Reply to Referee #1 (gmd-2022-203)

We thank referee #1 for the positive and constructive comments on our manuscript.
We took all comments of the reviewer into account. Below we (authors comment, AC) reply to the review (review comment, RC) and revised the manuscript accordingly. Additionally, we highlighted the changes of the manuscript, and attached them to the reply.

Here are our replies:

RC: "… more background information on the fundamental science of non-CO2 climate forcing could be beneficial here. For example, the less experienced reader may appreciate a more comprehensive explanation of (or references to) chemical reactions that lead to NOx-based effects, or the basis of contrail formation and persistence. A clearer explanation of these fundamentals in the beginning of the paper may help to justify decisions made later on regarding parameters used in aCCFs."

AC: Thank you for the feedback. In the introduction we now added some text to explain the NO_x-based climate effects. Additionally, we provide some references on NO_x -based effect and contrail formation for the interested reader (i.e. Stevenson et al., 2004; Terrenoire et al. 2022, Kärcher, 2008). Please refer to the track change in the revision.

RC: "… the discussion around the use of NOx EI and flown distance per kg fuel is not immediately obvious, based on wording. It took a good few reads to understand that these metrics were introduced purely to change units for the merged aCCFs. Better explanation around this unit conversion for both NOx aCCF and contrail aCCF might help to minimise confusion. See attached pdf for suggestions."

AC: Thank you for this helpful comment and your suggestions. We rephrased parts of this section, thus it should be easier to understand now (see tracked changes).

RC: "In the discussion on climate efficacy conversions, some more detail on how and why RF from different climate forcers results in different levels of warming could help too."

AC: As described in the text, the relation of constant climate sensitivity parameter fails especially for non-homogenous forcings. E.g., ozone change patterns inferred from precursor emissions of certain transport sectors (aviation, shipping, road traffic) are distinctly non-homogeneous (vertically and horizontally). In contrast to the forcing of the well mixed greenhouse gas CO_2, these non-homogenous forcings trigger feedbacks, that differ from those induced by CO_2 and thus give a climate response different from CO_2. We added some more description in the text.

RC: "A reference/link to the exact ECMWF ERA5 dataset used could aid the reader, should they decide to implement the tool themselves."

AC: We do not give the link in the text, but include in the data availability paragraph the sentence: "ERA5 reanalysis (Hersbach et al., 2020) data are available at the Copernicus Climate Change Service (C3S) Climate Data Store via https://doi.org/10.24381/cds.bd0915c6"

RC: "My research team and I do however, have one major area of concern in the technical implementation of the ozone aCCF: It is stated outright that the photochemical ozone formation does indeed increase with available sunlight. However, ozone aCCF does not take into account irradiance (table 2 states only temperature and geopotential are required to calculate ozone aCCF). How therefore, would these effects be captured in the generated maps? Note, this is less of a point about your findings, and more about drawing attention to *the fact that ozone aCCF formulation does not include solar radiation as input. The photolysis reactions pertaining to the formation of ozone are highly sensitive to solar radiation, so more information explaining why the derivation did not identify this sensitivity would be useful."*

AC: Of course, the ozone formation is highly sensitive to solar radiation. These aCCFs were developed by statistical methods relying on correlation to derive algorithms by linking the CCFs, which were explicitly calculated in comprehensive numerical chemistry climate model simulations, to local meteorological conditions (van Manen and Grewe, 2019). The publication of van Manen and Grewe provides a detailed description on how the approximations of the climate effect from NO_x-induced ozone are generated. Several candidates were selected for these correlations, also including solar incoming radiation. However, comparing the different correlations showed that in case of the ozone aCCF combining temperature and geopotential gives the best correlation (see Table 3 in the publication of van Manen and Grewe 2019 for the quantitative assessment of the correlations). With the geopotential in the ozone aCCF, we assume that this implicitly represents the expected latitudinal dependence. We shortly address this point in Appendix A, describing the aCCF formulations *RC: "One final area that has led to confusion in this paper is the aCCF limitations. Why is it stated that aCCFs are only configured for use in the North Atlantic Flight Corridor region, when all of the maps generated as examples are over mainland Europe? This contradiction between what is stated and what is shown in examples may lead to reader uncertainty."*

AC: The original CCFs, that led to the development of aCCFs, were calculated for the North Atlantic Flight Corridor during typical summer and winter days. This implies that using aCCFs for other locations or seasons should be carefully evaluated. Indeed, we here use the aCCFs over mainland Europe, which isn't included in the North-Atlantic Flight Corridor. However, the European airspace is highly impacted by the North-Atlantic dynamics, that is stretching to Europe. We evaluated the weather patterns over Europe carefully and came to the result that the classification of the weather patterns that was used for the North-Atlantic Flight corridor (classification after Irvine et al. 2013) are also valid for Europe. That's why we are confident, that aCCFs are valid over the European airspace. We now clarify this point in the text (Section 4).

