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An individual-based model of forest volatile organic compound emissions—UVAFME-VOC v1.0

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ABSTRACT

Forests produce and emit abundant non-methane volatile hydrocarbon species (VOCs) influencing the atmosphere chemistry and climate. Over a half century of research has produced significant understandings of the biochemistry and eco-physiology of biogenic VOCs. However, VOCs production is highly species-specific, and the impact of changes in species composition and abundance on VOCs emissions is unobservable in the time scales usually seen in field experiments. Prior modelling efforts are based on cases with an aggregate representation of vegetation. Individual-based models of forests simulate the dynamics of complex forest ecosystems based on birth, growth, and death of the individual trees comprising a simulated forest. Here an individual-based forest VOCs emissions model—UVAFME-VOC v1.0—is developed from the state-of-the-art individual-based forest gap model, UVAFME, coupled with a canopy VOCs emission model. UVAFME-VOC v1.0 implementation for the temperate deciduous forest in the southeastern United States is tested by comparisons to independent data in the region. A model application tested the hypothesis that the historical collapse of American Chestnut (*Castanea dentate*) resulted in the dominance of oak trees (*Quercus* spp.) and enhanced isoprene emissions. The model demonstrated a capability to simulate the forest compositional and structural dynamics and forest isoprene emission dynamics. The simulations show isoprene emissions depend heavily on forest successional stage and species composition, suggesting that environmental change can affect forest VOCs emissions primarily by influencing forest species composition. Prediction of isoprene emissions, of other phytogenic volatile organic compounds, and of impacts on atmospheric chemistry of various global change agents (e.g., warming, rising CO_2, ozone elevation, and herbivory) should explicitly consider forest diversity change. This individual-based model could provide widespread applications in addressing these problems.

1. Introduction

Since the discovery by Haagen-Smit, Went, and colleagues that plant-derived organic compounds can contribute to O_3 and haze formation (Haagen-Smit and Fox, 1954; Went, 1960) over half a century of research has shown the myriad ways that biogenic volatile organic compounds (VOCs) emissions from plants can influence both atmospheric chemistry and physical climate. Vegetation-derived VOCs enter the troposphere and are oxidized by reactions with hydroxyl radical (OH), nitrate radical (NO_3), and to a smaller extent, O_3 (Atkinson and Arey, 2003). These reactions affect the growth rate of methane (CH_4) and produce chemical products including O_3, secondary organic aerosol (SOA), and various forms of oxidized nitrogen, which profoundly affect the air quality and physical climate at regional and global scales, in particular the forested areas (e.g., Atkinson and Arey, 2003; Fuentes et al., 2000; Jacob and Wofsy, 1988).

A good understanding of the biochemical mechanisms and the eco-physiology of production and emission of abundant VOCs species has been developed with over half a century of research (e.g. Monson et al., 1995; Lerdau et al., 1997; Lerdau and Gray, 2003; Vickers et al., 2009). VOCs production and emissions are strongly regulated by light intensity and temperature variations among many other abiotic (e.g., rising CO_2, O_3 pollution, and drought) and biotic factors (e.g., herbivory) (e.g., Niinemets et al., 2013). These confine our understanding only to the low order levels, i.e., leaf and individual of the hierarchical ecosystems on short time scales.

However, how ecosystem-level VOCs emissions behave, in particular at decade-to-century time scales, is almost unknown. Changes in species composition could have profound impacts on phytogenic VOCs emissions because of the strongly species-

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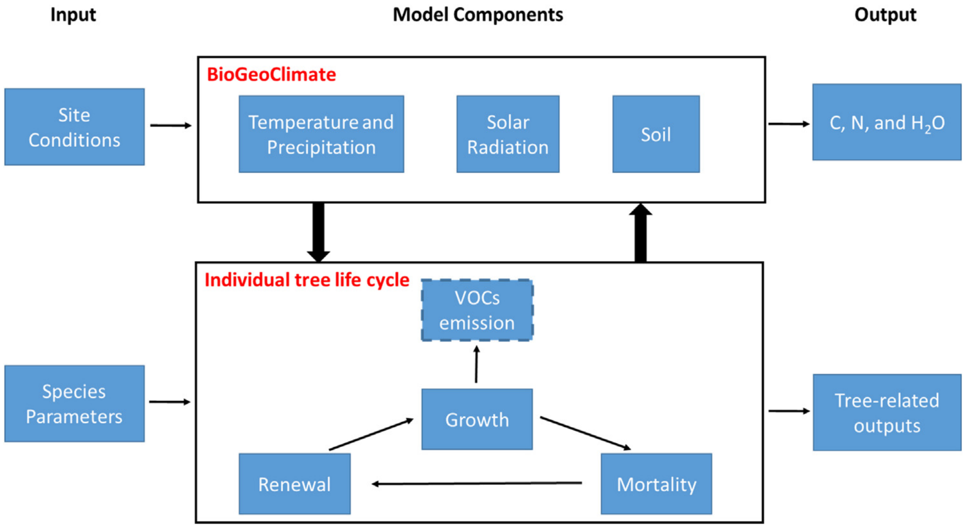

Fig. 1. A schematic of the main structure and components of UVAFME-VOC v1.0.

dependent nature of VOCs production (e.g., Lerdau et al., 1997; Loreto and Fineschi, 2014; Monson et al., 2013; Zimmerman, 1979). For example, in the eastern United States about one-third of tree species produce isoprene (Lerdau, 2007). Tropical systems have a similar proportion of emitting species, and even low diversity ecosystems, such as boreal forests, contain a mixture of emitting and non-emitting species (Lerdau, 2007). This inter-specific variability in VOCs production means that community dynamics (i.e., changes in species composition and abundance) could significantly affect an ecosystem's VOCs emission capacity (Lerdau and Slobodkin, 2002). Furthermore, recent work has shown that impacts of VOCs on the atmosphere can alter the trajectory of these community dynamics, feeding back to affect VOC emissions (Wang et al., 2016). A good understanding of VOCs emissions and controls at the community/ecosystem levels are critical for more accurate quantification of their impacts on global change-atmospheric chemistry feedbacks at larger temporal scales.

