Response to Reviews of "Updated Isoprene and Terpene Emission Factors for the Interactive BVOC Emission Scheme (iBVOC) in the United Kingdom Earth System Model (UKESM1.0)" by Weber et al.

We are grateful to both reviewers for their comments and efforts which have helped us improve this manuscript. Following the structure recommended by GMD, we have responded to each reviewers' comments sequentially below with italicised text showing the reviewer's comments and plain text showing our response. Text which has been added to the manuscript is coloured red. Original manuscript text is in blue and any text which has been removed from the manuscript is blue and has been struck through. The locations of changes are stated. We hope these revisions address the concerns of the reviewers.

Reviewer 1
SUMMARY AND GENERAL REMARKS

Biogenic Volatile Organic Compounds (BVOCs) play a key role in the composition of the atmosphere. They control the oxidizing capacity (abundance of OH) and contribute substatially to the formation of secondary organic aerosol (SOA). Therefore, acurate representation of BVOC chemistry and emissions in state-of-science Earth system models is imperative.

Weber et al. present a very comprehensive study of the inteactive BVOC emission model iBVOC in UKESM1. They identify a significant shortcoming in the selection of Emission Factors by mass (EFmass) for isoprene (IEFmass) and terpenes (TEFmass) for one particular Plant Funtional Type (PFT), namely C4 grasses. This leads to a massive overprediction of isoprene and terpene emissions from this PFT, while the global total budget remains relatively uneffected (compared to the literature). So, one could say right for the wrong reasons.

Weber et al. then analyse several alternative options and approaches of deriving improved EFs and evaluate the impact of their alternative EFs on emissions and atmospheric mole fractions of isoprene and terpenes. Some sensible reccomendations for fututure direction wrap up this very useful paper.

I think that this work represents a very valuable and useful contribution to the growing literature on the UK community Earth System Model UKESM. The authors have identified a significant shortcoming in the BVOC emission model and offer reasonable and useful alternatives. They also present a very detailed analysis of their suggested changes on UKESM, albeit limited mostly to the emissions and atmospheric abundance of BVOCs themselves. This is in my view where the paper falls a bit short of its potential. BVOCs pla a key role in tropospheric ozone production, the atmospheric oxidising capacity (OH abundance), and the formation of secondary organic aerosol (SOA) with substatial impacts on the radiation budget. This is a bit of a missed opportunity I feel, although I concede freely that the amount of work required is likely massive and probaly beyond the scope of this paper. I hope that future work along the lines detailed above will follow.

With the above said I recommend the publication of this paper in GMD after the minor issues, which I will outline in the following, have been addressed.

We are glad the reviewer finds this paper to be comprehensive and useful. We acknowledge the potential for expanding the analysis to examine the effect of changing the EF on other atmospheric and climatic variables, and the important insight this would bring. However, we note that such work is already underway for a follow up study examining the effect of wide scale land use change. We feel that separating out the technical description of emission factor development here from a wider analysis of the impact of BVOCs on atmospheric composition and climate will make both studies more accessible and easier to comprehend.

SPECIFIC REMARKS

p1l12: "future changes in land use and land cover (LULC) and change."; redundant, please revise.

We have removed the "and change".

p2l50: citation "Cao et al., 2021" does not appear to be in the list of references.

We have added Cao et al (2021) to the reference list.

p4ls99&100: please provide some refrences for JULES and UKCA.

We have added Best et al (2011) and Clark et al (2011) for JULES. For UKCA, while there isn't a single paper which describes all the processes, Archibald et al (2020) is the most relevant and we have included this.

p8l234: link; Is there perhaps another way of referencing these parameters (paper or technical documentation) that has a DOI? There is a potential risk that this link could break in future.

This is a fair point. To ensure long term access, we have included the relevant parameters in a new SI table (Table S1) and have made clear in the heading the source and revision number.

p11l333: reference to Table 3 should be to Table 4, I believe.

Yes, this has been corrected.

p11l349: "andorganic" should read "and organic"

This has been corrected.

p11l349: citation Mulcahy et al., 2020, doesn't appear to be in the list of references

We have added Mulcahy et al (2020) to the reference list.

p11l355,356: The first sentence in this paragraph seems a bit redundant, because it basically repeats what has been said in the previous paragraph.

We have made the following alteration, in conjunction with points raised by Reviewer 2.

UKESM1 has the capability to perform simulations using specified dynamics, also called "nudging", where certain offline meteorological fields from ECMWF (temperature and horizontal winds) are input (Dee et al., 2011), and free-running with online computed meteorology ~~from pre-industrial (PI), present day (PD) or future climates~~.

~~The UKESM1 simulations can be divided into~~ Our evaluation has three sections. Firstly, we perform present day (PD) simulations nudged to atmospheric reanalyses to compare the model simulations with different EF_{mass} values to observational data (Table 4). Secondly, we perform ~~from ECMWF (Dee et al., 2011) and~~ free-running simulations ~~of~~ using conditions from the pre-industrial (PI) and ~~, the PD,~~ Shared Socioeconomic Pathway SSP3-7.0, which represents a "regional rivalry" scenario, at 2050 (O'Neill et al., 2016) to assess the effect these different EF_{mass} values would have at these two periods (Table 4).

*p12l375: should read "timeseries **of** anthropogenic"*

This has been corrected.

p12l379: citation Sellar et al., 2019, doesn't appear to be in the list of references

This was an error in the date. It should have read Sellar et al., 2020 which is in the reference list. This has been corrected.

