



# Biodiversity matters in feedbacks between climate change and air quality: a study using an individual-based model

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**Abstract.** Air quality is closely associated with climate change via the biosphere because plants release large quantities of volatile organic compounds (VOC) that mediate both gaseous pollutants and aerosol dynamics. Earlier studies, which considered only leaf physiology and simply scale up from leaf-level enhancements of emissions, suggest that climate warming enhances whole forest VOC emissions, and these increased VOC emissions aggravate ozone pollution and secondary organic aerosol formation. Using an individual-based forest VOC emissions model, UVAFME-VOC, that simulates system-level emissions by explicitly simulating forest community dynamics to the individual tree level, ecological competition among the individuals of differing size and age, and radiative transfer and leaf function through the canopy, we find that climate warming only sometimes stimulates isoprene emissions (the single largest source of non-methane hydrocarbon) in a southeastern U.S. forest. These complex patterns result from the combination of higher temperatures' stimulating emissions at the leaf level but decreasing the abundance of isoprene-emitting taxa at the community level by causing a decline in the abundance of isoprene-emitting species (*Quercus* spp.). This ecological effect eventually outweighs the physiological one, thus reducing overall emissions. Such reduced emissions have far-reaching implications for the climate–air-quality relationships that have been established on the paradigm of warming-enhancement VOC emissions from vegetation. This local scale modeling study suggests that community ecology rather than only individual physiology should be integrated into future studies of biosphere–climate–chemistry interactions.

**Key words:** air quality; biodiversity; climate warming; individual-based model; isoprene; UVAFME-VOC.

## INTRODUCTION

Air quality change is closely linked to climate change (Jacob and Winner 2009, Wang et al. 2017a). Aside from the direct climatic effects initiated by the atmospheric physico-chemical processes (Jacob and Winner 2009, Weaver et al. 2009), the biosphere plays a key role by releasing large quantities of volatile organic compounds (VOC; Guenther et al. 1995, 2006), acting as precursors of tropospheric ozone (O<sub>3</sub>) in presence of relatively high concentration of nitrogen oxides (NO<sub>x</sub>; Atkinson and Arey 2003) and of secondary organic aerosols (SOA; Atkinson and Arey 2003, Kulmala et al. 2013). Climate-warming-initiated effects that cascade through this climate–biosphere–atmospheric chemistry chain have received the most attention (e.g., Ito et al. 2009, Weaver et al. 2009, Pacifico et al. 2012, Fu et al. 2015). Currently, it is widely accepted that warming can enhance forest VOC emissions (e.g., Sanderson et al. 2003, Heald et al. 2009, Pacifico et al. 2012) and thus aggravate O<sub>3</sub> pollution (Sanderson et al. 2003, Fu et al. 2015) and SOA formation (Kulmala et al. 2004, Paasonen et al. 2013). None of these studies, however, explicitly consider the role of terrestrial ecosystem species diversity change in influencing VOC emissions.

Impacts of temperature and other factors (e.g., radiation) on phyto-genic VOC production are now relatively well

understood at cellular-to-leaf scales over relatively short time scales with over half a century of research (Vickers et al. 2009, Loreto and Fineschi 2015, Sharkey and Monson 2017) since the descriptions in the mid-20th century by Haagen-Smit, Went, and colleagues of plant-derived organic compounds that could contribute to O<sub>3</sub> and haze formation (Haagen-Smit and Fox 1954, Went 1960). Ecosystem-level emissions have been extrapolated from this relatively good understanding of biochemical mechanisms and eco-physiological regulation via ecosystem models by aggregating vegetation into plant functional types (PFTs). For instance, well-defined, empirically derived, quantitative relationships between VOC emissions and environmental factors (notably temperature and light) have been obtained from extensive leaf-level measurements and constitute the cornerstone of regional and global VOC emissions models (Guenther et al. 1995, 2006). With the accumulation of biochemical and eco-physiological knowledge concerning phyto-genic VOC production and emissions, process-based models within the dynamic global vegetation model (DGVM) schemes have also been developed (e.g., Arneth et al. 2007). These models have been coupled with climate and atmospheric chemistry models to investigate climate–biosphere–chemistry feedbacks in the earth system and produced the conclusion that climate warming enhances VOC emissions and holds a positive relationship both with O<sub>3</sub> level (i.e., the so-called “climate penalty”; Sanderson et al. 2003, Ito et al. 2009, Fu et al. 2015) and SOA formation (e.g., Weaver et al. 2009). However, the lumped approach to representing vegetation in such global

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and regional models, either static or dynamic, cannot capture the hierarchical and dynamic nature of natural systems, neglecting the inherent interspecific heterogeneity and complex interactions (Huston et al. 1988, Purves and Pacala 2008, Scheiter et al. 2013). This aggregation of vegetation represents one of the major uncertainties in the current modeling of climate–biosphere–chemistry feedbacks (Lerdau 2007, Purves and Pacala 2008, Schurgers et al. 2011).

