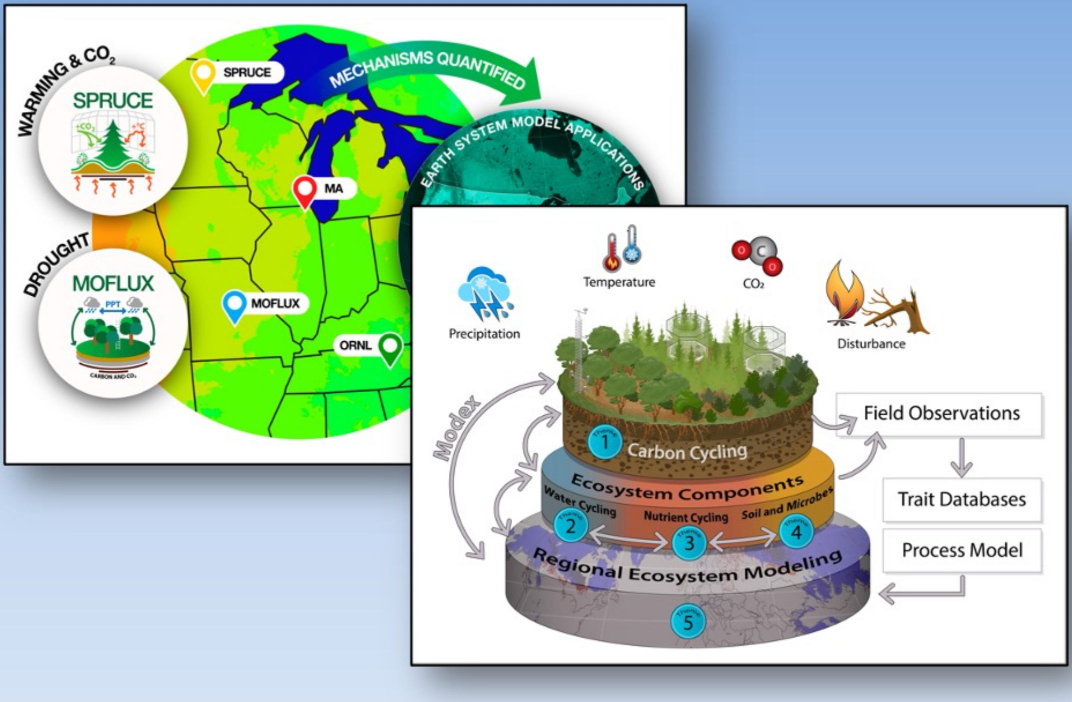
# Oak Ridge National Laboratory's Terrestrial Ecosystem Science Scientific Focus Area



## Fourth Review Report and Description of Proposed Plans for FY2024, FY2025, FY2026, FY2027 and FY2028

Submitted to the U.S. Department of Energy,
Office of Science, Biological and Environmental Research
1 April 2023

OAK RIDGE
National Laboratory

Inside Front Cover

# SCIENCE PLAN AND PROGRESS REPORT FOR THE TERRESTRIAL ECOSYSTEM SCIENCE SCIENTIFIC FOCUS AREA

Climate Change Science Institute, Environmental Sciences Division, Biological Sciences Division
Oak Ridge National Laboratory (ORNL)

Submitted to the Terrestrial Ecosystem Science, Biological and Environmental Research Program
DOE Office of Science
1 April 2023

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## Abstract

Understanding fundamental responses and feedbacks of terrestrial ecosystems to climatic and atmospheric change is the aim of the Terrestrial Ecosystem Science Scientific Focus Area (TES SFA). The proposed research efforts of the ORNL TES SFA seek to provide answers to the following overarching question: **How vulnerable to climate change are C stores of terrestrial ecosystems in eastern North America, and what are the implications for C–climate feedbacks?** The TES SFA focuses on ecosystems subject to water, energy, and nutrient constraints whose impacts are highly uncertain in Earth system models. Our proposed science includes manipulations, multidisciplinary observations, database compilation, and fundamental process studies integrated and iterated with modeling activities at multiple scales. The dominant manipulation is the Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment testing responses to multiple levels of warming at ambient and elevated $CO_2$ for a peatland ecosystem. Long-term observations of ecosystem function at an eddy covariance site in Missouri (MOFLUX) characterize ecosystem response to dominant hydrologic limitations. Research activities at SPRUCE and MOFLUX cover a spectrum of environmental drivers and complement each other. Process-level work occurs at smaller scales and aims to improve mechanistic representation of processes within terrestrial biosphere models. The TES SFA integrates experimental and observational studies with model building, parameter estimation, and data analytics to yield reliable model projections. This integrated model-experiment approach focuses on improving the land model (ELM) of DOE's Energy Exascale Earth System (E3SM) model and fosters enhanced, interactive, and mutually beneficial engagement between models and experiments.

## ORNL TES SFA Proposed Science Leadership Team

| Theme | Task | Description | Lead |
|---|---|---|---|
| **Co-Coordinating Investigators** | | | **Paul J. Hanson (2024-2025)**<br>**Melanie A. Mayes**<br>**Daniel M. Ricciuto** |
| **1** | | **Warming and Elevated $CO_2$** | **Natalie A. Griffiths**<br>**Paul J. Hanson** |
| | 1.1 | SPRUCE operations | Paul J. Hanson |
| | 1.2 | Carbon balance | Natalie A. Griffiths |
| | 1.3 | Physiology | J. Warren & D. Weston |
| | 1.4 | Peatland modeling | Xiaoying Shi |
| **2** | | **Water, Energy, and Carbon** | **Lianhong Gu**<br>**Jeffrey M. Warren** |
| | 2.1 | MOFLUX operations | Jeffrey D. Wood |
| | 2.2 | Energy balance | L. Gu & J. Wood |
| | 2.3 | Carbon processes | Melanie A. Mayes |
| | 2.4 | Water limitations | Jeffrey M. Warren |
| | 2.5 | LeafWeb | Lianhong Gu |
| **3** | | **Nutrient Feedbacks** | **Verity G. Salmon**<br>**Xiaojuan Yang** |
| | 3.1 | Decomposition | Verity G. Salmon |
| | 3.2 | Nutrient acquisition | Xiaojuan Yang |
| | 3.3 | Nitrogen balance | Matthew E. Craig |
| **4** | | **Microbial Soil Carbon** | **Melanie A. Mayes**<br>**Christopher W. Schadt** |
| | 4.1 | SPRUCE microbes and soil carbon | Christopher W. Schadt |
| | 4.2 | MOFLUX microbes and soil carbon | M. Mayes & M.Craig |
| **5** | | **Regional Modeling** | **Anthony P. Walker**<br>**Daniel M. Ricciuto** |
| | 5.1 | Model uncertainty | Daniel M. Ricciuto |
| | 5.2 | Regional modeling | Anthony P. Walker |
| | 5.3 | Ecosystem vulnerabilities | Jiafu Mao |
| **Data** | | **Data Management** | **Terri Velliquette** |

The Science Leadership Team listed above with invited SFA participants, will meet monthly to discuss science progress and continually update project planning. The Science Management Team will weigh in on all decisions regarding science and budget. There will also be an Executive Committee composed of the SFA Coordinating Investigators, the Data Manager, Theme and Task leads (TBD - perhaps rotating), and a representative from the Early Career Community (described below). The Executive Committee will meet regularly to discuss logistics, personnel development, and inclusion and equity within the group.

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# Abbreviations

| | |
|---|---|
| **AMR** | Automated Minirhizotrons |
| **BER** | Biological and Environmental Research |
| **BERAC** | Biological and Environmental Research Advisory Committee |
| **CADES** | Compute and Data Environment for Science computing cluster |
| **CCSI** | Climate Change Science Institute |
| **CIMER** | Center for the Improvement of Mentored Experiences in Research |
| **CIVE** | Compound Indicators for Vulnerable Ecosystems |
| **CMIP6** | Sixth iteration of the Climate Model Intercomparison Project |
| **CPPB** | Coupled Photophysical, Photochemical, and Biochemical |
| **CUE** | Carbon Use Efficiency |
| **DAAC** | Distributed Active Archive Center |
| **DAYMET** | Gridded daily meteorological data sets for modeling |
| **DMP or DMT** | Data Management Plan or Team |
| **DIC** | Dissolved Inorganic Carbon |
| **DOC** | Dissolved Organic Carbon |
| **DOE** | U. S. Department of Energy |
| **DOI** | Digital Object Identifier |
| **E3SM** | Energy Exascale Earth System Model |
| **ECC** | Early Career Community |
| **eCO$_2$** | Elevated CO$_2$ experimental treatments |
| **EC** | Eddy Covariance method for landscape flux observations |
| **ECC** | Early Career Committee |
| **ELM** | E3SM Land Model |
| **ELM-FATES** | Nutrient-enabled version of ELM |
| **ELM-SPRUCE** | ELM version for wetlands and peatlands specific to SPRUCE |
| **ELM-TAM** | ELM version with Transport and Absorptive fine roots and Mycorrhizal fungi |
| **EMSL** | DOE's Environmental Molecular Sciences Laboratory |
| **ESM** | Earth System Model |
| **ESS** | Earth System Science |
| **ESS-DIVE** | ESS Data Infrastructure for a Virtual Ecosystem |
| **ETC** | Electron Transport Chain |
| **FAME** | Fluorescence Auto-Measurement Equipment |
| **FATES** | Functionally Assembled Terrestrial Ecosystem Simulator |
| **FLUXNET** | Global confederation of eddy covariance research sites |
| **FRED** | Fine Root Ecology Database |
| **FY** | Fiscal Year |
| **FyCB** | Farquhar–von Cammerer–Berry |
| **GPP** | Gross Primary Production |
| **IAV** | Interannual Variation |
| **iLSTM** | Interpretable long short-term memory |
| **IMACSS** | Integrated Measurement and Control System for SIF |
| **INN** | Invertable Neural Network |
| **IPCC** | Intergovernmental Panel on Climate Change |
| **JGI** | Joint Genome Institute |

| | |
|---|---|
| **LAI** | Leaf Area Index |
| **LeafWeb** | Global trait data base for foliar photosynthetic and stomatal characteristics |
| **MA** | The Morton Arboretum |
| **MAAT** | Multi-Assumption Architecture and Testbed for models |
| **MCMC** | Markov Chain Monte Carlo method |
| **MEND** | Microbial Enzyme Decomposition model |
| **MIP** | Model Intercomparison Project |
| **ML** | Machine Learning |
| **MODEX** | model-experiment-observation |
| **MOFLUX** | Missouri Ozark eddy covariance flux site |
| **NASA** | National Aeronautics and Space Administration |
| **NGEE** | Next Generation Ecosystem Experiment |
| **NCE** | Net Carbon Exchange |
| **NEE** | Net Ecosystem Exchange |
| **NPP** | Net Primary Production or Productivity |
| **NPQ** | Non-photochemical quenching |
| **NSC** | Non-Structural Carbohydrate |
| **OLMT** | Offline Land Model Testbed |
| **ORNL** | Oak Ridge National Laboratory |
| **OSTI** | DOE Office of Scientific and Technical Information |
| **PAM** | Pulse-Amplitude Modulated fluorometry |
| **PFT** | Plant Functional Types |
| **PIER** | Plan for Promoting Inclusive and Equitable Research |
| **PMF** | Proton Motive Force |
| **PSI** | Photosystem I |
| **PSII** | Photosystem II |
| **PQ** | Plastoquinone |
| **QoI** | Quality of Interest |
| **SIF** | Solar Induced Fluorescence |
| **SOC** | Soil Organic Carbon |
| **SPAC** | Soil Plant Atmosphere Continuum |
| **SPRUCE** | Spruce and Peatland Responses Under Changing Environments experiment |
| **SPRUCEMIP** | SPRUCE project Model Intercomparison Project |
| **SSP** | Shared Socioeconomic Pathway |
| **SULI** | DOE Science Undergraduate Laboratory Internships |
| **TC** | Tethys-Chloris |
| **TES SFA** | Terrestrial Ecosystem Science Scientific Focus Area |
| **THx.x** | TES SFA Theme task number for proposed work |
| **TOC** | Total Organic Carbon |
| **TRY** | Global Plant Trait database |
| **USGCRP** | United States Global Change Research Program |
| **VPD** | Vapor Pressure Deficit |
| **WEW** | Whole-Ecosystem Warming |
| **WHC** | Water Holding Capacity |

# Executive Summary

*Understanding fundamental responses and feedbacks of terrestrial ecosystems to climatic and atmospheric change is the aim of the Terrestrial Ecosystem Science Scientific Focus Area (TES SFA). The proposed research efforts of the ORNL TES SFA seek to provide answers to the following overarching question:* ***How vulnerable to climate change are C stores of terrestrial ecosystems in eastern North America, and what are the implications for C–climate feedbacks?*** *The TES SFA focuses on ecosystems subject to water, energy, and nutrient constraints whose impacts are highly uncertain in Earth system models. Our proposed science includes manipulations, multidisciplinary observations, database compilation, and fundamental process studies integrated and iterated with modeling activities at multiple scales. The dominant manipulation is the Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment testing responses to multiple levels of warming at ambient and elevated* $CO_2$ *for a peatland ecosystem. Long-term observations of ecosystem function at an eddy covariance site in Missouri (MOFLUX) characterize ecosystem response to dominant hydrologic limitations. Research activities at SPRUCE and MOFLUX cover a spectrum of environmental drivers and complement each other. Process-level work occurs at smaller scales and aims to improve mechanistic representation of processes within terrestrial biosphere models. The TES SFA integrates experimental and observational studies with model building, parameter estimation, and data analytics to yield reliable model projections. This integrated model-experiment approach focuses on improving the land model (ELM) of DOE's Energy Exascale Earth System (E3SM) model and fosters enhanced, interactive, and mutually beneficial engagement between models and experiments.*

Terrestrial ecosystems store vast amounts of carbon (C) and globally these C stores are increasing in C density as ecosystems remove $CO_2$ from the atmosphere via physiological C feedbacks (Friedlingstein et al. 2020). However, climate change is expected to alter net ecosystem exchange (NEE) across biomes and mobilize vulnerable C stores (IPCC 2022). Earth system models (ESMs) predict that as temperature and precipitation regimes change climate–C feedbacks will overwhelm physiological–C feedbacks (IPCC 2021). Such climate impacts will make large terrestrial C stores vulnerable to loss in the form of greenhouse gas releases to the atmosphere, further exacerbating climate change. The mechanisms underlying climate-driven C losses remain uncertain, causing large inter-model variability in ESM ensemble simulations and strongly limiting Earth system predictability.

Temperature and water dynamics across space and time regulate processes at multiple scales from soil biogeochemical cycles to vegetation C uptake. Climate change is already increasing temperatures, shifting precipitation norms, and altering the timing, magnitude, and location of extreme events such that water availability and vapor pressure deficit (VPD) are increasingly driving ecosystem function. The water cycle is particularly important to future C–climate feedbacks because increased atmospheric demand and altered precipitation patterns could shift energy- and water-limited ecotones and will intensify climate extremes such as drought and fire (USGCRP 2018). Elevated $CO_2$, however, can ameliorate some effects of increased temperatures and reduced soil moisture. In the TES SFA, we target improved understanding of the C–climate feedback, focusing on mid-latitude temperate to boreal forest ecotones and ecosystems of eastern North America—systems that span wide gradients in moisture availability and temperature. Knowledge generated from these studies will be extended to other ecosystems though improved models.

The TES SFA focuses on ecosystems subject to water, energy, and nutrient constraints whose impacts are highly uncertain in ESM predictions. Key areas of uncertainty include the responses of cold, water-logged, high-C peatlands to a changing climate. At the other end of the spectrum, the responses of ecosystems on the ecotone between energy- and water-limited regions are also not well represented in models. In transition zones, plant species approach their biogeographical limits imposed by environmental stressors and/or interspecies competition, and they often experience extremely dynamic processes of mortality, natality, and growth (Gu et al. 2015, 2016a). Climate-driven increases in temperature or aridity can also drive increased atmospheric demand for water, which may exceed vegetation capacity for transport despite available soil water, leading to desiccation and reduced C uptake. Understanding of belowground coupled C, water, and nutrient biogeochemical cycling is particularly limited and imparts significant control on aboveground ecosystem structural and functional responses to changing climate.

We structure this proposal around the following theme-motivating questions that target key knowledge gaps and uncertainties in the climate and disturbance responses of boreal and temperate ecosystems:

1. *By how much and which mechanisms will warming affect southern boreal peatland ecosystem productivity, C storage, and greenhouse gas fluxes? Can elevated $CO_2$ ameliorate the likely negative effects of warming?*
2. *How do water availability and water cycle extremes interact with climate change to regulate net ecosystem exchange and energy balance within temperate and boreal forests?*
3. *How does environmental change alter nutrient distribution and dynamics, and what are the implications for understanding and predicting ecosystem C fluxes?*
4. *How do temperature, water availability, and plant inputs affect soil C and microbial functions, and what are the implications for ecosystem C storage and greenhouse gas fluxes?*
5. *Are the humid, high-C ecosystems of North America more vulnerable to changing climate and disturbance regimes than predicted by CMIP6? How does the collective knowledge gained from the TES SFA affect our understanding of the C feedbacks in the region?*

**Approach**

To answer each research question, we combine model–experiment–observation (MODEX) efforts to understand structure and function across a hierarchy of ecological scales for robust predictive understanding. We conduct manipulation experiments, observations, and modeling at the ecosystem scale. Finer, process-scale research in the field and laboratory in conjunction with hypothesis-driven process modeling enables better understanding of individual processes and informs ecosystem-scale predictions. Individual processes that warrant our attention may be (1) a well-understood process responsible for driving key ecosystem mass and energy flux exchanges that need better regional to global quantification, or (2) a process hypothesized to be of key importance for which understandings are inadequate and data are unavailable. Modeling, synthesis of existing data, and observations at broader landscape, regional, and global scales enable extrapolation and upscaling of finer-scale results to larger scales that are more relevant to regional understanding and Earth system modeling.

To address our research questions, TES SFA research methods and platforms include unprecedented ecosystem manipulation through the SPRUCE (Spruce and Peatland Responses Under Changing Environments) experiment, and a landscape-scale observation site at MOFLUX (Missouri Ozark eddy covariance flux site), which are positioned at opposing ends of soil water availability in eastern North America (**Fig. 1.1**). To disentangle diverse species response to environmental conditions and provide additional insight into above-belowground process-level linkages, we propose to make new observations across a phylogenetically and ecologically diverse suite of tree species from mature forestry plots at The Morton Arboretum (MA) in Lisle, IL. The MA site encompasses monoculture plots of 18 tree species, subdivided among gymnosperms and angiosperms, as well as species that associate with ectomycorrhizal fungi and arbuscular mycorrhizal fungi. Historical and current observations at the Walker Branch watershed at ORNL also provide key data to inform model parameterization.

Data from TES SFA experiments, observations, and process studies are integrated into models to identify and reduce uncertainties of terrestrial process and parameter in the global Earth system (**Fig. 1.2**). E3SM (Energy Exascale Earth System Model) and its land surface component (ELM) provide a framework for this model–data integration, uncertainty quantification, and spatial and temporal extrapolation. We engage other models linked into ELM to enhance prediction of vegetation demographics and competition, such as Functionally Assembled Terrestrial Ecosystem Simulator (FATES), and microbial production of $CH_4$, such as the Microbe model. We develop new peatland modeling capabilities in ELM that will be tested against model intercomparison projects (SPRUCEMIP), and eventually offered to the broader ELM community. Model predictions are continuously improved through parameterization, calibration, and the development of new process-based submodels focused on key aspects of wetland, boreal, and temperate forest systems, such as the Microbial Enzyme Decomposition (MEND) model and the Millennial model. Belowground strategies for plant nutrient acquisition will be explored by linking ELM with the TAM (Transport and Absorptive fine roots and Mycorrhizal fungi) model that includes a 3-pool fine root structure. Additional modeling platforms are developed and maintained to facilitate model analysis and uncertainty quantification, such as the Offline Land Model Testbed (OLMT) and the Multi-Assumption Architecture and Testbed (MAAT).