Investigating these issues, however, poses intrinsic challenges. Long tree generation times and slow forest dynamics mean that experimental studies would have to occur on time-scales of decades. Substituting space for time, a common practice in ecological studies of long-lived organisms, is difficult because of the spatial heterogeneity of tropospheric chemistry (Atkinson and Arey, 2003; Fuentes et al., 2000). Logistic difficulties with empirical studies dictate the need for predictive models. However, previous modelling studies examining long-term vegetation VOCs emissions dynamics in response to global changes have not explicitly considered species compositional dynamics within ecosystems. Current modelling frameworks mostly represent vegetation in an aggregate way without a consideration of species-specific changes (e.g., Purves and Pacala, 2008; Scheiter et al., 2013). This is the case from the earliest regional model, BEIS (Pierce and Waldruff, 1991), to the widely used global model, MEGAN (Guenther et al., 2006, 2012). Operating from regional through global scales, these models represent vegetation in coarse resolutions, genus to PFT statically with the emission factors empirically constrained by environmental fluctuations. In addition, built on DGVMs (Dynamc Global Vegetation Models; see review by Shugart and Woodward, 2011) process-based models that can explicitly consider the biochemistry and eco-physiology of VOCs production and emissions have also been developed (Sanderson, 2003; Arneth et al., 2007). Nonetheless, these dynamic models, with a representation of vegetation in the PFTs fashion, still cannot explicitly predict communities' compositional dynamics. Without an explicit consideration of ecosystems' compositional change, great uncertainties are intrinsic to these models in estimating the magnitude of VOCs emissions.

Forest gap models (Shugart and West, 1980) are a type of individual-based model (IBM) in use for over 40 years. They simulate forest compositional and structural dynamics through an explicit consideration of life cycles of individual trees, their interactions, and emergent behaviors at the ecosystem level (Shugart, 1984; Bugmann, 2001a; Grimm et al., 2005; Shugart and Woodward, 2011). IBMs provide a framework to develop an individual–based VOC emission model that can predict emissions at the ecosystem scale over time-scales relevant for community dynamics—decades to centuries. Our primary objectives are:

1. To introduce the development of a forest VOC emissions model initiated with the individual-based gap model of University of Virginia Forest Model Enhanced, UVAFME—UVAFME-VOC v1.0;
2. To evaluate this model's performance by implementing it for a temperate deciduous forest in the southeastern United States and then by comparing model outputs with independent field data. An additional test involves an application testing the hypothesis that the Chestnut Blight (*Cryphonectria parasitica*), which essentially eliminated American Chestnut, (*Castanea dentate*) as a dominant canopy tree in eastern North America, resulted in the oak-dominance and increased isoprene emission; and
3. Finally, to discuss the model's applicability and implications in addressing the feedbacks between global change and atmospheric chemistry bridged by the vegetation community ecology.

2. Methods

2.1. Description of UVAFME

UVAFME (Fig. 1) simulates the annual growth, death, and regeneration of each individual tree on a 1/20 ha plot. These processes are constrained by temperature, light, and soil moisture and nutrients at the individual-tree level, as well as by wind and fire disturbances at the stand level. Trees compete for light, nutrient, and water resources. The community dynamics and composition, including tree numbers of each species, basal area, leaf area, biomass carbon and nitrogen, and litter carbon and nitrogen can be derived from the sizes and species of individual trees, which are computed annually in the model. The soil carbon, nitrogen, and water dynamics, along with soil carbon and nitrogen storage, soil respiration,

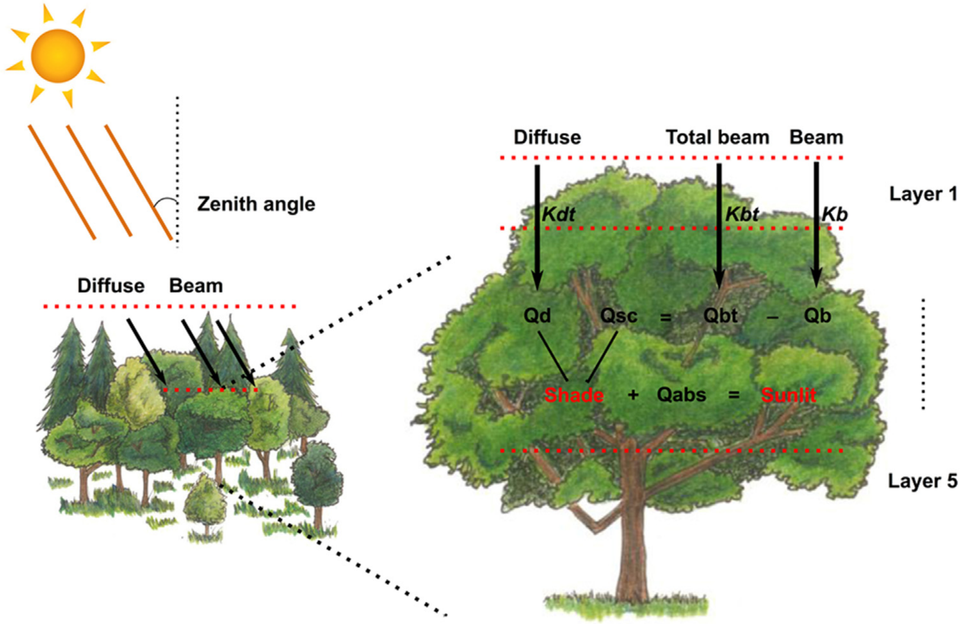

Fig. 2. A schematic of simulation of light transmission within stand and individual tree canopy. *Kdt*, *Kt*, and *Kb* represent the extinction coefficient for diffuse, total beam, and beam respectively. *Qsc* and *Qabs* denote the scattered and absorbed beam radiation, respectively.

and evapotranspiration, are calculated as state variables. The input data include species-related parameters, quantifying species' fundamental silvics and responses to environmental factors and site conditions, local soil physiochemical properties and meteorological temperature and precipitation. For details concerning the model algorithms, please refer to Yan and Shugart (2005).