*p13l392: should read "PFTs **as** discussed"*

This has been corrected.

*p15l366: should read "**are** at the lower end"*

This has been corrected.

p15l367: "total emissions" is redundant

I think this refer to original line 467.

"total emissions" has been removed.

p15l498: "land use cover" --> either "land use" or "land cover" or "land use and land cover"

This has been corrected to "land use and land cover".

p16l495: "Fig2b" should be Fig3b, I believe

Fig 2b is correct here as we are making the link between the spatial change in emissions in Fig 3 and the IEF change in Fig 2.

p16l502-504: how does this decrease of terpene emissions from needleleaf trees square with other models and observations, e.g., from Hyytialää? Haven't needle leaf trees always been thought to be important for terpene emissions at high latitudes. Please comment here and, if appropriate, in the text.

We agree that needleleaf trees are important sources of terpenes. We have taken the reviewer's suggestion to compare the simulated emissions of terpenes using the current and proposed TEF_{mass} values to measurements from the SMEAR II station at Hyytiälä (https://smear.avaa.csc.fi; last accessed 19th March 2023). We find that the observed emissions at Hyytiälä are lower than those simulated using the current TEF_{mass} values but higher than those simulated using the proposed updated TEF_{mass} values. However, it is important to note that while the measurement station at Hyytiälä is in a completely forested area, the corresponding grid cell in UKESM is only 54% trees (27% each needleleaf evergreen and needleleaf deciduous) with the remainder predominantly C3 grass, C3 crops and water (lakes), which have negligible or zero TEF_{mass}. Therefore, we expect UKESM1 to simulate lower terpene emissions than the fully forested region measurement site, but still within a factor of ~2-3. Given this reasonable agreement between the simulated and observed emissions, at least in the case of Hyytiälä and the surrounding boreal forest, we believe that the new TEF_{mass} values are reasonable.

Direct observations performed at this and other similar sites in Finland yield MT emissions of 3-10 ng m^{-2} s^{-1} (with a springtime peak of 50 ng m^{-2} s^{-1} in some species) from tree bark (Vanhatalo et al. 2015, Ghimire et al. 2016) and 0.34 ng m^{-2} s^{-1} from pine needles (Ruuskanen et al. 2005). This further supports the veracity of the new TEF_{mass} values proposed in this work.

2013 MT Emissions at Hyytiälä
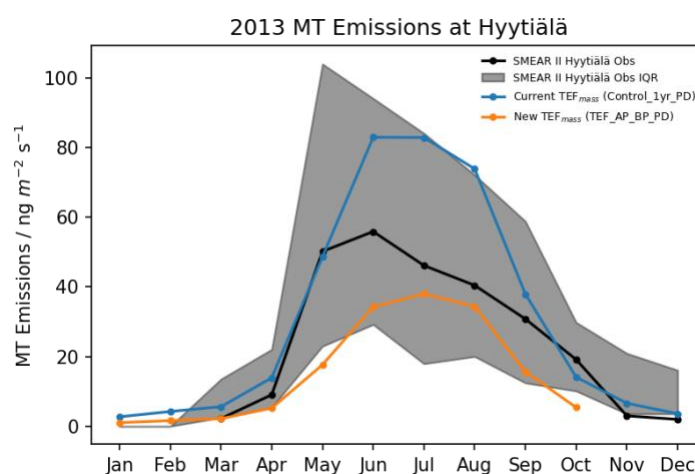
Given that the primary focus of our paper is the C4 grass EFs, we decided to include only a brief section on this analysis in the manuscript (new Section 4.4), highlighting that the new TEF$_{mass}$ values did a reasonable job. We have also included the above figure in the SI as new Fig S2. While it could be argued that validating all plant functional types would be ideal, we believe that the current analysis is sufficient for the scope and objectives of this paper. The additions are given below.

Section 3.3

We also used monoterpene emission data measured at the SMEAR II site in Hyytiälä (https://smear.avaa.csc.fi; last accessed 19th March 2023) to evaluate the change in terpene emissions

4.4 Terpene Emission Evaluation

While the primary focus of this paper is correcting the error with the emission factors for C4 grasses, we also performed a comparison of monoterpenes emissions measured by the SMEAR II station in Hyytiälä in the boreal forest with emissions from simulations using the current TEF$_{mass}$ (Control_1yr_PD) and updated TEF$_{mass}$ (TEF_AP_BP_PD) values. We found that new the TEF$_{mass}$ yielded emissions compared well to observations (Fig S2).

p16l508-511: how much could the bias be due to differences in climate between sim and obs? are those sims nudged? I believe they are, but maybe a comment on that fact may help. Even if nudged, there will be significant differences in climate. Important?

All simulations used for observation comparison are nudged for temperature and horizontal winds, greatly reducing whole atmosphere differences in climate between the model simulations and reality. Therefore, we think it is not fully appropriate to say there will be a "significant" difference in climate. However, we acknowledge that the lowest 11 model levels (approx. 700-1000 m) are not nudged so there will be some divergences here between model simulation conditions and reality although again this is tempered by the nudging applied to the higher levels.

To clarify this, we have made the following amendment to line 509 onwards.