One of the longest known and most robust results from studies of phytogenic VOCs is that their production and emissions are strongly contingent on species (e.g., Zimmerman et al. 1978, Lerdau et al. 1997, Monson et al. 2013). Across global biomes, a mixture of emitters and non-emitters of different VOC species in an ecosystem is ubiquitous (Loreto and Fineschi 2015). Changes in ecosystem composition that involve a shift in the relative abundance of species with differing VOC emission capacity can, in principle, be caused by climate warming or other disturbances from global environmental changes. Such changes in diversity have the potential to significantly influence the system-level emission capacity and even dominate physiological effects (Lerdau and Slobodkin 2002). Therefore, it is essential to explicitly incorporate the role of species diversity change when studying the effects of various environmental changes on forest VOC emissions, especially over long-term scales. Among the huge number of different VOC species, isoprene ( $C_5H_8$ , 2-methyl 1-3-butadiene) is the most abundant phytogenic VOC and plays the largest role in tropospheric oxidant dynamics (Jacob and Wofsy 1988, Atkinson and Arey 2003, Guenther et al. 2006, Pacifico et al. 2009). Isoprene is thus an ideal candidate for exploring roles of forest species diversity changes in influencing system-scale emissions.

Here we examine the impacts of climate warming on forest isoprene emissions over long time scales mediated both indirectly by compositional change and directly by leaf-level response. We hypothesize that compositional changes may either enhance or counteract the direct warming effects on leaves depending on the specific forest systems. Testing this hypothesis in field studies is logistically and methodologically challenging due to the long time duration required. Instead, a modeling experimental system of a temperate deciduous forest in the southeastern United States is built using an individual-based forest isoprene emissions model, UVAFME-VOC (v1.0; Wang et al. 2017b), which can estimate isoprene emissions based on an explicit simulation of the size and age of different species and their competition for light, water, and nutrient in a forest community. This model has demonstrated satisfactory simulation of forest compositional and structural dynamics and ecosystem level isoprene emissions in this region (Wang et al. 2016, 2017b). For example, with its prominent “individual-based” feature this model has been successfully applied to test the hypothesis that extinction of the American Chestnut (*Castanea dentata*) in the forests of the eastern United States in the late 19th and early 20th centuries enhanced isoprene emissions by favoring oak species (*Quercus* spp.; Wang et al. 2017b). Using this individual-based experimental system of a temperate forest, we investigated the impacts of climate warming on forest dynamics and isoprene emissions. The results presented demonstrate the utility of applying an individual-based model (Shugart 1984) to examine how biodiversity

responses may mediate climate change impacts on atmospheric chemistry via isoprene emissions.

## MATERIALS AND METHODS

### Model description

UVAFME-VOC (v1.0; Wang et al. 2017b) is an individual-based forest volatile organic compounds emissions model built from its predecessor, the University of Virginia Forest Model Enhanced (UVAFME), which is an individual-based model that unifies ecological theory of biodiversity and ecosystem function (Shugart 1984, Huston et al. 1988, Grimm et al. 2016). UVAFME-VOC simulates VOC emissions based on an explicit simulation of forest compositional dynamics by computing the growth, death, and regeneration of each individual tree of different species and their competition for light, moisture, and nutrients, from which system-level VOC emissions are modeled by explicitly computing and summing up each individual’s emissions with an explicit simulation of radiative transfer and leaf function through the canopy (Wang et al. 2017b). This individual-based modeling of forest dynamics enables UVAFME-VOC to apply species-based emission factors both explicitly and dynamically and distinguishes it from other PFT-based VOC models (e.g., Guenther et al. 2006, Arneth et al. 2007).

In detail, the simulation unit of an individual tree is described by tree geometry traits, including diameter at the breast height (DBH), diameter at the canopy height (DCH), tree height ( $H$ ), leaf area (LAI), and root depth (RD; Appendix S1: Fig. S1). These structural units are quantitatively linked by allometric relationships. Forest dynamics are thus simulated at an annual time step by computing the growth, mortality, and regeneration of such individual trees of different species. Tree growth is defined as an annual increment of DBH, which is computed by multiplying the optimal growth by scalars of available light, temperature, nutrient, and soil moisture. Tree death is a stochastic process, which is simulated by calculating the annual mortality probability taking into consideration both intrinsic mortality and environment-induced mortality. The annual establishment of new trees in terms of the number, size, and species is also a stochastic process that involves randomly selecting the species that establish in a given year from the candidate species pool, which consists of the species that can survive in a given environment and of the relative size of seedling bank of a species.

