Reply to Reviewer 2

We sincerely appreciate the two reviewers for their constructive comments to improve the manuscript. Reviewer 2's comments are reproduced below with our responses in blue. The corresponding edits in the manuscript are highlighted with track changes.

Major Comments

MOFLUX Point Comparisons – Much of this work is based around tuning the emissions scheme to observations at one location: the MOFLUX field site. Tuning a global model to one individual site is suboptimal, but necessary in this case given the limited data available on isoprene emissions and drought. However, more work should be done demonstrating that this tuning is not compensating for substantial model errors that lead to differences in prediction.

At minimum in order to assess the validity of this tuning factor, it would be useful to see the model performance on other variables necessary for predicting isoprene emissions. Example pertinent questions include:

Does the model properly simulate meteorological drivers of emissions at the MOFLUX site?

Response: Temperature is the main driver of biogenic isoprene (Mishra and Sinha 2020; Jiang *et al.* 2018). In response to the first reviewer, we included the timeseries showing daily averaged temperature compared to observed at the MOFLUX site during MAY-SEP 2012 in the updated supplement as **Fig. S10** and is included below as **Fig. R1**. ModelE does a reasonable job reproducing the temperature at the site which gives us confidence the meteorological drivers of biogenic isoprene are correct. We used nudged NCEP meteorology to simulate 2003-2013 and any changes in the meteorology are due to interactions in the model.

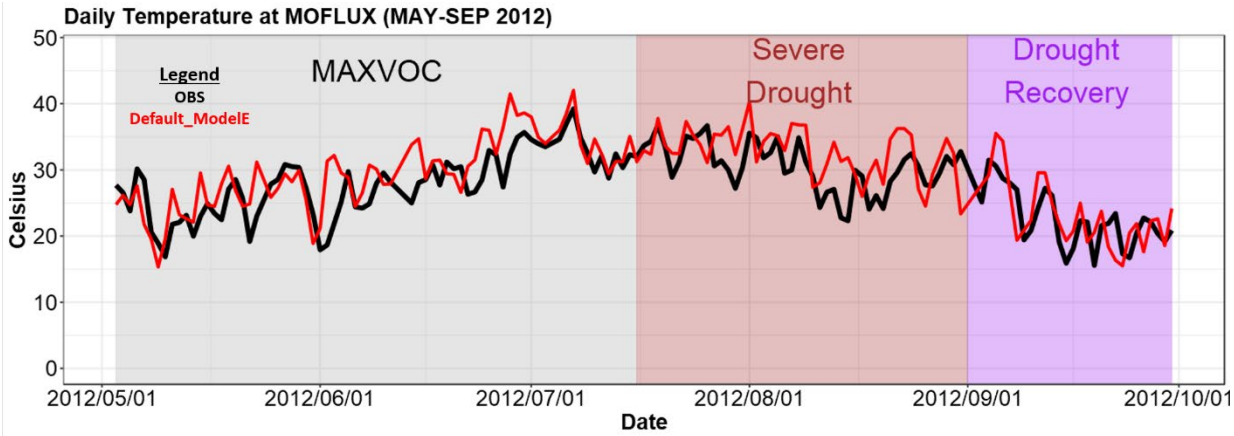

Figure R1: shows the timeseries of daily averaged (LST) temperature at MOFLUX site for MAY-SEP 2012 in Celsius. The observed temperature is shown in black and red shows Default_ModelE.

Gu *et al.* (2006) detail how the exchange of latent and sensible heat fluxes is one of the most important aspects of land-atmosphere coupling as these energy fluxes are affected by partitioning

of net radiation absorbed by the surface, which influence atmospheric dynamics, influence boundary layer structure, cloud development, and rainfall. Thus, we verified latent heat and sensible heat at the MOFLUX site and compared observed to simulated during MAY-SEP 2012, which we have included in the revised supplement as **Fig. S11**. We found from MAY-SEP 2012 Default_ModelE does a reasonable job reproducing hourly sensible heat with a correlation coefficient (R) of 0.83 and slope of 1. For MAY-SEP 2012, Default_ModelE has a R of 0.60 and slope of 0.52 when comparing to observed hourly averaged latent heat as shown below in **Fig. R2**.