We compare the output from the PD simulations to the CRiS observed isoprene columns (Section 3.3) for January, April, July and October 2013 (Fig 4). The use of nudging significantly reduces the difference in meteorology between the simulations and reality, greatly improving the comparability of modelled and observational data. However, the lowest 11 model levels (approx. 700-1000 m) are not nudged so there will be some differences between the model simulation conditions and reality in the boundary layer, although this is tempered by the nudging applied to the higher levels. ~~Figure 4 shows the comparison of observed and simulated isoprene columns from January, April, July and October 2013.~~

p17l530: The observations in are introduced without prior discussion. No references are offered. Please add references and discuss background a bit.

We agree with the reviewer that the introduction of observations could be clearer in the manuscript. We have included a reference to this new Section 3.3 when discussing comparison of the model data to observations (see amendment comment relating to p16l508-511). We have also added a reference to this section when discussing the C4 emission observation comparison in Section 4.3 (line 535 onwards).

Given the major change to the IEF$_{mass}$ values of C4 grass, the isoprene emissions from C4 grasses were compared to observations in southern Africa (Section 3.3, Fig 5).

In response to comments raised by Reviewer 2 we have also provided additional detail of the CrIS satellite product.

p17l335: I am not sure I understand the argument for introducing the scaling factor here. Isoprene emission are zero at night both at the observation sites and in iBVOC (there is a diurnal cycle in the model representing real

world conditions). So, why is the scaling need - and what data is scaled (I presume the reference is to the model). Please elaborate.

The field measurements were only taken during the day and missed the period where isoprene emissions would have been essentially zero at night. Klinger et al (1998) reports "All measurements were done during midday" (P.1444). Otter et al (2022) reports "Measurements were made between 7:30 and 11:30 a.m. and 14:30 and 16:30 p.m." (P.4267). Guenther et al (1996) reports "Midday net emission fluxes from the canopy were typically 3 to 5 mg C m^{-2} h^{-1}, although net isoprene deposition fluxes of-0.2 to -2 mgC m^{-2} h^{-1} were occasionally observed in early morning and late afternoon." (Abstract).

However, for this comparison we used monthly average model output which means that approximately half of the data points going into the model value would have been zero, halving the average value, hence the need for a scaling of 2. The following text was added from line 541 onwards.

(Emission measurements were only taken during the day while the use of model monthly average values mean that approximately half of the data points going into the model value will been zero, halving the model's average.)

p19l609-611: This sentence needs discombobulation and revision.

I have split this sentence into two. The first states that separating terpenes into α-pinene and β-pinene tracers and adding sesquiterpenes would be beneficial. The second explains why.

The expansion of iBVOC to speciate terpenes into separate α-pinene and β-pinene tracers ~~as~~ and the ~~well~~ addition of ~~as adding~~ new molecules, such as sesquiterpenes, would be beneficial for simulating atmospheric compostion. α-pinene and β-pinene display different chemical reactivity while sesquiterpenes can ~~influential~~ suppress ~~for~~ local O$_3$ and affect SOA formation by producing ~~including~~ highly involatile species which can nucleate new particles without sulphuric acid (e.g., Bianchi et al., 2019; Weber et al., 2020). ~~would also be beneficial.~~

p20: Data and Code availability. I appreciate that there are certain restrictions on the UM code and thus sharing is very complicated. However, this is not the case for all the data (and the code to process them), that heas been used in the plots and tables of this paper. All the data used to produce the plots and tablesas well as the code used to produce them must be made available publicly according to GMD policy. Ammend data availability section accordingly.

We have uploaded all data and analysis code to Zenodo with the following DOI 10.5281/zenodo.7741131.

We have added text to this effect in the Data Availability section.

p27: reference Weber et al., 2021 --> needs to be updated to Weber et al., 2022, I believe.

This reference has been updated.

Reviewer 2

The authors have worked from different perspectives to improve the estimation of BVOC emissions in UKESM1. They mainly accomplished this by integrating values, land cover fractions, and SLW from various sources into the model. The authors also compared the modeled isoprene column with satellite data, and compared modelled emission from C4 grass with field data.

This effort is likely seen as a noteworthy accomplishment by the UKESM community, as it improves the accuracy of emission magnitudes and responses to afforestation. However, further evaluation of the data sources used in the model and the model outputs are VERY necessary as the biases are even bigger after all these changes made in the model. Then, the authors' decision to scale certain variables, such as temperature, and not others raises questions. What scientific questions are they trying to answer, and how has this influenced their decision to only scale temperature and not other variables?

The method description needs a lot of clarity, since as I read it now, I have difficulties to understand the reasons to compare so many different setups in the model. Why can't you evaluate these different dataset first and then only take the best one into your model. Then in the Maxforest scenario, the authors have employed highly intricate methods in an attempt to isolate interactions between multiple factors by creating artificial scenarios. However, the current presentation of these methods can be challenging to comprehend, making it difficult for readers like myself to fully understand the information. A clearer text with the addition of a schematic diagram would greatly enhance the readability and overall understanding of these scenarios.

We thank the reviewer for the constructive comments and are pleased they find our manuscript useful for the UKESM community

Detailed comments:

The readability of the abstract needs to improve. By reading the current version of the abstract without reading the main text yet, I cannot understand the motivation to do these changes in the model, what "interactive" BVOC means, how these new EFs are calculated and why these are linked to LULC?