RC: "…technical details need to be addressed such as punctuation, wording and hyphenation, as there were lots of minor technical issues found in the manuscript….. The attached pdf attempts to address the specific areas that may need a second look, so that corrections can be made where deemed necessary."

AC: Thank you for the detailed corrections in the manuscript. All technical issues are addressed in the revised version of the manuscript.

Reply to Referee #2 (gmd-2022-203)

We thank referee #2 for the positive and constructive comments on our manuscript.
We took all comments of the reviewer into account. Below we (authors comment, AC) reply to the reviewer (review comment, RC) and revised the manuscript accordingly. Additionally, we highlighted the changes of the manuscript, and attached them to the reply.

Here are our replies:

RC: *"I find the description given in the manuscript rather difficult to follow. This might be related to the fact that the authors provide a mixture of technical description of the python tool and scientific explanation of the underlying assumptions."*

AC: Thank you for your feedback. We tried to clearly separate the technical description of the Library and the scientific background. That's why we first explain the underlying scientific background of the Library, before we actually introduce their technical details. By clarifying the specific comments of the reviewers and additional explanations on the scientific background, we hope that the descriptions are now better to follow.

RC: "*Furthermore, the authors refer to several studies that are still in preparation. This is very unfortunate as the reader is left with insufficient information and open questions, e.g., about the calculation of the climate metric conversion factors (sect. 2.4) or the updated set of algorithmic climate change functions, aCCF-V1.1."*

AC: Thanks a lot for this remark. We are fully aware of the problem that the publications are not available yet. Here the detailed answer to the two above mentioned publications:

1) In this work we provide metric conversion factors that were derived for this publication. These factors were calculated by the climate response model AirClim (Dahlmann et al., 2016): one simulation with pulse emission and one with future emission scenario. By simply comparing the two simulations the factors can be derived. In order to address the open question on the metric conversion we added some text in the manuscript. The publication in preparation (Dahlmann et al. 2023, in prep.) we refer to will introduce further metric conversion factors. We think that referring to this publication, that is still under preparation, has an added value to the reader, but it is not needed to understand the metric conversion factors.
2) The publication of aCCF-V1.1 (Matthes et al., 2023) is also not available yet, but it is in a very final state and will be submitted within the next two weeks to GMDD. Thus, it could be possible to provide the final reference during the type setting process. As aCCF-V1.1 is of particular interest to the potential user of the Library we additionally add the reference to the public Deliverable D1.2 of FlyATM4E "Report on expanded aCCFs including robustness and eco-efficiency aspect" H2020-SESAR-2019-2, where the AirClim calibration factors that are needed for aCCF-V1.1 are provided. However, the detailed explanation will be given in Matthes et al., 2023.
    - Matthes, S., Dietmüller, S., Dahlmann, K., Frömming, C., Yamashita, H., Grewe, V., Yin,F., Castino, F., 2023: Updated algorithmic climate change functions (aCCF) V1.1: Evaluation with the climate response model AirClim, submission to GMDD

RC: *"It might be helpful to restructure the manuscript by starting with the description of the tool, the required input data, the workflow etc., and only then describe the underlying scientific assumptions or simplifications. In particular the description of how the merged aCCFs are calculated (current Sect. 2) needs improvement and clarification. For the authors it is certainly clear what is behind all the parameters, conversion or efficacy factors, and where they come from, but for the inexperienced reader it can be very confusing."*

AC: Thank for the suggestion to further clarify the structure of the manuscript. We thought about your idea of restructuring the document. However, the current idea is to separate technical description of the Library from the scientific background, where we provide deep insights to e.g. physical climate metrics. Thus, we first explain the scientific background, as we think this information is needed to understand what the Library is doing. Second, we provided a detailed technical description. At the end of the introduction we follow your suggestion and stress the structure of the manuscript. Additionally, we made Section 2 more comprehensive by more detailed explanations.