Ecosystem-level isoprene emission,  $F_{ISO}$ , is calculated as a summation of the emissions from each individual tree at five canopy layers, with a differentiation between sunlit and shaded leaves at an hourly time step, according to the widely used empirical approach developed by Guenther et al. (1995, 2006)

$$F_{ISO} = \sum_{i=0}^n \sum_{j=1}^5 E_S(i) C_T(i) [L_{sun}(ij) C_L(j) + L_{shade}(ij) C_L(j)] \quad (1)$$

where  $i$  denotes one of  $n$  trees in the forest,  $j$  denotes one of five layers of each individual tree’s canopy,  $E_S$  represents the species-specific standard leaf-level emission rate of isoprene,  $L_{sun}$  and  $L_{shade}$  represent sunlit and shaded leaf area, and

$C_T$  and  $C_L$  account for light- and temperature-induced variability, respectively, which are calculated according to Guenther et al. (1995)

$$C_T = \frac{\exp\left(\frac{C_{T1}(T-T_S)}{R T_S T}\right)}{1 + \exp\left(\frac{C_{T2}(T-T_M)}{R T_S T}\right)} \quad (2)$$

$$C_L = \frac{\alpha C_{L1} L}{\sqrt{1 + \alpha^2 L^2}} \quad (3)$$

where  $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ ,  $C_{T1} = 95,000 \text{ J/mol}$ ,  $C_{T2} = 230,000 \text{ J/mol}$ ,  $T_M = 314 \text{ K}$ ,  $T_S = 303 \text{ K}$ ,  $\alpha = 0.0027$ , and  $C_{L1} = 1.066$ .  $T$  is hourly leaf temperature, which is assumed to be equal to hourly air temperature and constant through the canopy.  $L$  is hourly leaf-level PPFD (photosynthetic photon flux density;  $\mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ) at each canopy layer for sunlit and shaded leaves of each individual tree obtained with an explicit computing of light behavior within the stand and tree crown with a distinction between direct beam and diffuse radiation considering the shading by taller and surrounding trees, interception, reflection, scattering, and absorption.

Inputs required to drive this model include species-specific parameters quantifying species' fundamental silvics (including tree geometry, growth, mortality, and regeneration, as well as responses to environmental factors), site conditions (including soil physiochemical properties and topographical information), and climate data (including meteorological data of temperature and precipitation). The outputs include tree size, number, basal area, leaf area, biomass, and VOC flux, as well as other biogeochemical and hydrological variables. Model details and formulae can be found in the Appendix S1 and in Wang et al. (2017b).

#### *Building a modeling experiment forest system*

The temperate deciduous forest of eastern Tennessee, located in the southern Appalachian region in the southeastern United States, was selected as the modeling experimental system. This region is one of the most diverse forest

assemblages in the United States, with a climate typical of the humid southern Appalachian region (Johnson and Van Hook 2012). It was chosen because long-term forest compositional dynamics data are relatively rich, and species-specific isoprene data are complete in the region, facilitating model parameterization and validation (Shugart and West 1977, Wang et al. 2017b). Major species native to this region, 32 in total, including both deciduous and coniferous trees, are listed in Data S1, among which 10 are major isoprene emitters. All the parameters and values describing and quantifying each species required as inputs are listed in Data S1. In particular, the standard isoprene emission rates of these isoprene-emitting species are compiled according to the synthesis work by Geron et al. (2001). Sources of all the other parameter values are further described in the Appendix S1.

To build the experimental system, 30 years of historical meteorological data (1981–2010), including monthly precipitation (mm) and monthly maximum and minimum temperature ( $^{\circ}\text{C}$ ) accessed from the NOAA (National Oceanic and Atmospheric Administration) meteorological station at Oak Ridge ATDD, Tennessee, USA (GHCND: USW00003841; 36.0028 $^{\circ}$  N, 84.2486 $^{\circ}$  W; elevation 275.8 m above sea level), were used to drive the model on a plot size of 500  $\text{m}^2$  starting from bare ground for 500 yr (without a spin up). An average of 200 such simulations of independent plots, here presented in the form of forest compositional dynamics in terms of biomass, corresponds to a shifting-mosaic steady-state landscape (Bormann and Likens 1979, Shugart 1984, Bugmann et al. 1996) and captures well the forest composition in the field survey of the southern Appalachian mountain region (Braun 1950, Shugart et al. 1984). The detailed validation of this simulation has been presented in a previous study (Wang et al. 2017b).