We have improved the readability of the abstract as suggested by the reviewer. As for 'interactive', it is a common modelling term used to denote the fact that a process is calculated not by fixed input supplied to the model but by other diagnostics calculated by the model during its integration. In the abstract, we believe the reviewer refers to the name of the UKESM BVOCs scheme. To make the word "interactive" clearer, we have used italics. The abstract reads now:

Biogenic volatile organic compounds (BVOCs) influence atmospheric composition and climate and their emissions are affected by changes in land use and land cover (LULC). Current Earth System Models calculate BVOCs emissions using parameterisations involving surface temperature, photosynthetic activity, CO_2 and vegetation type, and use emission factors (EFs) to represent the influence of vegetation on BVOCs emissions. We present new EFs for the *Interactive* BVOC Emission Scheme (iBVOC) used in the United Kingdom Earth System Model (UKESM), based on those used by the Model of Emissions of Gases and Aerosols from Nature (MEGAN) v2.1 scheme.

Our new EFs provide an alternative to the current EFs used in iBVOC, which are derived from older versions of MEGAN and the Organizing Carbon and Hydrology in Dynamic Ecosystem (ORCHIDEE) emission scheme. We show that current EFs used by iBVOC result in an overestimation of isoprene emissions from grasses, particularly C4 grasses, due to an oversimplification that incorporates the EF of shrubs (high isoprene emitters) into the EF for C3 and C4 grasses (low isoprene emitters). The current approach in iBVOCs assumes that C4 grasses are responsible for 40% of total simulated isoprene emissions in the present day, which is much higher than other estimates of ~0.3-10%.

Our new isoprene EFs substantially reduce the amount of isoprene emitted by C4 grasslands, in line with observational studies and other modelling approaches, while also improving the emissions from other known sources, such as tropical broadleaf trees. Similar results are found from the change to terpene EF.

With the new EFs, total global isoprene and terpene emissions are within the range suggested by literature. While the existing model biases in isoprene column are slightly exacerbated with the new EFs, other drivers of this bias are also noted. The disaggregation of shrub and grass EFs provide a more faithful description of the contribution of different vegetation types to BVOC emissions, which is critical for understanding BVOC emissions in the pre-industrial and under different future LULC scenarios, such as those involving wide scale reforestation or deforestation. Our work highlights the importance of using updated and accurate EFs to improve the representation of BVOC emissions in Earth System Models and provides a foundation for further improvements in this area.

L58-62, It will be interesting for readers to know what types/magnitudes of impacts were found in Weber et al., 2022 study.

We have added the following sentence to line 62.

The warming effect of BVOC doubling was 43% smaller when using the more up to date BVOC chemistry in UKESM1.

L64-66, it is not clear. Many models, such as MEGAN, do simulate emissions' dependencies on meteorology, CO_2 and land surface cover. I did not understand this point! So what is lacking in the model at this stage?

This aim of this paragraph is to convey to readers the fact that while BVOC chemistry must be simulated accurately (as shown by the previous paragraph), BVOC emissions must also be simulated accurately. This sets up the importance of this paper's improvement to emission factors in UKESM1. We summarise the general approach to simulating emissions, providing readers with the necessary background to understand the detail in Section 2, and highlight the importance of emission factors in simulating BVOCs.

To increase clarity, we have amended the first sentence (line 64 onwards):

While the simulation of BVOC chemistry is important for model performance, ~~However, to improve overall model performance,~~ the emissions of BVOCs must also be simulated as faithfully as possible with inclusion of the dependencies on meteorology (temperature and solar radiation), atmospheric composition (CO_2) and land surface cover.

With regard to the reviewer's comment on models simulating the dependency of emissions on meteorology, CO2 and land surface cover since, we are in complete agreement with them, as shown by line 66 onwards.

Within climate models this simulation is often performed by specific modules such as iBVOC (Pacifico et al., 2011) or the Model of Emissions of Gases and Aerosols from Nature (MEGAN) v2.1 (Guenther et al., 2012). These modules combine external variables (temperature, CO_2, photosynthetic activity etc.) with the vegetation distribution and vegetation-specific emission factors (EF) in a grid cell to calculate emissions of various BVOCs for that cell.

To emphasise the importance of emission factors and link this paragraph to the main aim of this study, we have added the following sentence from line 73 onwards.

Thus, emission factors provide a link between vegetation cover (i.e. LULC) and BVOC emissions and are central to simulating emissions accurately with incorrect values driving model biases. Updating emission factors in UKESM is the major focus of this study.

We believe this clearly establish the state of the science approach to simulating BVOC emissions and makes clear to readers how this paper builds on this.

L81, so why does C4 have such a high emission factor in iBVOC then?

As we discuss in line 123 onwards, the erroneously high emission factor for C4 grass in the current version of iBVOC arose due to the adoption an unsuitable emission factor from the ORCHIDEE scheme when the modelling of the vegetation in UKESM went from 5 to 13 plant functional types (PFTs). The emission factor taken from ORCHIDEE was an amalgamation of the emissions factors of C4 grass (low emitters) and shrubs (high emitters) which was used in ORCHIDEE since that scheme does not differentiate between shrubs and grasses for this purpose (line 139 onwards). It is this error which this paper seeks to address.

L173-175, I think it is more justifiable if there are studies that actually evaluate the performance of MEGAN-modelled emissions for grass- or shrub-dominated areas, rather than directly using their values to your model because they have separated these PFTs. It might be the case that these EF values in MEGAN were assigned without ground measurements. By adding these 'unvalidated' EF could lead to adding another layer of uncertainties to your model.