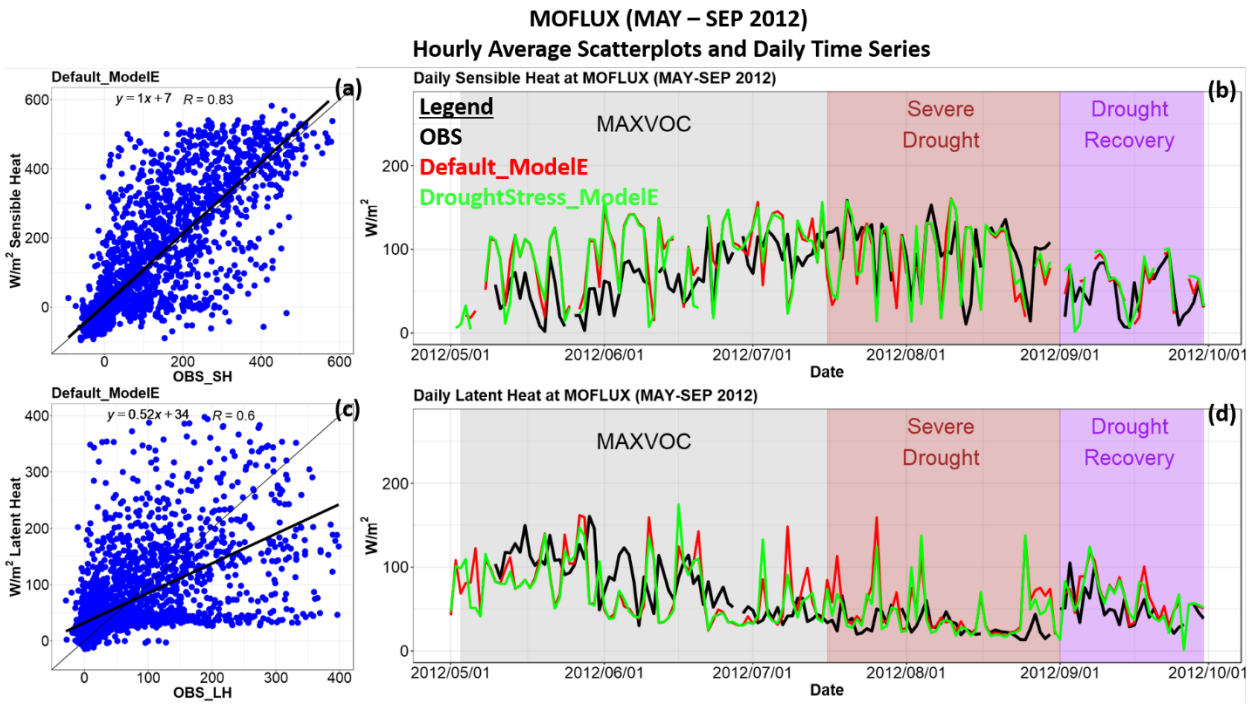

Figure R2: (a) shows the hourly averaged scatterplot comparing observed sensible heat (W/m2) to Default_ModelE for MAY-SEP 2012 at MOFLUX and (b) shows the daily averaged sensible heat timeseries comparing observed (black), Default_ModelE (red), and DroughtStress_ModelE (green) across the three periods of interest, MAXVOC (grey), Severe Drought (brown), and Drought Recovery (purple). (c) shows the hourly averaged latent heat (W/m2) of observed compared to Default_ModelE simulation for MAY-SEP 2012 at MOFLUX and (d) shows the timeseries of daily averaged latent heat.

Does the land classification in the model match the observed site?
Response: ModelE has MOFLUX grid as 30% deciduous broadleaf and 70% C4 crops. C4 crops such as corn, maize, sorghum, pearl millet do not emit large quantities of isoprene, so a majority of simulated isoprene emissions are from the deciduous broadleaf trees which comprise the MOFLUX site.

Does the model properly represent vegetation properties (e.g., LAI, PFT, etc.)?
Response: In our ModelE experiments, the Ent TBM (terrestrial biosphere model) uses prescribed satellite-derived vegetation canopy structure (plant functional type, canopy height, monthly leaf area index) (Ito *et al.* 2020). For our experiment and all GISS ModelE2.1 CMIP6

experiments monthly observed MODIS LAI is prescribed for the year 2004 for all simulated years (Ito *et al.* 2020). The Ent TBM PFTs are derived from the Moderate Resolution Imaging Spectroradiometer (MODIS) land cover and PFT products (Ito *et al.* 2020) and were remapped using a latitudinal distribution to the corresponding MEGAN PFTs. Ent TBM was also verified at several flux sites for several PFTs in (Kim *et al.* 2015).