#### *Modeling experiments of climate warming*

Climate warming experiments were conducted in the forest system simulated by the individual-based model, UVAFME-VOC, as described above. Specifically, two levels of warming (temperature increase by 2 $^{\circ}$  and 4 $^{\circ}\text{C}$  relative to

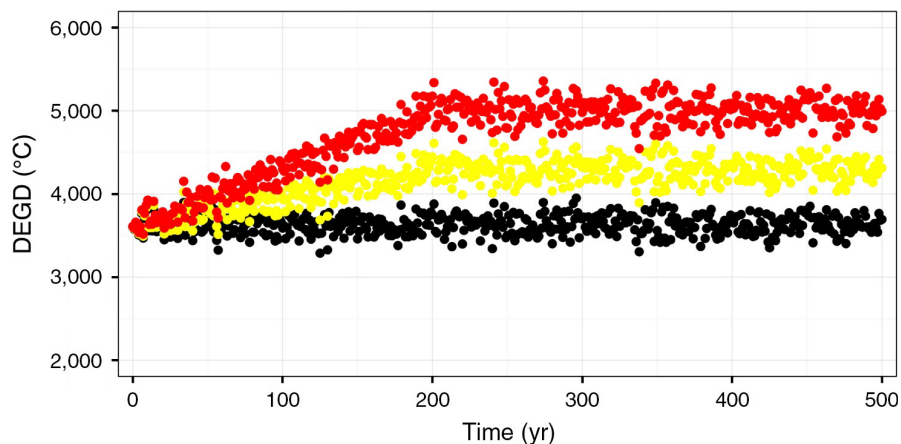


FIG. 1. Warming treatments (+2 $^{\circ}\text{C}$  shown as yellow dots and +4 $^{\circ}\text{C}$  shown as red dots) relative to the base climate in the simulation in terms of DEGD (growing degree days with a 5 $^{\circ}\text{C}$  base) in each year over the 500-yr simulation. The DEGD is calculated from the daily temperature interpolated from model input of monthly mean, maximum, and minimum temperature data. The variations reflect the inter-annual variability of the climate in the simulation.

the base climate) were exerted on this experimental system without changing any parameters and/or formulations. These temperature increases were achieved in 200 yr from year 0 to 200 linearly, with another 300-yr simulation with these stabilized climates (as per Shuman et al. 2011, which evaluated the sensitivity of Siberian larch forests to climate change using an earlier version of UVAFME). See Fig. 1 for the modeled climate warming dynamics over the 500-yr simulation across the three different warming treatments.

The capability of individual-based forest gap models to simulate climate change impacts on forests has been extensively demonstrated (e.g., Solomon 1986, Bugmann et al. 2001, Huth et al. 2005, Dale et al. 2010). Shugart and Woodward (2011) offer a review of the ability of different models (which all have similar formulations) to simulate climate change impacts on forest compositional dynamics. Many of these tests are against compositional changes in forests under paleo-climate conditions (e.g., Solomon and Webb 1985) or along altitudinal gradients (e.g., Yan and Shugart 2005). Moreover, the individual-based gap model, UVAFME, from which UVAFME-VOC (v1.0) was

developed, has also been successfully validated and applied to study forest dynamic changes in response to climate change (Shugart and Woodward 2011, Shuman et al. 2011). One major principle adhered to during the development of UVAFME-VOC is to keep the forest community dynamics simulation capability identical to the previous versions of the model so that changes in isoprene emissions can be viewed in the context of well validated results (Wang et al. 2017b).

## RESULTS

### Forest compositional changes resulting from warming

Successional dynamics of the modeling experiment forest system over 500 yr involve changes in 10 abundant species and 22 other species (Fig. 1a). Initially for a forest succession from an open plot, the “other” species category, mostly composed of pioneer species, dominates the forest with approximately 50% of the total biomass. Soon, both *Acer rubrum* and *Liriodendron tulipifera* become increasingly important, but *A. rubrum* eventually loses to the larger, faster-growing *L. tulipifera* trees, which persist and become dominant. After *L. tulipifera* declines over time, trees of four late-successional oak species (*Quercus alba*, *Q. velutina*, *Q. rubra*, and *Q. prinus*) become increasingly important, together accounting for approximately 75% of the stand biomass at year 300. The composition of the forest stabilizes and is eventually dominated by the aforementioned oaks, along with *L. tulipifera* and two maples (*A. rubrum* and *A. saccharum*).

