Replies to referee comments (RC1) on the scientific article "New Routine NLTE15μmCool-E v1.0 for Calculating the non-LTE CO_2 15 μm Cooling in GCMs of Earth's atmosphere" by A. Kutepov and A. Feofilov

Alexander Kutepov and Artem Feofilov

We would like to thank Reviewer 1 for his/her helpful comments and sincere desire to aid us to improve the manuscript.

We gratefully accept almost all technical comments and included corresponding changes in the manuscript (see below detailed replies).

We reply in detail here to general and specific comments of Reviewer 1. Unfortunately we may not accept some changes of the text suggested by this referee because our concept of this paper is different from how he/she sees it.

Below we reproduce the reviewer comments in a normal font and give our replies in italic.

OVERVIEW

The paper presents a new routine to calculate the Non-Local Thermodynamic Equilibrium (NLTE) cooling/heating for CO2 isotopes at 15um wavelength in the Mesosphere and Lower Thermosphere (MLT); the routine is called NLTE15umCool-E-v1.0. To sum up, the paper aims to show this routine as a parameterization alternative for General Circulation Models (GCMs) of Earth's atmosphere. The authors claim it is more accurate and faster than the previous parameterization.

We believe that there is a misunderstanding here. We do not claim that our routine is both more accurate and faster than the previous parameterization. We state clearly that it is ***slower*** *than Fomichev-1998 routine. But, it is much more accurate and flexible.*

GENERAL COMMENTS

The new routine represents a significant innovation and will be an important option for climate models simulating ancient atmospheres or performing projections based on CO2 increase trending. Still, the new routine brings advantages, such as an expanded volume mixing ratio (VMR) range, achieving 4000 ppmv, or even higher accuracy for temperature computed between 80 - 100 km height (non-LTE region).

Generally, it is an exact algorithm, which stems from our research code, so it may work with any CO2 VMR, for instance, for a Martian atmosphere, which consists 99% of CO2. It is a further development of our routine, which is since 2005 applied in the MPI MGCM (for Max Planck Institute Marc General Circulation Model) of Hartogh et al, 2005, [please see more also our replies to L. Rezac's comments (Kutepov and Feofilov, 2023b)]. We write in the text about 4000 ppmv as about an upper limit only because we show routine errors only up to this CO2 VMR.

Our routine is not limited by the altitude range 80-100 km. The non-LTE effects for the CO2 emission are particularly strong above 100 km. Our routine provides an exact solution of the non-LTE problem in the entire range of altitudes prescribed by the user. The upper boundary can be put at any altitude above about 110 km assuming corresponding atmospheric model inputs.

Despite the valuable scientific significance of the new methodology, the authors submitted the article without proofreading, which substantially affected my review. Overall, the manuscript introduction delivered an unusual approach at the beginning and along the other sections, where some crucial information was missed. In addition, the authors claim that the new combination of techniques (ALI + ODF) significantly reduced the time consumption during the simulations, as shown in Table 2 in the Ttot column. However, the manuscript doesn't provide the data and scripts used to compute each non-LTE technique comparison, making verifying the results impractical. Still, the authors compared the parameterizations KF23 and F98 with a reference model (WACCM6 CESM) but didn't explain why this model was chosen and what non-LTE parameterization is adopted within his source code. Another point is about the NLTE15μmCool-E v1.0 source code, where the users don't have a manual with instructions for users.

The issues discussed by the referee in this paragraph were addressed in our preliminary reply to his/her comments (Kutepov and Feofilov, 2023a). As for the lack of proofreading in the original version, we apologize for this and we provide a new version, which has been checked for grammar and typographical errors.

Due to the paper presentation demanding a substantial review and improvements, the authors should rewrite the paper to achieve the desired presentation quality and resubmit the manuscript as soon as possible. Anyway, I tried to perform a complete article review because I enjoyed the new routine purpose and intend to use it. Obviously, tt's not a proofread, but it will be useful to rewrite the paper. Below, I shared some specific comments. After that, I shared some minor comments. Then, I hope the authors resubmit the revised manuscript to the GMD journal.

We are grateful to this reviewer for his/her good will, detailed reading the manuscript, and for correcting grammar inconsistencies and typos. We tried to improve the text following the suggestions if they do not contradict with our concept of this manuscript as a technical paper.