The decision to recalculate emission factors using MEGAN values as a starting point was taken because the factor currently used in iBVOC for C4 grass is clearly incorrect. It is three times higher than the C4 grass emission factor in the original 5-PFT version of iBVOC (Pacifico et al., 2011) (originally 8, rising 24 $\mu gC\ g^{-1}\ hr^{-1}$), reasons for which are explained in the manuscript, and also contradicts the conclusions of other studies not affiliated with MEGAN or iBVOC; e.g., Loreto and Fineschi (2015) who state that isoprene emissions are "virtually absent" in C4 species based on measurements. Furthermore, the original 5-PFT iBVOC emissions factor for C4 grass is based on an earlier version of MEGAN (Guenther et al., 1995) so our approach is not only correcting a clear error introduced on going from 5 to 13 PFTs in iBVOC, but it also brings iBVOC into line with a newer version of the same scheme on which it was originally based.

In terms of the origin of the emission factors used by MEGAN, Guenther et al (2006) acknowledges that there are few measurements of isoprene emissions from grasses relative to trees (Section 3.1.2). However, the emission factors used by MEGAN for grasses are calculated using measured emissions (Guenther et al., 2006) and so, by extension, the emission factors proposed in this study are also based on measured emissions.

L182: what are the sources of these PFT distribution maps used for CESM and UKESM1?

In this section, the UKESM1 PFT maps comes from the land use simulated by the fully coupled historical simulations performed for CMIP6. In these runs, each land grid cell has set crop and pasture fractions with the remaining 9 PFTs (5 tree PFTs, 2 grass PFTs and 2 shrub PFTs) competing for spacing in the remainder of the cell (Sellar et al., 2020). The crop and pasture fractions were taken from CMIP6 Land Use Harmonization project v2h data set (LUHv2h) (Hurtt et al., 2020).

In CESM, the PFT maps come from the LUHv2 dataset for pre-2015 and the SSP3-7.0 land use data for the post-2015 runs.

L223-224: the degrees of impacts from different landcover datasets should be dependent on the area of study and also the differences in emission features of these PFTs. I wonder if the authors have actually tested the impacts from these different landcover datasets and if not, it needs justification.

We agree that the variation in simulated land cover will lead to variation in simulated isoprene and terpene emissions.

We did explore how the new EF values performed when LULC from CESM was employed (with the necessary lumping of PFTs). For the PD, the IEF_SLW_UKESM_PD EF values yielded emissions of 380 Tg yr⁻¹ while the IEF_SLW_CLM5_PD EF values yielded 420 Tg yr⁻¹. These are lower than the 457 Tg yr⁻¹ and 490 Tg yr⁻¹ simulated when same EF values were used with UKESM LULC but still well within the range of simulated emissions compiled in Fig 1 of Messina et al (2016) which runs from 310-680 Tg yr⁻¹. To clarify this, we have added two further rows to Table 4 with these results, denoting the runs IEF_SLW_UKESM_PD_CESM_LULC and IEF_SLW_CLM5_PD_CESM_LULC.

Thus, variation in LULC does make a difference to simulated BVOC emissions. However, since the iBVOC scheme is likely to be used exclusively in UKESM for the foreseeable future, its performance when coupled to UKESM land cover is of greatest importance. Therefore, having demonstrated to the reader the impact of LULC

uncertainty, we believe it is acceptable for this manuscript to focus on evaluating the new emission factors when UKESM LULC is used.

We have made the following additions to the manuscript:

Section 3, Line 380:
We also performed two UKESM1 simulations using LULC taken from a PD CESM2 simulation (with PFTs lumped as described in Section 2) to assess the influence of the underlying simulated LULC on emissions. These simulations, IEF_SLW_UKESM_PD_CESM_LULC and IEF_SLW_CLM5_PD_CESM_LULC (Table 4), used the same IEF values as IEF_SLW_UKESM_PD and IEF_SLW_CLM5_PD respectively.

Section 4, Line 488:

When UKESM1 LULC was replaced with CESM2 LULC, isoprene emissions are 380 Tg yr^{-1} (IEF_SLW_UKESM_PD_CESM_LULC) and 420 Tg yr^{-1} (IEF_SLW_CLM5_PD EF). These values are lower than the 457 Tg yr^{-1} and 490 Tg yr^{-1} simulated using the same IEF values and UKESM LULC, yet they are still well within the range of simulated emissions (310-680 Tg yr^{-1}) of Fig 1 of Messina et al (2016). This highlights the influence of uncertainty in LULC on BVOC emissions but, as iBVOC is chiefly for use with UKESM1, we will focus on the simulations using UKESM1 LULC.

We also reiterate the wider point about the importance of LULC on BVOC emissions in our summarising statements with the addition to Section 4.5.

Section 4.5

Simulation of external factors including land cover (cf. the effect of swapping UKESM and CESM LULC on simulated emissions; Table 4), surface temperature and meteorological conditions (e.g., droughts and floods) also affect BVOC emissions (eg, Sheil., 2018; Yáñez-Serrano et al., 2020).

L239-241, What are scaled and unscaled approaches? No explanation before.

The reviewer is correct to point out this inconsistency. In this case "unscaled" referred to the SLW from CLM5 which had not been scaled by a factor of 2 to account for the conversion between total mass and mass of carbon in the leaf. This was considered early in the work for comparison but the removed, as the texts states. We have removed this sentence.

