## Response to referee comment #3:

*This paper focused on estimating BVOC emissions in China for the year 2018 by using WRF-CLM-MEGAN. My main concern is about the 'new' knowledge brought up by this paper. The paper used the coupled version of model, but the current results are insufficient to present new knowledge from this simulation or the benefits of using WRF + CLM set up for running MEGAN. From the spatial and temporal pat-terns, we cannot simply see where the improvements are in comparation with previous estimations.*

**Response:** The manuscript was revised much according to three referees' comments.

The novelty in this study is that the BVOCs emission is estimated by including some PFT-specific physiological parameters. These parameters are derived from CLM4, but never considered in the previous BVOC estimation algorithms coupled in the weather forecasting models.

We found the improvements are important (more details could be found in the section 3.2). Firstly, the estimations by using leaf temperature in our study were about 20 % higher than those estimated based on air temperature as in the previous methods. Secondly, the separate treatments of sunlit and shaded leaves in this study, which affect within canopy solar radiation, lowered the estimations by a factor of 2 compared with estimates made by methods neglecting shaded canopy. Thirdly, in this study, leaf temperature and solar radiation were averaged over the past running time at each time step to estimate emission response to weather history. However, in the original code, this response was estimated based on fixed parameters. The improved representation in our study resulted in 50 % higher estimations than those based on fixed values.

The results were within a factor of 2 of most canopy-scale flux measurements and top-down isoprene inventories, indicating an overall good performance of the coupled model (section 4).

*Furthermore, the evaluation with the observation data compared the modelled result from 2018 with literature values from any another year, which is not rigid at all. The differences in measured and modelled site conditions, such as environmental conditions and plant composition were not discussed or compared in the evaluation, instead, the authors concluded that we need more measurement data.*

**Response:** Accepted. The monthly average or total emissions were used for comparison to minimize the influence of short-term differences in meteorological conditions. The differences in measured and modelled site conditions were also included in the revised manuscript.

**Revisions:** (Page 11, Line 329) "We evaluated the inventory against canopy-scale measurements conducted at different sites in China. Given that years of interest in the present study and observations are different, the average data or monthly total emissions were used for comparison.

Using eddy covariance technique, Baker et al. (2005) measured isoprene fluxes in Xishuangbanna, Yunnan Province (21.92°N, 101.27°E). Daytime

isoprene fluxes during the wet season (July 2002) was approximately 1 mg C $m^{-2}$ $h^{-1}$. Dry season (February and March) daytime fluxes averaged about 0.15 mg C $m^{-2}$ $h^{-1}$ and maximum fluxes were over 0.6 mg C $m^{-2}$ $h^{-1}$. Our model predicted a similar daytime average isoprene flux in wet season as 1.5 mg C $m^{-2}$ $h^{-1}$ at this site. The modeled flux for dry season was 1.19 mg $m^{-2}$ $h^{-1}$, higher than observed maximum value by a factor of 2.

Based on Relaxed Eddy Accumulation (REA) technique, emissions of isoprene and monoterpenes of a temperate forest in Changbai Mountain (42.4°N, 128.1°E) were measured during the summer seasons (June, July, August, September) in 2010 and 2011 (Bai et al., 2015). The mean isoprene emission flux was 0.889 mg $m^{-2}$ $h^{-1}$ and the mean total monoterpene emission flux was 0.143 mg $m^{-2}$ $h^{-1}$, and our results estimated emission fluxes of 1.97 for isoprene and 0.37 mg C $m^{-2}$ $h^{-1}$ for monoterpene. The average PAR and temperature during experimental periods were 837.5 μmol $m^{-2}$ $s^{-1}$ and 22.6 ℃, respectively. The simulation resulted in an average PAR of 1160.1 μmol $m^{-2}$ $s^{-1}$ and temperature of 22.23 ℃. The average leaf temperature was 23.37 ℃. The slight overestimation could be attributed to higher PAR simulated in the model.