SPECIFIC COMMENTS

1) The introduction starts abruptly from the radiative heat rate (h), also called radiative flux divergence (Eq.1).

The introduction is one of the most essential sections of a paper, where the authors bring an informative discussion within the article's scope. However, the current preprint introduction is similar to a subchapter of a book, which can push the readers away due to the need for more context.

We see the point, but we assume this time that our target reader is already prepared for this discussion, because it is very unlikely that the unprepared one will bother about the implementation of a complex code into a complex model. This manuscript is a technical paper, which suggests an advanced technical tool for the solution of a well-known problem of MLT cooling, which has been being discussed since the first publication of Paul Crutzen (Crutzen, 1970). To address this comment, we enhanced the introduction.

The paper should present some essential information, but I had to get the omitted information by reading other articles. For example, in the review "Infrared Radiation in the Mesosphere and Lower Thermosphere: Energetic Effects and Remote Sensing (Feofilov and Kutepov, 2012)" I found more precise information that is supposed to be present in the submitted preprint. The same in Kutepov et al. (2007) (https://doi.org/10.1029/2007GL032392) and Kutepov et al. (2016) (https://doi.org/10.5194/amt-10-265-2017, 2017).

As we have already written in our preliminary reply (Kutepov and Feofilov, 2023a) one cannot copy-paste our previous texts in this manuscript (nor paraphrase them – both are considered as self-plagiarism). It is normal when the reader, who develops the interest to the paper, follows the references to get more information. We thank the referee for this/her interest to our previous works which helped to write this report in a most objective and comprehensive way.

It's worth mentioning that in section 2, the authors describe the historical progress of some important iteration techniques along the century XX (e.g., Lambda Iteration (LI), Curtis-Matrix (CM), Accelerated Lambda Iteration (ILA), etc.). Thus, this section approaches the main article's subjects using a well-written structure despite minor details. On the other hand, the introduction is one of the preprint's weak points; to get around it, the authors must begin the paper by discussing attractive and interesting topics, considering increasing the article's readability. For instance, the Mars EXpression Mission (MEX) results or citing articles discussing the high levels of CO2 in the primitive atmosphere (4000 ppmv; threshold of the NLTE). After that, the authors would introduce the specific content gradually to present the general article's goals in the penultimate paragraph.

Please, see the answer to the 1st specific comment. The general interest will not help to promote the application of our routine in GCMs. One needs to develop the "feeling" that the correct non-LTE colling is important for the problem he/she solves. One usually starts with applying LTE cooling, then some simple non-LTE approximations, etc., and finally may come (or may not) to the need of a good non-LTE routine. The MPI MGCM developers appeal to us to give them a safe tool for the non-LTE cooling calculation only after they recognized they needed it to fit the observations.

Overall, I recommend moving the introduction (3 first paragraphs) to section 2 and writing more general paragraphs at the initial of the introduction (e.g., astrophysics, ancient atmosphere, SABER, PFS-MEX, etc.).

We tried improve the text following the reviewer comments.

2) Presentation and content connections

Please the authors must draw attention to the text's coherence and cohesion; once a well-written manuscript connects all the given information gradually. Another problem is the omitted nomenclature abbreviations, affecting the readability. For instance, the equation to compute the number of operations for the solution of radiating transfer (Nrad) is not declared as an abbreviation in the paper, only in Eq. 5. The same happens with the number of auxiliary operations (Naux). Ultimately, even though some readers can likely be familiar with this technical vocabulary, it's reasonable never to present abbreviations without declaring it properly before in the text, which occurs often in the manuscript (e.g., GCM, MLT, LIMA, ODF, VV, GRANADA, SABER, HITRAN, and others.).

We made all required corrections of the text.

3) GMD journal technical instructions

The document was prepared in disagreement with the technical instructions provided by the Copernicus/GMD journal. I recommend reading the author's guidelines and downloading the manuscript template file (Latex, Word, or R markdown). For example, the citation of Fomichev et al. (1993) is cited as Fomichev, Kutepov, Akmaev, and Shved (1993); it needs to be corrected. For articles with more than two authors, the citation needs to use the Latin acronym "et al". Otherwise, the readers could consider only the last name as a citation. For example, Fomichev et al. (1993) would be Shved (1993).

Done.

Another problem is that Tables 1 and 2 disagree with the technical instructions. Therefore, adjusting your tables before submitting the article again is necessary. Note that Table 2 can be combined to become only one.