Figure 1 shows the three SLW datasets with the CLM5 and ORCHIDEE values lumped into UKESM1 PFTs. We find reasonable agreement, particularly between UKESM1 and ~~scaled~~ CLM5 for the major emitting species. ~~Therefore, we dispense with the unscaled CLM5 approach (not shown) and only use scaled CLM5 SLW values (referred to hereafter simply as CLM5 SLW) along with the (scaled) ORCHIDEE and UKESM1 values.~~

Equation 4. I would imagine it should be more correct to directly calculate the emission factor of MEGAN at 30 celsius, and instead of getting a temperature scaling based on the temperature response of your model. As what has been implemented in the model now based on Equation 4, it forces MEGAN to follow the temperature response curves in your model. I don't think it makes sense.

We would not agree that applying the MEGAN v2.1 scaling is necessarily better than the using the temperature scaling considered by iBVOC. Both scalings are based on experimental parameterisations and represent different approaches to capturing the influence of temperature on BVOC emissions, and a range of parameter values is in this case desirable as a method of sampling uncertainty. The emissions factors and other parameterisations in MEGAN v2.1 (CO_2-inhibition, photosynthesis etc.) are independent of the temperature dependence. The iBVOC temperature dependence could just as readily be used in MEGAN v2.1, provided the reference temperature is corrected for which is what we aim to do with this scaling.

We also note that that the sophistication of the MEGAN temperature scaling hinders using the suggested approach. This is because MEGAN's temperature dependence, described by the activity factor γ, considers the current leaf temperature (T) as well as the average temperature over the last 24 (T_{24}) and 240 (T_{240}) hours (Eq. 8-10; Guenther et al., 2012).

Where T_s = 297 K (standard conditions), C_{T1}= 95, C_{T2}= 230 and C_{eo}= 2.

Thus $\gamma = f(T, T_{24}, T_{240})$

We do not believe it is appropriate to substitute 303.15 K for T_{24} and T_{240}, as this value for 24-hour or 240-hour averages is not representative of the actual temperatures experienced in most regions with high BVOC emissions, compared to the standard condition temperature value of 297 K in MEGAN. Thus, the parameterisation is likely to be less reliable if T_{24} and T_{240} were also set to 303.15 K.

Places where 24-hour average temperature can exceed 303.15 K are more likely to be in the middle of hot deserts than in rainforests or grasslands while places with a 240-hour average of 303.15 K are even more unlikely to have significant vegetation. For example, one of the hottest weather stations in the world is at Tamanrasset, in the Algerian Sahara, where the average daily mean at the height of summer is 29.2 °C (https://weatherspark.com/y/51498/Average-Weather-in-Tamanrasset-Algeria-Year-Round; last accessed 27th March 2023). By comparison, Manaus in the middle of the Amazon, has a daily mean of up to 28 °C (https://weatherspark.com/y/28814/Average-Weather-in-Manaus-Brazil-Year-Round; last accessed 27th March 2023).

L270-271: why are terpene emissions from broadleaf deciduous trees PAR-independent? Please clarify this!

While isoprene is generally emitted immediately after production, some plant species can store terpene and release them gradually over a period of time, greatly reducing the link between PAR/photosynthesis and terpene emission. Monoterpene emissions from needleleaf trees are mostly from stems and bark (Simpraga et al. 2019), whereas isoprene is mostly emitted from leaves (e.g., Sharkey et al. 2008) and is therefore more responsive to PAR.

In iBVOC, this PAR-independent approach for terpene emissions is assumed to be dominant for all PFTs except for tropical broadleaf deciduous trees where a 50:50 weighting is applied to represent the PAR dependent and PAR-independent emissions.

We acknowledge this could have been described more clearly in text and have made some amendments.

Line 274

iBVOC also applies a temperature dependence to terpene emissions (T_{terp}) in the 13-PFT setup for all PFTs, except for Broadleaf Deciduous trees whose parameterisation we describe later that are PAR-independent (Pacifico et al., 2011) (Eq. 5).

Line 285
In iBVOC terpene emissions for Broadleaf Deciduous trees have are assumed to have a PAR-independent component and a PAR-dependent component (terpene emissions for all other PFTs are assumed to be entirely PAR-independent). In a similar approach to MEGAN v2.1 (Section 2.2; Guenther et al., 2012), the PAR-independent component uses the terpene temperature dependence (T_{terp}; Eq 5) while the PAR-dependent component uses the isoprene temperature dependence (T_{isop}; Eq. 3) along with an additional term representing photosynthesis. These components have in a 50:50 weighting with the latter having the T_{isop} dependence We and we therefore use an average of T_{isop_scale} and T_{terp_scale} for the temperature scaling, $T_{terp\ BrDe\_scale}$, of this PFT (Eq. 7).

We have also corrected Eq.7 since it should have referred to the scaling factors, $T_{terpene\_scale}$ and T_{isop_scale}, not the temperature dependencies themselves.

$$\cancel{T_{terp_{BrDe}} = 0.5T_{terp} + 0.5T_{isop} = 1.79}$$

$$T_{terp\_BrDe\_scale} = 0.5T_{terp\_scale} + 0.5T_{isop\_scale} = 1.79$$

L282-283 Why PAR-dependent should correct for temperature response?

We believe this point is linked to the preceding point regarding our initial attempt to explain the PAR-dependent and PAR-independent pathways for terpene emissions from broadleaf deciduous trees.

As discussed above, in iBVOC the PAR-dependent and PAR-independent pathways have isoprene and terpene temperature dependencies respectively. This is why we applied an average of T_{isop_scale} and T_{terp_scale} for the temperature scaling for terpene emissions for this specific PFT. It is not a case of the PAR-dependent correcting for a temperature response.