2.2. Model development

Two principles guided the development of this individual-based VOCs emissions model. First, starting with the individual-based forest gap model, UVAFME, the overarching principle during model development was to keep the internal structure and functions of UVAFME unaltered. Second, in the simulation of VOCs emissions we applied the extensively used empirically based methodology (Guenther et al., 1995, 2006): that is, species-specific standard emission rate of different VOCs constrained by the leaf area of each individual tree and modified by environmental factors, e.g., light and temperature through the forest canopy profile with the central governing equation:

$$\mathrm{Evoc} = \mathrm{Es} * \mathrm{A_L} * \mathrm{C_L} * \mathrm{C_T},$$

where Es represents the standard leaf-level emission rate of VOCs, A_L represents leaf area, and C_L and C_T accounts for light- and temperature-induced variability, respectively. As will be discussed immediately below, the direct and diffuse light onto the leaf profile of each tree, in five canopy layers is simulated allowing the computation of each tree's VOCs emission as a summation of sunlit and shaded leaves production. Model structure and development are outlined in Fig. 1. Note the specific inclusion of the simulation of isoprene emissions. See Appendix A of Supplementary material for the simulation methodology of other VOCs species (e.g., monoterpenes).

The leaf area is assumed to be uniformly distributed throughout the crown of each tree [as with all the other vegetation models (Bugmann, 2001a; Sitch et al., 2003)] and updated annually. We assume that the leaf area in July of each year equals this year-step leaf area. To account for the light variation within the forest stand, the canopy of each tree is divided into five layers. Each layer is further subdivided into sunlit and shaded leaves. Isoprene emissions from the sunlit and shaded leaves of each layer of each tree are calculated (mg $\mathrm{m^{-2}\,h^{-1}}$) under constraints of air temperature and leaf-level PPFD (photosynthetic photon flux density) for both sunlit and shaded leaves with an hourly time step, as shown below. The sunlit-leaves flux and the shaded-leaves flux from each tree's five layers sum to the daily flux for each tree (mg $\mathrm{m^{-2}\,day^{-1}}$). The sum of isoprene emission over all trees represents the stand canopy isoprene flux (mg $\mathrm{m^{-2}\,day^{-1}}$).

Light-dependency algorithm follows Guenther et al. (1995):

$$C_L = \frac{\alpha C_{L1} \mathrm{L}}{\sqrt{1+\alpha^2 \mathrm{L}^2}}$$

where L is leaf level PPFD, μmol $\mathrm{m^{-2}\,s^{-1}}$, $\alpha = 0.0027$, and $C_{L1} = 1.066$. The hourly leaf-level PPFD at each canopy layer for sunlit and shaded leaves of each isoprene-emitting tree is obtained by three steps of calculation (Fig. 2):

First, the direct beam and diffuse PPFD above the forest stand is calculated from incoming total solar radiation. Second, considering the shading by taller and surrounding trees, the light intensity including total beam (unintercepted beam plus down scattered beam), beam (unintercepted beam), and diffuse PPFD above each individual tree canopy within the forest stand is then calculated. Third, the leaf area of sunlit and shaded leaves and the corresponding PPFD for each canopy layer are calculated. The sunlit leaf fraction and different flux densities are determined at each canopy layer using an exponential function of leaf area depth but with differing extinction coefficients based on a spherical leaf angle of 60°. The light intensity on shaded leaves is from both incoming diffuse light and scattered light from the direct beam inside the canopy, which plus the absorbed beam radiation equals the intensity on sunlit leaves surface. These calculations are described in Goudriaan and Van Laar (1994). See Appendix A of Supplementary material for more details concerning simulation of the sunlit and shaded leaf area and PPFD level.

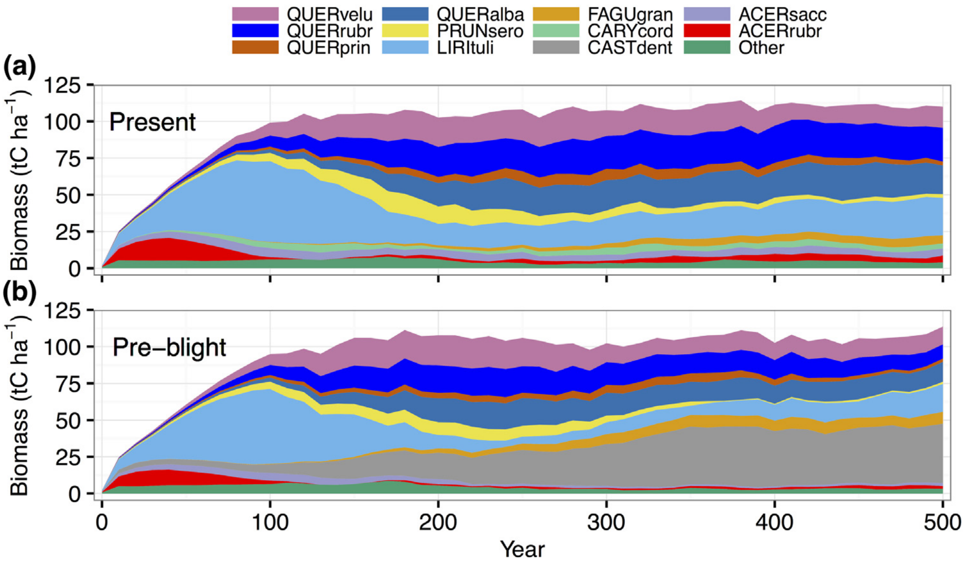

Fig. 3. Simulated forest dynamics in terms of biomass over 500 years for (a) the 'present' forest (i.e., without Chestnut) and (b) the 'pre-blight' forest (i.e., with Chestnut). The width of each color band represents the biomass (tC ha^{-1}) of different species at a specific year. QUERvelu: black oak; 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 following species simulated (see Appendix B of Supplementary material)).