We verified LAI at the MOFLUX site during 2012 using the NOAA Climate Data Record AVHRR (Advanced Very High Resolution Radiometer) LAI dataset (Vermote 2019) that we averaged on a monthly scale and regridded from 0.05°x0.05° to match ModelE's horizontal resolution. The timeseries of monthly averaged LAI for 2012 at the MOFLUX site is shown below as **Fig. R3b** and included in the supplement as **Fig. S12b**. ModelE simulates LAI quite well compared to observed prior to MAY 2012. During the MAXVOC period, Default_ModelE overestimates LAI, which is also when it is underestimating isoprene. During the severe drought period when Default_ModelE is overestimating isoprene, we still see an overestimation of LAI during JUL and AUG. During the drought recovery period, Default_ModelE shows the same decreasing trend as observed. The overestimation and underestimation of LAI do not appear to be linked to the underestimation/overestimation of isoprene emissions in the model.

Other monthly averaged meteorological drivers at MOFLUX during 2012 are available in the supplement and shown below in a stacked timeseries in **Fig. R3**. Variables shown include (temperature, LAI, relative humidity, shortwave incoming solar radiation, CO_2 flux, vapor pressure deficit (VPD), and canopy conductance) are compared to observed when observations are available in **SI Fig. S12**. Soil moisture by layer is shown in **SI Fig. S14** and below as **Fig. R4**. The model on the monthly scale is able to capture temperature, relative humidity (RH), and incoming shortwave solar radiation compared to observed at the MOFLUX site reasonably well. The model does overestimate monthly CO_2 flux during the MAXVOC period and severe drought periods as shown by **Fig. R3e**. Observed measurements were not available for vapor pressure deficit (VPD) nor canopy conductance, but are shown to characterize model performance in **Fig. R3f,g,** respectively. It is interesting to note canopy conductance is highly responsive to beginning drought conditions during MAXVOC period and shows minimum during severe drought period with recovery at the end of the period. This responsiveness suggests it could be used as a variable for future drought parameterizations.