Climate warming exerts significant impacts on the forest dynamics in terms of species composition and structure (Fig. 1b, c). The four major *Quercus* species (*Q. velutina*, *Q. rubra*, *Q. prinus*, and *Q. alba*) lose their position in the stand over the 500-yr simulation with continuous warming. In particular, *Q. prinus* almost totally disappears from the simulation when warmed by both 2° and 4°C. These significant changes are accompanied by changes in *L. tulipifera* and *A. rubrum*. *Liriodendron tulipifera*, a fast-growing, shade-intolerant species, does not show an apparent change with 2°C warming but does exhibit strong changes with 4°C warming. By contrast, *A. rubrum* shows a dramatic increase with continuous warming. Overall, with continuous warming this simulation presents compositional changes of an increase of red maple (*A. rubrum*) vs. oaks (*Quercus* spp.) declines. See Fig. S2 in the Appendix S1 for size distribution changes responding to climate warming.

### Changes in isoprene-emitting species and isoprene emissions

Ten isoprene-emitting species are present in this simulated forest, of which seven are oak (*Quercus*) species (Data S1). Among these isoprene-emitting species, the four oak species of *Q. prinus*, *Q. alba*, *Q. velutina*, and *Q. rubra* mostly determine ecosystem isoprene emissions over the long-term dynamics, and the remaining six species (hereafter referred to as “others”) only contribute substantially to the ecosystem-scale isoprene emissions at very early successional stages (Appendix S1: Fig. S3a). Climate-warming-induced forest compositional dynamics

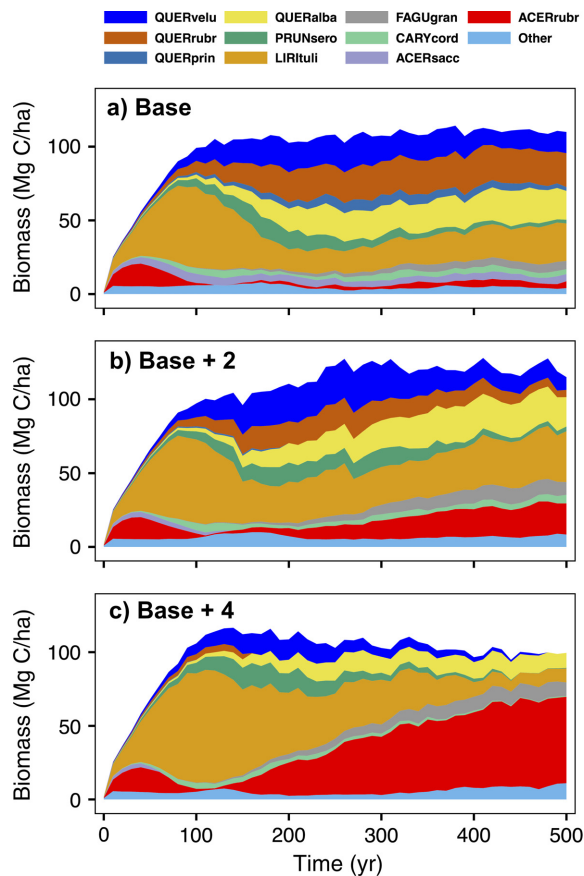


FIG. 2. Forest compositional dynamics in response to warming over a 500-yr simulation. Panes a–c show the base run, 2°, and 4°C warming, respectively. The width of each color band represents the biomass of different species at a specific year. QUERvelu, black oak; QUERrubr, red oak; QUERprin, Chestnut oak; QUERalba, white oak; PRUNsero, black cherry; LIRItuli, yellow poplar; FAGUgran, American beech; CARYcord, bitternut hickory; CASTdent, American Chestnut; ACERsacc, sugar maple; ACERrubr, red maple; and Other, all the remaining species simulated (see Data S1).

alteration, as described above, presents an apparent species diversity change in terms of emitters vs. non-emitters of isoprene. The relative changes of these isoprene-emitting species together are significant in the forest in terms of biomass, leaf area, and basal area (Fig. 3a; Appendix S1: Fig. S4). After an early successional stage, forests that are warming by 2°C start to show a decline of isoprene-emitting species. With further warming by 4°C, the emitters show a much earlier decline, and the percentage declines to less than 20% at a later successional stage. Moreover, warming significantly alters the relative abundance of individual species (Appendix S1: Fig. S3b, c). With continuous warming, except for the others category, *Q. velutina* and *Q. alba* become increasingly dominant while *Q. prinus* and *Q. rubra* gradually disappear from the forest. Overall, climate warming significantly inhibits the presence of the isoprene-emitting species at this location.