Larger-scale data products, synthesis, and modeling are used to broaden and scale mechanistic understanding beyond the confines of individual sites. Additional long-term observation sites (e.g., AmeriFlux) and information from trait analysis and databases (e.g., the Fine-Root Ecology Database [FRED], LeafWeb) are integrated into ELM along with knowledge gained from SPRUCE, MOFLUX, MA, and Walker Branch sites to provide regional-scale predictions and uncertainty quantification. In this proposal, the 10-year SPRUCE experiment will come to completion. Community engagement, data synthesis, and modeling will be key to understanding how the results of this ground-breaking manipulation can be extrapolated to the larger boreal ecotone, and to define the implications for future climate and peat C storage.

**Selected highlights for the previous research period March 2019 through March 2023**

- We produced 178 published, accepted, or in press papers since March 2019 (Appendix A).
- SPRUCE – We have completed 7 years of experimental warming and elevated $CO_2$ treatments. SPRUCE treatments over the first 6 years have led to net C losses from the peatland ecosystem at 34 to 35 gC $m^{-2}$ $y^{-1}$ $°C^{-1}$. Peatland elevation also decreased with warming (Hanson et al. 2020).
- SPRUCE – *Sphagnum* research over this funding cycling has provided three major insights: (1) warming at the SPRUCE site drastically alters the *Sphagnum*-associated microbial community composition and is correlated with reduced $N_2$-fixation (Carrell et al. 2019); (2) the main symbiotic partner with *Sphagnum*, *Nostoc spp*. ($N_2$-fixing cyanobacteria), is maintained through a unique exchange of C-, N-, and S-rich nutrients and is only mutualistic at low pH (Veličković et al. 2018, Carrell et al. 2022b); and (3) the ability for *Sphagnum* to acclimate to warming is highly dependent on its microbial community (Carrell et al. 2022a).
- Modeling – Multi-Assumption Architecture and Testbed (MAAT) v1.3 code was published open source on GitHub (https://github.com/walkeranthonyp/MAAT).
- Root Function – The impacts of roots and mycorrhizal hyphae on soil hydraulic parameters such as saturated hydraulic conductivity and soil water retention was highlighted in a recent paper published in *Rhizosphere* (Marcacci et al. 2022).
- Soil Carbon – A meta-analysis and incubation modeling study found that incubations and field-scale warming experiments conducted over short time frames predicts large losses of soil organic C stocks that are not sustained when experiments are run over longer periods (Jian et al. 2020).
- MOFLUX – Wood et al. (2023) reported a water availability threshold above which the forest was capable of actively regulating responses to environmental stress and below which this capability was lost.
- MOFLUX – Novel net flux partitioning approaches for eddy covariance data were developed, enabling better understanding of mechanisms controlling ecosystem component responses to environmental variations (Liu et al. 2022, Kira et al. 2021)
- MOFLUX – Models of photochemistry of electron transport were developed to model photosynthesis, explanation of chloroplast thylakoid structure and functions, and mechanistic expressions of solar-induced chlorophyl fluorescence (Gu et al. 2022 and 2023, Sun et al. 2023a).
- MOFLUX – The Fluorescence Auto-Measurement Equipment (FAME) technology developed by the SFA was patented by the US patent office, used in Next Generation Ecosystem Experiment (NGEE)-Arctic and NGEE-Tropics, and licensed to Campbell Scientific, INC.
- FRED – The third version of the Fine-Root Ecology Database (FRED 3.0) was released in March 2021 (data citation: Iversen et al. 2021), and data have been filtered and downloaded via the new user interface at https://roots.ornl.gov/public-release hundreds of times. FRED 3.0 has more than 150,000 observations of more than 330 root traits, with data collected from more than 1400 data sources. We highlighted FRED 3.0 as a community resource for belowground ecologists and modelers alike in an editorial that accompanies a Virtual Special Issue in *New Phytologist*, where we compiled more than 40 recent papers on the topic ‘Filling gaps in our understanding of belowground plant traits across the world’ (Iversen and McCormack 2021).

- LeafWeb – LeafWeb provided direct data support to the following studies: respiratory $CO_2$-refixation across species (Eckert et al. 2020, 2021); physiological basis and models for estimating photosynthesis with chlorophyll fluorescence (Han et al. 2022a & c, Li et al. 2020, Sun et al. 2023a); regulations of photosynthesis by photochemical and non-photochemical quenching (Han et al. 2022b); development of the bellows theory to explain the granal thylakoid structure and function of higher plants (Gu et al. 2022); development of a photochemical model for photosynthetic electron transport (Gu et al. 2023). The 2022 LeafWeb joint fluorometry and gas exchange data set is the largest ever released in the world (https://www.leafweb.org/information/data-publications/). LeafWeb is also providing C4 data support to C4 model synthesis led by Prof Danielle Way of Australian National University.

**Primary TES SFA, USDA Forest Service, and University Funded Participants for the period from September 2023 through September 2028.**

| Count | Person | Position/Institution |
|---|---|---|
| 1 | Anping Chen | Research Scientist, Colorado State University |
| 2 | Joanne Childs | ORNL Master Technician |
| 3 | Matt Craig | ORNL Associate Research Staff |
| 4 | Nancy F. Glenn | Professor, Boise State University |
| 5 | Natalie A. Griffiths | ORNL Senior Research Staff |
| 6 | Lianhong Gu | ORNL Distinguished Research Staff |
| 7 | Mark Guilliams | ORNL Technician |
| 8 | Paul J. Hanson | ORNL Corporate Fellow |
| 9 | Colleen M. Iversen | ORNL Distinguished Research Staff |
| 10 | Mihgzhou Jin | Professor, University of Tennessee, Knoxville |
| 11 | Randall K. Kolka | USDA Forest Service Researcher |
| 12 | David M. Kramer | Professor, Michigan State University |
| 13 | Misha B. Krassovski | ORNL Technical Professional |
| 14 | John Latimer | ORNL SPRUCE Subcontracted field technician |
| 15 | Yiqi Luo | Professor, Cornell University |
| 16 | Jiafu Mao | ORNL Senior Research Staff |
| 17 | Melanie A. Mayes | ORNL Distinguished Research Staff |
| 18 | M. Luke McCormack | Research Scientist, The Morton Arboretum |
| 19 | Karis J. McFarlane | Research Scientist, Lawrence Livermore National Laboratory |
| 20 | Keith C. Oleheiser | ORNL Technician |
| 21 | Kyle Pearson | ORNL Technical Professional |
| 22 | Daniel M. Ricciuto | ORNL Senior Research Staff |
| 23 | Andrew D. Richardson | Professor, Northern Arizona State University |
| 24 | Thomas A. Ruggles | ORNL Technical Professional |
| 25 | Verity G. Salmon | ORNL Research Staff |
| 26 | Christopher W. Schadt | ORNL Senior Research Staff |
| 27 | Geoff Schwaner | ORNL Technician |
| 28 | Stephen D. Sebestyen | USDA Forest Service Researcher |
| 29 | Xiaoying Shi | ORNL Research Staff |
| 30 | Terri Velliquette | ORNL Technical Professional |
| 31 | Anthony Walker | ORNL Senior Research Staff |
| 32 | Bin Wang | ORNL Postdoctoral Research Associate |
| 33 | Dali Wang | ORNL Senior Research Staff |
| 34 | Yaoping Wang | ORNL Postdoctoral Research Associate |
| 35 | Jeffrey M. Warren | ORNL Senior Research Staff |
| 36 | Sören E. Weber | ORNL Postdoctoral Research Associate |
| 37 | David J. Weston | ORNL Senior Research Staff |
| 38 | Jeffrey D. Wood | Assistant Research Professor, University of Missouri – Columbia |
| 39 | Xiaofeng Xu | Associate Professor, San Diego State University |
| 40 | Xiaojuan Yang | ORNL Research Staff |

# Narrative (Sections 1 Through 8)

## 1. BACKGROUND AND JUSTIFICATION

Oak Ridge National Laboratory's (ORNL's) Terrestrial Ecosystem Science Scientific Focus Area (TES SFA) conducts fundamental research in ecology and environmental science in support of the US Department of Energy (DOE) Office of Science Biological and Environmental Research (BER) Earth and Environmental System Sciences Division (EESSD) Environmental Systems Science (ESS) program. Our science is motivated by the grand challenges articulated in the EESSD Strategic Plan (DOE 2018) and the 2017 BERAC Grand Challenges Report (BERAC 2017) and supports a number of the pillars of the most recent US Global Change Research Program Strategic Plan (USGCRP 2022). The TES SFA addresses EESSD grand challenges by advancing our understanding of key ecosystem processes (including emphasis belowground) and components (soils, microbes, plants), their interactions, and their responses to climate change. TES SFA research is ambitious in its scope, effort, and resource requirements, undertaking the challenge of fully utilizing, testing, and extending broad interdisciplinary facilities of a DOE national laboratory. The ORNL TES SFA addresses complex multiscale, multidisciplinary scientific challenges with empirical, manipulative, and mechanistic modeling approaches enabled by long-term commitment and support from DOE. This project is unique in scope and depth, complements university and private sector efforts, and provides collaborative support for outside scientific endeavors.

### 1.1 Research Overview

Terrestrial ecosystems store vast amounts of C and globally these C stores are increasing in C density as ecosystems remove $CO_2$ from the atmosphere via physiological C feedbacks (Friedlingstein et al. 2020). However, climate change is expected to alter net ecosystem exchange (NEE) across biomes and mobilize vulnerable C stores (IPCC 2022). Earth system models (ESMs) predict that as temperature and precipitation regimes change, climate–C feedbacks will overwhelm physiological–C feedbacks (IPCC 2021). Such climate impacts will make large terrestrial C stores vulnerable to loss in the form of greenhouse gas releases to the atmosphere, further exacerbating climate change. The mechanisms underlying climate-driven C losses remain uncertain, causing large inter-model variability in ESM ensemble simulations and strongly limiting Earth system predictability.

Temperature and water dynamics across space and time regulate processes at multiple scales from soil biogeochemical cycles to vegetation C uptake. Climate change is already increasing temperatures, shifting precipitation norms, and altering the timing, magnitude, and location of extreme events such that water availability and vapor pressure deficit (VPD) are increasingly driving ecosystem function. The water cycle is particularly important to future C–climate feedbacks because increased atmospheric demand and altered precipitation patterns could shift energy- and water-limited ecotones and will intensify climate extremes such as drought and fire (USGCRP 2018). Elevated $CO_2$, however, can ameliorate some effects of increased temperatures and reduced soil moisture. In the TES SFA, we target improved understanding of the C–climate feedback, focusing on mid-latitude temperate to boreal forest ecotones and ecosystems of eastern North America—systems that span wide gradients in moisture availability and temperature. Ongoing and proposed research efforts in the ORNL TES SFA seek to provide answers to the following overarching question:

> **How vulnerable to climate change are C stores of terrestrial ecosystems in eastern North America, and what are the implications for C–climate feedbacks?**

The TES SFA focuses on ecosystems subject to water, energy, and nutrient constraints whose impacts are highly uncertain in ESM predictions. Key areas of uncertainty include the responses of cold, water-logged, high-C peatlands to a changing climate. At the other end of the spectrum, the responses of ecosystems on the ecotone between energy- and water-limited regions are also not well represented in models. In transition zones, plant species approach their biogeographical limits imposed by environmental stressors and/or interspecies competition, and they often experience extremely dynamic processes of mortality, natality, and growth (Gu et al. 2015, 2016a). Climate-driven increases in temperature or aridity can also drive increased atmospheric demand for water, which may exceed vegetation capacity for transport despite available soil water, leading to desiccation and reduced C uptake. Understanding of belowground-coupled C, water, and nutrient biogeochemical cycling is particularly limited and imparts significant control on aboveground ecosystem structural and functional responses to changing climate.

We structure this proposal around the following theme-motivating questions that target key knowledge gaps and uncertainties in the climate and disturbance responses of boreal and temperate ecosystems:

1. *By how much and by which mechanisms will warming affect southern boreal peatland ecosystem productivity, C storage, and greenhouse gas fluxes? Can elevated $CO_2$ ameliorate the likely negative effects of warming?*
2. *How do water availability and water cycle extremes interact with climate change to regulate net ecosystem exchange and energy balance within temperate and boreal forests?*
3. *How does environmental change alter nutrient distribution and dynamics, and what are the implications for understanding and predicting ecosystem C fluxes?*
4. *How do temperature, water availability, and plant inputs affect soil C and microbial functions, and what are the implications for ecosystem C storage and greenhouse gas fluxes?*
5. *Are the humid, high-C ecosystems of North America more vulnerable to changing climate and disturbance regimes than predicted by CMIP6? How does the collective knowledge gained from the TES SFA affect our understanding of the C feedbacks in the region?*

These five questions are tackled in five corresponding research themes (Section 1.3).

### 1.2 Research Philosophy

Our research philosophy is integrative, question-based, hypothesis-driven, and iterative to provide robust advances in Earth system predictability. Key uncertainties about vulnerable ecosystems and their impact on the Earth system arise from incomplete scientific knowledge and are identified through empirical research, literature synthesis, and model analysis. These uncertainties are a foundation for a high-level and specific research plan under a single overarching question which defines a research theme within this proposal (Section 1.3).

To answer each research question, we combine model–experiment–observation (MODEX) efforts to understand structure and function across a hierarchy of ecological scales for robust predictive understanding (**Fig. 1.1**). We conduct manipulation experiments, observations, and modeling at the ecosystem scale. Finer, process-scale research in the field and laboratory in conjunction with hypothesis-driven process modeling enables better understanding of individual processes and informs ecosystem-scale predictions. Individual processes that warrant our attention may be (1) a well-understood process responsible for driving key ecosystem processes that need better regional to global quantification, or (2) a process hypothesized to be of key importance for which understandings are inadequate and data are unavailable. Modeling, synthesis of existing data, and observations at broader landscape, regional, and global scales enable extrapolation and upscaling of finer-scale results to larger scales that are more relevant to regional understanding and Earth system modeling.

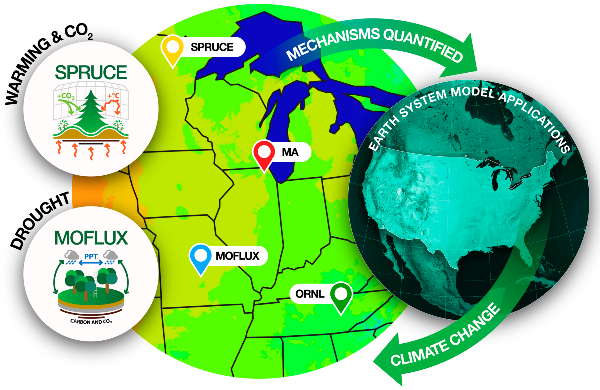

**Fig. 1.1 Image capturing TES SFA Thematic areas of research driven by global climate and environmental change issues. Study sites in the focus region represent important areas of North America. Major field studies are located at ecotone boundaries for moisture (SPRUCE upland–wetland; MOFLUX forest–prairie). Process research is carried out at ORNL and the Morton Arboretum (MA). Modeling/MODEX efforts are located primarily at ORNL with the support of key subcontracted groups.**

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Within each research theme, we deploy a mixture of interactive approaches to yield new understanding and improve models for each focused topic (**Fig. 1.2**). These approaches are (1) empirical: manipulation and observation; (2) data-based: extracting published and unpublished measurements within and beyond the SFA; (3) process-based: a focus on incorporation of key above- and belowground processes; and (4) scale/hierarchy: extending our work across scales. Within each research Theme, we also include Tasks that reflect these different scales and data types.

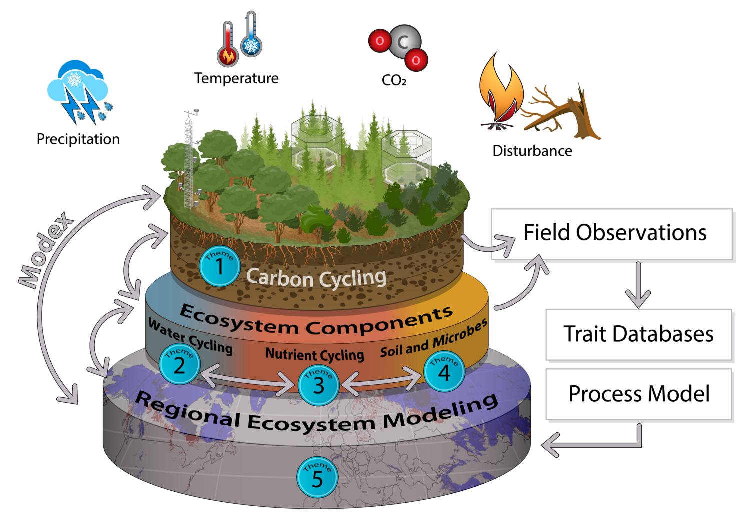


**Fig. 1.2 A representation of the model-experiment dialog that takes place across the SFA research themes as we characterize key ecosystem responses to climate drivers across important natural gradients for eastern United States ecosystems. Disturbance of many types are represented by fire and a broken tree in the figure.**

Open science is a key component of our research philosophy. Science and society benefit the most when scientific data, tools, and methods are open access. We plan for and expend effort on data management, data archival, and open access to model and software tools and research publications. We also aim to build a diverse research community and provide our research platforms as an open resource.

Open science also means open to everyone. The TES SFA will be managed by an Executive Committee composed of the Co-PIs and Theme/Task leaders, the data manager, and an early career staff representative to ensure open communication and engagement through all levels of the project. We will develop a new Code of Conduct to ensure equity and inclusion; enhance training to prevent possible harassment and bullying throughout our lab activities, field work, conference attendance, and scientific publications; and to provide mentoring and growth opportunities for everyone on the project (Section 6). We are engaging with historically black colleges and universities (HBCUs) and minority serving institutions (MSIs) to ensure their participation in the TES SFA and to provide important job training activities and increase community engagement regarding the effects of climate change and the potential for mitigation.

## 1.3 Research Approaches

To address our research questions, TES SFA research methods and platforms include unprecedented ecosystem manipulation through the Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment, and a landscape-scale observations the Missouri Ozark eddy covariance AmeriFlux site (MOFLUX), which are positioned at opposing ends of soil water availability in eastern North America. On the higher soil water side, SPRUCE is a large-scale environmental change experiment focusing on the response of a *Picea mariana* (black spruce)–*Sphagnum* peat bog in northern Minnesota to multiple levels of warming at ambient or elevated $CO_2$. Boreal and temperate peatlands and forests are significant global C stores that if lost are irrecoverable within the time scale needed to mitigate climate change through decarbonization (Noon et al. 2021). Loss of boreal forest C represents one of nine key global tipping points (Lenton et al. 2019) and loss of boreal and temperate peat could be even more significant. SPRUCE offers an in situ experimental platform for testing mechanisms that control vulnerability of organisms and ecosystem processes to temperature and elevated atmospheric $CO_2$ and provides data for model development and testing. A recent short-term drought at SPRUCE showed the added benefits of interannual variability for testing additional hypotheses.

On the lower soil water end of the spectrum in the eastern United States, the TES SFA supports long-term monitoring of landscape-scale C and energy flux and solar-induced chlorophyll fluorescence (SIF) measurements at the MOFLUX forest–prairie transition site. MOFLUX exemplifies upland hardwood forests in which a balance of water and energy controls C cycling. Being on the forest–prairie ecotone, MOFLUX is subject to periodic droughts that can alter plant productivity, mortality, and soil respiration, and thereby ecosystem C storage. Both SPRUCE and MOFLUX research platforms support and benefit from smaller-scale, process-level observations of mechanistic processes ranging from soil C cycling to root function to photosynthesis, while attracting and maintaining a large community of outside collaborators contributing a myriad of research projects within these platforms.