The temperature-dependency algorithm of isoprene emission (Guenther et al., 1995) is:

$$C_T = \frac{\exp \frac{C_{T1}(T-T_S)}{RT_S T}}{1+\exp \frac{C_{T2}(T-T_M)}{RT_S T}}$$

where $R = 8.314\,J\,K^{-1}\,mol^{-1}$, $C_{T1} = 95{,}000\,J\,mol^{-1}$, $C_{T2} = 230{,}000\,J\,mol^{-1}$, $T_M = 314\,K$, and $T_S = 303\,K$. T is leaf temperature, which is assumed to be equal to hourly air temperature and constant through the canopy. Hourly temperature is calculated from daily minimum and maximum temperature, the previous-day maximum temperature, and the following-day minimum temperature (Goudriaan and Van Laar, 1994). See Appendix A of Supplementary material for detailed procedures to calculate the hourly temperature.

2.3. Model performance evaluation

To evaluate the performance of UVAFME-VOC v1.0, we implemented it to simulate the forest successional dynamics and VOCs (isoprene) emission in the southern Appalachian Mountains region located in the southeastern United States. This region has an extensive field record of forest inventory data (e.g., Fowells, 1965; Hardin et al., 2001), and, in particular, extensive research on VOCs production and emissions make species-specific information readily available (e.g., Geron et al., 2000, 2001). Historically, the Chestnut blight (*Cryphonectria parasitica*), a fungus parasite introduced from Asia (Braun, 1950; Woods and Shanks, 1959) of the late 19th and early 20th centuries, caused a massive change in forest composition in the eastern United States. American Chestnut (*Castanea dentate*), which had comprised as much as 50% of East Coast lowland forests, disappeared almost completely and was replaced to a large extent by oaks (Braun, 1950). Unlike oak, American Chestnut does not emit isoprene (Guenther et al., 1996) and it has been hypothesized that the Chestnut Blight has produced an approximate doubling of the biomass of isoprene-emitting species and a significant increase of isoprene emission (Lerdau et al., 1997). To date, however, this hypothesis has not been tested. A community/ecosystem-scale IBM is an ideal vehicle for explicitly testing the question of how changes in species composition might alter VOC emissions.

2.3.1. Model parameterization

Thirty-two species including both deciduous and coniferous trees native to the southern Appalachian region in the southeastern US, plus chestnut, are included in the simulation (Appendix B of Supplementary material). Twenty-five parameters describing silvical properties of each species required as inputs were drawn from the literature. Specifically, wood bulk density values were from global wood density data compiled by Zanne et al. (2009). Species response to nutrient availability is according to Weinstein (1982). All the remaining parameters are estimated according to Fowells (1965) and Hardin et al. (2001). Major isoprene-emitting species and their standard emission rates were according to Geron et al. (2001).

Thirty years of meteorological data for monthly precipitation, mm and monthly maximum and minimum temperature (°C) ranging from 1981 to 2010 were obtained from the NOAA (National Oceanic and Atmospheric Administration) meteorological station at Oak Ridge ATDD, Tennessee, USA (GHCND: USW00003841; Latitude/Longitude: 36.0028°/-84.2486°; Elevation: 275.8 m) to compute monthly average precipitation, monthly maximum and minimum temperature, and their standard deviations. Soil-related parameters including organic layer carbon and nitrogen, active layer carbon and nitrogen, and base soil layer carbon are estimated according to Johnson and Van Hook (2012). Values of 25 cm and 12.5 cm were used for soil field capacity and soil permanent wilting point, respectively.

2.3.2. Simulation methodology

We applied a Monte Carlo simulation of a landscape of indeterminate size sampled with a system of independent sample plots with the same climate and soil conditions. Therefore, the average of the simulation corresponds to a shifting-mosaic steady-state landscape (Bormann and Likens, 1979). An analysis of convergence of average species-specific biomass values indicated that 150–200 replicate plots are needed to provide a sample which approximates a statistically quasi-stable landscape response of the forest landscape (Bugmann et al., 1996). The model was run for a plot size of 500 m^2 starting from bare ground (i.e. gaps with ample active seeds where secondary succession occurs, and which in field such gaps can be created from the death of a canopy-dominant tree resulting

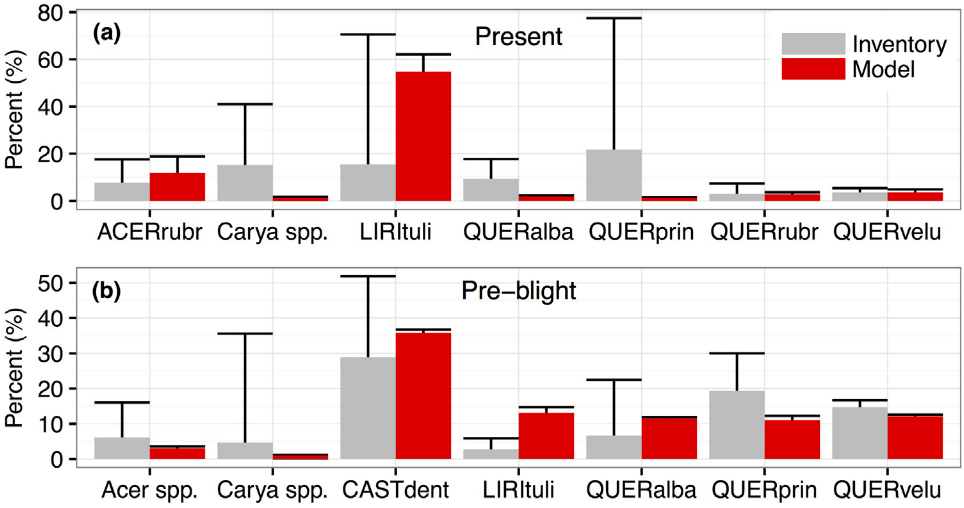

Fig. 4. Comparisons between model simulation and field survey in terms of percent species composition in basal area (m^2 ha^{-1}). (a) Comparison of major species in the present forest between the average of model simulation output from 10 to 90 year and field data describing the forest composition at a successional age of about 40 year at Walker Branch Watershed in eastern Tennessee (35°58′ N and 84°17′ W) acquired from Grigal and Goldstein (1971); (b) Comparison of major species in the pre-blight forest between the simulation (average of 400–500 year output) and field data describing the composition of eastern Tennessee before the outbreak of chestnut blight acquired from Shugart and West (1977). The error bars show the upper 95% confidence interval. Species code is same with Fig. 3.

