessible description of the model, its modules and components and their interaction, and focus on several most important improvements in the new version and demonstration of their effect on the model performance. This way the above criteria can be met.

 \rightarrow Yes, we agree with remark: an article needs to be clear and concise. We think it is the purpose of our conclusion as: The new CHIMERE version called v2023r1 was presented in this article. It contains both new processes and new numerical tools. More precisely for the researchers, the pollen emissions are now distributed and can be used for any local studies in Europe, the turbulence and the transport were updated with more recent parameterizations and the impact of the fires on the surface was added. For the users performing long simulations or forecast, the integration of the XIOS model enables to have a faster model, with a computational cost 40% less than the previous version. It is also possible to easily manage the output, including the possibility to write sub-hourly fields such as the maximum of concentration during an hour.

4.1 General comments:

1. The manuscript is poorly written. Quite a few phrases have unclear meaning. It has to be heavily edited to become understandable by a wide community of geoscientists. I have highlighted few such phrases for the first page only (see minor comments), but the problem exists for the entire text.

 $\rightarrow~$ Thanks a lot for the comments. The manuscript was edited by all co-authors and is now more clear.

2. Introduction lists a lot of changes and updates, lists various modules, mechanisms and pieces of data provided with the model. Some table summarizing these changes would be of help, but bot in the introduction. Many of the modules are given with abbreviations and names etc without references. Each point there leaves more questions than gives answers.

 $\rightarrow\,$ All abbreviations are now explained and references were added. Note that CHIMERE is NOT an abbreviation.

3. Introduction does not specify what "CHIMERE v2023v1" actually is. Is it just a CTM code, a code bound with a specific emission datasets, a bunch of setups for several different applications? Does it include initial and boundary conditions for all possible use cases?

 \rightarrow OK, it is now better explained. CHIMERE is a chemistry transport model. It is distributed with additional codes to help users to prepare mandatory input data. But the article here is only related to the CTM.

4. The paper describes the new state of the model without describing the old state, which makes it difficult to understand what has been improved, why and how significant each improvement is. Some table summarizing these changes would be of help.

 $\rightarrow\,$ Everything in this article is new between the previous version v2020r3 and this version.

5. The paper attempts to cover all the changes to the model, effectively not covering anything in sufficient details. It would be beneficial to highlight few main changes, describe in details why they were needed, what has been changed to what, describe use cases when they bring the most improvement and illustrate the improvements due to them separately. To mention several: Urban correction, subgrid dust emission, effect of fires on ozone deposition and dust emission, several implementation for ragweed pollen etc. Does each of them improve the model performance? How much? Those interested in complete list and chronology of changes during last couple of decades should be referred to a changelog.

 \rightarrow As noted to the Referee #2, this model is complex and it is not possible to isolate processes one by one to describe a benefit or not. There's little point in making a chronological changelog, as the development team works in parallel on different aspects, each being more specialized in certain areas.

6. Specific keywords, data formats, namelist syntaxes, files, variables, classical equations used to diagnose meteorological parameters, implementations of specific schemes/modules, ways to organize subroutines etc. should be left to the model documentation, where they should be properly described.

 \rightarrow There is a lot in the model documentation (250 pages) and this article is already a very simplified and synthetic version of all changes made in the model since the last version.

7. The conclusions essentially say that the new version is faster, more accurate and more flexible. How does this information advances geoscientific model development in general?

 $\rightarrow\,$ Faster code means more simulations, or longer simulations with fewer errors because the code is more accurate.

4.2 Specific comments (1st page only):

- p1.15: "The impact of fires on wind speed, soil properties and LAI was added." Do fires affect the wind speed? → Yes. Details are given in the article.
- p1.17.: "..Europe with 60x60 km..." The model has been run as a part of a CAMS-REGIONAL ensemble with 10-km resolution for the whole Europe. The project makes a whole-year assimilated run at the same resolution. Why so coarse resolution for the evaluation of non-assimilated simulation?

 \rightarrow The CAMS domain called "whole Europe" by this Referee is smaller than the domain used here. With this resolution, we were able to perform many simulations for the validation (we performed tens of simulations to test all processes in many configurations). And we probably don't have the same computing resources as CAMS. Which puts us on the same level as most of the users of the model for which this article is intended.

- p1,l12: "models have proven their interest ..."
 - \rightarrow Changed to:

Regional deterministic models have proven their value for studies about climate change...

• p1.,113: "These models have to be accurate and efficient, with at the same time a good accuracy and a low computational time." Same message twice?

 \rightarrow Changed to:

These models have to be both accurate and with a low computational time.

• p1., 118: "the possibility to read emission fluxes from fires" Hopefully, "fluxes from fires" not "reading from fires". What makes these emission fluxes different from other emission fluxes?

 \rightarrow The chemical emissions from fires is a complete research topic. We can try to summarize this in a few words but it is difficult. We propose this sentence:

Version v2014 included, the possibility to read emission fluxes from fires, calculated using a specific model in pre-processing, reading daily satellite data of Fire Radiative Power and burnt areas and converting these informations in chemical species hourly fluxes by using additional informations as vegetation type and related fuel load for each.

• p1. 118: "the SAPRC chemical mechanism" Non-introduced abbreviation.

 \rightarrow It was corrected.

• p1.,119: ".. version included ... new datasets for the chemical boundary conditions" Does the model include a full datast needed to run it? Can it be used with other datasets?

 \rightarrow Yes, the model is distributed with several full datasets and it is the user's choice of use one of them or to build its own one.

- p1,l.20: What makes a hemispheric run so specific?
 - \rightarrow The following sentence was added:

Version v2017 (Mailler et al., 2017) added the possibility to use an hemispheric domain (and the way to manage the grid and the transports schemes), \dots

• p1,l.21: Fast-JX is not introduced properly. What is "resuspension scheme"?

 \rightarrow We have to keep in mind that this introduction is just an overview of was done in the previous version and is not intended to be exhaustive and very detailed on everything described. Fast-JX is a code name not an acronym. A resuspension scheme is the parametetrization for the resuspension of aerosols.

• p1,l.22: WRF abbreviation, no reference

 \rightarrow OK, it was corrected.

• p1,l.22: OASIS3-MCT abbreviation

 $\rightarrow\,$ The following explanation was added: OASIS: Ocean Atmosphere Sea Ice Soil and MCT: Model Coupling Toolkit

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