The authors mention the unit of measurement for cooling rate in the document, sometimes adopting K/day and K/Day, but the correct is K/d. Please fix it.

We checked several papers from various journals and some books, for instance the book by Lopez-Puertas and Taylor (2001). We found that various authors prefer using different cooling/heating rate unit presentations: K/Day, K/day, K day^{-1} , etc. among them K/d it is perhaps the rearrest variant used. Therefore, we have chosen to use in our manuscript "K/day" as the most widely used and clearly red and to avoid misunderstanding, for example, reading K/d as K/decade, which is used in some papers dealing the climate change. We leave this issue open for the discussion with the journal's technical team.

4) Figure 1: CO2 vibrational levels diagram …

Figure 1 is based on Feofilov and Kutepov (2012) but is slightly different. The first problem in Figure 1 is the abbreviations FH, SH, TH, and FB. I didn't find the abbreviation meaning in the document, but in Feofilov and Kutepov (2012) review, each one is declared: First Hot (FH), Second Hot (SH), Third Hot (TH), and Fundamental Band (FB). Another problem is the CO2 isotopes code 626, 627, 628, and 636. The authors should declare explicitly the isotopes just like in Feofilov and Kutepov (2012) in section 2.2.3 ("*... The isotopes are marked using the lower digit of the atomic weight: 16O 12C 16O corresponds to 626 …"*). Additionally, the authors should declare and distinguish the main isotopes of the minor CO2 isotopes in the text section 2.

Done

I realized that the HITRAN codes (10002 and 02201) are in different positions than Figure 7 in Feofilov and Kutepov (2012). Thus, my question is: does it affect something in the diagram?

We corrected Fugure 1.

Please include the missed unit on the left side of the figure: Energy (cm^-1).

Done

The Figure 1 caption is identical to Figure 7 in Feofilov and Kutepov (2012). I recommend using other words to avoid plagiarism issues.

Done

5) Figures legends

Figures 4, 5, and 6 must contain a box legend declaring the latitude with your corresponding color, such as Figures 2 and 3.

Done

6) Model evaluation

The authors present the KF23 and F98 routines errors compared to a reference model (WACCM6 CESM). Only the graphical plots and interval range aren't enough to validate KF23. I recommend employing the *Root Mean Square Error* (RMSE) to show that KF23 is more accurate than F98.

Please, see the preliminary reply (Kutepov and Feofilov, 2023a).

Well, I have some important questions:

1) Why did the authors use the WCACCM6 CESM as a reference Model?

Please, see the preliminary reply (Kutepov and Feofilov, 2023a).

2) What is the parameterization adopted within the reference model? Please declare it in the manuscript.

Done. *This is the Fomichev et al, 1998 algorithm.*

3) What are the advantages and/or disadvantages of the KF23 compared to the parameterization adopted in the reference model?

The paper discusses in detail advantages and disadvantages of the KF23 compared to the Fomichev et al, 1998 algorithm.

The manuscript does not mention anything about the WCACCM6 CESM. If possible, request additional information from Dan Marsh.

Done

6) Comments about the NLTE15μmCool-E v1.0 source code

The program can be compiled using a Makefile, but during the first attempt, the compilation fails due to a deprecated GCC flag "g77" (Line 53 of the Makefile). I solved it by updating it to "gfortran", which can recognize all previous GNU Fortran versions (77, 90, 95, etc.). After that, I tested the program, and at a glance, everything worked well. A minor issue is in the file main.f at line 124, where I needed to provide additional space for Pressure (P) and Temperature (T) strings; otherwise, the value number would remain print merged with P and T in the console.

Thanks for reporting these issues. We fixed them in the updated version of the code.

Additionally, I would like to change some parameters to run different simulations, but the code "read_parameters.c" does not provide the parameter CO2 VMR. Thus, having a namelist to set CO2 values easier would be interesting. For instance, I am setting from 400 to 4000 ppmv.

We see the point, but the problem here is twofold – first, the code already receives the CO2 VMR vertical profile from the model and there's no need to replace it with a single value, knowing that CO2 is well-mixed up only to 70-75 km in Earth's atmosphere. Second, such a namelist will require either a recompilation or a reading routine. Both will decelerate the testing and/or running the code. We suggest the reviewer to change the input parameters including the VMRs of CO2 and O through the inputs of the interface.