To disentangle diverse species response to environmental conditions and provide additional insight into above-belowground process-level linkages that inform models, we propose to make new observations across a phylogenetically and ecologically diverse suite of tree species from mature forestry plots at The Morton Arboretum (MA) in Lisle, Illinois. The MA site encompasses monoculture plots of 18 tree species, subdivided among gymnosperms and angiosperms, as well as species that associate with ectomycorrhizal fungi and arbuscular mycorrhizal fungi. Historical and current observations at the Walker Branch watershed at ORNL also provide key data to inform model parameterization.

Data from TES SFA experiments, observations, and process studies are integrated into models to identify and reduce uncertainties of terrestrial process and parameter in the global Earth system (**Fig. 1.2**). E3SM (Energy Exascale Earth System Model) and its land surface component (ELM) provide a framework for this model–data integration, uncertainty quantification, and spatial and temporal extrapolation. We engage other models linked into ELM to enhance prediction of vegetation demographics and competition, such as Functionally Assembled Terrestrial Ecosystem Simulator (FATES), and microbial production of $CH_4$, such as the Microbe model. We develop new peatland modeling capabilities in ELM that will be tested against model intercomparison projects (SPRUCEMIP), and eventually offered to the broader ELM community. Model predictions are continuously improved through parameterization, calibration, and the development of new process-based submodels focused on key aspects of wetland, boreal, and temperate forest systems, such as the Microbial Enzyme Decomposition (MEND) model and the Millennial model. Belowground strategies for plant nutrient acquisition will be explored by linking ELM to the TAM (Transport and Absorptive fine roots and Mycorrhizal fungi) model that includes a 3-pool fine root structure. Additional modeling platforms are developed and maintained to facilitate model analysis and uncertainty quantification, such as the Offline Land Model Testbed (OLMT) and the Multi-Assumption Architecture and Testbed (MAAT).

Larger-scale data products, synthesis, and modeling are used to broaden and scale mechanistic understanding beyond the confines of individual sites. Additional long-term observation sites (e.g., AmeriFlux) and information from trait analysis and databases (e.g., the Fine-Root Ecology Database [FRED], LeafWeb) are integrated into ELM along with knowledge gained from SPRUCE, MOFLUX, MA, and Walker Branch at ORNL to provide regional-scale predictions and uncertainty quantification. In this proposal, the 10-year SPRUCE experiment will come to completion. Community engagement, data synthesis, and modeling will be key to understanding how the results of this ground-breaking, long-term manipulation can be extrapolated to the larger boreal ecotone, and to define the implications for future climate and peat C storage.

## 1.4 Research Themes

This section provides an overview of the five TES SFA research themes. Associated hypotheses, primary tasks, and key deliverables for each theme are described in Section 3.

### 1.4.1 Theme 1: Peatland C Cycle Responses to Warming and Elevated $CO_2$

The goal of Theme 1 is to provide mechanistic understanding and model improvements to understand the impacts of warming associated with climate change on peatland ecosystem C cycle and balance leading to uptake from or release of C to the atmosphere. We use consistent above- and belowground manipulations of the ecosystem climate and atmosphere to examine plausible future conditions that ecosystems will be exposed to under a warming climate with elevated $CO_2$ atmospheres. With this proposal, we seek support to complete a decade of operation of the SPRUCE experiment (Hanson et al.

2017; https://mnspruce.ornl.gov/). This manipulation examines sustained temperature increases across a broad range of warming conditions (+0°C to +9°C) with and without the addition of elevated $CO_2$ atmospheres (+500 ppm). We focus on temperate peatland ecosystems because they store a disproportionately large amount of terrestrial C and are expected to be vulnerable to climate change. Smaller-scale process efforts in other TES SFA Themes and the results from other warming research studies around the world are important to the interpretation of SPRUCE-specific observations and proposed syntheses will seek to identify and quantify universal response mechanisms applicable to wetlands in general, and these findings will be shared with the broader community in an international workshop in 2024. Modeling efforts synthesize our experimental results over time and across spatial scales and provide the basis for a functional wetland land surface model applicable to the SPRUCE peatland and related wetland ecosystems.

### 1.4.2 Theme 2: Water, C, and Energy Processes under Compounding Climatic Stressors

The goal of Theme 2 is to develop predictive understanding of coupled ecosystem water, energy, and C-cycle processes that can be transferred directly to improving the performance of ecosystem and land surface models. Theme 2 also uses the understanding of complementary ecosystem processes (e.g., nutrient cycling, microbial activities) gained in other TES SFA themes to inform representations of land surface processes in climate models. Research will emphasize the SPRUCE and MOFLUX field sites in sensitive ecotones at the two ends of a forest ecosystem water availability spectrum. For energy processes, we propose to answer the long-term question of why state-of-the-art measurement techniques cannot close the land surface energy budget. Theme 2 will test the hypothesis that the transient energy storage in photophysical, photochemical, and biochemical reactions of photosynthesis, particularly the proton motive force (PMF; the electric and proton concentration gradients across the thylakoid membrane established by photosynthetic electron transport), are sufficiently large to affect leaf and land surface energy balance and temperature regimes. For C processes, Theme 2 will develop advanced, mechanism-based methods that partition observed net fluxes into contributions from different pathways across scales (gross primary production [GPP], autotrophic/heterotrophic above/belowground respiration, point to ecosystem scales) and innovative analysis approaches such as coupled photophysical, photochemical, and biochemical (CPPB) modeling and machine learning (ML). For water processes, we will target uncertainties in limitation through the soil-plant-atmosphere continuum (SPAC), ranging from pore-level assessment of soil–root connectivity to ecosystem-level exchanges of water and C with the atmosphere. Theme 2 will also support improvements to the web-based analytical and archive tool LeafWeb so that it may continue to be a comprehensive automated online tool to support cutting-edge environmental photosynthesis research and monitoring for the global community. Data collected by LeafWeb will be used in Theme 2 studies of ecosystem energy, water, and C processes.

### 1.4.3 Theme 3: Nutrient-C Feedbacks

The goal of Theme 3 is to quantify the role that nutrients play in modulating C cycle feedbacks. We will use empirical data collection, database curation, and an array of field sites to improve the ability of nutrient-enabled ESMs to predict ecosystem response to climate change. The role of N in limiting C sequestration is especially unclear in simulations of boreal ecosystems. Initial results from the SPRUCE experiment indicate that trees and shrubs do not consistently take advantage of observed increases in nutrient availability, and the decline in *Sphagnum* biomass and productivity has caused a net decrease in the plant biomass N and P pools after 6 years of experimental manipulations (Section 2). To improve the representation of nutrient cycling in ESMs requires expanding our scientific scope beyond the boreal zone and the SPRUCE experiment. Comprehensive nutrient budgets and dynamics need to be quantified from a variety of ecosystem types so that a clear understanding of plant nutrient acquisition strategies and microbial nutrient use during decomposition can be attained. In this theme, we propose to expand observations at MOFLUX to include plant and soil nutrient dynamics, downslope leaching, erosion, and litter chemistry. At MA, we aim to complement ongoing process measurements of above- and belowground plant phenology in monospecific forestry plots with measurements of resin-available N and P in soils. Lastly, we will support continued development and expansion of the global trait database FRED with an emphasis on data curation from underrepresented biomes underlain by organic soils (e.g., bogs) as well as fine-root traits that inform the representation of root nutrient acquisition in models across a variety of plant functional types (PFTs). Model refinement of nutrient acquisition, allocation algorithms, nutrient resorption for whole ecosystems, plants, and microbes will take place by linking ELM with TAM, enabling dynamic vegetation feedbacks with FATES, and testing process hypotheses in MAAT. Our proposed research will incorporate data collection from experimental manipulation (SPRUCE), natural climate variation (MOFLUX), monospecific stands, and FRED into a wide array of nutrient-enabled models. These models will be evaluated to quantify the effects of environmental change on nutrient distribution and dynamics and strengthen our predictive understanding of nutrient constraints on ecosystem C fluxes.

### 1.4.4 Theme 4: Microbial and Soil-forming Processes

The goal of Theme 4 is to determine the influence of microbial and soil-forming processes on soil C storage and greenhouse gas emissions, given the effects of climate change on soil temperature, moisture, and plant inputs. For at least a decade, the role of the microbial community in soil C storage and greenhouse gas emissions has been highly debated. Traditional first-order models remain unable to capture many nonlinear processes such as priming, changes in inputs, microbial community shifts, and acclimation of microbial physiology to climate changes. However, models that explicitly include microbial pools and functions retain artifacts of their structural configuration. These structures vary widely and encompass different representation of soil aggregation; partitioning of microbial community into bacteria, fungi, and archaea or functional groups; representation of microbial uptake and leaching of dissolved organic C (DOC); types of DOC; and whether to include enzymes explicitly. Consequently, different microbial-explicit models will produce different predictions of future soil C stores and greenhouse gas emissions. In this Theme, we seek to use new observations and the long-term data collection at MOFLUX within the multi-model environment of MAAT to determine optimal model configurations to best predict the future trajectory of soil C storage in the context of long-term climate changes and short-term climate events at the forest–prairie ecotone. A major outcome of this effort will be to discover the efficacy of including different structure, pools, and parameters in microbial models and thereby provide appropriate and tested model configurations to the ELM community. At SPRUCE, we will take advantage of a wealth of existing microbial data, ongoing and new regular data collections from multiple decomposition experiments, higher frequency microbial biomass estimates using multiple methodologies, and new automated real-time greenhouse gas emission measurements to understand and predict how different microbial functional groups, such as bacteria, fungi, and archaea, contribute to observed high-frequency $CH_4$ and $CO_2$ emissions as a function of experimental treatments, seasons, and time.

### 1.4.5 Theme 5: Regional Integration and Extrapolation

The goal of Theme 5 is to implement our improved process knowledge in a regional modeling framework to quantify and understand the broader scale vulnerability of ecosystem C and C feedbacks of humid ecosystems of North America under climate change. The regional domain includes our core and secondary sites (**Fig. 1.1**: SPRUCE, MOFLUX, MA, Walker Branch), covers key C stores over a large range of potentially vulnerable temperate and boreal ecosystems, and sits on what is currently the humid side of the strong continental gradient in aridity index. Integration and extrapolation activities leverage ELM developments in Themes 1–4 and integrate them to make multi-site and regional simulations. We also leverage high-resolution observations to support vulnerability assessments where models may be missing key processes or structures. These regional simulations and analyses using improved process knowledge of peatlands and forest processes will be assessed against state-of-the-art C cycle climate models to assess how knowledge gained within the SFA changes our understanding of climate-C feedbacks and future projections. We will use advanced multi-site model calibration to estimate PFT parameters for ELM and FATES-enabled ELM across our study domain. We will develop high-resolution data sets to drive the model and run high-resolution simulations to help capture fine spatial variability and better represent nonlinearity in ecosystem responses to climate change. High-resolution observations and model data will be utilized to provide detailed quantification of model uncertainty and comprehensive assessment of ecosystem vulnerability across North America.

## 2. PROGRESS MARCH 2019 THROUGH DECEMBER 2022

This section summarizes accomplishments of the ORNL TES SFA since the 2019 review. Over that period, we have published 178 peer-reviewed articles in leading national and international scientific journals, sustained SPRUCE experiment science and operations, continued long-term MOFLUX landscape C flux and energy balance observations, developed cutting-edge SIF measurements and associated mechanistic models, conducted process-based research on root function and microbial soil C cycles, improved process-based predictive models as potential inputs into Earth system landscape models, and continued the development of publicly available data sets of global importance. We also provided leadership in national and international ecological and climate change–related workshops and meetings, and in numerous interactions with the public. Publications for the reporting period cited here are enumerated in Appendix A, and data products listed in Appendix B are denoted in the text using a "D" after the publication date (e.g., Heiderman et al. 2018D) to distinguish them from publication citations.

### 2.1 SPRUCE Experiment

The SPRUCE experiment, established in August 2015 (Hanson et al. 2017), is the first whole-ecosystem, forest-scale experiment to increase temperatures from deep soils throughout tree canopies in combination with increasing atmospheric $CO_2$ concentrations. The decade-long experiment is being carried out in an ombrotrophic bog peatland ecosystem of northern Minnesota (S1 Bog on the USDA Forest Service Marcell Experimental Forest) dominated by trees, *P. mariana* and *Larix laricina* (larch); ericaceous shrubs, *Rhododendron groenlandicum* (Labrador tea) and *Chamaedaphne calyculata* (leatherleaf); sedges; and mosses in the genus *Sphagnum*. The SPRUCE experiment consists of 10 specially designed, enclosed plots that are 12.8 m in diameter and outfitted with heating infrastructures for air- and deep-soil warming, as well as a range of biological and environmental monitoring sensors (Griffiths and Sebestyen 2016D, Krassovski et al. 2015, 2018, Hanson et al. 2015D, 2016D).

The SPRUCE study was established to address the primary and supplemental overarching hypotheses presented in Section 1.3 with a focus on cycling and storage of C and its potential release to the atmosphere in the form of $CO_2$ or $CH_4$. The ecosystem-scale observations of SPRUCE further enable testing the role and importance of belowground process (rooting, water and nutrient acquisition, microbial community structure and function) and aboveground community structure (*Sphagnum* vs. shrub-layer vegetation vs. trees).

Hypothesized increases in $CO_2$ and $CH_4$ release to the atmosphere in response to temperature increases across a broad range (+0 to +9°C) have been supported by data (Hanson et al. 2020). Reductions in net primary production (NPP) dominated by the loss of *Sphagnum* contributions (Norby et al. 2019) and enhancements in decomposition and methanogenesis drive the linear declining function with warming (Hanson et al. 2020, Kluber et al. 2020, Liang et al. 2021, Wilson et al. 2021a). A hypothesized role for elevated $CO_2$ as an offset to such losses has not been found to be significant, presumably because of nutrient limitations present in the ombrotrophic peatland even though nutrient availability has increased with warming (Iversen et al. 2023).

The following text provides succinct descriptions of SPRUCE science accomplishments since March 2019. Published works are described and recent results are highlighted and referenced to publicly available data sets. Prior descriptions of SPRUCE are also available at http://mnspruce.ornl.gov/content/spruce-project-documents. A full description of SPRUCE infrastructure and operations is included in Appendix E.

#### 2.1.1 SPRUCE C Cycle Changes

The SPRUCE study of long-term, whole-ecosystem warming (WEW) enabled ecosystem-level analysis of changes in the peatland C cycle (Hanson et al. 2020). Warming caused variable responses for vegetation and consistent net losses of both $CO_2$ and $CH_4$ for a linear response of $-31.3$ gC $m^{-2}$ $y^{-1}$ $°C^{-1}$. Carbon losses with warming of +2.25°C to +9°C were found to be 4.5 to 18 times faster than the historical rate of peatland C accumulation. Through 3 years of sustained active season exposure to elevated $CO_2$, we did not observe a dominant and hypothesized increase in C uptake, likely due to nutrient limitations on the photosynthetic process.

Component annual net C exchange (NCE; gC $m^{-2}$ $y^{-1}$) data for all plots are now available through the first 6 years of the SPRUCE study. The 6-year results suggest that autotrophic decreases for *Sphagnum* and trees are partially offset by gains by the shrub community and fine root processes belowground. Nevertheless, the overall C sink capacity continues to decline with warming driven mostly by heterotrophic C losses. The combined plot-level estimate of NCE shows that loss rates per degree C are similar through 6 years of manipulation without a strong elevated $CO_2$ ($eCO_2$) effect consistent with Hanson et al. (2020) as shown in **Fig. 2.1**.

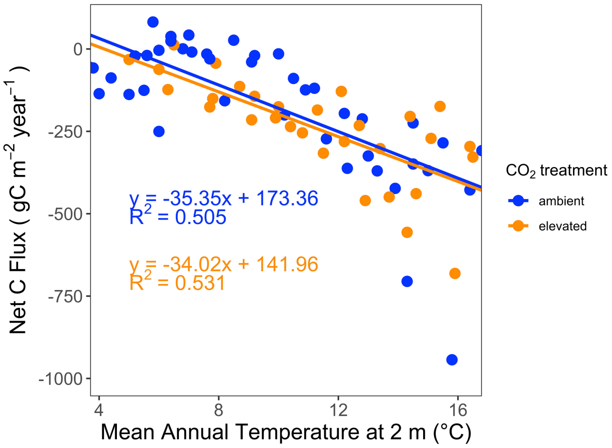


**Fig. 2.1. Estimated ecosystem net C exchange (NCE) for all treatments and years plotted against the mean annual air temperature at +2 m for each plot in 2016, 2017, 2018, 2019, 2020, and 2021. NCE was calculated as the difference in measures of above- and belowground net primary production (NPP) C losses via heterotrophic $CO_2$ efflux, net $CH_4$ efflux, and combined total organic C and dissolved inorganic C efflux. Treatment plots receiving ambient or elevated $CO_2$ atmospheres denoted by color symbols.**

Helbig et al. (2022) contrasted the SPRUCE experimental warming results with multiyear eddy covariance NEE estimates for multiple peatland sites. The reported data demonstrate that simple interannual variation in temperatures for natural systems are unable to inform warming level responses enabled by the SPRUCE experiment.

S1 Bog phenology – Phenological observations of tree, shrub, and sedge spring growth and flowering (*P. mariana, L. laricina, R. groenlandicum, C. calyculata, Maianthemum*, sedges), foliar senescence (*L. laricina, Smilacina*), and snow-cover metrics are being recorded. A daily photographic record of tree-, shrub-, and instrument-level monitoring has been compiled into phenology movies (https://mnspruce.ornl.gov/node/594), and phenology images are being incorporated into the PhenoCam network (https://phenocam.nau.edu). Richardson et al. (2018) published the first 2 years of phenology results in *Nature,* which reported that WEW linearly correlated with an unexpected delay in autumn green-down and an expected advance in spring green-up of the dominant woody species. Updated analyses of continued operations show sustained warming impacts on metrics of phenology.

### 2.1.2 Changing Peat Profile C Stocks and Related Processes

McFarlane et al. (2018) examined the historical peatland accumulation rates for the S1 Bog. The authors found that the bog has been accumulating C in peat for 11,000 years, but accumulation rates changed over time with a period of low C accumulation—likely a result of warmer and drier environmental conditions. These results suggest that experimental warming treatments, as well as a future warmer climate, may reduce net C accumulation in peat in this and other southern boreal peatlands. In 2021, 5-year post-treatment samples of peat were collected but showed no dramatic changes in peat characteristics based on traditional metrics (e.g., bulk density, C concentration). Additional analyses based on isotopic changes in the surface peat have been reported (Wilson et al. 2021a). Additional assessments of the bulk peat profile are pending.

*Related bog elevation measurements* – Because warming and $eCO_2$ treatments are hypothesized to have dramatic effects on peat C stocks, we have tracked changes in bog elevation over time using standard elevation transects (two groups per enclosure). Since the initiation of WEW treatments, control and ambient (non-enclosed) plots have continued to gain elevation, but there is a significant and progressive decline in elevation with warming treatments, especially in the hollows (**Fig. 2.2**). Elevation reductions may result from mass loss (i.e., gaseous C loss through enhanced respiration or methanogenesis, or loss of dissolved C through outflow), volume loss due to drying (esp. 2021), collapse of the *Sphagnum* layer (see next section), or loss of hummock–hollow microtopography due to reduced root production that provides architectural structure for the hummock–hollow complex. If solely from mass loss, the 5 cm decline in elevation exhibited in the +9°C treatment would equate to a major C loss of approximately 1.4 kg C per m$^2$.