Reply to specific comments:

L15: which non-CO2 emissions?

- ➔ **AC:** To be clearer we know reformulated the text. See tracked changes.

L51/52: I find this sentence a bit confusing. On the one hand the authors talk about climate optimal trajectories, on the other hand they consider only non-CO2 climate impacts. How about additional CO2 emissions that might arise from a re-routing to reduce non-CO2 impacts?

- ➔ **AC:** CO2 is also considered for re-routing, however as CO2 does not depend on the geographical location of emission, their aCCF is just a constant value. To make it clearer we rephrased the sentence to "…quantitative estimate of CO2 as well as of total non-CO2 climate effect. The latter is needed as four-dimensional data set ...." (see tracked changes).

L90/91: What do you mean by "NOx induced methane"? To me, NOx induced methane sounds like CH4 produced from NOx, but as far as I know NOx emissions from aircraft lead to a reduction of CH4 via NOx induced OH formation, right? So maybe "NOx induced CH4 loss"?

- ➔ **AC:** Yes, that is right, CH4 is destructed via NOx. In the manuscript we understand the NOx -induced methane change as a methane decrease. To make it less confusing we now shortly explain the NOx- based effect of ozone production and methane destruction in the introduction (see Line 16-22). Moreover, we here changed the text to: "….NOx-induced ozone (production), NOx-induced methane (destruction) ….". However, in the manuscript we use the wording NOx-induced ozone aCCF and NOx-induced methane aCCF.

L94/95: As stated here, the contrail aCCFs are obtained from contrail radiative forcing calculations based on ERA-Interim reanalysis data, but in the example given in the manuscript ERA5 data are used as meteorological input. Do you expect any errors/biases arising from the different meteorological data sets?

- ➔ **AC:** The statistical approach that provides the contrail aCCFs is based on a Lagrangian trajectory simulations that are using ERA Interim Data (for details see supplement of Yin et al. 2022). On the contrary, the mathematical formulation of the water vapour, ozone and methane aCCF is based on comprehensive chemistry climate model simulation. The derived aCCF formulations can be applied to every data set (ERA5, ERA-Interim, or any other NWP, or climate data).
  Generally speaking using different meteorological input data introduces additional uncertainties requiring further evaluation. However, comparing ERA5 and ERA-Interim, we expect only marginal differences.

L100: Please provide some more details/examples on the assumptions and simplifications. And how do these affect the results of your tool?

- ➔ **AC:** First, the development of aCCFs is based on a statistical approach where assumptions were taken (van Manen et al., 2019). Moreover, the CCFs data, that are the basis of the aCCF formulation are calculated within a climate model (here simplification of atmospheric processes is needed). All these assumptions made during the development of the aCCFs don't affect the tool. But, the aCCFs are subject of these uncertainties.

L106/107: This sentence is not clear to me. How do the different units of the individual aCCFs affect the weighting for different aircraft/engine classifications? Please clarify.

- ➔ **AC:** I rephrased the sentence and hope it is clear now. See tracked changes.

L147-149: How is this statement related to the values provided in Table 2?

- ➔ **AC:** This value is also derived by the emission inventory of the DLR project "Transport and Climate" (TraK). As mentioned in the text the uniform value of 0.16 km/kg(fuel) is given by averaging over the ten most frequent routes in the North Atlantic Flight corridor with the ten most used aircraft types in the year 2012. As mostly wide-body aircraft types are used over the NAFC, this value is similar to the in Table 2 provided wide-body values at typical flight altitudes

Table 1: This table provides altitude-resolved average specific NOx emission indices for three different aircraft categories. The values are provided with three decimal places, which implies a high accuracy. However, I would assume that these numbers are associated with some (large?) uncertainties. For example, the wide-body aircraft type seems to include a wide range of different aircrafts. I would be interested to see some uncertainty ranges of these emission indices. Same holds for table 2.

- ➔ **AC:** Thanks for the feedback. We now extended both table 1 and table 2 by including the standard deviations of the emission indices.

L182/183: Is the statement on the different emission scenarios a more general comment related to climate metrics or is this directly related to the aircraft emissions? In general, it is not quite clear to me which emission scenarios are meant in Sect. 2.4. Aircraft emissions along a flight track or climate scenarios like the RCPs in general?