Using REA method, Bai et al. (2016) measured emissions from a bamboo (*Phyllostachys violascene*s) plantation in Zhejiang Province (30.3°N, 119.57°E) and the average isoprene emission fluxes were 2.8, 1.1, 0.2, 0.1 mg $m^{-2}$ $h^{-1}$ for the experimental periods in July, August, September and October. The predicted monthly average fluxes of these four months were 2.4, 2.3, 3.2, 0.46 mg $m^{-2}$ $h^{-1}$, respectively. Estimations for July and August were within a factor of 2 of observed values. Large discrepancies were found in September and November. The comparisons indicated an overall good performance of the WRF-CLM4-MEGAN in forest areas during wet seasons. However, the large difference associated with estimations for dry areas and seasons clearly suggested that additional investigation and improvements are needed."

*The structure of this paper is not well organized. For example, the data information L151 – 154 were placed in the results section; large amount of model description was placed in the introduction part. The aim or hypothesis of this study is not clear.*

**Response:** Accepted. We rewrote the Introduction and Method and Data sections.

**Revisions:** (Page 2, Line 51) "The MEGAN algorithms have been incorporated into Community Land Model (CLM), the terrestrial component of the earth climate system model, as one step toward integrating biogeochemical processes in the model. In the coupling of MEGAN and CLM, all the physical and biological variables required by BVOC estimation are determined by comprehensive ecological and physiological processes parameterized in CLM at each time step (Levis et al., 2003; Oleson et al., 2010; Lawrence et al., 2011). Process-based models are typically coupled within dynamic vegetation models that have a mechanistic model for leaf

photosynthesis at their core (Arneth et al., 2007; Pacifico et al., 2011; Yue and Unger, 2015). In general, these coupled models are employed to investigate the long-term interactions and feedbacks between terrestrial vegetation and climate change with spin-up and simulation time from tens to thousands of years.

Instead of coupling detailed algorithms within the land surface parameterizations, a simplified version of MEGAN algorithm, the parameterized canopy emission activity (PCEEA) algorithm, has been coupled with weather and climate forecasting models as an independent module to generate online biogenic emission inventory for atmospheric chemistry simulation (Guenther et al., 2006; Sakulyanontvittaya et al., 2008; Fu and Liao, 2012; Henrot et al., 2017). Instead of using a detailed canopy model to calculate leaf temperature and leaf-level photosynthetic photo flux density (PPFD), the PCEEA algorithm parameterizes the modification of these plant physiological variables on emission rates based on ambient temperature and canopy above solar radiation. Although leaf temperature is strongly related to ambient temperature, it is also affected by other ecological conditions such as irradiation and evapotranspiration. Subin et al. (2011) indicated that the strong advection and boundary layer mixing during the day decoupled the air temperature from the vegetation temperature to a great extent, making daytime surface energy budget the primary controlling factors of vegetation temperature changes. Furthermore, due to the different morphological and physiological properties, relationships between air temperature and leaf temperature, and between canopy above PPFD and leaf-level PPFD, vary significantly among tree species. Since the PCEEA algorithm was based on standard MEGAN canopy model simulations for warm broadleaf forests, using the same equations for representations of other plant types leads to unpredictable uncertainties. Leaf temperature and PPFD averaged over the past 24 and 240 h are used in MEGAN algorithm to account for effects of medium-term weather history. However, the PCEEA algorithm obtains the past conditions from a prescribed climatological monthly mean dataset, which could be much different from the real meteorology (Zhao et al., 2016). Therefore, reasonable plant-specific physiological variables are needed to improve the BVOC estimation in weather models.

CLM version 4 (CLM4) was coupled and released with the Weather Research and Forecasting model (WRF), a mesoscale numerical model designed to simulate regional weather and climate, since version 3.5 as one of the land surface scheme options to better characterize land surface processes (Jin and Wen, 2012; Jin et al., 2010; Subin et al., 2011). Because MEGAN has been embedded within CLM as mentioned above, the coupling of WRF-CLM4-MEGAN allowed regional weather forecasting models to estimate BVOC emissions within a comprehensive ecological climatology framework. Besides improvements result from real-time plant physiological

variables derived from land surface parameterizations, sub-grid vegetation compositions represented in CLM4 are also expected to provide a more reasonable estimation in view of the significant variability in basal emission ability among tree species. However, few studies employed the coupled mode to estimate regional BVOC emissions (Zhao et al., 2016)."