L290: MEGAN did not consider photosynthesis.

MEGAN does consider photosynthesis. The dependence on photosynthesis and its parameterisation via consideration of photosynthetic photon flux density is documented in Section 2 of Guenther at al (2012). Our point is that the parameterisation of the dependence on photosynthesis differs between MEGAN and iBVOC.

L289: it needs some descriptions about the differences in CO2 inhibition between iBVOC and MEGAN. And how about the light response?

This is a good point. We have added further detail about the source of each CO_2-inhibition and photosynthesis parameterisations. A direct comparison for the CO_2-inhibition schemes is difficult due to the parameterisations' different dependencies: iBVOC takes the ratio of internal leaf CO_2 concentration to a PFT-specific value while MEGAN v2.1 uses a single parameterisation for all equations which considers atmospheric CO_2.

However, we have added further discussion based on Cao et al (2021) as this work found the CO_2-inhibition effect to be stronger in UKESM/iBVOC (line 291 onwards).

Both models simulate reductions in isoprene emissions with CO_2. The CO_2 inhibition parameterisation in iBVOC follows that of Arneth et al (2007), considering the ratio of the plant's internal CO_2 concentration to a PFT-specific reference value, while MEGAN uses the parameterisation of Heald et al (2009) which is not PFT-specific. Cao et al (2021) found the CO_2 inhibition in UKESM (using iBVOC) to be almost twice that of CESM (using MEGAN) when considering isoprene emissions in the late 21st century.

We have also added extra detail regarding the photosynthesis parameterisation in both schemes (line 295 onwards). We now direct the readers to relevant sections in the MEGAN and iBVOC documentation and emphasise that the two schemes use different approaches when it comes to this parameterisation.

MEGAN parameterises the effect of photosynthesis with a scaling term composed of a light dependent fraction (LDF) and light independent-fraction (LIDF = 1-LDF) with the former a function of the photosynthetic photon flux density averaged over a 24-hour period for both shaded and unshaded leaves (Section 2.2, Guenther et al., 2012). By contrast, iBVOC describes the impact of photosynthesis from the perspective of electron transport, following Arneth et al (2007) as described in Section 2.2 of Pacifico et al (2011).

L394-395: what do you mean by using "PD emission" for this Maxforest scenario. So BVOC emissions were also kept in the present day conditions? Or do you only mean other gas emissions?

We acknowledge this needs to be clarified. All anthropogenic and biomass burning emissions were kept at PD levels, but isoprene and monoterpenes emissions were allowed to change based on LULC change. To clarify this, we have made the following change from line 407 onwards.

All these simulations used PD anthropogenic and biomass burning emissions and GHG concentrations but BVOC emissions were allowed to respond to LULC change ~~to isolate the impact of LULC change on BVOC emissions~~.

L396: I don't understand this paragraph. Why set CO2 to be a constant? What do you mean "CO2 is not emitting", how could these influence the CO2 inhibition effects on isoprene and monoterpene emissions? Is there a run where you have all these interactions turned on? I understand the authors want to isolate the impacts from LULC only, but different environmental conditions, such as CO2, at present and future can influence/determine the magnitudes of impacts from LULC.

Given the large uncertainties in the carbon cycle, it is standard practice for climate models to run with prescribed surface concentrations of CO_2, rather than CO_2 emissions. For timeslice runs, such as the free-running simulations performed under PI and SSP3-7.0 conditions, this means setting a constant CO_2 value appropriate for the specific period (e.g., 280 ppm for the PI, 530 ppm for SSP3-7.0 at 2050). This CO_2 concentration is still used to calculate the effect of CO_2 inhibition of isoprene emissions (i.e., the inhibition is greater in SSP3-7.0 at 2050 than in the PI).

We acknowledge that CO_2 changes between 2010 and 2050 will have an influence on BVOC emissions. However, the aim of the simulations detailed in Table 5 is to compare the change in BVOC emissions between 2010 and 2050 Maxforest LULC when using the current iBVOC emissions factors and when using the proposed updates to these emissions factors. We also want to compare these changes to those simulated by CESM. The key conclusion is that the change in BVOC emissions goes from the unrealistic reduction in emissions when using the current emission factors to a change which much closely resembles CESM. We are not arguing that these simulated changes are what is going to happen, rather we are showing the new emission factors in UKESM produce a more sensible result which more closely aligns with the results in another model using the established MEGAN v2.1 scheme when the same experiment is performed. We chose to use consistent CO_2 in the simulations to avoid the added complication of varying CO_2 inhibition. We do not have a run where all interactions were turned on.

We have added the following text to line 408 onwards.

We compare the change in BVOC emissions between 2010 and 2050 Maxforest land use when the default EF_{mass} values were used to when the new EF_{mass} values were used. We also performed the same experiments in CESM2 (Section 3.2) and compare the change in BVOC emissions between 2010 and 2050 Maxforest land use to the UKESM simulations.

About evaluation dataset:

L438-439: It needs to be described what the CrIS isoprene columns provide and how this data has been used for evaluation. Which runs were used to compare with the CrIS data.

We have added further detail on the CrIS technique from line 443 onwards:

The CrIS is a longwave infra-red Fourier transform spectrometer onboard a satellite which can measure two isoprene IR absorption features. The absorption data collected by the spectrometer are then combined with an artificial neural-network to calculate monthly mean isoprene columns with further detail provided in Wells et al (2020).

Alongside our response to Reviewer #1's comment "*p16l508-511*" we have added the following text from line 514 onwards, which clarifies what runs were compared to CrIS data.