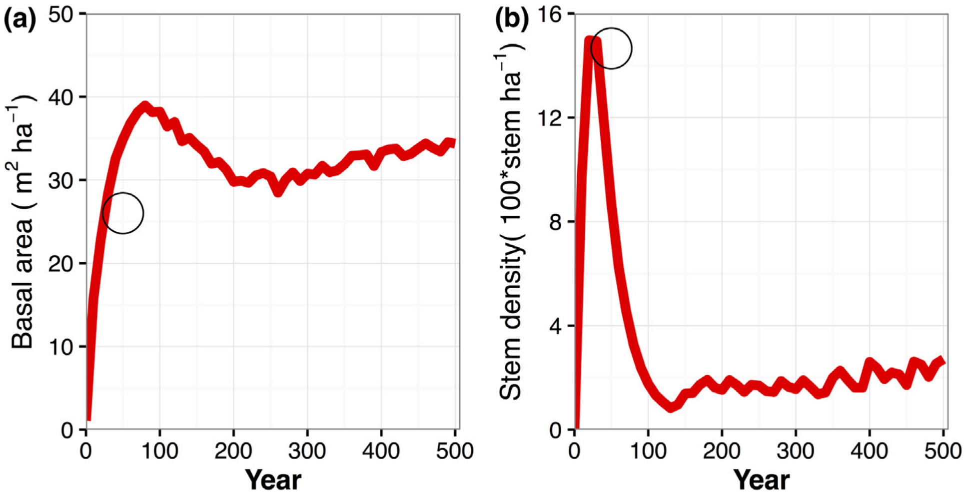

Fig. 5. Stand basal area (a) and stem density (b) dynamics over the 500-year simulation of the present forest. The open circle represents a value of basal area (26 m^2 ha^{-1}) and stem density (1466 stem ha^{-1}) at a successional age of 50 years at Walker Branch Watershed in eastern Tennessee (35°58′ N and 84°17′ W) acquired from Lafon et al. (2000) and Bugmann et al. (2001b), respectively. Trees with a diameter larger than 2.5 cm are included.

from wind, fire, or other disturbances) and lasting for 500 years for 200 independent plots. All the results presented are the average of 200 such runs. Specifically, the simulation without and with the chestnut tree was defined as ‘Present’ and ‘Pre-blight’, respectively.

2.3.3. Validation criteria

As recommended by Grimm et al. (2006), the validation of an IBM should include individual, community, and system level inspections emphasizing the hierarchical structure of an ecological system. We compared simulation results with a series of independent observations involving community composition, basal area, stand density, biomass, productivity, and isoprene emission. Several criteria were applied to demonstrate the reliability of this model:

(1) ‘Present’ simulation outputs including composition, stand basal area, stem density, biomass, productivity, and soil respiration generally match empirical data;
(2) ‘Pre-blight’ forest composition is similar to the historical record;
(3) Proportion of isoprene-emitting species within the forest community was much lower in ‘Pre-blight’ than in ‘Present’; and
(4) Correspondingly, isoprene emission is much higher from ‘Present’ forest than from the ‘Pre-blight’ forest.

3. Results

3.1. Forest successional dynamics in the southeastern United States

Successional dynamics of the ‘Present’ forest over 500 years involves changes in 10 abundant species and 22 other species (Fig. 3a). 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-

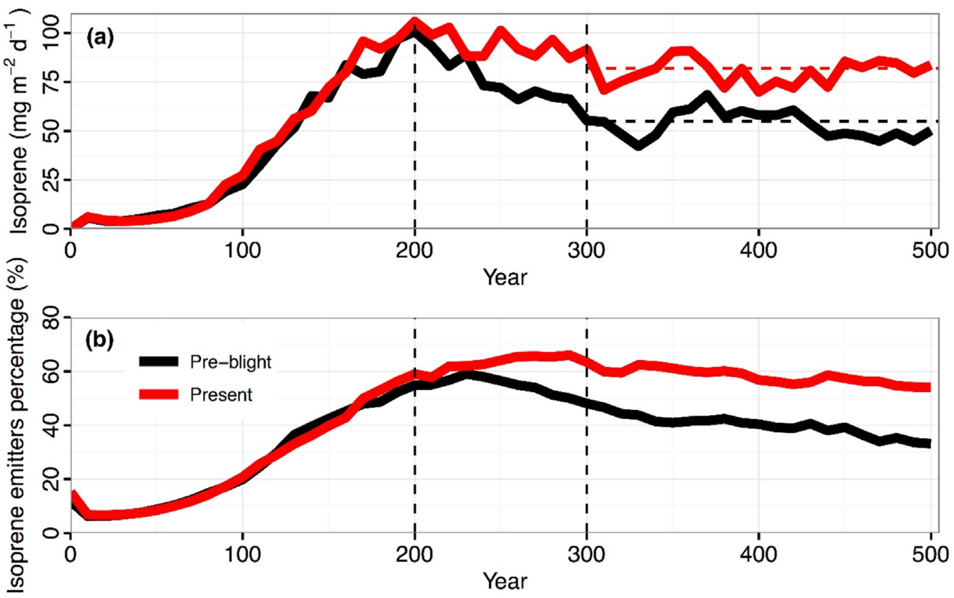

Fig. 6. Comparisons of isoprene emission rate (a) and percentage of isoprene-emitting species' biomass within the forest stand (b) between the 'Present' (red) and 'Pre-blight' forest (black) over the 500-year simulation. The isoprene emission rate represents the average of daily isoprene emission rate from July of each year.

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 500. The composition of the forest stabilizes and is eventually dominated by aforementioned oaks, along with *L. tulipifera* and two maples (*A. rubrum* and *A. saccharum*). This simulated composition matches the description in southeastern United States qualitatively (Shugart, 1984). Moreover, the average percent composition over the first 100 years of simulation was compared with available field species survey data (Fig. 4a). Generally, composition was statistically not different with field inventory data (overlap between 95% confidence intervals). These results suggest that the model can capture the forest succession composition.