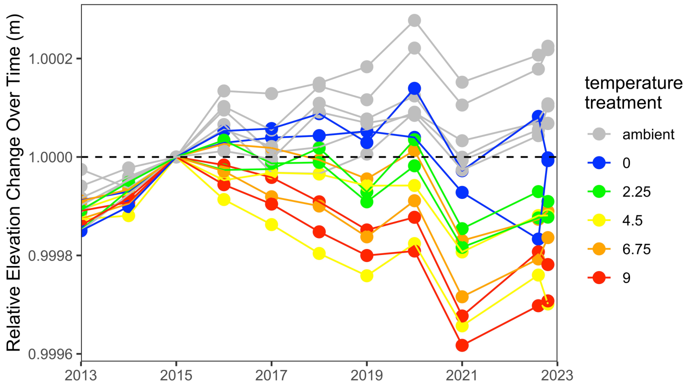


**Fig. 2.2. Relative change in peat elevation by treatment temperature since pretreatment assessments in 2015 are plotted through 2022. The reference elevation is at 1 m = 412.5 m. Warmer colors indicate warmer temperature treatments.**

*Decomposition* – After 6 years of in situ placement, litterbags continue to reveal no clear effect of warming on the decomposition of aboveground litter in the 10 SPRUCE enclosures. Decomposition rates of fine roots (primarily *Rhododendron* fine roots) continued to show a positive response to warming. Samples from the year 6 litterbag collection are being analyzed for microbial community composition and chemical composition (C, N, P content). One final (10 year) retrieval is planned in 2025.

Shelley et al. (2022) conducted a 5-year decomposition study outside of the enclosures and examined the effect of intrinsic (litter quality) vs. extrinsic (soil moisture, temperature, porewater chemistry) drivers on moss decomposition. They found that litter chemistry was the main driver of the early phases of decomposition, and environmental drivers became more important in the later phases. These findings suggest that warming effects (an extrinsic driver) may become more apparent as the SPRUCE decomposition measurements continue.

Biannual cotton strip retrieval (a stable and uniform surrogate for plant tissues composed of 95% cellulose) reveals strong effects of warming on labile C decomposition, with faster decomposition in warmer enclosures throughout the peat profile (**Fig. 2.3**). However, soil moisture is the predominant driver in the near-surface peats, which has implications for interpreting decomposition drivers in our litterbag study (the litterbags are deployed in the top 0–20 cm of peat). A manuscript describing the cotton strip results is being drafted.

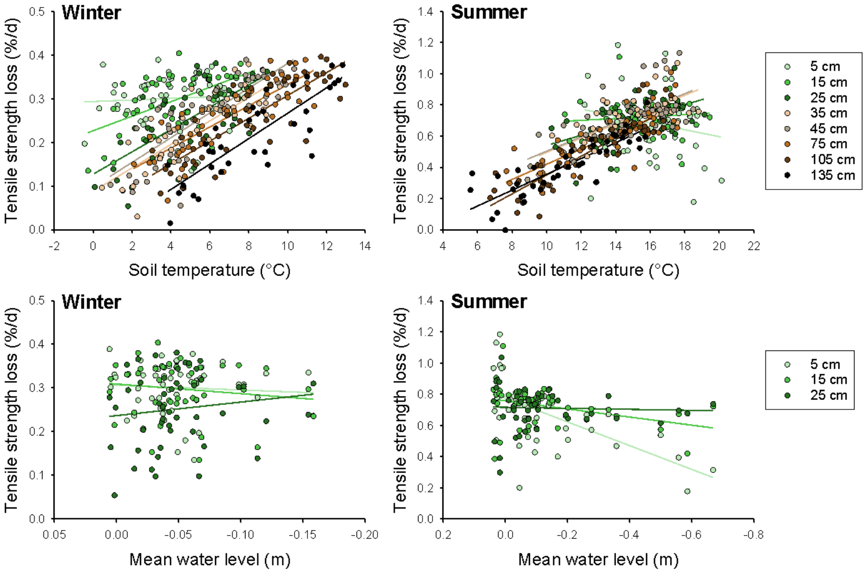


**Fig. 2.3. Relationships between soil temperature and tensile strength loss (cotton strip decomposition) from 5 to 135 cm deep in the (top left) winter and (top right) summer, and relationships between water level (an indicator of soil moisture) and tensile strength loss in near-surface peats from 5 to 25 cm deep in the (bottom left) winter and (bottom right) summer.**

### 2.1.3 Nutrient Cycling and Feedbacks

Pretreatment N and P budgets (Salmon et al. 2021) serve as an important benchmark for ELMv1-SPRUCE, a site-scale version of ELM version 1 that includes peatland processes for simulating SPRUCE treatments. They also serve as a reference point for comparing ecosystem stoichiometry under SPRUCE manipulative treatments. Pools and fluxes for ecosystem N and P cycles under ambient conditions were synthesized from more than a dozen water, peat, and vegetation SPRUCE data sets, as well as historic data from the USDA Forest Service Marcell Experimental Forest. Analysis of pretreatment plant N:P indicate varying degrees of N vs. P limitation across PFTs, with trees exhibiting the highest degree of N limitation. On an annual basis, N accumulates in the bog ecosystem at $0.2 \pm 0.1$ g N $m^{-2}$ $y^{-1}$, similar to annual N-fixation rates within the *Sphagnum* moss layer. Annual P inputs are generally balanced by losses from the bog ecosystem. *Sphagnum* biomass represents a large and dynamic pool of N and P at the S1 Bog; the observed decline of this species in response to SPRUCE WEW (Norby et al. 2019) is therefore expected to dramatically affect ecosystem N and P cycles.

The first indications of how SPRUCE treatments have influenced N and P cycles were published in a study tracking plant-available nutrients in SPRUCE plots from 2014 to 2018 (Iversen et al. 2023, Iversen et al. 2017D). Iversen et al. (2023) found that WEW exponentially increased plant-available ammonium and phosphate, but that nutrient dynamics were unaffected by $eCO_2$. The WEW response increased by an order of magnitude between the first and fourth year of the experimental manipulation, perhaps because of mortality of *Sphagnum* mosses in the warmest treatments. However, neither the magnitude nor the temporal dynamics of the responses were captured by ELMv1-SPRUCE. Key results from these additional years of data include a developing interaction between warming and $eCO_2$, where ammonium availability is depressed under $eCO_2$ in the warmest plots (Petro et al. in press).

### 2.1.4 Autotrophic Organism Growth Responses

Growth and contributions to NPP are being characterized for trees (*P. mariana, L. laricina*), woody shrubs (e.g., *R. groenlandicum, C. calyculata, Vaccinium oxycoccos, Kalmia polifolia*), a forb (*Maianthemum trifolium*), and graminoids (e.g., *Eriophorum vaginata*). Special attention is also paid to the production and presence of *Sphagnum* spp. across the bog surface. We continue to evaluate belowground primary production by tree, shrub, forb, and graminoid roots.

Aboveground vegetation production – Initial hypothesized responses for rooted trees, shrubs, forbs, and graminoids were that low temperatures would enhance decomposition and free nutrients for use by plants with roots in the affected peat profile locations. Such a “fertilization” was expected to enhance rooted vegetation growth and NPP. At higher temperatures, heat and water stress combined were expected to lead to reduced growth. A study on shrub-layer production growth through the first four seasons of manipulations (McPartland et al. 2020) demonstrated mixed responses, with some species showing increases with warming (*Rhododendron*, an ericaceous shrub) and others showing dramatic losses (*Maianthemum*, a forb). These patterns continue to be expressed in annual data collections.

Tree growth data showed initial negative responses for *P. mariana* in early years of the treatments that have dissipated with time. Current cumulative data suggest developing positive responses for *L. laricina*; observed changes are hypothesized to be driven by nutrient availability increases under warming.

Belowground dynamics – Building on our work to understand fine roots in an ombrotrophic bog prior to initiation of climate change treatments (Iversen et al. 2018), we leveraged ongoing data collection (e.g., from manual and automated minirhizotrons [AMRs], root ingrowth cores, and ion-exchange resins; Childs et al. 2019D, 2020D, Iversen et al. 2017Da, 2017Db, 2021D, Malhotra et al. 2020D, Malhotra et al. 2020, Defrenne et al. 2021, Iversen et al. 2023) to address the key question, **How does warming affect root and fungal growth, and how are belowground dynamics related to edaphic and environmental conditions?**

Our work in recent years has highlighted increases in ericaceous shrub root growth with warming (using root ingrowth cores; Malhotra et al. 2020), as well as increases in ectomycorrhizal fungi growth and an extended belowground growing season with warming (using AMRs; Defrenne et al. 2021). A new effort led by Sören Weber (postdoc) began in July 2022 and focuses on changes in rooting depth distribution, root phenology and production with warming using the manual minirhizotron data.

Sphagnum production and community response – No *Sphagnum* growth response to warming or $eCO_2$ treatments was observed in 2016, but we observed a curvilinear response to temperature in 2017 with maximum growth in the +4.5°C plots, and a linear decline with temperature in 2018 to 2021. Warming had a profound effect on *Sphagnum* percent cover, in which declines began in 2016 and increased through 2017–2021, increasing the area of ground with no live *Sphagnum* cover (Norby et al. 2019; **Fig. 2.4** left). NPP of *Sphagnum* declined with increasing temperature in 2017 and 2018, and was lower in $eCO_2$ plots in 2018 (**Fig. 2.4** right), with similar responses in 2019 to 2021. The response to temperature is related to drying of the hummocks. Shading from increased shrub production in the warmer enclosures also contributed to declining growth, which was confirmed in another experiment in 2021. The loss of productivity, amounting to 18 to 37 g C $m^{-2}$ per degree warming, will have important impacts on the C budget and structure and function of this ecosystem.

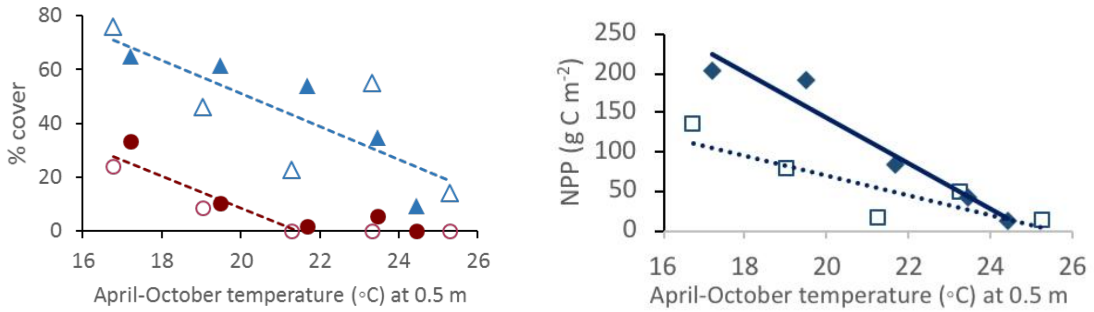


**Fig. 2.4. (left) Fractional cover of *S. angustifolium/fallax* (blue) and *S. magellanicum* (red) in 2018; closed symbols: ambient $CO_2$; open symbols: $eCO_2$. (right) Net primary production (NPP) of *Sphagnum* in 2018 in ambient $CO_2$ (closed symbols) and $eCO_2$ (open symbols).**

Understanding how Sphagnum microbiome interactions influence warming acclimation and nutrient cycling – The importance of microbial associates on *Sphagnum* growth and productivity has been recognized in the scientific literature for more than a century. However, how warming influences the *Sphagnum* microbiome and the role that it has on $N_2$-fixation and host plant productivity have received far less attention. Therefore, research over the past funding cycle targeted these knowledge gaps and are briefly described here.

To investigate how *Sphagnum*-associated microbial community composition changes and functions in response to SPRUCE-imposed warming treatments, we conducted a large-scale 16S rDNA amplicon profiling, *nifH*-qPCR, and $N_2$-fixation study. The results show that warming manipulations drastically alter microbial community composition by decreasing diversity and decreasing the abundance of $N_2$-fixing taxa. Furthermore, maximal rates of $N_2$-fixation decreased with increasing warming (Carrell et al. 2019). This finding has important implications as $N_2$-fixing microbial associates are critical for *Sphagnum* production and competitive success, along with the provision of N inputs to the ecosystem.

We decided to follow up these results with laboratory experiments examining the environmental conditions and metabolic basis for *Sphagnum* symbiosis with its main microbial associate—cyanobacteria (**Fig. 2.5**). Previous research has shown that peatland $N_2$-fixation activity is stimulated by the addition of pH-raising bicarbonate, whereas *Sphagnum* growth remained unaffected, suggesting that *Sphagnum*–cyanobacteria symbiosis is decoupled at high pH. To test this hypothesis, we conducted a pH gradient study and found that the *Sphagnum*–cyanobacteria symbiosis was only mutualistic at low pH, whereas high pH resulted in competition and dysbiosis (Carrell et al. 2022b). To investigate the nutrient basis of the symbiosis, we investigated metabolic profiles both spatially and from cross-feeding experiments. Results show that trehalose is the main carbohydrate source released by *Sphagnum*, which was depleted by cyanobacteria along with sulfur-containing choline-O-sulfate, taurine, and sulfoacetate. In exchange, cyanobacteria increased exudation of purines and amino acids (Veličković et al. 2018, Carrell et al. 2022b), providing metabolic support for the presumed C and N nutrient exchange along with evidence for sulfur (S) in this key peatland symbiosis.

In addition to $N_2$-fixation, microbes can enhance growth benefits to their plant hosts. To test this within the *Sphagnum* microbiome system, we collected *Sphagnum* from SPRUCE enclosures, mechanically separated the associated microbiome, and transferred them onto germ-free laboratory *Sphagnum* for temperature experiments. Host and microbiome dynamics were assessed with growth analysis, Chl*a* fluorescence imaging, metagenomics, metatranscriptomics, and 16S rDNA amplicon profiling. Microbiomes originating from +9°C enclosures imparted enhanced thermotolerance and growth acclimation at elevated temperatures (**Fig. 2.5**). Metagenome and metatranscriptome analyses revealed that warming altered the microbial community structure in a manner that induced the plant heat shock response, especially the HSP70 family and jasmonic acid production. The heat shock response was induced even without a warming treatment in the laboratory, suggesting that the warm microbiome isolated from the field provided the host plant with thermal preconditioning (Carrell et al. 2022a). Our results demonstrate that microbes, which respond rapidly to temperature alterations, can play key roles in host-plant acclimation to rapidly changing environments.

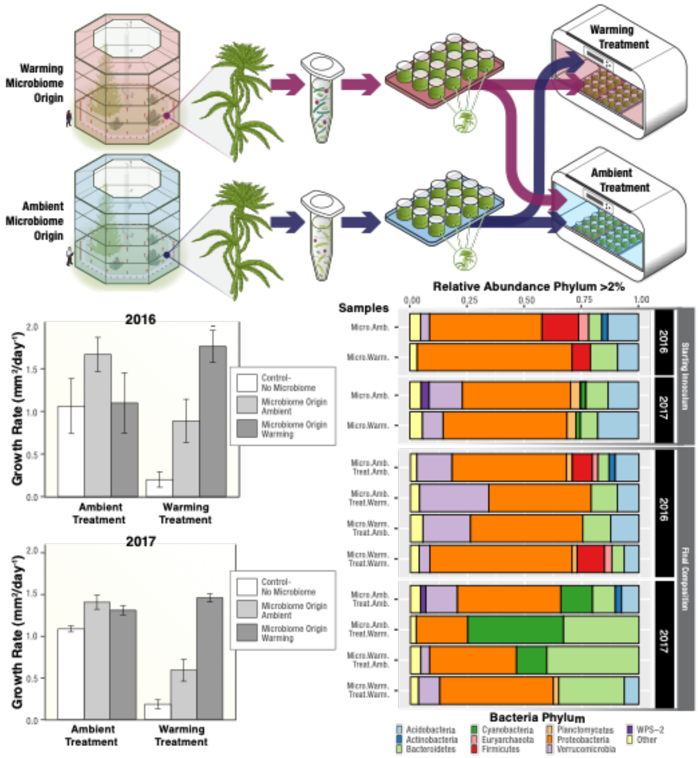


**Fig. 2.5. (a) Experimental approach and design: field-collected donor moss microbiomes collected from ambient or warming conditions were transferred to germ-free recipient moss (*Sphagnum angustifolium*), and the resulting communities were placed in an ambient or warm growth chamber. (b) Average moss growth rate under ambient or warming treatments as a function of the thermal origin of the microbiome. Error bars represent standard error of the mean of *n* = 6 for 2016, *n* = 12 for 2017. (c) Relative abundance of microbiome phyla, determined by 16S rDNA amplicon sequencing of the starting field-collected inoculum (*n* = 3 of each composite sample) from ambient or warming experimental plots, and the final compositions of experimental samples (*n* = 6 for each condition). An asterisk indicates statistical significance ($P < 0.05$) based on a Tukey's HSD post hoc test of the percentage change of total growth between moss with a microbiome and moss without a microbiome within the same chamber.**

### 2.1.5 Woody Plant Physiology

*Sap flow* – Ongoing measurements of sap flow, stomatal conductance, and twig water potential indicate significant species-specific increases in water use by the trees. There was no apparent temperature or $CO_2$ treatment effect on *P. mariana* water use, but significant increases in water use with temperature occurred in *L. laricina* (**Fig. 2.6**). The *P. mariana* strategy is conservative, maintaining hydraulic safety at the expense of C uptake, even as C losses increase through increased temperature-dependent respiration rates. In contrast, *L. laricina* increased C uptake with warming but pushed the bounds of hydraulic safety, reaching and exceeding its turgor loss point (Warren et al. 2021). As a result, in the warmest plots, there has been some tree mortality, including top dieback and branch tip damage in some individuals of both species. In 2019, the sap flow network was expanded to additional trees, up to six per plot. Initial analysis of sap flow in summer 2019 (wet year) and 2021 (drought year) indicates a reduction in stand level water use during drought, with less transpiration in warmer plots.

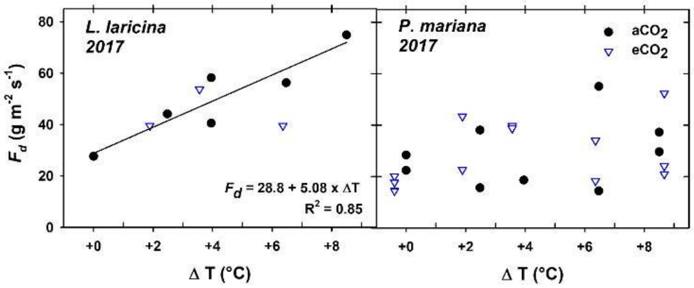


**Fig. 2.6. Differential tree water use ($F_d$) in response to temperature but not $eCO_2$ at the SPRUCE site illustrates different hydraulic strategies by *Picea* and *Larix*. *Picea* reduced stomatal aperture, maintained safe leaf water potentials, and stable water use. *Larix* kept stomata open, increased water stress, and increased water use.**

<u>*Phenology*</u> – Sap flow has been used to assess the vegetation phenology. Based on multiple years of sap flow, we found a strong temperature effect (but no effect of $eCO_2$) on spring phenology, accelerating spring initiation of sap flow by ~1 to 3 days per degree warming and extending sap flow into the fall by ~1 day per °C of warming for *L. laricina*, and more than 3 days per °C of warming for *P. mariana*, depending on timing of the first hard freeze event. Sap flow results complement and support the PhenoCam image-based analysis (Richardson et al. 2018, 2018D).