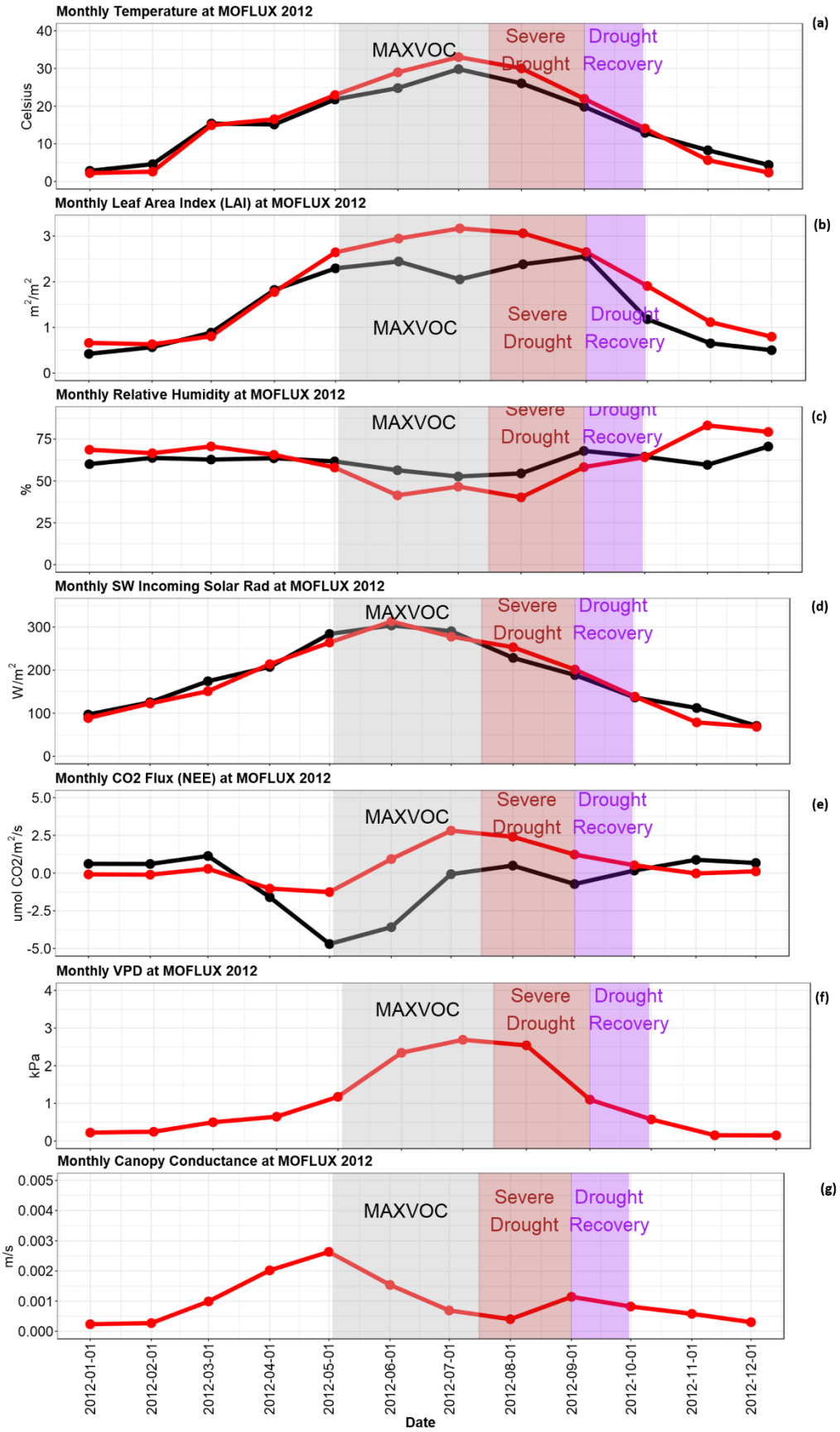
Monthly Temperature at MOFLUX 2012
(a)
Celsius
MAXVOC
Severe Drought
Drought Recovery
Monthly Leaf Area Index (LAI) at MOFLUX 2012
(b)
m²/m²
Monthly Relative Humidity at MOFLUX 2012
(c)
%
Monthly SW Incoming Solar Rad at MOFLUX 2012
(d)
W/m²
Monthly CO2 Flux (NEE) at MOFLUX 2012
(e)
umol CO2/m²/s
Monthly VPD at MOFLUX 2012
(f)
kPa
Monthly Canopy Conductance at MOFLUX 2012
(g)
m/s
2012-01-01
2012-02-01
2012-03-01
2012-04-01
2012-05-01
2012-06-01
2012-07-01
2012-08-01
2012-09-01
2012-10-01
2012-11-01
2012-12-01
Date

Figure R3: monthly stacked timeseries of meteorological variables at MOFLUX during 2012: (a) temperature (Celsius), (b) LAI (m^2/m^2), (c) relative humidity (RH) (%), (d) shortwave incoming solar radiation (W/m^2), (e) CO_2 Flux (Net Ecosystem Exchange) (NEE) μmol $CO_2/m^2/s$, (f) vapor pressure deficit (VPD) (kPa), and (e) canopy conductance (m/s). Monthly averaged observed is shown in black for when observations are available and Default_ModelE simulated is shown as red. The periods denoted MAXVOC (grey), severe drought (brown), and drought recovery (purple) are labeled on the timeseries.

Shown below in **Figure R4** is monthly averaged soil moisture by layer and is included in the supplement as **SI Fig. S14**. The upper layers (layers 1-4) show the largest response to beginning drought conditions in MAXVOC period with decreasing soil moisture. The severe drought period continues this behavior with decreasing soil moisture, while the drought recovery period shows an increase in soil moisture due to precipitation events at the end of August. The lower layers (5-6) show the least response in soil moisture with nearly linear behavior.