Similar to the species composition changes, total biomass becomes relatively less variable, beginning around year 100 (Fig. 3a). Over succession, the total basal area and stand density quickly reached a maximum of almost 40 m^2 ha^{-1} and 1400 stem ha^{-1} within 100 years, respectively (Fig. 5). Subsequently, total basal area declined until around the 200 year to about 30 m^{-2} $year^{-1}$, and then stayed relatively stable with a slight increasing trend (Fig. 5a). The stem density sharply declines and then keeps relatively stable at about 200 stems ha^{-1} (Fig. 5b). These patterns result from the initial rapid stand establishment, followed by thinning from competition. The simulation matches very well with the available field survey data at a succession age of around 50 years (Fig. 5). Further, three principal carbon cycling processes, net primary productivity, soil respiration, and net ecosystem production and the forest carbon stock through dynamic development show reasonable resemblance over successional time (see Appendix A of Supplementary material for details).

With the American Chestnut included, i.e., 'Pre-blight' forest, the successional dynamics were quite different in forest composition from the 'Present' forest (Fig. 3b). Chestnut was dominant in 'Pre-blight' forests and oaks (*Quercus* spp.) dominant in the 'Present' forest. Chestnut was a canopy-dominant, shade-tolerant tree in these forests (Braun, 1950). These simulated changes in forest composition accord well with the description of forest change in response to the chestnut blight in the southeastern United States (Keever, 1975; Nelson, 1955; Woods and Shanks, 1959). Moreover, such dominance and the composition of other species by the model simulation matched the historical field survey data quantitatively. As shown in Fig. 4b, the percentage of each species in the simulation at the later successional stage were not statistically different with field survey data except for only *L. tulipifera* [see Shugart and West (1977) for more details on historical forest composition].

3.2. VOCs, isoprene emission dynamics

Isoprene emissions following the 'Present' forest dynamics (Fig. 6) showed an initial increase with the isoprene producers gradually accumulating in the forest. After the plateau at around the year 200 with an emission rate of about 100 mg m^{-2} d^{-1}, isoprene emission rate slightly declined until around year 300 when the emission settled at around 85 mg m^{-2} d^{-1} with the stabilization of forest composition and structure (for diurnal dynamics, see Appendix A of Supplementary material).

The magnitude of isoprene emissions simulated here was a little lower than was found in the simulation by MEGAN in the southeastern US (Guenther et al., 2006). MEGAN and other models (e.g., BEIS) assign an emission factor to each plant functional type or genus (Guenther et al., 2006; Pierce and Waldruff, 1991). By contrast, the UVAFME-VOC v1.0 uses species-specific emission factor, which could contribute to this difference in simulated isoprene emission.

The ecosystem level emissions are comprised of emissions from different species and leaf types (sunlit and shaded) with differing proportions (Fig. 7). Initially, the total isoprene emissions attributed to the 'others' reached nearly 50% percent, but this contribution source declined in importance very quickly and was nearly zero after about 60 years. The eventual contribution, ranked by the percentage, was from *Q. prinus*, *Q. alba*, *Q. velutina*, and *Q. rubra* (Fig. 7a). This dynamic change was accompanied by change in leaf area of sunlit and shaded leaves over the succession. The total isoprene emissions were also separated into sunlit leaf- and shaded leaf-derived production, hereafter called sunlit and shaded flux, respectively (Fig. 7b). During the early successional stage, the sunlit flux and shaded flux remained stable and contributed almost equally (~50%) with the sunlit flux being slightly higher. The contribution by sunlit leaves relative to shaded leaves gradu-

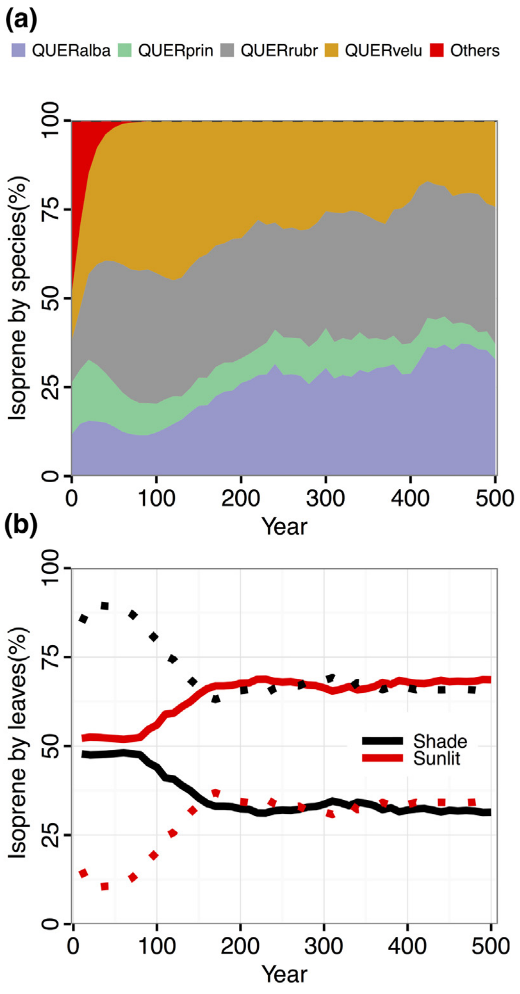

Fig. 7. Total isoprene emissions contributed by species and leaf type (sunlit and shade leaf). (a) Total isoprene emissions comprised by different species, among which the 'others' refer to the isoprene emitters besides the four oak species. (b) Percent contribution to total isoprene emissions (solid lines) and to total leaf area (dashed lines) from sunlit (red) and shaded leaves (black). Note the dynamics presented in (b) starts from the year 10. See species code in Fig. 3 and the leaf area in units of $m^2\ m^{-2}$ in Appendix A of Supplementary material).

ally increased, and eventually increased to about 75%, sunlit leaves against 25%, shaded leaves at the later successional stage.

