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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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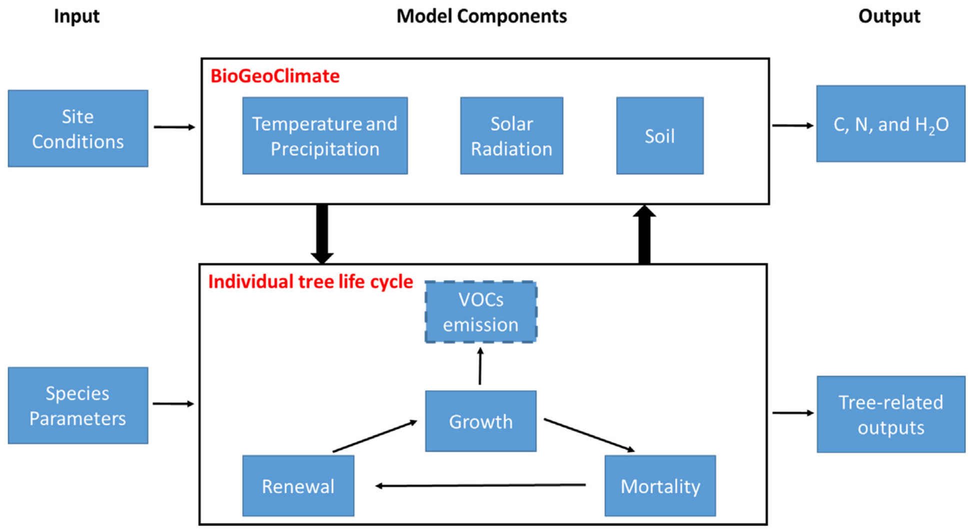

Fig. 1. A schematic of the main structure and components of UVAFME-VOC v1.0.

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,