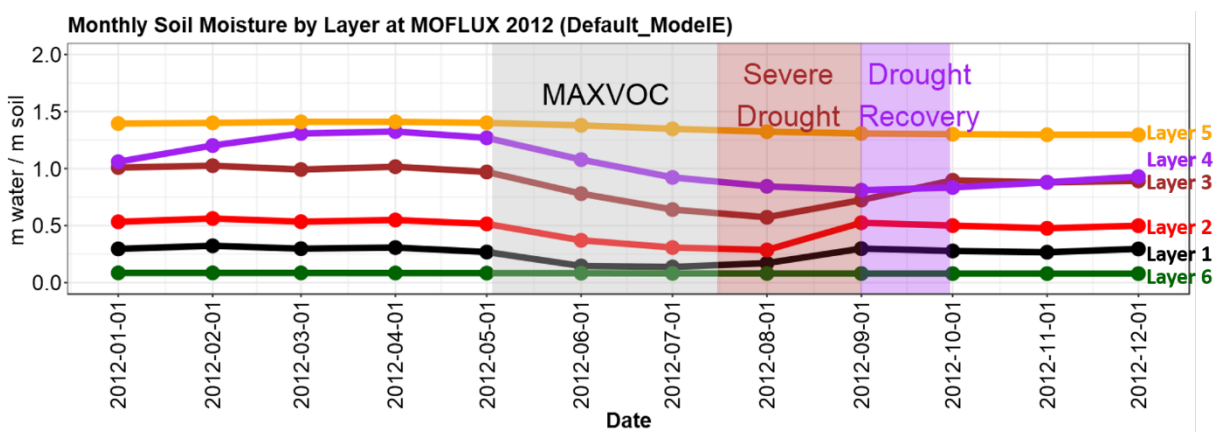

Figure R4: monthly averaged soil moisture for the individual layers of the soil during 2012. Layer 1 (black), layer 2 (red), layer 3 (brown), layer 4 (purple), layer 5 (gold), and layer 6 (green). Simulated soil moisture values are from the simulation (Default_ModelE).

How do the differences in simulated emissions and observations compare with the substantial uncertainty estimates in the MEGAN model (Guenther et al., 2012)?

Response: Guenther *et al.* (2012) states that MEGAN global annual totals are within a factor of 2 of top down emission estimates, so a factor of 2 uncertainty is likely in MEGAN2.1. Arneth et al. (2008) evaluated several global models for isoprene and found for 14 models the isoprene ranged from 460-570 Tg C (including one standard deviation of 55 Tg) a year which is close to our global average from 2003-2013 was ~533 533 Tg yr^{-1} of in Default_ModelE and ~~518 Tg yr^{-1} in DroughtStress_ModelE. The differences in isoprene estimates compared to observed at MOFLUX during the severe drought period of 2012 have a normalized mean bias of 76.10% overestimate, which is less than a factor of two uncertainty that is possible in the MEGAN2.1 model.

The scatterplot in Figure 2 and associated discussion shows a very limited improvement in R2

(0.03). Since this work is entirely focused on water stress, it would be useful to have those metrics only for the water stressed time periods.
Response: Thank you for the comment. Yes, this paper shows a small improvement in R of 0.05 between Default_ModelE and DroughtStress_ModelE for MAY-SEP 2012 at MOFLUX. I have made changes on line 686-687 to make it clearer that the improvements in mean bias and normalized mean bias are reported for the severe drought/water stress period.

Shown below in **Fig. R5** and included in the updated supplement as **Fig. S13** is the scatterplots of hourly isoprene at MOFLUX during the 2012 severe drought period, with the points color coded by water stress values for the simulations, Default_ModelE, DroughtStress_MEGAN3_Jiang, and DroughtStress_ModelE. When comparing the severe drought period in Default_ModelE to DroughtStress_ModelE we do not see an improvement in R despite seeing large improvements of mean bias, but we do see a decreasing slope and lower y intercept. Default_ModelE during severe drought period has a mean of 5.10 mg/m^2/hr ISOP and DroughtStress_ModelE has a mean of 3.31 mg/m^2/hr of ISOP. Shown below in the scatterplots is reduction and tighter fit around 1:1 line. When we examine the daily correlation coefficient the R increases from 0.40 (Default_ModelE) to 0.48(DroughtStress_ModelE) for the severe drought period.