This dynamic change pattern of ecosystem level isoprene emissions originated from the compositional and structural changes of the simulated forest over natural succession. The annual growth environment, including air temperature and in-coming radiation which were primary controlling factors for isoprene production, did not change during the 500-year succession (see Appendix A of Supplementary material) for diurnal and annual temperature and radiation cycles). However, the within-canopy environment experienced significant modifications resulting from the compositional and structural changes, which can affect isoprene production and emission (e.g., Bryan et al., 2015). This model explicitly simulated shaded and sunlit leaf area and the corresponding leaf-level PPFD variations of each individual tree within the canopy. Here an individual white oak , *Q. alba* tree within the forest stand is used to illustrate the changes (Fig. 8). At 10 year, when succession just started from bare ground, the white oak tree is still small and shaded by other trees (as indicated by the leaf area and PPFD in Fig. 8a and b), which results in an almost linear decline of sunlit leaf area fraction (Fig. 8a) and light extinction within the canopy (Fig. 8b). By contrast, at 300 year the white oak (*Q. alba*) tree has grown much bigger and become canopy dominant (as indicated by the leaf area of >4 $m^2\ m^{-2}$ and above-canopy PPFD of nearly 600 umol $m^{-2}\ s^{-1}$). At this point the sunlit leaf area proportion (Fig. 8c) and sunlit and shaded leaf level PPFD exponentially decline within the canopy (Fig. 8d).

When the American Chestnut was included (i.e., 'Pre-blight'), the isoprene emission followed similar successional dynamics, but the magnitude is much lower than the 'Present' forest (Fig. 6a). At a later successional stage (300–500 year), the 'Pre-blight' forest isoprene emission was lower than the 'Present' forest by as much as 50%. This is mostly from isoprene-emitting species in the 'Pre-blight' forest being much less common than in the 'Present' forest (Fig. 6b). The presence of American Chestnut significantly suppresses the growth and dominance of isoprene-emitting species (mostly *Quercus spp.*) in the pre-blight forest, as shown in Fig. 2. These results are congruent with the hypothesis that the Chestnut blight increased the dominance of *Quercus spp*. and isoprene emissions (Lerdau et al., 1997).

4. Discussion

4.1. *Forest compositional dynamics simulation in southeastern United States*

The simulated successional changes resemble expected changes in forest composition, basal area, and stem density in the southeastern United States. The model's reconstruction of historical forest composition with American Chestnut also reasonably reproduced the historical forest compositional change in the eastern United States caused by the Chestnut Blight. These results suggest that UVAFME-VOC v1.0 is able to simulate the dynamic changes of secondary temperate deciduous forests in the southeastern United States. This motivates applications of this model to simulate the temperate forest dynamics in the southeastern United States in response to anthropogenic disturbances [e.g., impacts of pollutant ozone on forest diversity change by Wang et al. (2016)].

As is often the case, more detailed model tests are limited by the lack of detailed long-term (century time-scale) forest records with the associated weather records. In addition, the forests in the eastern United States regenerated from farmlands that were abandoned after disturbance by European colonists (McEwan et al., 2011). However, it is seldom a simple succession process because of human disturbances and climate change (McEwan et al., 2011; Oliver, 1980; Pederson et al., 2014). This is a common challenge in the evaluation not only of this specific model but of individual-based models in general (Harrison and Shugart, 1990; MacPherson and Gras, 2016).

4.2. *VOCs emissions simulation in southeastern United States*

Results presented suggest that UVAFME-VOCs 1.0 can simulate forest isoprene emission capacity change in the eastern United States. Simulation by this model offered a clear dynamic pattern of isoprene emission capacity over long-term forest succession. This ecosystem behavior is totally determined by forest community change in terms of species composition and structure, indicating the essential role of forest systems themselves in determining VOCs emission capacity. Moreover, the application with this model—a test of the hypothesis of significantly enhanced isoprene emissions from the present forest compared with the forest prior to the Chestnut Blight—clearly shows that ecosystem composition change plays an important role in determining ecosystems' VOCs emissions. This conclusion to some extent is supported by the postulation from the current short-term field surveys or experimental studies (Purves et al., 2004; Valolahti et al., 2015). The current widely used global and regional vegetation VOCs emissions model frameworks, e.g.,

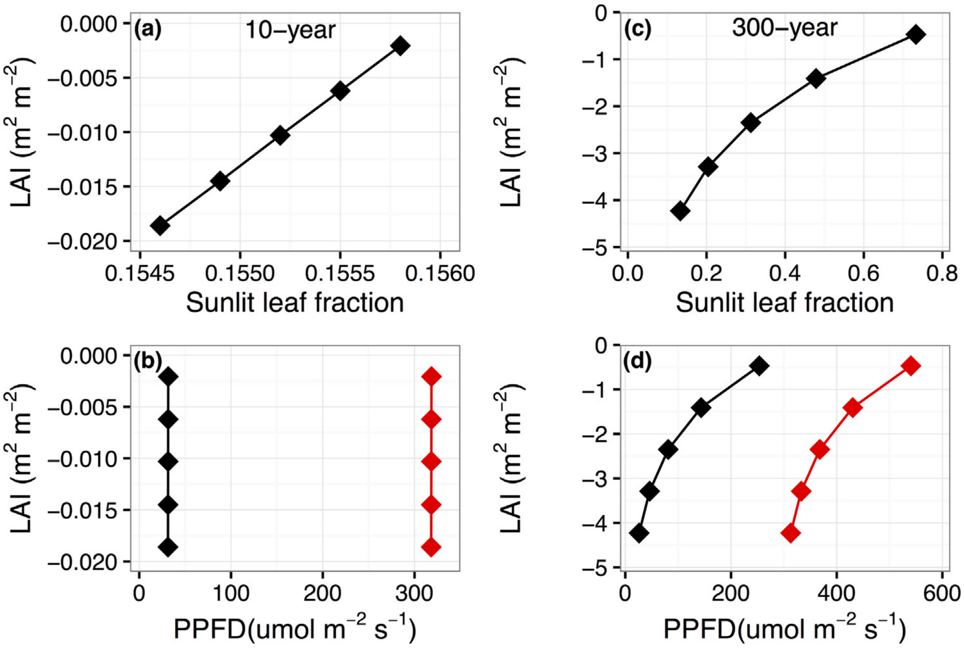

Fig. 8. An example of profile of fraction of sunlit leaf area and PPFD on the sunlit and shaded leaves across a white oak (*Q. alba*) tree canopy within the stand. The white oak tree was randomly chosen from the simulated forest stand at a successional age of 10 (a, b) and 300 (c.d). A spherical leaf angle of 60° is assumed. The negative values on Y-axis indicate an increasing canopy depth. Red lines denote the light intensity on sunlit leaves.