*English needs to improve in this paper.*
**Response:** Accepted.

*L35-37, please use more recent global estimations.*
**Response:** Accepted.
**Revisions:** (Page 2, Line 37) "Globally speaking, biogenic volatile organic compounds (BVOCs) emitted by terrestrial vegetation are estimated to be 500 ~ 1100 Tg C $yr^{-1}$, corresponding to about 90 % of the emission total (Guenther et al., 1995; Arneth et al., 2011; Henrot et al., 2017)."

*L45-46, What do you mean with '. . .as an insolated step outside the whole terrestrial ecosystem processes'? Do you actually mean that BVOC processes are not linked to photosynthesis? Another issue here is that the references the authors listed here were just based on one model. It is not a good idea to conclude this is a general problem for modelling BVOCs only based on one model.*
**Response:** Accepted. We reworded the sentence and added other references.
**Revisions:** (Page 2, Line 51) "The MEGAN algorithms have been incorporated into Community Land Model (CLM), the terrestrial component of the earth climate system model, as one step toward integrating biogeochemical processes in the model. In the coupling of MEGAN and CLM, all the physical and biological variables required by BVOC estimation are determined by comprehensive ecological and physiological processes parameterized in CLM at each time step (Levis et al., 2003; Oleson et al., 2010; Lawrence et al., 2011). Process-based models are typically coupled within dynamic vegetation models that have a mechanistic model for leaf photosynthesis at their core (Arneth et al., 2007; Pacifico et al., 2011; Yue and Unger, 2015). In general, these coupled models are employed to investigate the long-term interactions and feedbacks between terrestrial vegetation and climate change with spin-up and simulation time from tens to thousands of years.

Instead of coupling detailed algorithms within the land surface parameterizations, a simplified version of MEGAN algorithm, the parameterized canopy emission activity (PCEEA) algorithm, has been coupled with weather and climate forecasting models as an independent module to generate online biogenic emission inventory for atmospheric chemistry simulation (Guenther et al., 2006; Sakulyanontvittaya et al., 2008; Fu and Liao, 2012; Henrot et al., 2017). Instead of using a detailed canopy model to calculate leaf temperature and leaf-level photosynthetic photo flux

density (PPFD), the PCEEA algorithm parameterizes the modification of these plant physiological variables on emission rates based on ambient temperature and canopy above solar radiation. Although leaf temperature is strongly related to ambient temperature, it is also affected by other ecological conditions such as irradiation and evapotranspiration. Subin et al. (2011) indicated that the strong advection and boundary layer mixing during the day decoupled the air temperature from the vegetation temperature to a great extent, making daytime surface energy budget the primary controlling factors of vegetation temperature changes. Furthermore, due to the different morphological and physiological properties, relationships between air temperature and leaf temperature, and between canopy above PPFD and leaf-level PPFD, vary significantly among tree species. Since the PCEEA algorithm was based on standard MEGAN canopy model simulations for warm broadleaf forests, using the same equations for representations of other plant types leads to unpredictable uncertainties. Leaf temperature and PPFD averaged over the past 24 and 240 h are used in MEGAN algorithm to account for effects of medium-term weather history. However, the PCEEA algorithm obtains the past conditions from a prescribed climatological monthly mean dataset, which could be much different from the real meteorology (Zhao et al., 2016). Therefore, reasonable plant-specific physiological variables are needed to improve the BVOC estimation in weather models."

*L113-115, it is not clear for me why the authors decided to use MODIS LAI, instead of the modelled LAI and dynamic vegetation, and also why not consider CO2 impacts on emissions? Please clarify. MODIS LAI is 8 days intervals, how the author deal with the days between 2 LAI images. Another issue is that: did the authors consider quality flag for the LAI product?*

**Response:** The effects of variations in $CO_2$ concentration was neglected in this study because the simulation was performed for only one year and studies indicated that accounting for $CO_2$ inhibition has litter impact on predictions of present-day isoprene emission (Heald et al., 2009). The main purpose is to improve BVOC estimations in weather forecasting models by using plant-specific physiological parameters. Modeling dynamic vegetation was beyond the scope of this study and required more computing resources and more time for spin up. Compared with the prescribed monthly LAI in the default CLM4, MODIS data provide LAI data for a specific year with high spatiotemporal resolution. We used one LAI image for 8 days. Because the MODIS LAI Collection 6 product shows higher than 90 % main algorithm retrieval rates for most biome types (Yan et al., 2016) and relatively small influence of LAI as described in the Uncertainty section, the quality flag was not considered in our study.