- ➔ **AC:** Different emission scenarios can be used – this statement is not related to aircraft emissions only. However, in section 2.4 we mean the time development of aircraft emissions, when we talk about emission scenarios. The emission scenarios include pulse emission (emission at certain time, leading to temperature change; this metric is used if one compares the future impact of an emission in a certain year), sustained or future increasing emission scenario. Future emission scenario is representing the growth of the air traffic and is used to evaluate temperature change (emission continue to develop) at a given year. We clarified this point in the manuscript.

L191: Why is the climate metric P-ATR20 not suited for some questions? And why are FATR20/50/100 better suited? Please explain

- ➔ **AC:** The question on the choice of a suited metric is essential. For details the reader is referred to the cited publication of Grewe and Dahlmann 2015. The P-ATR20 metric gives the information about the climate impact of an emission in a certain year. However, if you want to answer the question of the climate effect reduction of steadily applying a certain routing strategy, the P-ATR20 would not give you the right answer and future emission scenario are more suitable. To be clearer we rephrased the text accordingly.

Table3: Why are the conversion factor for H2O aCCF and O3 aCCF identical? Same for CH4 aCCF and PMO aCCF?

- ➔ **AC:** The conversion factor converts the ATR20 from a pulse emission into ATR from a future increasing emission. An important issue for the conversion factor is the time development of the forcing. As we use the impact on an annual basis the time development of O3 and H2O forcing is the same. Therefore, also the conversion factor for O3 and H2O are the same. The conversion factors of PMO and CH4 are the same, as the time development (and forcing) of PMO is coupled with the time development (and forcing) of CH4. We added some text in the manuscript. Please see the tracked changes in the resubmission

L239/240: "… compatible and tested with the standard of European Centre for MediumRange Weather Forecasts (ECMWF) data…" What exactly does this mean? Format, naming conventions, meta data? And what is meant by "standard ECMWF data"? Reanalysis? Forecasts? And what would be necessary to use the library with different meteorological data?

- ➔ **AC:** With standard we mean "Standard format" (naming conventions, meta data, …). We tested the Library for the different product types of ECMWF reanalysis data (i.e. reanalysis of ERA5, ensemble of ERA5, ERA-Interim, forecast). We didn't test the Library with input from other meteorological data sources. But of course, in the future we aim to make the Library consistent with input from other meteorological data sources, thus the user could specify the source of the data product he wants to use. Such an implementation should be straight forward, only small adoptions in the Library would be necessary. We also addressed this point in the Section "Conclusions" where we give an outlook. Moreover, we delete "standard" and replace it by "several data products of ECMWF (i.e. ERA5, ERA-interim, forecast)"

L274: What is meant by "provided default data set"? Does the python library come with a climatology of meteorological data? And if so, where does the default data set come from?

- ➔ **AC:** Thanks for recalling this point. In fact, with this sentence, we meant that with CLIMaCCF, there is a possibility to calculate the required meteorological variables (in case of missing) by using other alternative variables included in the input dataset. For instance, the potential vorticity unit required for aCCF of water vapor can be calculated by temperature and components of wind (see Table 5 of the revised paper). In the manuscript we now replace "default data set" by "input data set".

L289: Why is the PCFA-SAC more accurate and how does is consider aircraft and engine properties? In L282/283 it is written that SAC uses rel. humidity over ice and temperature.

- ➔ **AC:** Thanks, the text is not correctly formulated here. The SAC states, that a contrail will form when the exhaust-air mixture in the expanding plume reaches water-saturation. This depends on ambient air pressure, humidity, fuel and aircraft properties. Thus, using SAC is more accurate than simply using ISSR, that uses the temperature threshold of 235K. However, to exactly calculate SAC one needs to know additional aircraft specific parameters. Rephrased it in the text.

L368: What is meant by "MET information"? Is MET an abbreviation? If so, please explain.

- ➔ **AC:** Meteorological product, we now spell it out

L404: Is there any specific reason for using 15 June 2018 as an example?

- ➔ **AC**: No there is so specific reason for that choice. It is just an example for a typical summer day. See "as application example" (line 339).

Fig. A1: Is there any difference in the H2O aCCFs for the different aircraft categories? To me, the plots look identical.