<u>*Gas exchange*</u> – Initial responses of foliar gas exchange after the first year of WEW indicated species-specific shifts in thermal acclimation of both photosynthesis and respiration with warming, and corresponding shifts in leaf N content, but no effect of $eCO_2$ (Dusenge et al. 2021). New analyses indicate that the thermal optimum of photosynthesis ($T_{\mathrm{opt}}$) in both conifers increased with warming, but these increases were largely insufficient to keep pace with warming. However, there was some benefit of $CO_2$ addition for *L. laricina,* likely due to suppression of photorespiration. While both species can thermally acclimate photosynthesis to maintain C uptake under mild warming, acclimation will be limited under more extreme temperature shifts (Dusenge et al. under review). Thermal acclimation of photosynthesis was correlated with changes in the $T_{\mathrm{opt}}$ of $V_{\mathrm{cmax}}$ and $J_{\mathrm{max}}$ for both tree species, and for the shrub species *C. calyculata* in late summer, but no change in $T_{\mathrm{opt}}$ was exhibited by the shrub species *R. groenlandicum*. Elevated $CO_2$ also led to a downregulation of photosynthetic capacity in *R. groenlandicum,* as displayed by a reduction in $V_{\mathrm{cmax}}$ at 25°C. Surprisingly, there was little acclimation of tree foliar respiration to WEW (although respiration was correlated to maximum carboxylation capacity of Rubisco).

<u>*Damage and hydraulics*</u> –We initiated additional tree monitoring on selected trees that vary in visible foliar discoloration or loss. We are linking measurements of sap flow to water potential, hydraulics, gas exchange, nonstructural carbohydrates (NSCs), and infrared and hyperspectral remote sensing. Through this integrated experimental approach, we are assessing the trade-offs among growth, acclimation, and defense, and consequences of each strategy. A damage index for the tree and shrub species was added to the weekly phenology survey to provide additional information on degree and timing of damage. New assessments of multiyear water potential dynamics indicate that the warming-induced water stress observed in the first few years (Dusenge et al. 2021, Warren et al. 2021) continues. The percent loss of xylem conductivity increased with warming for both tree species, with native embolism at growth temperatures ranging from 10% to more than 20%. Results illustrate the mechanism for observed water potential stress under WEW. Using the past 4 years of plant water stress, we continue to see divergent hydraulic strategies between the two tree species; *P. mariana* exhibited a more conservative response to warming through reduced stomatal aperture and reduced water stress, whereas *L. laricina* maintained open stomata, which led to greater water stress—a strategy that favors C uptake but at greater hydraulic risk.

### 2.1.6 Hydrology and Porewater Chemistry

*Hydrology* – After 6 years of WEW, lateral water flux (i.e., stream flow/outflow) continues to respond to warming treatments. Specifically, outflow decreased with warming, likely because of increased evapotranspiration. Water table recession analysis (conducted by Jonathan Stelling, University of Minnesota) showed that recession rates from 2019 to 2021 increased approximately 0.6 mm $d^{-1}$ $°C^{-1}$ of warming. When comparing the 2021 drought to the historic low water table in the S1 Bog of >1 m below the surface (i.e., 1976), this depth was nearly reached in the highest-temperature enclosures. Specifically, over the 2021 summer season, the +9°C plots experienced nearly 80 cm of water table drop, and the +0°C plots approximately half that. A drought that lowers bog water tables to this severity occurs approximately 11 times per 100 years, so it can be representative of a decadal drought regime.

*Porewater chemistry* – After the first 6 years of WEW, total organic C (TOC), and cation concentrations remained elevated in shallow porewater (0–10 cm, 30–40 cm depths) in warmer enclosures. Minimal chemistry changes have been observed in deeper porewater (50 cm depth and below) to date.

*Enclosure outflow* – Solute concentrations in outflow continue to respond to warming. Higher TOC concentrations (**Fig. 2.7**), along with some cations and metals (i.e., Ca, Al, and Fe), were observed in warmer enclosures, and the responses of total N and total P concentrations to warming were variable. Although the concentrations of some solutes have increased in outflow with warming, the fluxes of these solutes are generally lower from the warmest enclosures (**Fig. 2.7C**) since fluxes are driven primarily by changes in flow rather than changes in chemistry.

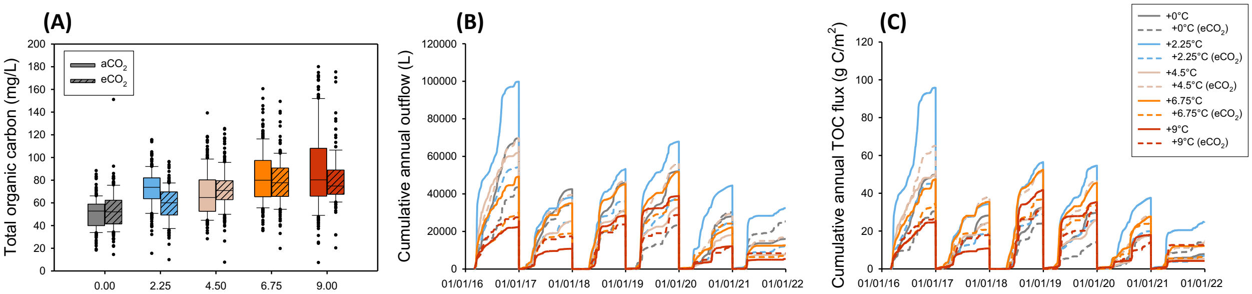


**Fig. 2.7. (A) TOC concentrations in lateral outflow, (B) cumulative annual lateral outflow, and (C) cumulative annual TOC flux from SPRUCE enclosures and responses to warming over 6 years (2016–2021).**

### 2.1.7 Microbial Community Response

*Microbial community responses* – Initial studies of the responses to in situ experimental warming of the SPRUCE chambers indicated that the peat microbial communities and decomposition rates were resistant to elevated temperatures in the first years of experimental warming (Wilson et al. 2016). A more recent in-depth analysis using combined evidence from metagenomics, proteomics, and metabolomics analysis has shown that while abundance profiles have not changed, a distinct shift has occurred in the microbial activity toward methanogenic metabolisms (Wilson et al. 2021b) that is shifting deeper within the peat profile with both temperature and $CO_2$ treatments. Analyses of metagenomes completed in collaboration with JGI over the past year from peat sampling in August 2018 show that across all years analyzed to date (2014, 2016, and 2018), microbial communities deeper in the peat profile are changing in composition. Approximately 10% of all the 800+ metagenome-assembled genomes recovered from the peat profiles show significant changes in relative abundance with time and treatment. These include most of the metagenome-assembled genomes occurring in high abundance and across multiple depth layers.

Peat decomposition communities show decreased diversity with depth, but within depths, microbial communities shifted and have become more diverse over the course of the 3-year decomposition study. The deepest depth of the peat decomposition study (40 cm) also shows an increase in the abundance of methanogenic archaeal lineages with temperature. Data are currently being compared with mass loss, C/N content, and Fourier-transform infrared–based characterization of organic matter remaining after the 3-year in situ incubation.

*Net $CH_4$ and $CO_2$ efflux and associated microbial processes* – In a new study interpreting the response of microbial processes and the flux of both $CH_4$ and $CO_2$ from the SPRUCE experiment, Hopple et al. (2020) in *Nature Communications* reported on long-term warming and $eCO_2$ impacts on anaerobic C cycling and $CH_4$ emissions in the S1 Bog. Large increases in the production and emission of $CH_4$ and $CO_2$, not present early in the warming experiment, are now observed after 5 years of warming, with microbial respiration becoming more methanogenic. The entire peat profile is experiencing greater rates of decomposition with warming, but elevated $CO_2$ continues to show limited effects on soil C cycling to date. While the massive soil C pool in peatlands has accumulated over millennia, these data suggest that it will be destabilized under prolonged warming and become more methanogenic.

#### 2.1.8 SPRUCE Publications and Data Sets

Since February 2019, SPRUCE efforts have produced 42 publications on the preceding results, including 2 papers in the *Proceedings of the National Academy of Sciences* and 3 in the Nature family of journals. In total, 25 new data sets from SPRUCE activities were developed, and 6 were updated.

### 2.2 MOFLUX and SIF Studies

Since March 2019, MOFLUX research has focused on coordinated ecophysiology, eddy covariance (EC), and SIF studies to advance integrative ecosystem science. This focus has led us to explore a wide range of scientific issues, including the photophysics, photochemistry, and biochemistry of photosynthesis; ecosystem-scale hydraulics and water relations; and innovative, multi-way partitioning of NEEs observed by EC. Major advances have been achieved in all tasks proposed in MOFLUX research, leading to some unexpected findings and development of new models, theories, and unplanned applications. Here we provide a summary of a few examples of these advances, and additional examples are given in Appendix D.

#### 2.2.1 MOFLUX Infrastructure and Operation

MOFLUX has been measuring ecosystem fluxes continuously with the EC technique, and a broad array of complementary ecophysiological and biometric data. Given the importance of drought as a driver of intra- and inter-annual flux variability, we have maintained detailed records of predawn leaf water potential of major tree species in the forest—a unique data set (Gu et al. 2015) in and of itself, but all the more powerful because it is coordinated with ecosystem flux and biometric observations.

Through the availability of the rich historical data records and ongoing data collection, we successfully leveraged MOFLUX as a validation supersite for forest water stress research. Through a collaborative effort with scientists at CalTech and Stanford University, a NASA-funded project has enabled the deployment of additional sensors at MOFLUX for ~3–4 years. These sensors include two GPS units that enable novel GNSS-based retrieval of canopy vegetation optical depth and water content, and a Moni-PAM system with 7 sensor heads to measure leaf-level active chlorophyll-*a* fluorescence. Additionally, a spectrometer with a broad spectral range will be deployed alongside our Fluorescence Auto-Measurement Equipment (FAME) system that measures SIF.

We also significantly augmented the capacity to monitor subsurface climate through an initiative associated with the AmeriFlux Management Project’s Year of Water, enabling 3 profiles of volumetric water content and temperature to 1 m depth (9 depths) and 3 profiles of collocated soil matric potential measurements (to 50 cm depth; 5 depths). We also installed another two water content profiles to achieve 5 profiles. This will greatly enhance our understanding of subsurface moisture dynamics and associated implications on belowground C cycling and ecosystem function.

#### 2.2.2 MOFLUX Technology Development

Progress in science-enabling technology – We further improved the design of FAME and its controlling software Integrated Measurement and Control System for SIF (IMACSS). Both FAME and IMACSS were originally developed by MOFLUX project members supported by the TES SFA during previous research and development efforts for easy integration with the EC technique (Gu et al. 2019a). Improvements achieved since March 2019 focused on the operator–machine interface. Switches were added to give the operator easy options to control FAME functions, and LED lights were added to indicate FAME operational statuses. These improvements allow a single operator to conduct calibration and maintenance of FAME. FAME has been granted patent protection by the US Patent Office (US011287381B2) and IMACSS has been copyrighted by DOE. Both FAME and IMACSS have been licensed to Campbell Scientific Inc. For these efforts, Lianhong Gu was awarded the Technology Commercialization Award (2020) and received two Inventor’s Awards (2022) from ORNL.

### 2.2.3 MOFLUX Progress in Science

*Enhancing understanding of ecosystem C cycling* – We developed a novel three-way method for partitioning NEE of $CO_2$ into GPP, and above- ($R_{above}$) and belowground ($R_{below}$) ecosystem respiration (Liu et al. 2022). We applied this algorithm to MOFLUX measurements and found that, at the annual time scale, $R_{below}$ dominated over $R_{above}$, with the former accounting for 66.9%–86.4% and the latter 13.6%–33.1% of the total ecosystem respiration ($R_{eco}$). The ratio of $R_{below}$ to $R_{above}$ varied seasonally, ranging from 1.77 to 7.25 in the growing season, and 1.02 to 4.57 in the non-growing season. We also found that $R_{below}$ was significantly more sensitive to temperature than $R_{above}$. These novel partitioning results and method enable improved constraints for validating C cycle simulations by ecosystem models.

We have also conducted analyses in which we synthesize litter and leaf area index (LAI) data sets with predawn leaf water potential and ecosystem flux observations. Leaf litter, which comprised 83% of total litter on average, decreased over the 11 years (Sen’s slope = $-7.9$ g $m^{-2}$ $year^{-1}$, $p = 0.06$) and independent measurements also showed a decreasing trend in seasonal peak LAI. Leaf litter production showed a lagged response to drought stress. Meanwhile, reproductive litter production exhibited acute sensitivity to extreme climate events. Flowering was strongly suppressed when a hard freeze occurred after early green-up (2007), and there was decreased fruiting following periods of summer drought stress.

*Developing knowledge of ecosystem water relations and hydraulics* – A novel ecosystem pressure–volume analysis was developed to derive the water potential at the ecosystem wilting point ($\Psi_{EWP}$), an ecosystem analog of the leaf turgor loss point (Wood et al. 2022). The $\Psi_{EWP}$ is an integrated ecosystem trait that balances vegetation’s ability to access water with the capacity for leaves to maintain turgor. The $\Psi_{EWP}$ defines marked shifts in ecosystem functional state—when community predawn leaf water potential ($\Psi_{pd}$) falls below $\Psi_{EWP}$, there is a breakdown of vegetation–environment interactions. For example, GPP and surface conductance ($G_S$) become highly insensitive to light. A bottom-up analysis of the root density distribution and soil moisture release characteristics suggest that these traits define the vegetation’s ability to acquire water and are key determinants of $\Psi_{EWP}$ and leaf wilting. We conducted novel analyses in which we also measured midday leaf water potential ($\Psi_{md}$) to estimate the efficiency of root-to-leaf water transport through the forest plant community. By combining leaf water potentials and transpiration ($T$) inferred from EC measurements, we estimated the community hydraulic conductance: $K_{com} = \frac{-T}{(\Psi_{md}-\Psi_{pd})}$. On a unit leaf area basis, $K_{com}$ values were consistent with whole-tree conductance values inferred from sap flow probes, and gas exchange ($G_S$ and GPP) was coordinated with $K_{com}$. Moreover, we found a seasonal basis for hydraulic control of ecosystem gas exchange (**Fig. 2.8**). Taken together, these findings concerning ecosystem-scale water relations and hydraulic conductances indicate the importance of hydraulic processes in governing the dynamics of ecosystem water and $CO_2$ exchange, and they represent novel constraints that can be used for model benchmarking.

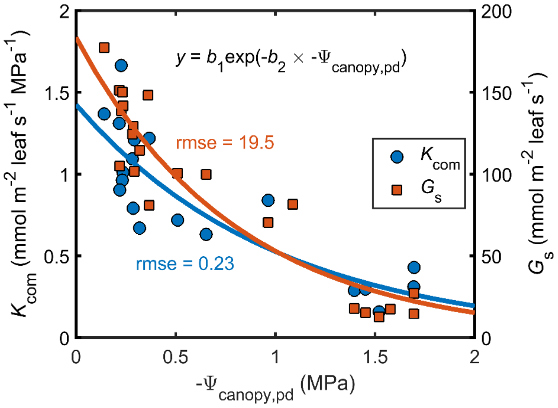
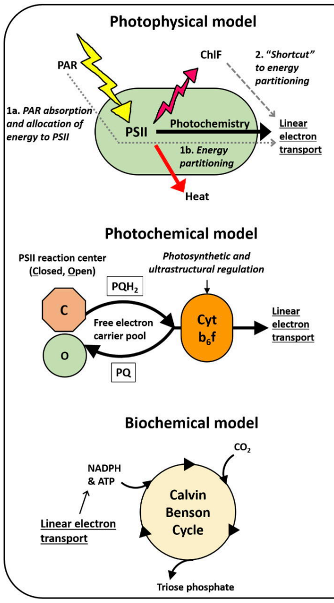


**Fig. 2.8. The ecosystem-scale hydraulic vulnerability curve demonstrates a hydraulic basis for seasonal gas exchange.**

*Formulation of a complete photosynthesis modeling strategy* – The MOFLUX research objectives required us to first formulate a strategy to model the complete system of photosynthesis from light harvesting to $CO_2$ assimilation because SIF is emitted from the antenna complexes of reaction centers. This also means that we will need to develop a broadly applicable model that can mechanistically predict essentially all variables of photosynthesis of potential interest to ecologists and land-atmosphere interaction modelers. This effort would represent a major advance since the development of the widely used Farquhar–von Caemmerer–Berry (FvCB) biochemical model of photosynthesis (Farquhar et al. 1980, Sharkey 1985). Photosynthesis is commonly divided into two stages of broad reactions—the light (or light-dependent) reactions and the C (i.e., dark, light-independent, or Calvin–Benson cycle) reactions (Buchanan 2016). To achieve our objectives, we realized we must further divide the light reactions into the photophysical reactions and photochemical reactions because these two groups of reactions are spatially separated, follow different laws, and operate at vastly contrasting time scales. A similar view was first proposed by Kamen (1963) but mostly ignored in general photosynthesis modeling efforts. The photophysical reactions cover the stages of light harvesting in the antenna complexes, partitioning of the harvested energy among different dissipation pathways, and the transfer of excitation energy to the reaction centers of photosystem II (PSII) and photosystem I (PSI). The photochemical reactions cover the subsequent electron transport. They include water splitting in the oxygen evolving complex, charge separation, acquiring of electrons by acceptors in the reaction centers, and subsequent transfer of electrons by mobile carriers within the bilipid core of thylakoid membrane, lumen, or stroma, to the eventual acceptor NADP+ in the C reactions to produce NADPH in the stroma. A broadly applicable photophysical model was already developed in our previous efforts (Gu et al. 2019b). To link the model of Gu et al. (2019b) with the FvCB model for complete modeling of photosynthesis, we would still need a model to bridge the gap between them—a photochemical model. For the final complete model of photosynthesis to be broadly applicable, the photochemical model would have to be similar to the photophysical model of Gu et al. (2019b) and the FvCB model in rigor and complexity. In **Fig. 2.9**, Box 1 depicts our strategy for complete modeling of photosynthesis. This strategy has guided our successful development of a broadly applicable photochemical model (the middle section of Box 1, Gu et al. 2022, 2023 and Appendix D).



**Box 1. Modeling framework**

*There are two photophysical model routes to predict linear electron transport rate:*

1a. The absorption of PAR photons, and allocation of energy to PSII
1b. Energy partitioning in PSII
2. A ChlF shortcut to modeling energy partitioning

*The photochemical redox model represents linear electron transport from PSII to Cyt $b_6f$ based on:*

1. *The states of PSII reaction centers and the free plastoquinol/plastoquinone pool*
2. *Capacity of Cyt $b_6f$ to support linear electron transport depends on:*
   a. *Influence of thylakoid lumen pH on the reaction of $PQH_2$ with RieskeFeS*
   b. *Influence on the linear electron transport rate on Cyt $b_6f$*
   c. *Competition of cyclic electron transport rate*
   d. *Ultrastructural control through macromolecular crowding effects from shrinking/swelling of thylakoid*
3. *Marcus theory of temperature effects on redox reactions*

*The classic FvCB biochemical model describes photosynthesis in terms of three canonical limitation states:*

1. *Rubisco activity*
2. *RuBP regeneration*
3. *Triose phosphate utilization*

**Fig. 2.9. A framework for a complete model of photosynthesis including both photophysical and photochemical components.**

<u>*Optimization of the photosynthetic electron transport chain (ETC)*</u> – The successfully developed photochemical model has applications beyond TES. For example, it can be used to provide insights on how the photosynthetic ETC can be genetically optimized to sustainably improve photosynthesis. Many components of the photosynthetic apparatus have been targeted for genetic modification to improve photosynthesis. Successful translation of these modifications into increased plant productivity in fluctuating environments will depend on whether the ETC can support the increased electron transport rate without risking overreduction and photodamage. Under the present atmospheric conditions, the ETC appears suboptimal and will likely have to be modified to support proposed photosynthetic improvements, and to maintain energy balance. For TES SFA work we derived photochemical equations to quantify the transport capacity and corresponding reduction level based on the kinetics of redox

reaction along the ETC. Using these theoretical equations and measurements from diverse C3/C4 species across environments, we identified several strategies that can simultaneously increase the transport capacity and decrease the reduction level of the ETC (**Figs. D13** and **D14**). These strategies include increasing the abundances of reaction centers, cytochrome b6f complex, and mobile electron carriers; improving their redox kinetics; and decreasing the fraction of secondary quinone-nonreducing PSII reaction centers. Our findings will facilitate the development of sustainable photosynthetic systems for greater crop yields.