MEGAN (Guenther et al., 2006, 2012), could benefit from including this community dynamical perspective.

Clearly, uncertainties still exist. First, long-term empirical data on VOCs emissions dynamics following ecosystem successional development are rare. Very recently, a simple, stable, and affordable method toward ecosystem-level long-term VOCs flux measurements was proposed (Rinne et al., 2016), potentially providing long-term data to better evaluate this model. Second, algorithms used in this current version of model for simulating light- and temperature-induced variations can be further improved (Guenther et al., 2006; Sharkey et al., 1999). Other factors influencing VOCs production, e.g., drought, nitrogen deposition, and CO_2 elevation, could be useful future additions, as would consideration of VOCs chemistry within the stand canopy. Certainly, the latter has been suggested to be important in quantification of actual forest VOCs emissions capacity (Bryan et al., 2015; Fuentes et al., 2000).

4.3. Generality and implications of UVAFME-VOC

We did not fine-tune model parameters to meet the field observation. Rather, general silvical properties and standard VOCs emission rate of the North America temperate tree species were used to implement the simulation. Although the evaluation of performance of this model was currently limited to the temperate deciduous forest in the southeastern United States, it could apply to other forests around the world. Individual-based gap models have been extensively verified, validated, and applied to simulate local-, landscape-, and regional-level forest dynamics in many environments (Shugart and Woodward, 2011). With the recent technical advances in computer and remote-sensing infrastructures, a large-scale testing of individual-based forest models has become feasible (Shugart et al., 2015). Additionally, although this model currently only introduces the isoprene emission simulation, it provides a convenient framework to conduct simulations on other species of VOCs (e.g., monoterpenes). This is facilitated by the accumulating and readily available species-specific emission data of various VOC species around the world (e.g., Geron et al., 2000).

This individual-based model can be a powerful tool in studying the VOCs emissions dynamics by integrating individual metabolism differences, community, and ecosystem ecology. These are potentially important contributions to the over half a century of research on vegetation VOCs emissions. Global change agents, including, for example, rising CO_2 level, climate change, nitrogen deposition, ozone pollution, biotic invasions, altered disturbance regimes, and land-use change, have modified and will continue to modify ecosystems' composition and species diversity (Franklin et al., 2016). How these changes can affect vegetation VOCs emissions because of diversity change has only rarely been studied. For example, UVAFME-VOC v1.0 has been applied to study forest-isoprene-ozone feedbacks (Wang et al., 2016). A positive feedback loop between tropospheric ozone pollution and forests is simulated, which is mediated by favoring isoprene-emitting species because of their overall stronger resistance to ozone's oxidative pressure (Wang et al., 2016). This feedback mechanism could maintain the ecosystem-level carbon fixation capacity in the face of increased ozone in the eastern United States (Wang et al., 2016).

Further, the sort of massive community-scale changes seen in the case of American Chestnut because of Chestnut Blight invasion are not uncommon in mid- and high-latitude forest systems. For instance, eastern hemlocks (*Tsuga Canadensis*), oaks (*Quercus* spp.), and other species have also been heavily impacted by pathogens and/or herbivores in North America (Orwig et al., 2002; Rizzo and Garbelotto, 2003). In particular, a similar change is ongoing in both North America and Europe as the emerald ash borer (*Agrilus planipennis*) and, in Europe, the chalara fungus, (*Hymenoscyphus fraxineus*) wreak havoc on ash (*Fraxinus* spp.) populations (Poland et al., 2015; Thomas, 2016). *Fraxinus* does not emit large amounts of VOCs, while several of the species likely to replace it, e.g., *Populus spp.* in higher latitudes and *Quercus spp.* in lower ones, are large emitters of isoprene (Harley et al., 1999; Lerdau and Gray, 2003). Any replacement of *Fraxinus* by these genera will likely lead to large increases in system-level VOCs emissions and thus a large change in the troposphere's redox potential. *Fraxinus* also is more sensitive to ozone damage than *Populus* and *Quercus* (Landolt et al., 2000), which creates the possibility for a positive feedback where increases in these two genera lead to higher levels of VOCs emissions to the atmosphere and higher ozone concentrations, which, in turn, can accelerate the decline of *Fraxinus*. Estimating the extent, magnitude, and impacts of these changes requires a formal modeling approach that explicitly considers species identity, and the model developed here should be considered.

Therefore, individual-based model, UVAFME-VOC v1.0, should be applied in studying global environmental change effects on forest VOCs emissions and the complex mechanisms underlying climate change-air quality feedbacks mediated by the vegetation, in particular the role of forest composition dynamics in influencing ecosystem-scale VOCs emissions.

5. Conclusion

This work introduces the development, evaluation, and application of an individual-based forest VOCs emission model—UVAFME-VOC 1.0. With an explicit consideration of individual metabolic and functional differences and their interactions, this model simulates forest succession impacts on isoprene emissions in the southeastern United States. Results of this model imply that the disappearance of American Chestnut as a canopy tree from the Chestnut Blight resulted in a dominance of oak trees (*Quercus* spp.) and increased isoprene emissions in today's forests. UVAFME-VOC provides a flexible framework to simulate not only isoprene but also other phytogenic volatile compounds from forests, and as an experimental system, could see widespread applications in studying feedbacks among global change, forest diversity, and atmospheric chemistry.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.ecolmodel.2017.02.006.

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