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Author(s)	陳, 展灼
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氏名 陳 展 灼

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A Study on Process-based Modeling of Monoterpene Emission from Terrestrial Ecosystem
(陸域生態系からのモノテルペン排出量のプロセスベースモデルによる推定)

1. Introduction

Terrestrial ecosystems are major sources of biogenic volatile organic compounds (BVOCs), including isoprene, monoterpenes (MTs), and sesquiterpenes, which play critical roles in atmospheric chemistry and climate regulation. These compounds undergo chemical reactions that contribute to forming secondary organic aerosols (SOA), photochemical smog, and ground-level ozone, influencing air quality and human health (Peñuelas & Staudt, 2010). Climate change can alter BVOC emissions through shifts in the environment of vegetation, such as temperature, precipitation, and atmospheric CO₂, affecting regional and global climate feedback mechanisms (Arneth et al., 2011). Integrating BVOC dynamics into climate models is crucial for improving atmospheric composition and environmental change predictions.

Modeling BVOC emissions is essential for understanding their spatial and temporal variations. Empirical models, such as the Model of Emissions of Gases and Aerosols from Nature (MEGAN), estimate emissions based on observed relationships with environmental factors like temperature and light (Guenther et al., 2012). On the other hand, process-based models, including Lund–Potsdam–Jena General Ecosystem Simulator (LPJ-GUESS), simulate the physiological and ecological mechanisms driving BVOC production and emission, providing insights into climate-driven changes (Arneth et al., 2007; Schurgers et al., 2009). While empirical models offer accurate short-term predictions, process-based models enhance mechanistic understanding, highlighting the need for improved observational data to refine model accuracy.

Soil BVOC emissions, originating from litter decomposition, microbial activity, and root processes, also contribute to atmospheric composition and ecosystem interactions (Tang et al., 2019). These emissions vary depending on soil properties, vegetation traits, and climate conditions. In some regions, such as the Arctic or tropical rainforests, soil BVOC fluxes can be significant, influencing local air chemistry and biogeochemical cycles (Kramshøj et al., 2016; Yáñez-Serrano et al., 2020). Additionally, soil BVOCs mediate plant-microbe interactions, affecting root development, plant competition, and ecosystem resilience (Ndah et al., 2024).

Despite growing recognition of BVOC emissions from both vegetation and soil, uncertainties remain regarding their contributions to global carbon and nutrient cycles. Future research should focus on refining process-based models, expanding field measurements across diverse ecosystems, and improving the integration of BVOC emissions into climate simulations. A comprehensive understanding of these emissions will enhance predictions of their climate feedback effects and inform strategies for mitigating atmospheric pollution and environmental change.

2. Research objectives

This study aims to model MT emissions from both vegetation and soil and incorporate these processes into a terrestrial modeling framework.

(1) The first part of the thesis focuses on simulating MT emissions from a Japanese larch forest ecosystem using the land ecosystem model called the Vegetation Integrative Simulator for Trace gases (VISIT) model, considering plant photosynthesis and the effects of future climate change at a half-hourly scale. It aims to capture BVOC dynamics, assess the sensitivity of emissions to environmental factors, and explore emission changes under different climate scenarios.

(2) The second part of the thesis integrates laboratory-based litter MT emission observations with site-level flux data to develop a process-based representation within LPJ-GUESS. It quantifies litter MT emissions to temperature and moisture and links them with vegetation dynamics and soil biogeochemical processes.

3. Methods and materials

3.1 Study sites and datasets

The study sites for this research include the Fuji Hokuroku (FHK) Flux Observation site (for modeling vegetation MT emission by VISIT) in Japan and the Norunda and Hyltemossa sites (for modeling litter MT emission by LPJ-GUESS) in Sweden.

At the FHK site (35°26'N, 138°45'E), MT emissions were measured using the relaxed eddy accumulation method at a height of 35 m above ground from May to September 2011, with a 30-minute interval, totaling 665 sets of observations. The site, situated at 1100 m elevation with volcanic ash soil, is dominated by *Larix kaempferi* (Japanese larch) in the overstory and ferns in the understory. For model simulations (2006–2012), half-hourly meteorological data specific to the site was used, while a 300-year spin-up employed harmonized National Centers for Environmental Prediction (NCEP) Climate Forecast System Reanalysis (CFSR) data (1979–2005), fitted to a half-hourly resolution using a squared sine function for temperature and radiation adjustments. We obtained climate data from the sixth version of the Model for Interdisciplinary Research on Climate dataset (MIROC6) for future projections at the FHK site.