These changes in species composition mean that the forest system's isoprene emissions do not simply show an increase as expected from the direct scale-up of leaf-scale warming-enhancement effects to the ecosystem level circumventing the community level (Appendix S1: Fig. S5). With 2°C warming isoprene emissions are enhanced initially until the system sees an emission reduction resulting from a decline of isoprene emitters (Fig. 3b). With the isoprene emitters further decreasing and thus warming-enhanced emissions being offset by the reduction arising from a decline of isoprene emitters, no difference is seen between the base and 2°C warming (Fig. 3b). By later in succession, the reduction resulting from a decline of isoprene emitters starts to exceed the direct warming-enhancing effect, resulting in suppressed isoprene emissions (Fig. 3b). When warmed by 4°C, the forest's compositional change of emitters decline completely dominates the warming-enhancement effect, strongly inhibiting the isoprene production (Fig. 3b). These results demonstrate that, over long time scales, a

forest ecosystem's isoprene emission capacity depends on species composition.

## DISCUSSION

### *Warming-induced forest compositional changes*

The temperate deciduous forests across the eastern United States have been experiencing dramatic changes in composition during the past century. Red maple, a “super-generalist” that has characteristics of both early- and late-successional species (Abrams 1998), has been widely documented with a large expansion (e.g., Abrams 1998, McDonald et al. 2002, Fei and Steiner 2007), which is in stark contrast to a decline of oaks (e.g., Abrams 1998, McDonald et al. 2002, Crosby et al. 2014, Nowacki and Abrams 2015) and sugar maple (Iverson et al. 2008, Bishop et al. 2015). Several factors have been proposed to explain such changes including fire suppression, forest management, preferential browsing, insect and disease outbreaks, and climate change (Abrams 1998, Iverson et al. 2008, Pederson et al. 2015, Nowacki and Abrams 2015).

This model-based local-scale study, focusing on the single factor of increasing temperature, supports the view that climate warming has contributed to these observed trends (Davis 1983, Abrams 1998, Speer et al. 2009). The temperature-induced changes in composition emerging from this modeling experiment feature dramatic red maple increases vs. oak declines. This better performance under increasing temperatures by red maple (Appendix S1: Fig. S6) is in accord with its super-generalist characteristics (Abrams 1998). This strong tolerance gives red maple a competitive advantage over other species during forest development, resulting in the declines of other species, especially the isoprene-emitting *Quercus* spp. Moreover, these simulated compositional changes are congruent with other modeling work studying future climate change impacts on forest composition (Solomon 1986, Dale et al. 2010).

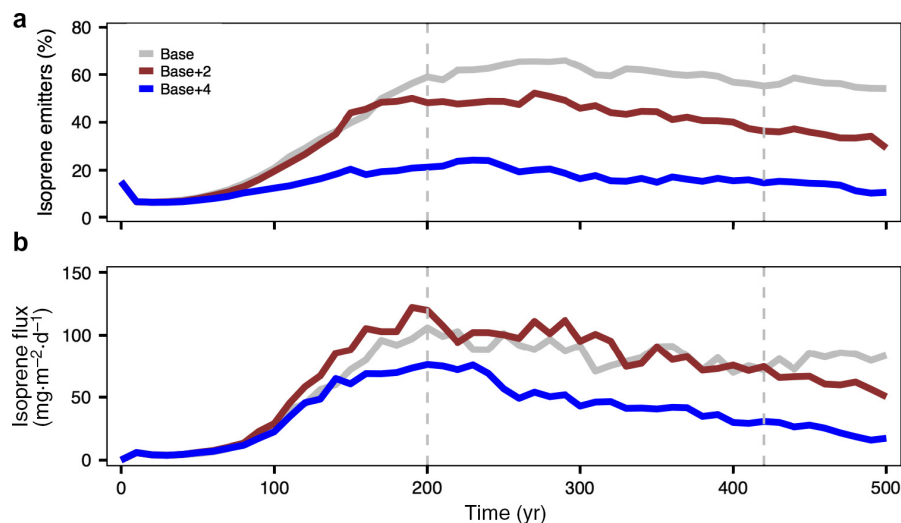


FIG. 3. Dynamics of isoprene-emitting species abundance and isoprene flux in response to warming. (a) The abundance of isoprene-emitters is calculated as the percentage of total isoprene emitters (10 species in total listed in Data S1) in the forest in terms of tree biomass (Mg C/ha). (b) The isoprene emission rate represents the average of daily isoprene emission rate from July of each year. Results shown are the average of model runs on 200 plots of 500 m<sup>2</sup> size loaded with same species information.