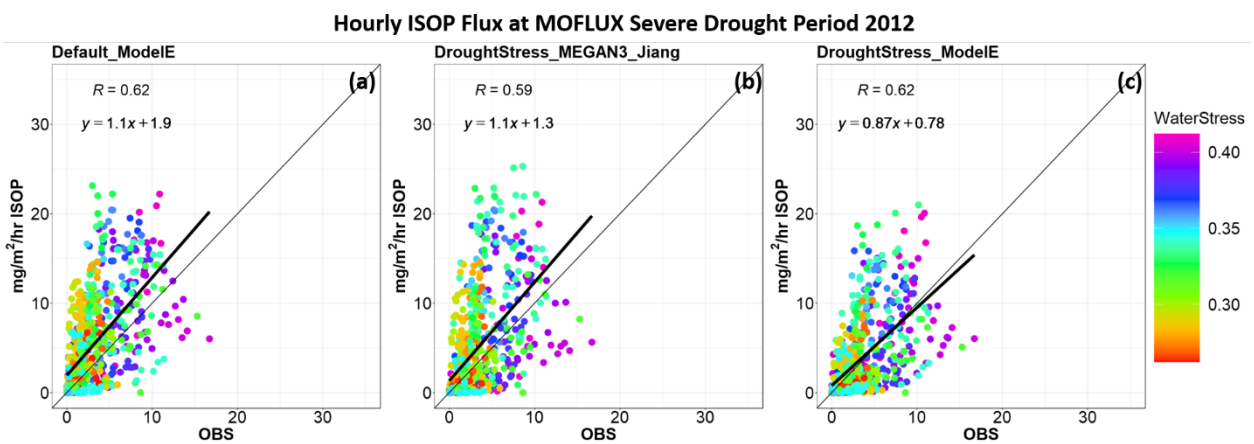

Figure R5: reports the metrics comparing observed hourly isoprene at the MOFLUX site during the severe drought period of 2012 to simulated isoprene (LST). (a) Default_ModelE, (b) DroughtStress_MEGAN3_Jiang, and (c) shows DroughtStress_ModelE with points color coded by the value of water stress.

Model Tuning
The authors recommend applying the drought stress when the model grid cell water stress is in below the 4th percentile. I understand the logic for this choice, but it should be contextualized further. Is there reason to expect that vegetation respond to relative or absolute water stress?
Response: Please see line 257-264 where we include how vegetation respond to water stress. "Vegetation responds to high water stress by undergoing physiological, morphological, and biochemical changes (Seleiman *et al.* 2021). During high water stress plants experience decreasing photosynthetic rate due to stomatal closure, decreasing stomatal conductance,

transpiration, and evaporative cooling. There is also during drought decreasing rubisco efficiency, which is the enzyme used for carbon fixation of atmospheric CO_2 into useable sugar molecules during photosynthesis (Seleiman *et al.* 2021). If stress leads to leaf wilting or excess demand on carbon stores, leaf senescence can occur and hence reduction in leaf area. These are just a few of the ways vegetation respond to water stress, which impact isoprene emissions."

Just like for soil moisture used in previous isoprene drought stress parameterization by (Guenther *et al.* 2012) there is a threshold where the water stress shuts down physiological processes leading to decreasing isoprene emission and eventually cessation, using the MOFLUX site data we tried to pin point when this occurs and how frequently it occurs at the site in order to develop our DroughtStress_ModelE parameterization.

In the model, the Ent TBM simulates response to water stress as a linear reduction in stomatal conductance in response to relative extractive water content in the soil, which results therefore in a reduction of net carbon assimilation of leaves (Kim et al. 2015). The Ent TBM does not simulate a reduction in carboxylation capacity of RubisCO, but this leaf physiological parameter only is responsive to temperature in the model. Since observed LAI is prescribed in the model, any leaf senescence due to stress is not explicitly simulated.

Is this tuning representative of any physical or biological process, or simply statistical?
Response: Please see line 654 where we clarify it is statistical.

Formaldehyde Comparisons – The analysis of formaldehyde retrievals in this work may be lacking relative to the state-of-the-science and does not support the conclusions in the manuscript. For apples-to-apples comparisons between satellite observations of formaldehyde and models, the Air Mass Factor (AMF) should be recalculated and applied to the observations. That was not done in this work. At the very least that point and the associated limitations imposed should be discussed.
Response: Please see line 750–753 where we discuss the limitation of not applying a model calculated air mass factor to the observations. "As this is the first evaluation of tropospheric ΩHCHO in ModelE, a gridded level 3 dataset was used for analysis without applying air mass factor (AMF) using ModelE predicted HCHO profiles, which according to Zhu *et al.* (2016) can lead to an increase in ~38% uncertainty in the southeast U.S.."

As this was the first time the tropospheric HCHO column were analyzed in ModelE the results were unexpected. For the first look at tropospheric HCHO column in this paper we used the already gridded Level3 data, which air mass factors cannot be applied to. If we were to use the L2 daily product from (https://www.temis.nl/qa4ecv/hcho.html) then air mass factor calculation could be applied, but this would require many factors at a high temporal and vertical resolution than the version of ModelE used here and to convert from track swath to lat-lon grid; due to storage constraints was not attempted. Zhu *et al.* (2016) stated that applying AMF could reduce OMI uncertainty in southeast U.S. by ~38% which is still not enough to account for ModelE's overestimation. We have found that there are large differences in tropospheric HCHO column when using NCEP nudged winds versus free-running model winds with less overestimation in free-running simulations. There needs to be more work done to analyze where this disconnect in model performance is coming from, but it is beyond the scope of this work.