### 2.2.4 MOFLUX Publications and Data Sets

Since February 2019, MOFLUX and SIF task efforts have produced 44 peer-reviewed publications on the preceding results, including 1 paper in the *Proceedings of the National Academy of Sciences* and 1 in *Nature Geosciences*, and the patent and copyright and commercial licensing of two inventions. Quality assured MOFLUX flux data are released to AmeriFlux annually by May of the next year. Other datasets (e.g., pre-dawn leaf water potential, litter production, and LAI) are regularly updated and publicly released via https://tes-sfa.ornl.gov/node/80.

## 2.3 Mechanistic C Cycle modeling

This task incorporates model development and MODEX activities at point scales, at regional to global scales, and at the level of mechanistic functional units to identify process contributions to global climate C cycle forcing from terrestrial ecosystems.

*Canopy processes* – We improved understanding and quantified the relationship between SIF and GPP, and used the new knowledge to inform model processes in ELM. We derived the GPP:SIF ratio from multiple data sources as a diagnostic metric to explore its global-scale patterns of spatial variation and potential climatic dependence. We found that the growing season GPP:SIF ratio varied substantially across global land surfaces, with the highest ratios consistently found in boreal regions; spatial variation in GPP:SIF was strongly modulated by climate variables; and the most striking pattern was a consistent decrease in GPP:SIF from cold-and-wet climates to hot-and-dry climates. Furthermore, GPP:SIF can be empirically modeled from climate variables using a ML random forest framework, which can improve the modeling of ecosystem production and quantify its uncertainty in global terrestrial biosphere models. Relevant work is detailed by Chen et al. (2020) and is highlighted in a commentary by Jeong and Park (2020).

Remote-sensing SIF offers a unique proxy for the evaluation and calibration of ELM GPP. We trained different ML models with satellite-based SIF data and in situ GPP observations from 49 EC towers. These trained ML GPP-SIF models were fed into the ELM to generate ELM-simulated global SIF estimates, which were benchmarked against satellite SIF observations with a surrogate modeling approach (**Fig. 2.10**). We found good modeling performance of the ML-based GPP. When fed with the ML GPP-SIF models, ELM can well predict the spatial-temporal SIF variations. Model parameter sensitivity analysis suggested that the fraction of leaf N in RuBisCO is the most sensitive parameter to

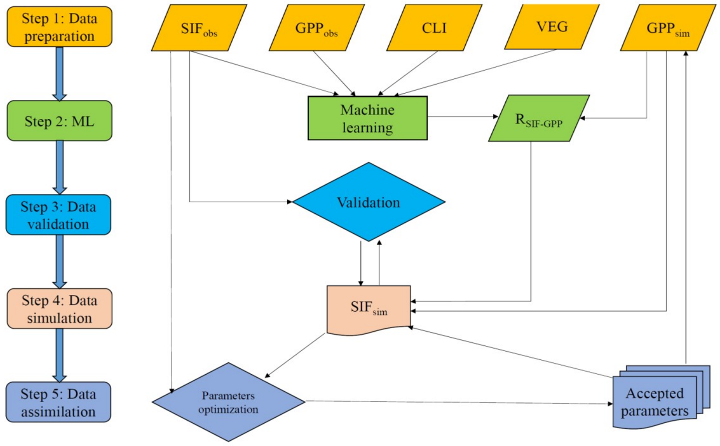


**Fig. 2.10. The schematic of improving ELM photosynthesis parameterization via satellite SIF, ML, and surrogate modeling.**

SIF; other sensitive parameters include the Ball–Berry stomatal conductance slope and the $V_{\mathrm{cmax}}$ entropy. The posterior uncertainty in simulated GPP was greatly reduced after benchmarking, and the model produced improved spatial patterns of mean GPP relative to other global GPP products. Our integrated approach provides a new avenue for improving land models and using remote-sensing SIF, which can be further improved in the future with more ground- and satellite-based observations. A relevant manuscript has been submitted (Chen et al. in review).

*Phenology modeling* – We evaluated and improved the above- and belowground phenology of ELMv1-SPRUCE using SPRUCE phenological observations. For the evergreen phenology, we introduced an explicit green-up controlled by temperature and degree-day thresholds in spring, and we changed the default constant for litterfall to an intensive offset in autumn via an exponential function. The results show that the new models reduced biases in start of season (SOS) and end of season (EOS), and improved temperature responses compared to default models. The timing of root growth and mortality is well-known to differ from leaf onset and senescence in all biomes. We thus fitted an empirical function to the SPRUCE minirhizotron observations to enable a longer and more gradual onset period in spring and adjusted the root litterfall parameters to induce earlier root litterfall. Compared with limited root growth observations, the revised ELMv1-SPRUCE can better reproduce the belowground SOS and EOS than the original model. Moreover, with optimized parameters of both roots and photosynthesis, the new root phenology schemes produced slightly lower gross primary productivity but higher heterotrophic respiration in late summer compared to the original model. More robust assessment using latest observations is needed to evaluate the phenological feedbacks and temperature responses.

We also introduced new seasonal-deciduous phenology schemes into ELMv1-SPRUCE and evaluated their performance against the SPRUCE PhenoCam observations from 2015 to 2018 (Meng L et al. 2021a). We found that phenology simulated by the revised model (i.e., earlier spring onsets and stronger warming responses of spring onset and autumn senescence) was closer to observations than simulations from the original algorithms for both the deciduous conifer and mixed shrub layers (**Fig. 2.11**). Moreover, the revised ELM generally produced higher C and water fluxes during the growing season and stronger flux responses to warming than the default ELM. A parameter sensitivity analysis further indicated the significant contribution of phenology parameters to uncertainty in key C and water cycle variables, underscoring the importance of precise phenology parameterization.

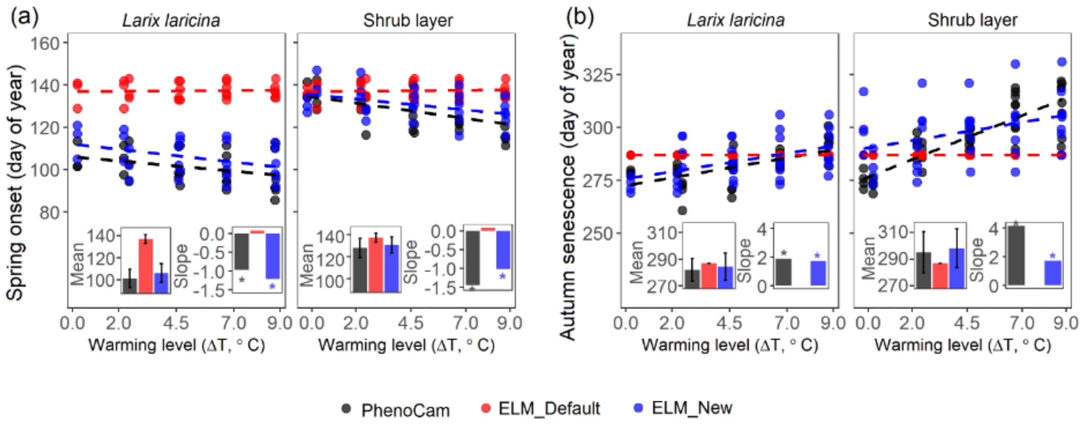


**Fig. 2.11. Observed and simulated responses of (a) spring onset and (b) autumn senescence to warming at SPRUCE. Linear regression lines are shown as dashed lines. The mean phenology across all warming and $CO_2$ levels and slopes of phenology against warming levels are shown in the subfigures. The error bars in the subfigures represent the standard deviations of phenology across all warming levels. Significance $P < 0.1$ from two-tailed Student's *t* test. Spring onset was studied during 2016 to 2018, and autumn senescence was studied during 2015 to 2018.**

*Disturbance* – Natural and anthropogenic driving mechanisms underlying the changes of peat fire remain to be explored. We investigated major affecting factors and predictability of peatland fires for 1997 to 2016 using multi-source environmental data sets and the two-step-correcting ML framework, a combination of multiple ML classifiers, regression models, and a self-correcting technique. We found that

(1) the oversampling algorithm worked for the unbalanced data and improved the recall rate by 26.88% to 48.62%; (2) the random forest performed best across multiple fire data sets; (3) temperature, air dryness, seasonality, and frost day frequency dominated the peat fires, overriding the impacts of biomass, soil moisture and human activities; and (4) the seasonality and frost day frequency was further identified as the critical factor that could change the physical characteristics and thermal hydrology in peatlands, thus favoring peat fire occurrences.

Using recent satellite-derived wildfire products and ELM simulations driven by three different climate forcings, we investigated the interannual variation (IAV) of burned area and its climatic sensitivity globally from 1997 to 2018 (Tang et al. 2021). We found that (1) the ELM simulations generally agreed with the satellite observations in terms of the burned area IAV magnitudes, regional contributions, and covariations with climate factors, confirming the robustness of the ELM to the usage of different climate forcing sources; (2) tropical savannas, tropical forests, and semi-arid grasslands near deserts were primary contributors to the global burned area IAV; and (3) precipitation was a major fire suppressing factor and dominated the global and regional burned area IAVs, and temperature and shortwave solar radiation were mostly positively related with burned area IAVs. This study reveals the spatiotemporal diversity of wildfire variations, regional contributions, and climatic responses, and can provide new insights for wildfire modeling, prediction, and management.

*SPRUCE $CH_4$ and hydrology modeling* – A new manuscript using ELMv0-SPRUCE, a site-specific version of ELM version 0 that includes a mechanistic $CH_4$ model, was published describing the hydrological feedbacks on peatland $CH_4$ emissions under the SPRUCE treatments (Yuan et al. 2021a). This study found that reduced water table levels from increased evapotranspiration mitigates the warming effect on $CH_4$ emissions. An improved approach to simulating ebullition was integrated into the SPRUCE terrestrial ecosystem model, and the authors found that including ebullition improved predictions of porewater $CH_4$ concentrations (Ma et al. 2022). We also examined the sensitivities of ELMv0-SPRUCE C and hydrology outputs to uncertainties in microtopography parameters, including hummock height, horizontal separation, and hollow fraction (Graham et al. 2022). The model experiment showed that the model outputs were typically most sensitive to hummock height, and that NEE was overall the most sensitive model output to the microtopography parameters. Hummock height also influenced the partitioning of C into above- and belowground pools.

A series of two papers reporting the $CH_4$ module of the ELMv0-SPRUCE model introduced the incorporation of the microbial-functional group-based $CH_4$ module into the ELMv0-SPRUCE model and its application to the warming and $eCO_2$ impacts on $CH_4$ processes at the S1 Bog (Ricciuto et al. 2021, Yuan et al. 2021a). The model reproduced the observed vertical distributions of DOC and acetate concentrations, the seasonality of acetoclastic and hydrogenotrophic methanogenesis, and $CH_4$ concentration along the soil profile. Meanwhile, the model estimated that plant-mediated transport, diffusion, and ebullition contributed to approximately 23.5%, 15.0%, and 61.5% of $CH_4$ transport, respectively.

The model application to the S1 Bog examined the mechanistic processes of how warming and $eCO_2$ affect methanogenesis and methanotrophs along soil profile. We found that warming and $eCO_2$ stimulate peatland $CH_4$ emissions through different mechanisms. The stimulating impact of warming is primarily through the stimulation of microbial processes. The stimulating impact of $eCO_2$ is primarily through enhanced substrate availability by increased photosynthesis. Although warming significantly increased $CH_4$ emission, the hydrological feedbacks leading to a reduced water table mitigated the stimulating effects of warming on $CH_4$ emission (Yuan et al. 2021b).

The isotopic component of the $CH_4$ module has been successfully developed (**Fig. 2.12**). The pools and fluxes of $^{13}C$ and $^{14}C$ are added to all C pools and processes associated with $CH_4$ processes in ELMv0-SPRUCE. For example, the DOC has additional pools of $^{13}C$ and $^{14}C$.

Ongoing efforts are also evaluating the interactive impacts of drought and warming on $CH_4$ flux. Field observations showed substantial warming impacts on $CH_4$ emission post-2020, much stronger than pre-2020. Opposite this pattern, the 2021 drought strongly suppressed $CH_4$ emissions. The present ELMv0-SPRUCE model has captured the stimulating impacts of warming on $CH_4$ emission in early years of the experiment, but was unable to capture the stronger warming response in later years, perhaps because of warming-induced substrate flush or microbial growth.

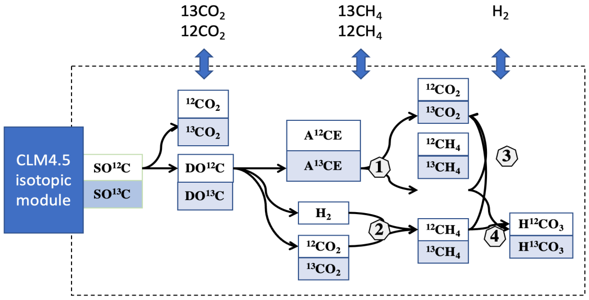


**Fig. 2.12. Isotopic processes and in ELM-SPRUCE CH$_4$ module. ACE: acetic acid; SOC: soil organic C; DOC: dissolved organic C; $^{14}$C is not shown but is kept in the code.**

*Model–data integration/uncertainty quantification* – We developed an invertible neural network (INN) to calibrate ELM with observed flux data from MOFLUX. The INN in this example was trained on 1,000 simulations of ELM with different values of 7 parameters related to allocation, leaf properties, and phenology. The INN can efficiently address forward and inverse modeling simultaneously; in inverse mode, it can perform model calibration by producing posterior distributions for the ELM parameters; in forward mode, the INN generates ELM predictions of a model output of interest, such as latent heat flux. The INN is much more computationally efficient than past approaches, producing similar posterior estimates of latent heat flux to the Markov Chain Monte Carlo (MCMC) method but 30 times faster. The INN may be used to quickly evaluate the role of new measurements or reduced measurement uncertainty in reducing model prediction uncertainty, potentially speeding up the MODEX cycle at our study sites.

We developed an interpretable long short-term memory (iLSTM) network for daily NEE predictions based on time series observations of seven environmental variables, including nighttime temperature (Tn), daytime temperature (Td), shortwave radiation (Ra), VPD, precipitation (P), soil water content (SWC), and atmospheric CO$_2$ concentration. By exploring internal network structures iLSTM enables interpretability of variable importance and variable-wise temporal importance to the prediction of targets. We applied iLSTM to predict NEE at the Morgan Monroe State Forest site. The results (**Fig. 2.13**) indicate that iLSTM not only improves prediction performance by capturing different dynamics of individual variables but also reasonably interprets the different contribution of each variable to the target and its different temporal relevance to the target.

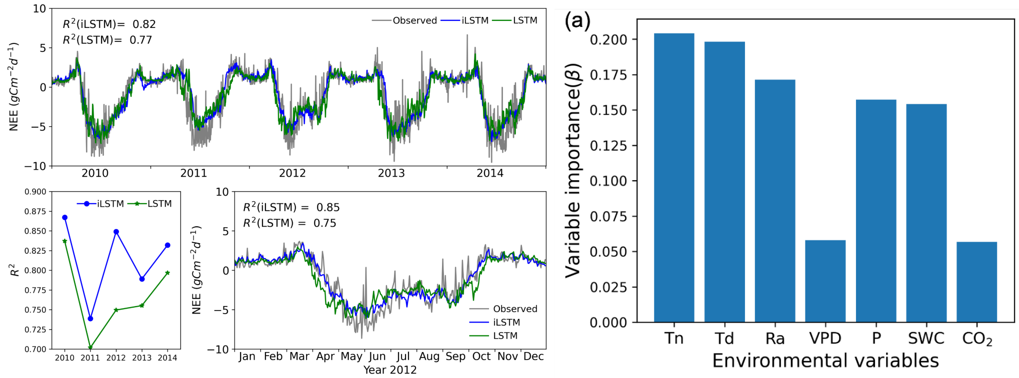


**Fig. 2.13. (left) The comparison between our iLSTM method and the standard long short-term memory (LSTM) method shows superior prediction performance of iLSTM. (right) iLSTM indicates that temperature and radiation are the two most important drivers of NEE at this site.**

We are developing ML workflows to enable uncertainty quantification at SPRUCE, MOFLUX, and other observation sites of interest. A new method has been developed for model-independent data assimilation (Huang et al. 2021). OLMT (https://github.com/dmricciuto/OLMT) has been updated to include automated parameter sensitivity analysis and model calibration techniques. It is currently being applied at SPRUCE to visualize model uncertainty. We are also developing an artificial intelligence enabled ELM diagnostic and validation framework that will speed up the ELM function validation at different spatial-temporal scales. This leverages work being done in the E3SM next-generation development, taking advantage of GPU architectures that we will use to increase the efficiency of MODEX at regional scales.

*ELM-SPRUCE soil and vegetation modeling* – Using the comprehensive measurements at SPRUCE, we evaluated model performance at the process level. ELMv1-SPRUCE simulated net carbon exchange (NCE) responses to warming consistent with field observations under ambient $CO_2$ conditions. However, ELMv1-SPRUCE failed to capture the observed general lack of response to $eCO_2$ concentrations (Hanson et al. 2020). A more detailed analyses of model results suggest that model-simulated $eCO_2$ responses occur mostly because of increased allocation to the nonstructural carbohydrate (NSC) pool. Ward et al. (2019) showed that NSC in two shrub species increased significantly under $eCO_2$ conditions. Preliminary data for spruce and larch also showed a significant increase of NSC under $eCO_2$ (J. Warren, unpublished data). We also compared simulated aboveground NPP responses to warming with field observations for each PFT at SPRUCE. Although ELMv1-SPRUCE–simulated shrub NPP compares well with observations at lower-temperature treatments, ELMv1-SPRUCE fails to capture the observed increasing productivity with warming. Malhotra et al. (2019) suggested that the increased productivity of shrub is mainly due to the significant increase of fine root length, which allows greater access to soil nutrients. ELMv1-SPRUCE does not explicitly represent root traits such as specific root length and the linkage between root traits and nutrient uptake. Therefore, we designed two simulations to test if the increased shrub productivity is caused by greater access to nutrients: (1) the default shallow root profile and (2) a deeper fine root profile to allow greater access to nutrients. Simulations results show that with deeper fine roots, shrub productivity is greatly increased, consistent with observations. This suggests that it is critical to improve the representation of fine root traits and nutrient uptake in ELMv1-SPRUCE.

*Sphagnum mosses modeling* – We developed a *Sphagnum* moss PFT and associated processes within the ELM-SPRUCE models (both v0 and v1) and used the updated model to examine the bog ecosystem response to warming and $eCO_2$. The new model can capture the seasonal dynamics of moss *Sphagnum* GPP and predict reasonable annual values for *Sphagnum* NPP. The model predicts that different PFTs responded differently to warming levels under both ambient and $eCO_2$ concentration conditions. The NPP of two dominant tree PFTs showed contrasting responses to warming scenarios (increasing with warming for *Larix* but decreasing for black spruce), while shrub NPP had similar warming response to *Larix*. *Sphagnum* in hummocks vs. hollows showed opposite warming responses: *Sphagnum* in hollows showed generally higher growth with warming, while the growth of *Sphagnum* in hollows was more variable and was strongly dependent on water table height. The ELMv0-SPRUCE predictions further suggest that the effects of $eCO_2$ can change the direction of the warming response for the bog peatland ecosystems (Shi et al. 2021).