*Physiology, ecology, and the responses of forest isoprene emissions to climate warming*

Contrary to the widely seen scale-up from the temperature-dependent leaf-level response that other modeling studies have shown (e.g., Sanderson et al. 2003, Goldstein et al. 2009, Heald et al. 2009, Pacifico et al. 2012), this modeling experiment demonstrates that climate warming may not enhance isoprene emissions totally because of a balance between the temperature-driven physiological increases in isoprene emission and decreases in emission due to ecological changes in species composition. This combination of physiological and ecological controls implies that there may be a threshold for the forest system examined here in terms of isoprene emission capacity in response to climate warming (Fig. 4). Prior to this threshold, climate warming can stimulate isoprene emissions whereas, beyond this threshold, isoprene emissions can be reduced because of a largely diminished occurrence of isoprene-emitting species. Similar threshold phenomena are widely seen in ecosystem functioning under environmental disturbances (Groffman et al. 2006).

Such reduced isoprene emissions under climate warming could have significant implications for the atmospheric chemical processes regionally in the southeastern United States (Fig. 4). First, climate warming may not aggravate O<sub>3</sub> pollution because of a decline of O<sub>3</sub> formation precursors (that is, a possible disappearance of “climate penalty”), although the warming–O<sub>3</sub> relationship is also influenced by other factors including O<sub>3</sub> advection and anthropogenic NO<sub>x</sub> emissions (Atkinson and Arey 2003, Fiore et al. 2005, Fu et al. 2015). Such a decline of O<sub>3</sub> level induced by reduced isoprene emissions has been suggested by the study

of Drewniak et al. (2014), who suggested reduced O<sub>3</sub> formation resulting from the red maple expansion at the cost of oak shrinkage in the eastern United States. Second, declines in isoprene emissions may reduce the formation of SOA, which has a cooling effect. Goldstein et al. (2009) has suggested a significant contribution of vegetation isoprene emissions to SOA formation in the southeastern United States. Reduced isoprene emissions herein potentially form a new positive rather than negative feedback mechanism to climate warming (Kulmala et al. 2004, Goldstein et al. 2009, Paasonen et al. 2013). Moreover, the lifetime of methane in the atmosphere could also be locally reduced by this decline of isoprene emissions, which would tend to decrease overall greenhouse-gas-induced warming (Jacob and Wofsy 1988, Atkinson and Arey 2003).

*Uncertainties*

As with other modeling and empirical studies, which can never consider all the factors affecting the process being considered, this study of warming impacts on isoprene emissions does not consider all possible factors (e.g., extreme weather events such as heat waves). Such neglect creates potential uncertainties in evaluating results. The challenge is to consider, based on our best understanding, which of these neglected factors may be most important and how they may create uncertainty. In the case of warming impacts on isoprene emissions, two factors that are associated with higher temperatures, in particular, may be significant water stress and elevated ambient CO<sub>2</sub> concentrations. Each of these could affect leaf-level function and alter isoprene on physiological scales and may also affect species interactions and thus alter isoprene emissions on ecological time scales.