Another question is about instructions to install the routine and explain some technical aspects of the program, such as the role of the objects and libraries. Otherwise, it might be hard to couple the routine in climate models. I strongly recommend preparing a readme file.

As for the libraries, we do not use something external, all the matrix operations and other functions are coded in the framework of our code. Regarding the objects, they are created during the compilation, but it's the main executable, which is called by the interface. For obvious reasons, we cannot foresee all possible cases of coupling of our routine to GCMs, but our experience with

Martian GCM and WACCM tells us that this is doable with a little effort. We added a readme file explaining the installation procedure.

MINOR COMMENTS

Line 3: Typo, replace "nigh" with "night". ***Done.***

Line 3: Cooling rate "K/Day -> "K/d" and so on along the text.

Please see our reply to the comment in the section "3) GMD journal technical instructions"

Line 13: "… with the opposite sign" replace by "… with the opposite sign:" ***Done.***

Line 17: "… LTE 15 um band cooling" replace by "… LTE 15 um band cooling:" ***Done.***

Line 21: "Declare what is the GCM abbreviation" ***Done.***

Line 22: where (Curtis and Goody, 1956; …) use (e.g., Curtis and Goody, 1956; …). You should do the same in other parenthesis examples along the text. ***Done.***

Line 40-41: The citation format is wrong, change it for Fomichev et al. (1993). ***Done.***

Line 48: Please avoid using terms like "below" and "above" within the document. After the typesetting stage of the manuscript, the final version will modify the position of the paragraphs, equations, tables, and figures. ***Done.***

Line 54: Declare what is MLT. ***Done.***

Line 55: Declare what LIMA is. ***Done.***

Line 63: Such as the Fomichev et al. (1998) parameterization is called F98; it would be reasonable to call the Kutepov and Feofilov (2023) parameterization of KF23. Please consider adopting KF23 instead of KF2023. ***Done.***

Line 69: ARMS wasn't declared before in the introduction, therefore, it should be explained in the manuscript as a full nomenclature: Atmospheric Radiation and Molecular Spectra (ARMS). ***Done.***

Line 71: ODF means Opacity Distribution Function, but it wasn't declared before. ***Done.***

Line 74: Please consider putting the citation (Hubeny and Mihalas, 2015) at the end of the sentence, Line 76. ***Done.***

Line 82: Add a missed comma after "… non-LTE problem …" -> "… non-LTE problem, …"

In the same line, you should change "… that in case …" -> "… that in the case …". ***Done.***

Line 88: Put the citations in the final of the sentence. ***Done.***

Line 94: Gramma -> Change “However, the convergence of both algorithms depends, strongly on the way the local non-linearity is treated, see next section.” By “However, the convergence of both algorithms depends strongly on how the local non-linearity is treated, see next section.” ***Done.***

Line 99: What is GRANADA? Declare the nomenclature in the sentence. ***Done.***

Line 113: What is VV? Please declare VV as the intermolecular Vibrational-Vibrational. ***Done.***

Line 139: What do you are comparing in “This way of treating the radiative transfer is about 50-100 times than the 140 classic LBL approach”. You mean “…more than the…”, “…faster than then…”. ? ***Done.***

Line 147: Clarify how it can be standard and modified simultaneously. ***Done.***

Line 150: … “ generalized …” : remove the space at the beginning. ***Done.***

Line 152: Put the citation at the final of the sentence. ***Done.***

Line 160: ALI-ARMS should be declared before. ***Done.***

Line 163: What is PFS? Declare it in the text (Planetary Fourier Spectrometer) ***Done.***

Line 164: What is SABER? Declare it in the text (Sounding of The Atmosphere Using Broadband Emission Radiometer) ***Done.***

Line 175: What is VT? Declare it (Vibrational-Translational). ***Done.***

Line 176: in Lopez-Puertas and Taylor (2001), add DOI and ISBN in the references. ***Done.***

Line 179: Please, change “ro-vibrational” to “rotational-vibrational”. ***Done.***

Line 207-209: Consider including 1) time for solving the radiative transfer (Trad) … 2) time for auxiliary (Taux) … 3) time for matrix inversions (Tinv). ***Done.***

Line 210: After (Kutepov et al., 1998) add “:” . Please do the same before other equations. ***Done.***

Line 211: Remove the comma at the final of the equation. Do the same in other equations. ***Done.***

Line 217-218: Please make sure to regard the architecture name of the processor. Usually, x86 is 32-bit, whereas x64 is 64-bit. Do the same in Line 279.