*Modeling at other sites* – We are also using the point version of ELM (version 1) at MOFLUX and additional AmeriFlux sites relevant for the TES SFA. We are currently developing a site-level benchmarking package focused on model–data comparison with AmeriFlux data, which will complement the International Land Model Benchmarking Project package and will serve as a useful tool for SFA model development tasks. These model development tasks at SPRUCE to improve model physiology, nutrient cycling, phenology, and root function are being evaluated across sites covering a wide range of environmental conditions using this framework. An uncertainty quantification framework jointly developed by E3SM and the ORNL TES SFA provides critical information about model parameter sensitivity (Ricciuto et al. 2018) and can be used to improve model performance through calibration of model parameters with observations. Lu et al. (2018) demonstrated that calibrating ELM using a surrogate modeling approach combined with a parameter optimization method significantly improved predictions of LAI and C fluxes at MOFLUX.

*Ultrahigh-resolution ELM data preparation and simulation* – We have developed an ultrahigh-resolution (1 km) ELM simulation capability over dedicated regions to improve our predictive understanding of terrestrial system processes and their feedbacks to climate. We used the 3-hourly meteorological forcing data (Kao et al. 2022), generated from DAYMET (Thornton et al. 2021), and the sub-daily temporal information from other meteorological reanalysis data sets (such as the Global Soil Wetness Project Version 3; Yoshimura and Kanamitsu 2013). We also developed a dynamic surface properties data set to represent the heterogeneity of landscape surface at 1 km resolution. We also implemented a computational framework to conduct the ultrahigh-resolution simulations over any regions within the North American continent (Yuan et al., in preparation).

### 2.3.1 Modeling Publications and Data Sets

Since February 2019, science efforts on mechanistic C-cycle modeling have produced 35 publications.

## 2.4 Multi-Assumption Modeling

The multi-assumption modeling task was set up to tackle the question, ***What processes are responsible for structural uncertainty in terrestrial ecosystem models (TEMs), and how can structural uncertainty be estimated rapidly and accurately?*** For TEMs, the state of the art is to run ensembles of different models in model intercomparison projects (MIPs). However, MIPs take a long time to generate results, rarely identify the processes responsible for the variability, and do not represent the full range of model structural variability. We developed the open-source MAAT model and protocol (Walker et al. 2018) to help address structural uncertainties of models. MAAT is a general modeling software architecture that modularizes system models into their component parts and automates switching among different model structures (e.g., theory, hypotheses, assumptions). This generalization and automation allow different models to be specified from input files and enables a full model ensemble to be run in a single execution of the code. Breaking TEMs down into their component process hypotheses and assumptions connects them directly with the language of experiments and observations (Medlyn et al. 2015), facilitating the connection between modeling and experiment science.

TEMs rely on leaf-scale photosynthesis models, which exhibit substantial structural uncertainty. Walker et al. (2021) applied a novel formal model sensitivity analysis (previously developed with TES SFA support in collaboration with Florida State University and Pacific Northwest National Laboratory; Dai et al. 2017) to identify the key processes responsible for leaf-scale photosynthesis model structural uncertainty. Surprisingly, we found that the method for selecting among photosynthetic rate-limiting processes dominated this uncertainty. We showed that this sensitivity to the limiting-rate selection method, a single process polymorphism, propagated through to global simulations in ELM and FATES, causing a difference in global photosynthesis equivalent to 50%–160% of anthropogenic $CO_2$ emissions. In collaboration with Brookhaven National Laboratory, we devised novel high-resolution $A$-$C_i$ measurements to discriminate among alternative hypotheses for the limiting-rate selection process. Using novel $A$-$C_i$ measurements to constrain parameters using state-of-the-art MCMC methods (coded into MAAT by Science Undergraduate Laboratory Internship [SULI] intern Abigail Johnson), we identified the Farquhar hypothesis as the most likely mechanism. Our results represent a complete MODEX loop by suggesting that adoption of Farquhar limiting rate selection by TEMs will reduce model uncertainty.

In collaboration with the microbial C task, we developed a multi-assumption soil C model to help answer the question, ***How does structural variability in microbial soil C decomposition models influence steady-state responses of soil C to a change in input rates?*** Using the first generation of the multi-assumption soil C model in MAAT, we assessed a new hypothesis that soil C saturation (i.e., the limits to soil C storage as organic inputs increase) could be driven by microbial population constraints on soil microbes in addition to soil texture, which is typically assumed in TEMs (Craig et al. 2021). Literature data synthesis provided evidence of microbial population limits as organic inputs increase, supporting our hypothesis. These results suggest that additional mechanistic studies of soil C saturation are warranted.

We have also recently published empirical results suggesting that microbial decay of the mineral-associated organic matter pool can be stimulated by organic inputs (Craig et al. 2022). Access to this pool is a key structural difference across many state-of-the-art soil decomposition models. To assess the impacts of this variation and other key processes, we have incorporated many of these models from the DOE sphere (MEND, Wang et al. 2013; MIMICS, Wieder et al. 2014; MILLENIAL, Abramoff et al. 2022; CORPSE, Sulman et al. 2014; RESOM, Tang and Riley 2015; and CENTURY, Parton et al. 1987) into MAAT.

The MAAT efforts supported a well-attended session at the 2019 AGU Fall Meeting in December on "H13Q—Advances in Stochastic, Multi-hypothesis, and Other Data-Driven Methods for Environmental and Earth System Modeling" to provide a forum for building the multi-hypothesis modeling community.

We also collaborated on existing MIPs to provide results for the Global Carbon Project (e.g., Friedlingstein et al. 2020).

### 2.4.1 Multi-Assumption Modeling Publications and Data Sets

Since February 2019, science efforts on multi-assumption modeling have produced 12 publications, three datasets, and two intermediate software releases (MAAT versions 1.2 and 1.3).

## 2.5 Linking Root Traits to Function

The root function task was developed to improve understanding of root function and implications for modeling. Our research focused on assessing root function in situ, including a focus on the root rhizosphere, where there are dynamic interactions and exchanges among roots, soil pores, and soil surfaces. Of particular interest was how hydraulic conductivity from the bulk soil to the root changes as soils dry and if there is a loss of preferential pathways, or development of air gaps that prevent water uptake. Such root data are critical for modeling water availability to plants, especially in process-based models such as ELM or FATES.

We continue to leverage the unique capabilities of the neutron imaging facilities at ORNL including the High Flux Isotope Reactor and the Spallation Neutron Source to assess root traits, functions, and interactions with soil microbes and soil physicochemical attributes. Our work quantified water uptake rates of individual roots in situ and linked those to root traits such as diameter or order (Dhiman et al. 2019, Warren et al., being revised). Subsequent modeling of these data revealed that roots and mycorrhizae affect soil hydraulic properties. Therefore, model use of root-free soil hydraulic parameters leads to greater model uncertainty. This led to an experiment to assess how roots or mycorrhizal hyphae affect soil hydraulic properties, which revealed significant influence on soil water release parameters, such as saturated hydraulic conductivity, the slope of the soil water release curve, and saturated water content (Marcacci et al. 2022).

We are also looking at novel techniques to improve sub-mm assessment of root soil water dynamics, including use of ML to improve quantification of 3D dynamics (Venkatakrishnan et al. 2021), and development of ultrafast computed tomography techniques (**Fig. 2.14**). In June 2022, Jeff Warren hosted a session on future application of neutrons to soil, rhizosphere processes, and plant–soil interactions. Workshop conclusions will be used to inform development of future beamlines, such as the Spallation Neutron Source's VENUS and CUPI$^2$D beamlines (Brügger et al. in press), that could enable unprecedented insight in soil, rhizosphere, and root function in situ.

The Root Function Task of the ORNL TES SFA has been awarded three successful DOE Office of Science Graduate Student Research Program fellowships—one on neutron imaging, and two on how root traits and respiration vary in response to drought or temperature, or seasonally across different species (Ficken et al. 2019, Hogan et al. 2021). In one of these studies, we focused on seasonal respiration using a novel measurement system that assessed a single third- or fourth-order root system while attached to different mature temperate tree species; rates of root system $CO_2$ efflux ranged between 10 and 90 µmol $m^{-2}$ $s^{-1}$, and ectomycorrhizal species had slightly greater rates than arbuscular mycorrhizal species (Hogan et al. 2023). In collaboration with the Root Traits Task (i.e., FRED), we recently established a relationship with MA to assess mature tree root, mycorrhizal, and heterotrophic microbial respiration dynamics *in situ* for 10 species that vary across evergreen and deciduous, and ectomycorrhizal and arbuscular species. Seasonal respiration measurements of respiratory efflux from 108 root/fungal exclusion collars are currently being measured across the active season. Results will provide novel root functional data for models that increasingly consider root and mycorrhizal function (such as FATES).

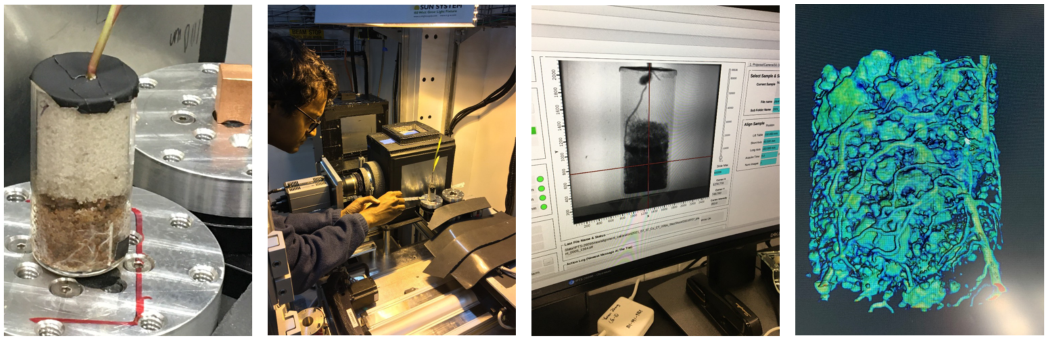


**Fig. 2.14. Testing ultrafast neutron computed tomography and ML in July 2021 using maize with deuterium injections. More than 160,000 images were collected to assess capability to measure three-dimensional soil–root water dynamics in situ (1.8 TB of data). Initial results suggest a 90 s run with 0.1 s image exposure may be an optimal setting. Our earlier research with neutron computed tomography collected images over multiple hours, precluding understanding of short-term dynamics.**

### 2.5.1 Publications on Root Traits and Function

Since February 2019, science efforts on root traits and function have produced 14 publications and 1 data set on the preceding results.

## 2.6 Microbial Processing of Soil C

Experimental and modeling studies continued to focus on the key role of microbial activity in influencing $CO_2$ emissions and soil C cycling, and in particular, to understand the role of soil moisture which has been somewhat neglected in comparison to temperature. Microbial data collection at both MOFLUX and SPRUCE was used by the MAAT modeling approach (Section 2.4).

Following our work with ELM at MOFLUX (Liang et al. 2019), our MEND model was parameterized with 11 years of observations to predict soil organic C (SOC) dynamics under five extreme moisture scenarios with different frequencies and severities over 100 years (Liang et al. 2021). A nonlinear response of SOC decomposition to soil moisture changes decreased decomposition by microbes under drying that was not compensated by increased decomposition under wetting conditions. In 2017, we trenched four of MOFLUX's continuous LI-COR chambers to isolate heterotrophic respiration. Since then, we collected soil cores to measure pH, total C and N, microbial biomass C and N, texture, moisture content, and root length and density data on a quarterly basis. We used these data streams for artificial intelligence and wavelet coherence analysis to examine the effects of environmental factors and their time scales on soil respiration and its partitioning. Key results were that (1) heterotrophic respiration was responsive to soil temperature at daily and seasonal time scales, whereas autotrophic respiration was most responsive to aboveground productivity (using LAI as a proxy) and time of year; (2) the time of year and LAI were most influential for determining the partitioning between heterotrophic and autotrophic respiration; and (3) soil moisture was most relevant to soil respiration on synoptic weekly to monthly time scales.

We investigated the effects of soil texture and changing water content at the laboratory and field scales under steady-state and transient conditions using soils of three distinct textures (sandy soils, loamy soils from MOFLUX, and clayey soils) (Singh 2020). Soil texture strongly influenced respiration rates, and sandy soils showed the lowest respiration rate, followed by loamy and clayey soils (Singh 2020, Jagadamma et al. 2021). We found higher cumulative SOC loss under the transient moisture state compared with the steady state, and different mechanisms contributed to the "Birch effect" in different textured soils. In sandy soil, metabolite accumulation and changes in bacterial community structure were the most important drivers of the Birch effect, whereas in loamy and clayey soils, metabolite accumulation and release of aggregate-protected C were more important (Singh et al. 2023). A moisture manipulation experiment—drought, rainfed, and irrigated—in a soybean field in western Tennessee showed decreases in $CO_2$ emissions, microbial biomass, and enzyme activity under the imposed drought compared with rainfed and irrigated conditions (Singh 2020, Mayes et al. 2021a), consistent with model results (Liang et al. 2021). Therefore, the response of microbial respiration to changing soil moisture will strongly depend on the sensitivity to textural differences and the mechanisms underpinning increased SOC turnover from different soils upon wetting and drying must be discerned to improve the understanding of terrestrial C cycling in response to extreme events.

For modeling SOC decomposition, the extent to which model microbial parameters can be extrapolated across time and sites may govern the ability of models to routinely include microbial functions. We used ORNL incubation experiments (Kluber et al. 2020) to find that 3 major microbial parameters controlling microbial uptake, growth and maintenance are highly site-specific, but if additional parameters involving enzyme production and turnover are also optimized as well, the model parameters can be distinctly generalized for different soil series (Jian 2020). On the other hand, we found that parameters from short-term incubations (<1 year) are most applicable to predicting changes in SOC stocks associated with short-term warming experiments (<1 year), and parameters from long-term incubations (>1 year) are most applicable to predicting changes in SOC stocks associated with long-term warming experiments (>1 year to decades). The implications are that both incubations and field-scale warming experiments conducted over short time frames will tend to predict large losses of SOC stocks that are not sustained when experiments are allowed to continue over longer time frames (Jian et al. 2020). Microbial community acclimation and the subsequent changes in fitted microbial parameters with time are the most likely causes for these model–data interactions.

Finally, we developed comprehensive data sets to enable modeling of microbial functions in soils. We collected core samples from SPRUCE in June 2021, August 2021, and June 2022, and determined microbial biomass C and N from chloroform fumigation extraction; gene copies of total, bacterial, fungal, and archaeal microbes using qPCR; and total, bacterial, fungal biomass using phospholipid fatty acid in collaboration with Jessica Gutknecht at the University of Minnesota. Microbial biomass C is the most common type of data used in models, but it also requires large volumes of soil and provides no details regarding numbers of bacteria, fungi, and archaea. This TES SFA task has an existing data set from different soil types from around the world comparing the three kinds of data, and we initially found a high degree of correlation between the microbial metrics, with one exception—organic soils. The SPRUCE samples will therefore enable development of broad correlations between the different kinds of microbial data and thereby expand the kinds of microbial data available for modeling the SPRUCE site. This work is also an important contribution to the literature by providing a validated relation for different kinds of microbial analyses in global soils.

### 2.6.1 Publications Microbial and Soil C

Since February 2019, the microbial and soil C task has produced 13 publications on the preceding results and supported 2 PhD student dissertations. Two data sets have also been released.

## 2.7 Global Traits Databases

### 2.7.1 FRED

FRED (https://roots.ornl.gov/) has been and will continue to be a freely available resource for the broader community of root and rhizosphere ecologists and terrestrial biosphere modelers (Iversen et al. 2017; *New Phytologist*). Building on the recent releases of FRED versions 2.0 (McCormack et al. *2*018) and 3.0 (Iversen and McCormack 2021), our progress to date has focused on improving our understanding and model representation of fine-root trait variation around the world by asking the following questions.

1. **How can we leverage data in FRED to improve our understanding of root trait variation around the world?**

The FRED team has continued to be involved in international collaborations (https://roots.ornl.gov/synthesis-activities). For example, the sROOT working group within the German Centre for Integrative Biodiversity Research from 2018 to 2020 leveraged FRED 2.0 to develop a Ready to Use database that is a species-specific subset of FRED and TRY, a global plant trait database (Guerrero-Ramirez et al. 2021, Guerrero-Ramirez et al. 2021D), resulting a series of publications focused on the global variation in fine-root traits within the multidimensional Root Economics Space (Bergmann et al. 2020) and along environmental gradients (Laughlin et al. 2021), and within and among above- and belowground plant traits (Weigelt et al. 2021). This collaboration continues within the international RootFUN working group, which is focused on the links among root traits and ecosystem function (Barry et al., in preparation). Furthermore, a number of groups have also used FRED as a resource to answer their own scientific questions (https://roots.ornl.gov/publications).

To develop a more holistic view of belowground resource acquisition strategies, we used the empirical root trait relationships derived via FRED 2.0 to parameterize a heuristic model that includes the traits and functional contributions of mycorrhizal fungi (McCormack et al. *2*019). We are also conducting a global assessment of the variation in root traits by implementing a hierarchical Bayesian model that simultaneously considers the major controls of root-trait variation in FRED 2.0, including fine-root functional class, plant–species phylogeny, mycorrhizal associations, and environmental conditions (Liu et al., in preparation).

2. **What root trait data are missing from FRED and what additional data synthesis activities or data harvest from the literature are needed to fill these gaps?**

We released the third version of the FRED in March 2021 (Iversen et al. 2021D). We worked with web developers within ORNL's Information Technology Services Division to encode the observations in FRED into database form (Microsoft Azure), and to develop a user interface (programmed using Vue.js for the user interface and Node.js for the data interface) that allows users to filter the observations in FRED according to their scientific needs. The user interface is accessed from https://roots.ornl.gov/public-release. Data have been filtered and downloaded via the new user interface nearly 300 times through 15 June 2022. FRED 3.0 has more than 150,000 observations of more than 330 root traits, and data are collected from more than 1,400 sources. We highlighted FRED 3.0 as a community resource for belowground ecologists and modelers alike in an editorial that accompanies a Virtual Special Issue in *New Phytologist*, where we compiled more than 40 recent papers on the topic "Filling gaps in our understanding of belowground plant traits across the world" (Iversen and McCormack 2021).

Like any ecological database, FRED 3.0 contains hundreds of thousands of root trait observations (**Fig. 2.15**), but these observations are sparsely spread across multiple categories of root traits and locations from around the world, highlighting areas new observations are needed. The FRED team is helping to fill knowledge gaps in multiple ways. First, FRED 3.0 is providing the foundation for new, biome-specific working groups to synthesize root trait observations from underrepresented biomes such as the Arctic ("Arctic Underground," PIs Hewitt and Mack) and the tropics ("Tropical Forest Root Traits," PI Cusack). Second, the root trait framework developed by the FRED team has been leveraged to develop a Root Traits Handbook and companion paper advocating for increased quantification of functional root traits (Freschet et al. 2021a, 2021b). Third, FRED has been integrated with aboveground traits, soil characteristics, and across the phylogenetic tree via integration with the TRY plant trait database (Kattge et al. *2*020), collaboration with the International Soil Carbon Network (Malhotra et al. *2*019), and participation in the Open Traits Network (Gallagher et al. *2*020).

3. **How can we inform and improve model representation of root form and function?**

Leveraging FRED, we are seeking to reduce ESM uncertainty by replacing the current 1-pool representation of fine roots in ELM with a 3-pool belowground model structure representing both transport and absorptive fine roots, as well as mycorrhizal fungi to model vertically and temporally resolved fine-root systems. This framework balances the complex, high-dimensional variability of fine-root systems with empirical support from databases of explicit root and fungal traits (e.g., FRED). We have submitted a demonstration of this 3-pool root structure in ELM (ELM-TAM; Transport and Absorptive fine roots and Mycorrhizal fungi) showing robust impacts on model predictions (Wang et al. accepted).

### 2.7.2 FRED Publications and Data Sets

Since February 2019, science efforts related to FRED have produced 12 publications and 4 data citations on the preceding results.