The ModelE simulated formaldehyde column disagrees substantially with observations (e.g., Figure 6). It appears as though the column is overestimated by at least a factor of 3. This enormous overestimation is not common across other models of atmospheric chemistry (e.g., GEOS-Chem), and calls into question the validity of ModelE simulated formaldehyde concentrations. While adding the drought stress does improve the simulation, that result alone is not interesting as anything that reduces formaldehyde concentrations would improve the simulation. The authors should make a stronger case as to why the ModelE formaldehyde simulations should be trusted as a useful assessment tool for isoprene emissions changes.
Response: You are correct ModelE in these nudged simulations is overestimating HCHO column. We have added a section explaining the limitations on line 769-773, "It was found that nudged simulations show a large overestimation of HCHO column compared to free-running simulations using model winds. As this study only shows modest decreases in HCHO column we can only conclude that adding isoprene drought stress into a model may reduce HCHO column depending on atmospheric chemistry, but under certain NO_x and VOC limited environments may have another effect."

We have found a discrepancy between nudged and free-running simulations and their HCHO columns in ModelE. We need to explore more where the discrepancy and overestimation is coming from in the nudged simulations as the free-running simulations do not have as large an overestimation as shown below in **Fig. R5**. As shown below in Fig. R5a this is an experiment equivalent to Default_ModelE and shows the eleven-year average of tropospheric HCHO column from 2003-2013 across North America, which falls closer to reported studies of (Zhu *et al.* 2016; Kaiser *et al.* 2018) of 0 to 3.5×10^{16} molecules/cm^2.

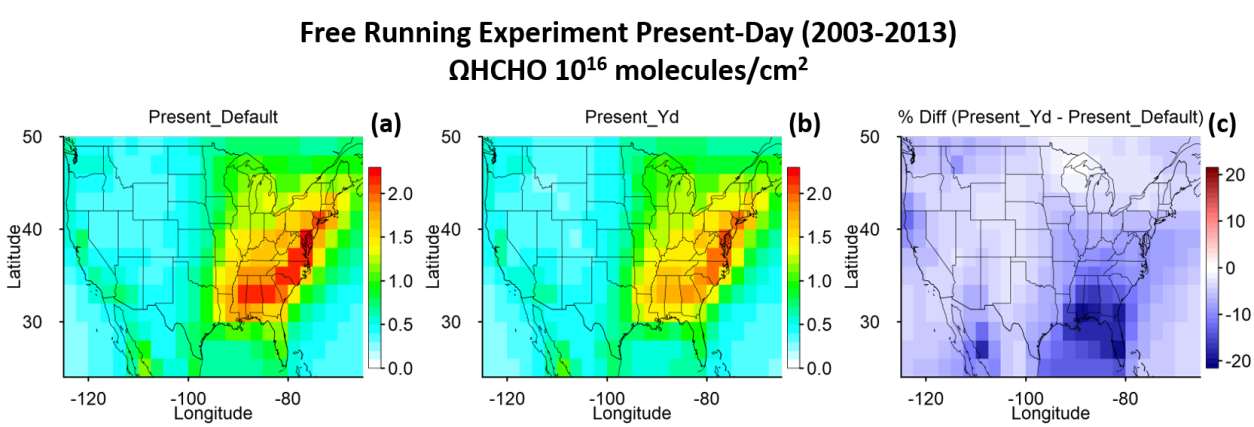

Figure R5: (a) tropospheric HCHO column in free running simulation with same experimental setup as Default_ModelE, (b) tropospheric ΩHCHO for experiment equivalent to DroughtStress_ModelE, (c) shows the percent difference between experiments.

Statistical significance of results

Many of the results here are lacking detailed statistical treatment to understand if the results are either statistically or practically useful, in particular Figure 2, Figure 4, Figure 5, and Figure 7. All these figures and associated discussion describe noisy results. I am sympathetic to

the challenges related to non-drought variability in constraining the process the authors are addressing, but substantially more rigorous assessment is needed before these results can be assessed in depth. For example, the trends shown in Figure 4 do not appear to be significant in any way. They visually look to be a random sampling of points scattered about y = 0, and do not appear to show "decreasing isoprene emissions" as claimed in the text.