*L121, ". . . and each run covered 31 days . . . " where these runs refer to? Please clarify.*

**Response:** Accepted. We reworded the sentences.

**Revisions:** (Page 6, Line 172) "The meteorological fields were initialized at the start of each model run, which covered one month in order to account for the effects of past canopy climate."

*L148, not clear for me what modification/process have been implemented.*

**Response:** Accepted. We reworded this section.

**Revisions:** (Page 4, Line 117) "The coupling of CLM4-MEGAN improves the BVOC estimations through reasonable driving factors and detailed sub-grid representation, as briefly introduced below. We refer the reader to the description of Oleson et al. (2010) for the details of computations.

1. leaf temperature

Variations in leaf temperature are influenced by net radiation absorbed/emitted by the vegetation and sensible and latent heat fluxes from vegetation. The two-stream approximation is applied to vegetation when calculating solar radiation reflected and absorbed by the canopy. Leaf temperatures are determined by the canopy energy balance equations. Due to the dependence of heat fluxes on vegetation temperature, the Newton-Raphson iteration is used to solve for folia temperature and the vegetation fluxes simultaneously.

2. sunlit and shaded fractions of canopy

The canopy in CLM4 is treated as sunlit and shaded leaves. The leaf fractions of different plant types are determined according to leaf and stem area index and the solar zenith angle at each time step. CLM4 assumed that sunlit leaves receive the absorbed direct beam radiation and the absorbed diffuse radiation apportioned by $f_{sun}$ (the sunlit fraction of the canopy), and that shaded leaves receive the absorbed diffuse radiation apportioned by $f_{sha}$ (the shaded fraction). This division into sunlit and shaded leaves is important in modeling canopy processes, since the sunlit leaves will receive a much higher light flux density than shaded leaves under sunny conditions (Dai et al., 2004).

3. the medium-term weather history

Current MEGAN algorisms use average leaf temperature, solar radiation and leaf fractions over the past 24 and 240 h to account for the influence of past canopy climate. CLM4 contains an accumulation module used to calculate the average of user-specified variables over user-defined time intervals. However, the accumulation of past time leaf temperature and PPFD are commented out in the default CLM4 code and fixed values are assigned to those coefficients based on conditions during previous days. After activating this module, we found a decrease in average temperature and PPFD with increasing simulation time. That was because these two variables were not being accumulated but still being averaged over the total running time. We corrected the accumulation code so that the average leaf temperature, PPFD and leaf fraction are calculated at each time step.

4. sub-gird heterogeneity

In CLM4, the surface heterogeneity is represented using a sub-grid tile approach in which grid cells are composed of multiple landunits (glacier, wetland, lake, urban and vegetated area), snow/soil columns and plant functional types (PFTs). Vegetated surfaces are comprised of up to 4 plant

functional types (PFTs). An explicit canopy layer represents the PFTs with specific leaf and stem optical properties, root distribution parameters, aerodynamic parameters and photosynthetic parameters. The detailed representations of sub-grid improve the accuracy of land surface parameterizations and lower the uncertainty from plant distribution in BVOC estimation (Zhao et al., 2016; Schultz et al., 2016)."

**References:**

Heald, C. L., Wilkinson, M. J., Monson, R. K., Alo, C. A., Wang, G., and Guenther, A.: Response of isoprene emission to ambient CO2 changes and implications for global budgets, Global Change Biology, 15, 1127-1140, 10.1111/j.1365-2486.2008.01802.x, 2009.

Yan, K., Park, T., Yan, G., Liu, Z., Yang, B., Chen, C., Nemani, R. R., Knyazikhin, Y., and Myneni, R. B.: Evaluation of MODIS LAI/FPAR Product Collection 6. Part 2: Validation and Intercomparison, Remote Sensing, 8, 10.3390/rs8060460, 2016.