- ➔ **AC:** No, there is no difference here as the specific aCCF of H2O is given in K/kg(fuel), thus there is no need to be converted the H2O aCCF. Moreover, this is also clear from equation 1 and we also addressed the point, that the H2O aCCF is already fuel related and does not need to be multiplied by the emission index of water vapour in Section 2.2. Moreover, we added a short note in the caption of Fig. A1.

L408: ".. gets somehow more important…" This formulation is not very scientific and should be rephrased.

- ➔ **AC:** Deleted "somehow".

Climate hotspots: I am wondering how meaningful the usage of percentiles as threshold values is? If I understand this approach correctly, it will always identify climate hotspots, no matter how strong the absolute climate impact is, but a re-routing could lead to additional CO2 emissions, so I am wondering how applicable this feature is in practice?

- ➔ **AC:** Of course, an efficient overall implementation will rely on combining fuel penalty and climate effects with mitigated non-CO2 effects during the trajectory optimization process. And yes, it is right, that with this approach climate hotspots are always identified. We also tested constant thresholds (this is also an option included in the Library), however these constant thresholds are not representative for different altitudes, seasons, geographical locations. Thus, we decided to use percentiles as threshold value. Future development could of course provide different concepts of identifying climate hotspots (e.g. tabulated geographical and time dependent fixed threshold values). By the selection of the 99% or 95% percentiles the regions that are identified are small, we expect that the re-routing (from fuel optimal route) will not need much additional fuel (and thus additional CO2).

Section 5.3: I think this section would benefit from a more quantitative discussion of uncertainties. For example, what is the uncertainty range of the non-CO2 climate effects?

- ➔ **AC:** This section underlines, that several sources of uncertainties are associated with the calculation of aCCF. As mentioned in the text Lee et al., 2021 summarizes the quantitative estimate of aviation RF (their Fig. 3 illustrates the confidence intervals of these RF estimates). We do not see the need to repeat these values here, however we directly refer to Fig.3 of Lee et al., 2021 in the text now.

Although it is a bit unsatisfying that the authors strongly refer to a paper that is still in preparation. What is the status of Matthes et al, 2022?

- ➔ **AC:** Thanks a lot for pointing that out. As mentioned in the comment above this paper is still not available yet, but in a very final state. Note that *Matthes et al. 2022* is now separated into two papers. One is about the updated aCCF version (aCCF-V1.1), explaining in detail their development (submission to GMDD within the next two weeks). The other one is the paper on the FlyATM4E concept of identifying robust eco-efficient aircraft trajectories (submitted to Meteorologische Zeitschrift, TAC special issue).
    - Matthes, S., Dahlmann, K., Dietmüller, S., Yamashita, H., Grewe, V., Soler, M., Simorgh, A., González Arriba, D., Linke, F., Lührs, B., Meuser, Maximilian, C. F., and Yin, F.: Concept for identifying robust eco-efficient aircraft trajectories: methodological concept of climate-optimized aircraft trajectories in FlyATM4E, Meteorologische Zeitschrift, 2023, submitted
    - Matthes, S., Dietmüller, S., Dahlmann, K., Frömming, C., Yamashita, H., Grewe, V., Yin,F., Castino, F., 2023: Updated algorithmic climate change functions (aCCF) V1.1: Evaluation with the climate response model AirClim, submission to GMDD
    - We will additionally refer in the manuscript to the public Deliverable D.1 of the FLyATM4E project, that provides the AirClim calibration factors, needed for aCCF-V1.1. However, we hope that these publications are available as preprint within the typesetting phase.

5.4: Would you expect different results for meteorological input data other than ERA5? How sensitive are the calculated aCCFs to the meteorological data?

- ➔ **AC:** How sensitive the aCCFs are for different meteorological data, depends on how the input data (e.g. temperature, geopotential) differ between the used dataset and the ERA5 data. Moreover, the vertical and horizontal resolution of the used data product also influences the granularity of the aCCFs. We added a comment on that in Section 5.4.

L536/537: What would be necessary to use other meteorological data than ECMWF products in CLIMaCCF? Is it only a coding issue or would the calculation of the aCCF require additional adaptations?

- ➔ **AC:** Yes, that is only a coding issue. All NWP data, providing the input variables that are needed to calculate aCCFs, could be used. We only tested it for ERA ECMWF data - however, with some small coding adoptions the Library could also use other data products. Rephrased to be clearer.