We compare the output from the PD simulations to the CrIS observed isoprene columns (Section 3.3) for January, April, July and October 2013 (Fig 4). The use of nudging significantly reduces the difference in meteorology between the simulations and reality, improving the comparability of modelled and observational

data. However, the lowest 11 model levels (approx. 700-1000 m) are not nudged so there will be some differences between the model simulation conditions and reality in the boundary layer, although this is tempered by the nudging applied to the higher levels.

L485-487: do you know why they differ so largely in terms of the coverage of evergreen tropical trees? Which one is closer to the observation-based landcover maps?

A major driver of the difference between the simulated land cover will be the differences in the parameterisations used by the Joint United Kingdom Land Environment Simulator (JULES) used in UKESM and the Community Land Surface Model version 4 (CLM4) used in Guenther et al (2012), including the different PFTs employed.

CLM4 has two types of tropical tree (broadleaf evergreen and broadleaf deciduous) while JULES/UKESM only has one (broadleaf evergreen). The sum of the area of the two types of tropical tree PFTs in Guenther et al (2012), 28.5×10^6 km^2, is much closer to the 26.0×10^6 km^2 area of the single tropical tree PFT in UKESM. We focused on the direct comparison between the broadleaf tropical evergreen tree PFTs in UKESM and CLM4 because the emission factor from the CLM/MEGAN PFT was used directly to calculate the new the emission factor for the UKESM PFT. We acknowledge this could be made clearer in the text and have made the following change to line 495.

This contribution is greater than the 46% estimated by MEGAN v2.1 (Guenther et al., 2012). However, the area of this PFT in UKESM1 is 67% greater than CLM4 (26.0 vs. 15.6×10^6 km^2). (While this difference in area may seem large, the total areas of tropical trees in UKESM and CLM4 are much more similar if the area of CLM4's deciduous evergreen tropical tree PFT, for which is there is no direct analogue in UKESM, is included.) On an emissions per unit area basis for ~~this~~ the broadleaf evergreen tropical PFT, isoprene emissions in UKESM1 are within 5% of that from Guenther et al. (2012) while terpene emissions are ~25% lower.

CLM4 draws its land cover from Version 1 of the Land-Use History A product (LUHa.v1., Hurtt et al. 2006) while JULES/UKESM uses interactive land cover (as described in the response to the comment pertaining to L.182) so is likely to perform well for Year 2000 conditions. While UKESM uses an interactive approach, we note that UKESM also does reasonably well in tree placement (https://ukesm.ac.uk/portfolio-item/the-virtual-trees-of-ukesm/, last accessed 16th March 2023).

Further evaluating the differences between different land cover simulations and their drivers is beyond the scope of this study.

L517-519: As CrIS data is the only global datasets that are used for evaluation, it is difficult to argue that the changes on emission factors are better if the biases are increased. Please clarify.

We acknowledge that switching to the new EF$_{mass}$ values results in an increase in biases, and we have made this clear to our readers (line 535 onwards). However, it is important to keep in mind that the increase in model bias is much smaller when going from the original to new EF$_{mass}$ values than when transitioning from the standard chemistry in UKESM (Strat-Trop) to the updated isoprene chemistry (CRI-Strat 2), as shown in Weber et al., (2021). Additionally, we emphasise that just because one approach may do better under specific circumstances (such as the PD), this does not mean that it is better overall, as shown by the non-sensical results suggesting that wide- scale tropical tree planting would reduce isoprene emissions when using the original EF$_{mass}$ values in UKESM (Fig 6(a)).

L561: What do you mean that CLM5 SLW approach can capture the SLW of the MEGANv2.1.

We refer here to the final paragraph of Section 2.3.2, specifically the fact that when CLM5 values are used, we can calculate the EF$_{mass}$ values first using Eq.1, and then perform the necessary PFT lumping. By contrast, when UKESM SLW values are used, the lumping of PFTs must occur before the EF$_{mass}$ values are calculated, potentially increasing the uncertainty in the calculated EF$_{mass}$. To clarify this, we have made the following amendment to line 587.

~~The CLM5 SLW approach also captures the SLW of the MEGAN v2.1 PFTs before lumping while the UKESM1 SLW does not.~~ The CLM5 SLW approach allows PFT-specific SLW values to be used to calculate the

L583: the authors never mention how the light responses differ between iBVOCs and MEGAN. How valid is your method that only focuses on temperature scaling, but not the others, like CO2 or light?

In response to the comment regarding L289, we have provided greater detail regarding the parameterisations for light and CO_2 in both schemes and pointed readers to the relevant sections in the documentation papers. We have also highlighted the substantial challenges in comparing the parameterisations for CO_2-inhibition and photosynthesis due to the differences in their implementations in MEGAN v2.1 and iBVOC. Additionally, we want to emphasize that the updated emissions factors presented in this study are not definitive and that further improvements to the CO_2-inhibition and photosynthesis parameterisations in iBVOC may be also necessary. This point has been made clear in Section 4.5 of the text.

Our approach of converting variables from one scheme to another is not without uncertainties. However, we have extensively evaluated the performance of the model with our approach in both present day and other scenarios (PI, SSP3-7.0 at 2050 and the Maxforest scenarios) and have shown that our approach produces sensible results. Importantly, our approach is expected to improve UKESM1's ability to capture the effect of LULC change on BVOC emissions, which is currently limited by the use of the current emission factors.