Response:
Figure 2 is crucial to show as it shows a quantitative comparison of simulated to observed hourly isoprene for the three simulations Default_ModelE, DroughtStress_MEGAN3_Jiang, and DroughtStress_ModelE and how isoprene values relate to water stress. This figure is needed for the paper, because it is crucial for understanding the distribution of the data for any researchers that may attempt to integrate isoprene drought stress using MOFLUX observations into their model, because it can be used as a comparison for literature purposes.

Figure 4 is a way to statistically show how the distribution of global isoprene is changing in four isoprene emitting hotspots in relationship to SPEI which indicates drought or non-drought conditions. This figure represents the challenge of parameterizing drought stress in global models as the isoprene reductions are not strongly correlated with negative SPEI to indicate drought. SPEI and water stress do not have a very strong relationship and this figure is to show the wide distribution of changes shown due to implementing an isoprene drought stress to other global regions.

Figure 5 shows the percent the difference of isoprene and HCHO column for Eastern and Western U.S. This figure is useful for showing across two very different isoprene emitting regions, which greatly vary in magnitude of emissions how large the reductions in isoprene which are mimicked on a lesser scale by reductions in HCHO column are. This figure is useful for gaining a broad picture perspective of what is occurring across these two regimes.

Figure 7 Shows the relationship between the maximum percent isoprene changes in relation to what is occurring with ozone during these drought periods as a way to see how much the change in the precursors BVOC affects ozone mixing ratio. This figure is crucial to explore if the implementation of isoprene drought stress improves or worsens the simulation of ozone in the model.

Figures R1, R2, R3, and R4 are now included in the Supplementary Materials and related discussions added on line 175-251.

<u>Minor Comments</u>
The introduction includes substantive discussion of drought impacts on SOA, but the analysis does not assess SOA at all, this is confusing.
Response: Our original intent was to analyze $PM_{2.5}$ and compare to observations, with a focus on determine if applying isoprene drought stress improved or worsened simulation of $PM_{2.5}$. However, we found the model underestimated $PM_{2.5}$ and the underestimation made quantifying improvements due to applying isoprene drought stress negligible, so this analysis was not included. Our mentions of SOA are for background literature information.

L548: How was the selection of an alpha value of 100 made? "Best fit" by what metric?
Response: Please see line 595-597 for context. "α =100 had the lowest NMB closest to zero during the severe drought period, and the most improved slope, y-intercept, and correlation coefficient during the summer of 2012."

L657: "there is model agreement" is far too strong of a statement given the large scatter in Figure 2.
Response: This was also addressed by the first reviewer and we have included a revision, so it is not such as strong a statement in line 712-714. "Overall, there is an acceptable level of agreement between measured and modeled fluxes in DroughtStress_ModelE indicating it is a suitable model-tuned parameterization for estimating isoprene emissions during severe drought at the MOFLUX site."

L695-698: This sentence around HCHO overestimation is confusing. Are there any reasons why the authors suspect these reasons are the culprit for overestimation? If so, why were they not addressed in more detail during model development?
Response: Please see line 765-766, and 769-773 for corrections. "It was found that nudged simulations show a large overestimation of HCHO column compared to free-running simulations using model winds. As this study only shows modest decreases in HCHO column we can only conclude that adding isoprene drought stress into a model may reduce HCHO column depending on atmospheric chemistry, but under certain NO_x and VOC limited environments may have another effect."

We did not know when developing the isoprene drought stress parameterization of the severe overestimation of HCHO column in ModelE as this is a climate model and it had never been explored the current HCHO columns during present-day. This overestimation problem will require further analysis and was beyond the scope of this paper.

L747: "clear decreases" are not evident given the substantial variability in the figure. See discussion of statistical significance above.
Response: Please see line 826-827, for correction "For the Eastern U.S. (East) there are visible decreases in the percent reduction of isoprene emission and ΩHCHO during the 2007, 2011, and 2012 drought years."

L823: These changes in HCHO and O3 are very small relative to the large biases that still exist, particularly in rows 2 and 3 of Figure 7.
Response: Yes, the changes in HCHO column and O_3 are small, but there is no worsening of the biases in the model due to including isoprene drought stress and even small improvements are shown.

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