In Sweden, the Norunda site (60°05'N, 17°29'E) is a managed mixed evergreen forest dominated by *Pinus sylvestris* (Scots pine) and *Picea abies* (Norway spruce). MT emissions were measured using an eddy covariance system and a proton transfer reaction time-of-flight mass spectrometer (PTR-TOF-MS), providing hourly flux data during multiple observation periods between 2020 and 2022. The forest floor MT emissions were measured using a soil chamber and collected litter biomass from June to October 2015. Given that the understory vegetation was a non-MT emitter, it was assumed that the forest floor emissions primarily originated from the litter decomposition of the dominant tree species. Besides, the Hyltemossa site (56°06'N, 13°25'E) provided litterfall biomass data from 2019 and 2020, collected using 20 traps and processed to obtain daily biomass values.

Leaf-level MT emission capacities for Scots pine and Norway spruce were determined based on branch chamber measurements using gas chromatography-mass spectrometry (GC-MS) in 2013 and 2014. Litter MT emissions were further analyzed through controlled experiments using a factorial design with different temperature and humidity conditions. In this experiment, fresh litter was incubated under these conditions, and VOCs were collected and analyzed using GC-MS. The emission capacity was parameterized using an exponential function, with standard conditions set at 13°C and 86% moisture, allowing the integration of litter MT emissions into the model framework.

3.2 Land ecosystem models

The VISIT model is a process-based terrestrial model that simulates trace gas fluxes between the atmosphere and ecosystems, with a focus on carbon, nitrogen, and water cycling components (Ito, 2019; Ito & Oikawa, 2002). It integrates biogeochemical interactions and uses ecophysiological relationships and environmental responsiveness to model processes like photosynthetic CO₂ assimilation, autotrophic respiration, litterfall, and heterotrophic respiration (Ito & Inatomi, 2012). Plant photosynthesis is simulated using a biochemical model coupled with radiation transfer. This model is designed to assess ecosystem-level gas fluxes and the dynamics of various components based on dry-matter production theory.

The LPJ-GUESS model is a process-based ecosystem model that simulates vegetation dynamics, carbon, and nutrient cycling across global terrestrial ecosystems. It accounts for plant photosynthesis, respiration, vegetation dynamics, and phenology, as well as soil biogeochemical processes (Smith et al., 2014). The model simulates forest succession, land-use change, and environmental responses by representing ecosystem compartments like canopy, soil, and litter. BVOC emissions, including isoprene and monoterpenes, are modeled based on photosynthetic electron flux and influenced by environmental factors like temperature, light, and CO₂ concentration (Arneth et al., 2007; Schurgers et al., 2009). The model requires a 500-year spin-up and uses a variety of climate datasets, including the Climate Research Unit – National Centers for Environmental Prediction (CRU-NCEP) dataset, for site-specific simulations, such as those at the Swedish sites.

4. Results

4.1 Modeling vegetation MT emission by VISIT

The VISIT model was evaluated for its ability to simulate ecosystem-level monoterpene (MT) emissions from a Japanese larch (*Larix kaempferi*) forest. The model successfully captured daily and seasonal variations in key carbon fluxes, including gross primary production (GPP), ecosystem respiration (ER), and net ecosystem exchange (NEE). The comparison between simulated and observed GPP showed a strong correlation (RMSE = 1.77 gC m⁻² d⁻¹, R² = 0.88), while ER was slightly underestimated by approximately 15%, possibly due to an incomplete representation of soil microbial respiration processes. The model's ability to simulate seasonal changes in leaf area index (LAI) was also validated against MODIS LAI data, showing good agreement during the growing season.

For MT emissions, the VISIT model was compared against the empirical MEGAN model, a widely used BVOC emission model. While both models performed similarly in terms of Willmott's index of agreement (VISIT: 0.61, MEGAN: 0.63), the VISIT model showed lower mean bias error (MBE = 0.29) and root mean squared error (RMSE = 0.43), indicating more accurate emission predictions. The MEGAN model exhibited a stronger response to temperature, often overestimating emissions during peak temperature periods, whereas the VISIT model accounted for storage-based emissions, resulting in a more balanced response to environmental fluctuations. To further evaluate the VISIT model's response to environmental factors, short-term changes in MT emissions were analyzed. The model demonstrated a strong correlation between MT emissions and photosynthetically active radiation (PAR), suggesting that emissions are tightly linked to plant photosynthetic activity. Additionally, a detailed analysis of 30-minute intervals showed that when temperature increased but PAR decreased, the MEGAN model predicted a rise in emissions, whereas the VISIT model accurately captured the observed decline.