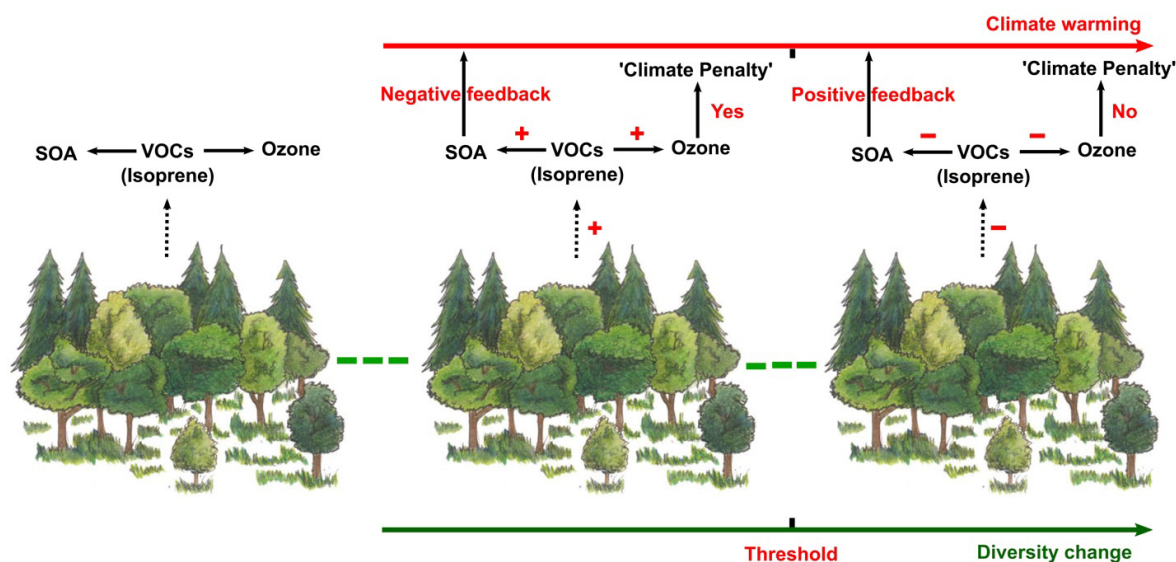


FIG. 4. Schematic of climate warming impacts on atmospheric chemistry mediated by forest compositional changes. A threshold exists for forest systems in terms of isoprene production in response to climate warming, where the indirect warming effect (suppression of isoprene emissions from a decline of isoprene-emitting species) offsets the direct effect (enhancement of isoprene production and emission by increasing temperatures). Prior to and beyond this threshold, distinctive feedback mechanisms between climate and atmospheric chemistry mediated by the forests may occur at least regionally in the southeastern United States. Plus (+) and minus (–) signs denote the positive and negative effect, respectively, and it is noteworthy that the isoprene–O<sub>3</sub> relationships described here are based on a relatively high level of nitrogen oxides. Note the forest in this figure is for illustrational purpose only and does not necessarily indicate actual composition changes.

Water stress could increase isoprene emission by reducing stomatal conductance and thus increasing leaf temperature and decreasing internal CO<sub>2</sub> concentration (e.g., Rosenstiel et al. 2003) or it could decrease isoprene emission by reducing the availability of carbon for isoprene synthesis. Many studies of water stress impacts have been conducted on different species, and the responses of isoprene emissions to such stress have not been consistent across studies, suggesting that the underlying mechanisms are not well understood. For example, the recent synthesis study by Fini et al. (2017) found that some isoprene emitters do not respond to mild and moderate drought-induced depressions of stomatal conductance, while some decrease, and others increase, their emissions. There is a clear need for added research on VPD and drought impacts on VOC emissions with an emphasis on understanding the basic mechanisms that may explain such heterogeneity among species. Water stress, especially over long periods, is also a major factor determining species composition and may affect system-scale isoprene emissions (Clark et al. 2016).

As regards elevated ambient CO<sub>2</sub>, its impacts on both ecological and physiological processes would be influential for isoprene emissions. It has been shown that elevated CO<sub>2</sub> inhibits leaf-level isoprene emissions when temperatures are not elevated (Sharkey et al. 1991, Sharkey and Monson 2014). Recent work, however, has shown that this CO<sub>2</sub>-caused reduction in isoprene emission disappears under higher temperatures and has presented convincing evidence for the mechanism underlying the temperature dependency of the CO<sub>2</sub> suppression (Sun et al. 2013, Potosnak et al. 2014, Niinemets and Sun 2015, Monson et al. 2016). If the current physiological mechanistic models are correct, then elevated CO<sub>2</sub> will not suppress isoprene emissions under high temperatures. At the ecological scale, how elevated CO<sub>2</sub> affect forest compositional dynamics over long-term scales (Bazzaz 1990) and thus isoprene emissions are unknown.

#### *Broader implications*

Two broader implications emerge from this study. First, ecological effects and species composition, especially over decadal and longer time scales, can play a significant role in the biosphere's responses and feedbacks to global change. By explicitly considering forest compositional changes, this study adds complexity into the climate-warming-air-quality feedback mechanisms mediated by the terrestrial biosphere. Although this local-scale computational study focused on one specific forest area in the southeastern United States, it suggests that species diversity change and community-level interactions among individuals (community ecology), not just individual-level metabolism (physiology), are of great significance in influencing system-level isoprene and, most likely, other VOC emissions and thereby atmospheric chemical processes and air quality in the context of global environmental changes over long-term scales. For example, the importance of diversity is also evidenced by a 13-yr field warming study conducted in the subarctic ecosystems showing that warming-induced changes in vegetation composition are a major factor affecting the monoterpene and sesquiterpene emission potentials, but with overall enhanced emissions (Valolahti et al. 2015).

Second, with a recognition of the importance of ecological effects arising from diversity, this modeling work also highlights the importance of going beyond grouping of organisms by functional type in modeling studies. This is true in particular for vegetation VOC emissions, for which the Plant Functional Type classification system does not map onto the variability of VOC emission capacity among species. This modeling study with UVAFME-VOC demonstrates that individual-based models that consider interspecific dynamics provide a promising modeling strategy to explicitly incorporate such fine scale heterogeneity. A challenge, however, in applying such models on large spatial scales is the paucity of species-specific data in most of the ecosystems across the world. This challenge, however, should not deter efforts to improve the resolution of Earth system models so that they can better predict biosphere/atmosphere impacts across long time scales.

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