We agree that the typical nomenclature of the processor's architecture is as suggested by the reviewer. But, these very processors are capable of operation both in 32-bit and in 64-bit

architecture, that is specified in the corresponding /proc/cpuinfo files: Architecture: x86_64, CPU op-mode(s): 32-bit, 64-bit. We compiled the code to use them in 64-bit mode.
To exclude possible ambiguities, we updated the text as follows: We performed this study at two different machines, with x86_64 Intel and Intel Xeon Gold processors operating at 2.2 and 2.5 GHz, respectively. We compiled the ALI-ARMS code to be used in 64-bit architecture with the help of a standard gcc compiler and we ran it on a single processor

Line 219: declare the gcc compiler nomenclature: gnu compiler collection. ***Done.***

Line 226: I suggest changing "Whereas N is …. " to "Thus, whereas N is defined by the mathematical nature of the problem and the algorithm applied, the coefficient C may depend on many factors, such as the quality of programming, language used, operational system, interpreter, computer architecture and performance, etc." ***Done.***

Line 237: It is worth remembering NL meaning (number CO2 vibrational levels) once the readers see NL declared only in line 23 on the second page. ***Done.***

Line 245: Change to "…. is approximately N^3" and where is "Therefore," change to "Thus, we have the following equations:" ***Done.***

Line 253: Include DOI and ISBN of the Book Press et al. (2002). ***Done.***

Line 271: After compared to the nighttime… include a comma. ***Done.***

Line 286: What is the reference model? Please, declare your name as well as justify the reasons to use it. In addition, declare the abbreviation Volume Mixing Ratio (VMR) here; otherwise, this abbreviation will appear suddenly at line 307. ***Done.***

Line 289: Change the word above to before. ***Done.***

Line 290: What do you mean about "various waves"? If you are talking about gravity waves, declare it explicitly in the paragraph. !!!!

Page 13: In Figure 3, there is a typo in the caption: Solis, change to Solid. ***Done.***

Line 319-321: Update the sentence to "For instance, the test for the nighttime for a roughly twice smaller set of bands, which does not include weak first and second hot bands of 626 and 636 isotopes, shows that the maximal cooling rate error for 400 ppmv may increase up to 3 K/d; however, computing time becomes only 10% shorter (see also Table 2)." ***Done.***

Line 333: include a comma after "… absorption and assimilation" ***Done.***

Line 335: You don't declare before what is VT and VV. ***Done.***

Line 370: The authors say, "… many previous studies (e.g., Lopez-Puertas and Taylor (2001)). I was expecting to cite at least three papers. Add more citations or modify "… many previous studies". ***Done.***

Line 377-378: Consider changing the sentence to "The accuracy tests of the KF23 routine were performed for a 1 km step grid with the upper boundary of the atmosphere at 130 km." ***Done.***

Line 380: Add a comma after However ***Done.***

Line 395: Please consider updating the last conclusion paragraph to "The KF23 routine provides accurate cooling calculations in a vast range of k and O(3 395 P) variations. It also works well for very broad variations of CO2, both below and above the current density, up to 4000 ppmv. Consequently, this allows us to use this routine to model the Earth's ancient atmospheres and the climate changes caused by increasing CO2."

Done.

Line 424: Typo, replace "…. User to switch on an off" with "… User to switch on and off"?

Done.

References

Crutzen, P. J.: Discussion of paper "Absorption and emission by carbon dioxide in the atmosphere" by J. T. Houghton, Quart. J. Roy. Met. Soc., 96, 767–770, 1970.

Hartogh, P., A. S. Medvedev, T. Kuroda, R. Saito, G. Villanueva, A. G. Feofilov, A. A. Kutepov, and U. Berger, Description and climatology of a new general circulation model of the Martian atmosphere, J. Geophys. Res., 110, E11008, doi:10.1029/2005JE002498, 2005.

Kutepov, A.A., and Feofilov A.F., "Reply on Comment on gmd-2023-115 of referee 1", https://doi.org/10.5194/gmd-2023-115-AC1, 2023a.

Kutepov, A.A., and Feofilov A.F., "Reply on Comment on gmd-2023-115 of Ladislav Rezac", https://gmd.copernicus.org/#AC2, 2023b.