Moreover, the VISIT model was used to project future MT emissions under different Shared Socioeconomic Pathway (SSP) scenarios, ranging from low-emission (SSP119) to high-emission (SSP585) scenarios. The model predicts that under SSP585, MT emissions will increase significantly, reaching approximately 0.18 nmol m⁻² s⁻¹ by 2100, compared to 0.12 nmol m⁻² s⁻¹ under SSP119. This increase is primarily driven by rising CO₂

concentrations, which indirectly affect MT emissions by altering plant photosynthesis and biomass accumulation. It is noted that temperature is the dominant factor influencing short-term MT emissions, while CO₂ concentration plays a more significant role in long-term trends. Under SSP585, the correlation between MT emissions and GPP weakens over time, suggesting that rising CO₂ levels may alter the balance between carbon assimilation and BVOC production. This highlights the need for future studies to explore the direct biochemical effects of elevated CO₂ on BVOC synthesis pathways. Despite its strong performance, the VISIT model has several limitations. First, it only accounts for MT emissions from *Larix kaempferi*, ignoring BVOC contributions from the soil layer, which may explain discrepancies between observed and simulated emissions in early spring and late autumn. Second, the parameterization of MT production is based on empirical relationships rather than a fully mechanistic representation of enzymatic processes, which could introduce uncertainties under changing climate conditions.

To improve future simulations, several recommendations are proposed: (1) incorporating soil BVOC emissions into the model to account for non-vegetation sources; (2) refining the scaling of ambient temperature to leaf temperature, as BVOC emissions are strongly temperature-dependent at the leaf level; and (3) integrating water stress effects into the BVOC production scheme to better capture drought-induced emission variations. These refinements would enhance the accuracy of the VISIT model in predicting ecosystem-scale BVOC emissions under future climate change scenarios.

4.2 Modeling litter MT emission by LPJ-GUESS

This section investigates the contribution of litter to ecosystem-level monoterpene (MT) emissions in a Swedish boreal forest using the process-based LPJ-GUESS model. Results indicate that litter contributes around 2% of total ecosystem MT emissions, a relatively small but non-negligible fraction. The acceptable weighted relative root mean square error (wrRMSE) indicates reasonable agreement between model predictions and observed litter MT fluxes. However, variations in emission capacities across different litter types suggest that decomposition-based emissions are influenced by factors such as litter quality, microbial activity, and environmental conditions, particularly temperature and moisture.

Analysis of temperature and moisture dependencies revealed that litter MT emissions are primarily controlled by abiotic factors, with temperature exerting a stronger influence than moisture content. Scots pine litter exhibited higher MT emissions than Norway spruce, particularly for α -pinene and carene, likely due to differences in stored BVOCs and decomposition rates. The model also identified substantial variability in litter MT emissions across seasons, with peaks occurring in warmer months due to enhanced microbial activity and volatilization. Despite these insights, uncertainties remain regarding the role of litter biochemical composition (e.g., PH, lignin content) and soil organic matter dynamics, which were not explicitly parameterized in the model. Further refinement in litter quality representation could improve predictive accuracy.

To enhance litter MT emission simulations, future work should focus on incorporating high-resolution observational data, particularly under extreme weather conditions that could impact microbial decomposition and BVOC release. Additionally, refining the representation of wind-driven litterfall dynamics and integrating soil BVOC processes into the LPJ-GUESS model could provide a more comprehensive understanding of BVOC fluxes at the ecosystem level. Given the increasing recognition of litter-derived BVOCs in atmospheric chemistry and climate interactions, these improvements would contribute to more accurate Earth System Model (ESM) representations of biogenic emissions.

5. Summaries of the thesis

This thesis explores process-based modeling of MT emissions from both vegetation and litter in terrestrial ecosystems, with a focus on Japanese larch forests in Japan and boreal forests in Sweden. By integrating observational data with process-based models (VISIT and LPJ-GUESS), the study improves the representation of MT production, storage, and emission dynamics under varying environmental conditions. The results highlight the key role of temperature, light, and CO₂ concentration in influencing emission patterns, while also revealing the contribution of litter decomposition to overall BVOC fluxes. The thesis underscores the importance of linking vegetation activity with BVOC emissions to enhance ESM and better predict ecosystem-climate interactions.

Despite the advancements, uncertainties remain in capturing species-specific emission variability, the influence of soil BVOCs, and the effects of litter quality on emissions. Future research should focus on refining model parameterization, integrating soil BVOC processes, and incorporating additional environmental stress factors such as drought. These improvements will further enhance the accuracy of process-based BVOC modeling, contributing to a more comprehensive understanding of biogenic emissions in global terrestrial activities and climate feedback systems.

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