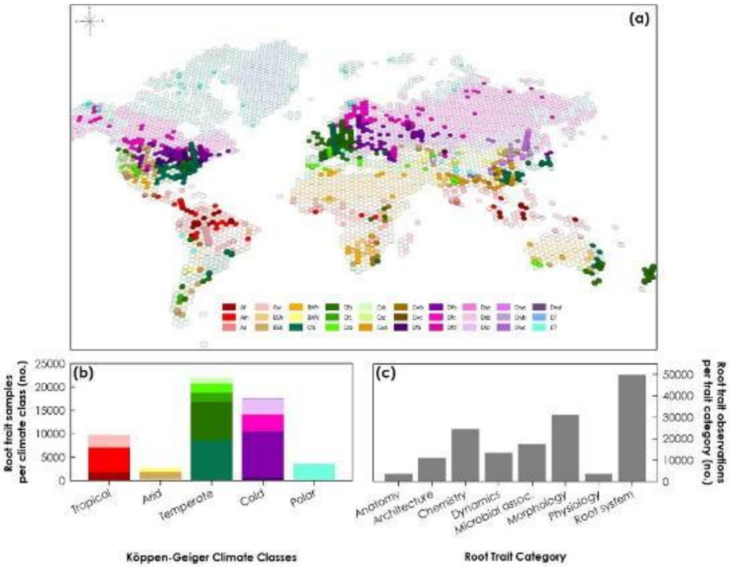


**Fig. 2.15. (a) FRED 3.0 observations are distributed unevenly around the world (map from Iversen and McCormack 2021). For the purposes of this map, land cover within a Köppen-Geiger climate classification zone (Kottek et al. 2006) was aggregated into hex bins extruded in 3D space based on the number of root trait samples collected in each bin. Map courtesy of Chris DeRolph. (b) Number of root trait samples collected from each Köppen-Geiger climate subclass, summed within each climate class. (c) Distribution of observations in FRED 3.0 across broad categories of root traits; for more information about the trait categories (https://roots.ornl.gov/data-inventory).**

### 2.7.3 LeafWeb

LeafWeb (https://www.leafweb.org/) is an online automated research tool that supports cutting-edge analyses and modeling of photosynthesis by plant scientists. We have updated LeafWeb to accept joint or separate measurements of pulse-amplitude modulated (PAM) fluorometry and gas exchange for C3 and C4 photosynthetic pathways. With the new development of photophysical and photochemical models by Section 2.2.3, it is now possible to use joint measurements of PAM fluorometry and gas exchange to improve photosynthesis modeling.

We have also been conducting offline tests on ways to increase the flexibility in data formats that LeafWeb users are allowed to use. The purpose is to reduce the time needed and potential errors produced by users in preparing their data sets for analyses by LeafWeb. In offline tests, we now use keywords to define variable names. Users can place a variable in any column as long as the keyword for that variable is used as the header name for that column. LeafWeb automatically searches for that keyword to determine the column in which the variable value is stored. The start and end of the metadata and actual PAM fluorometry and gas exchange data are automatically determined. To support this effort, a standard LeafWeb data dictionary has been created and sent to LeafWeb users for comments and suggestions (https://www.leafweb.org/information/data-publications/). These added flexibilities reduce the time users need to prepare for data submission and analyses by LeafWeb.

In offline efforts, we have started to integrate codes for the models of photophysics of Gu et al. (2019) and photochemistry of Gu et al. (2022, 2023) into the LeafWeb code system for both C3 and C4 photosynthetic pathways. This integration will enable the joint optimizations of photophysical, photochemical, and biochemical parameters of photosynthesis by LeafWeb when joint measurements of PAM fluorometry and gas exchange are submitted by users. With the new efforts, we aim to enable LeafWeb to estimate essentially all photophysical, photochemical, and biochemical parameters of photosynthesis that are of interests to ecophysiologists, modelers, and remote sensing scientists. These new functionalities will greatly expand the capability of LeafWeb to support cutting-edge photosynthesis research.

We are also working to update the C4 photosynthesis model in LeafWeb. The current version of LeafWeb uses the simple empirical C4 model of Collatz et al. (1992). Although this model is commonly used in large-scale C cycle models, it is rarely used by plant scientists because it is too simplistic and cannot represent full responses of C4 photosynthesis to climate change. Our aim in this aspect was to replace it with the state-of-the art biochemical model of C4 photosynthesis commonly used by plant scientists (Yin and Struik 2021, von Caemmerer 2021). Furthermore, we have been working in LeafWeb to couple the state-of-the-art C4 biochemical model with the photophysical model (Gu et al. 2019) and the photochemical model of Gu et al. (2022, 2023) so that complete analyses of C4 photosynthesis can be performed despite difference in biochemistry of C3 and C4 plants.

*Progress in LeafWeb user interface development* – LeafWeb support libraries have been updated. More than 30 support libraries have been updated with bug and security fixes, including Umbraco 7.15.3, Hangfire 1.7.7, Bootstrap 3.4.1 to 4.3.1, and Entity Framework to 6.3. The Bootstrap upgrade made LeafWeb usable on mobile devices. We added a LeafWeb search interface to the Search and Manage Queue pages. More than 100 uploaded data samples with errors were analyzed to find common formatting issues for users. A document was added to explain how to avoid these errors. Such analyses also led to developing additional coding strategies that are more tolerant to nonlethal formatting errors. User accounts have been created for frequent users so that they can manage their data submissions. A batch download function has been added to allow fast and easy download of LeafWeb inputs and outputs.

*Progress in LeafWeb data support to scientific research* – Examples where LeafWeb provided direct, significant support include: Control of biochemistry on respiratory $CO_2$-refixation (Eckert et al. 2020); Variations of respiratory $CO_2$-refixation across species (Eckert et al. 2021); Physiological basis for estimating photosynthesis with chlorophyll fluorescence (Han et al. 2022a); Seasonal variations in SIF and its relationship with photosynthetic capacity (Li et al. 2020); Regulations of photosynthesis by photochemical and non-photochemical quenching in fluctuating light environments (Han et al. 2022b); Influence of redox states of reaction centers on the inference of photosynthetic capacity from fluorescence (Han et al. 2022c); The development of the bellows theory to explain the granal thylakoid structure and function of higher plants (Gu et al. 2022); The development of a photochemical model for photosynthetic electron transport (Gu et al. 2023); The development of theoretical framework for SIF research and application (Sun et al. 2023a and b). Even though LeafWeb is a free online service tool for global photosynthesis researchers, we do not track how users use LeafWeb analysis results of their own data in their research.

*Progress in publicly released LeafWeb data sets* – LeafWeb users, not LeafWeb, are the owner of both the original data submitted and LeafWeb analysis results of the data. By using LeafWeb services, users agree to grant the LeafWeb operator access to their original data and LeafWeb results. Any use of the original data and LeafWeb analysis results by anyone other than the data owner is contingent upon permission from the data owner. LeafWeb releases only the data sets that have been undergone manual quality assurance and control and used in peer-reviewed publications that have major TES SFA contributions, according to journal and DOE data policies.

For the past funding period, LeafWeb released a comprehensive data set that consists of 261 data files (Han et al. 2022D). This data set contains measurements of leaf gas exchange and PAM fluorometry of light, $CO_2$, $O_2$, and temperature responses from 26 C3 and 4 C4 species measured by independent researchers in Canada, China, Finland, the Netherlands, and the United States in different years. To our knowledge, this is the largest data set ever collected that contains simultaneously obtained PAM fluorometry and gas exchange measurements.

#### 2.7.4 Publications for LeafWeb

Since February 2019, science efforts associated with LeafWeb have directly supported 10 publications and 1 publicly released data set.

### 2.8 Data Management, ESS-DIVE, and Collaboration

#### 2.8.1 Data Submission and Publication

As summarized in Appendix B, the TES SFA has published 170 data products (including 97 total from SPRUCE which includes 5 products currently available to the project team only while awaiting associated manuscript publication). All incoming data were assigned digital object identifiers (DOIs) using the DOE Office of Scientific and Technical Information (OSTI) Elink tool; archived at the project archive or other program-specific archive (e.g., MOFLUX at AmeriFlux); and made publicly available on the TES SFA and SPRUCE websites. Team members were highly encouraged to include full data set citations in their manuscript's references. Updates are made to data sets with ongoing data collection typically on an annual basis. In FY 2022, six data sets from the SPRUCE experiment were updated to include new data.

#### 2.8.2 Website and Data Access

The FRED, SPRUCE, and TES SFA websites were upgraded to the latest version of the website content management system Drupal 9. With this upgrade came improved security measures and changes to the look of the websites. To resolve some technical issues on the SPRUCE website with file access and download capabilities, the decision was made to transfer the file host to Dropbox and install a Dropbox module directly on the data set landing page that also improved the backend workflow and the ability to transfer large data files to the data management team (DMT).

### 2.8.3 Code and Software Sharing

Public release of SPRUCE-specific E3SM code was managed by the E3SM project as part of a collaboration agreement between the ORNL TES SFA and E3SM and subject to E3SM policies and licensing (https://e3sm.org/resources/policies/). Development branches of the E3SM code for research purposes are available on GitHub (https://github.com/E3SM-Project/E3SM/). The most recent release was assigned a DOI through DOECODE (10.11578/E3SM/dc.20210927.1) with a 3-Clause BSD license. The Multi-Assumption Architecture and Testbed (MAAT v1.3.1) is open source and available on GitHub (https://github.com/walkeranthonyp/MAAT).

### 2.8.4 ESS-DIVE Repository

DMT collaborated with the DOE ESS Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) (https://ess-dive.lbl.gov/) staff and initiated the mirroring of data packages at the ESS-DIVE long-term repository (**Fig. 2.16**). These project data and metadata were reviewed and updated to meet Findable, Accessible, Interoperable, and Reusable (FAIR) principles (https://doi.org/10.1038/sdata.2016.18) and other repository requirements. To date, there are 58 TES SFA (including 24 SPRUCE) data packages mirrored at the repository and available within project portals developed by the DMT. ESS-DIVE staff were invited to present about the repository at the SPRUCE monthly meetings.

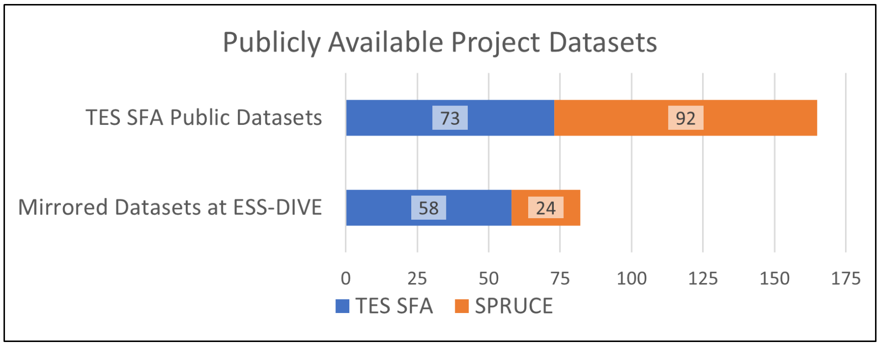


**Fig. 2.16. The total number of publicly available TES SFA data sets and number of data sets mirrored at ESS-DIVE.**

### 2.8.5 Collaboration

Collaboration across BER projects continued with TES SFA participants Paul Hanson and Daniel Ricciuto, who initially served on the ESS-DIVE Archive Partnership Board; Terri Velliquette took over that role in 2021. Terri continued to serve as the Data Management co-lead on the DOE ESS Cyberinfrastructure Working Group and builds relationships with colleagues both within DOE and externally through interactions with the ESS community, Earth Science Information Partners, OSTI, and ESS-DIVE. From these interactions, the TES SFA can stay current with community archiving expectations, maintain awareness of data management best practices, and present project challenges and requests for improvements.

## 3. RESEARCH PLANS FOR FY 2024, FY 2025, FY 2026, FY 2027, AND FY 2028

This section describes our research plans by TES SFA Themes and tasks during five fiscal years from FY2024 through FY2028. An overview is provided in Section 1. For ongoing research tasks, we refer the reader to Section 2 describes recent TES SFA activities. Cited articles therein and past annual and triennial review reports on the TES SFA web page (https://tes-sfa.ornl.gov/node/17) provide more details.

### 3.1 Theme 1: Carbon Cycle Responses to Warming and Increased Atmospheric $CO_2$ Concentration

*By how much and by which mechanisms will warming affect southern boreal peatland ecosystem productivity, C storage, and greenhouse gas fluxes? Can elevated $CO_2$ ameliorate the likely negative effects of warming?*

Recent review articles (Crowther et al. 2016, Gallego-Sala et al. 2018, Haff et al. 2021, Patel et al. 2022, Yan et al. 2022) continue to underscore the need for research on warming in peatlands and high-latitude regions to provide the quantitative mechanistic understanding necessary to scale observations and experimental results within ESMs. The motivation for SPRUCE (Hanson et al. 2017) is to develop quantitative information on high-C boreal ecosystem responses to warming and elevated atmospheric $CO_2$ as a prerequisite for the development of ecological forecasting tools for policy makers to evaluate safe levels of greenhouse gases in the atmosphere. The SPRUCE experiment provides a platform for testing mechanisms controlling the vulnerability of organisms and ecosystems to important climate change variables. The ongoing SPRUCE experiment (Hanson et al. 2017) is sited in a southern boreal peatland and has five WEW treatments, initiated in August 2015, and two $CO_2$ treatments, initiated in June 2016. The SPRUCE experiment is set up to address the following major hypotheses:

- Warming will enhance microbial functions to increase decomposition and lead to peatland C losses and the release of greenhouse gases to the atmosphere.
- Warming will extend the growing seasons and enhanced vegetation and moss physiological activity may both increase C gain by peatlands.
- Warming-induced decomposition will release stored essential nutrients that can be used by vegetation to enhance previously nutrient-limited primary production and thereby enhance peatland C storage.
- If not limited by nutrient supplies or water stress, elevated $CO_2$ may enhance photosynthesis, help alleviate water stress, and limit peatland C losses.

The TES SFA has completed 7 of 10 years of the planned decadal operation of SPRUCE. With support from the proposed work under Themes 2–5, Theme 1 will bring SPRUCE continuous operations to completion at the end of the 2025 calendar year, measure response variables in years 8, 9, and 10, and complete post-treatment characterization. Theme 1 research activities focus on the measurable C cycle responses addressed by the SPRUCE experiment, along with associated process studies and model algorithm development. SPRUCE measurement objectives include all components of NPP above- and belowground, net exchange of $CO_2$ and $CH_4$ and their autotrophic and heterotrophic components, C flux via lateral outflow, physiological and hydraulic processes driving photosynthesis and respiration contributions to the C cycle, and SIF characterization of GPP. Seasonal changes in phenology of, and long-term changes in, vegetation community composition are addressed as a part of Theme 1 as they establish the component contributions to the C cycle. Warming-induced changes in peat C stocks measured by traditional C concentration bulk density assessments and interpretations of isotopic change with time are also a focus. Full archiving of the vast amount of empirical data, samples, and model results for future scientific consideration and public dissemination will be a key activity through 2028.

Theme 1 tasks include the operation of the SPRUCE experiment investigating the responses of peatland ecosystems to warming and elevated $CO_2$ (TH1.1), evaluation of changes in net C balance for peatlands and their C stocks (TH1.2), changes in phenology of physiological processes and growth under warming and elevated $CO_2$ (TH1.3), and the development of process models and landscape-scale wetland models enabling peatland ecosystems to be better represented in models (TH1.4).

### 3.1.1 SPRUCE Experiment Operations (Task TH1.1)

Key Personnel: Pearson and Hanson

<u>SPRUCE operations</u> – Operation of the SPRUCE WEW treatments and associated environmental observations (e.g., half-hour air and soil temperatures, relative humidity, water table depth, $CO_2$, and $H_2O$ concentrations in air) will continue 24 h a day through December 31, 2025. The $eCO_2$ treatments will be operated during daytime hours throughout the active growing season (typically May through October) in 2023, 2024, and 2025. Performance data for WEW and $eCO_2$ treatments are available from Hanson et al. (2016D) and Appendix E.

Beginning in 2026, we will invest sequestered funds (estimated at $2 million) to decommission the SPRUCE experimental site consistent with expectations of our research agreement with the Marcell Experimental Forest. Under a memorandum of understanding between ORNL and the USDA Forest Service, components of the infrastructure associated with the SPRUCE field experimental manipulations need to be removed following active research on the S1 Bog. The dominant experimental enclosures, propane and $CO_2$ pipelines and storage tanks, fenced infrastructure, storage containers, and the experimental control building will all be removed on a schedule that will allow progress while not impeding the important post-treatment science in FY 2026 and FY 2027. The USDA Forest Service has the discretion to retain as much of the infrastructure as needed to support sustained or future research activities at this site.

Current discussions suggest that the four access boardwalks will be retained for future research activities, but we would be expected to remove active systems for air warming (HVAC systems, aboveground enclosures, propane pipelines, and storage tanks), infrastructure associated with elevated $CO_2$ exposures (pipelines and storage tanks), and within-bog electrical service. The timing of removals and the development of associated subcontracts (bid-based) will be planned and solicited in 2025 and executed on a schedule spread across 2026 to 2028 as some facilities will be needed to support final observations and destructive sampling.

### 3.1.2 Changing C Balance and Peat Stocks under Warming and $eCO_2$ (Task TH1.2)

Key Personnel: Griffiths, Hanson, Iversen, Mayes, Weston

The primary questions driving Task TH1.2 are as follows:

1. *Will belowground warming reverse 10,000 years of C accumulation in peatlands that store one-third of the Earth's terrestrial C?*
2. *If the peatland turns into a C source, how much C release will occur?*
3. *Will the released C be in the form of $CO_2$, or $CH_4$ with about 30 times the global warming potential of $CO_2$, at the end of this century (Myhre et al. 2013)?*

Key activities under this task include the integration of measures of NPP (current year growth), live biomass pools, peatland stocks, lateral losses of TOC, and the net exchange of greenhouse gases ($CO_2$ and $CH_4$) necessary to calculate annual net C gains or losses for the peatland (Griffiths et al. 2017, Hanson et al. 2020). Modeling activities are addressed in Task TH1.4.

<u>*Shrub-layer NPP and tree growth (Griffiths, Hanson et al.)*</u> – Nondestructive evaluation of shrub community composition and cover will be executed by R. Montgomery, University of Minnesota with B. Palik USDA Forest Service, at annual, mid-summer events. Following those assessments, 1.2 $m^2$ destructive assessments of shrub-layer vegetation stocks and annual production (Hanson et al. 2018Da) will be collected in August 2023 and August 2025. For this purpose, we will begin partial sampling of random ends of the 3 community plots per enclosure. Nondestructive tree-level basal area growth for all ambient and treatment plots will be continued annually (Hanson et al. 2018Dc). We will also continue to support contracted annual terrestrial laser scanning in May and August for canopy height and volume change assessments (Nancy Glenn et al., Boise State University).

<u>*Sphagnum moss physiology, productivity, and community interactions (Weston et al.)*</u> – *Sphagnum* mosses are a key genus at the SPRUCE site and throughout boreal and sub-arctic peatlands, where they dominate plant productivity and exert an outsized influence on nutrient cycling and C storage as

recalcitrant peat. Key observations have included *Sphagnum* NEE, percent cover, NPP, and microbial community composition and N-fixation. *Sphagnum* net photosynthesis and response to warming has been difficult to assess thus far using automated open-top chambers, which are complicated by simultaneous measurement of soil respiration and differential hydration. As such, novel gas exchange chambers will be used in campaigns to further assess *Sphagnum* photosynthetic temperature response in field and laboratory campaigns across a range of leaf water content for mosses. Measurements will address the following questions: 1) How is *Sphagnum* growth and productivity influenced by long-term warming and $CO_2$ treatments? 2) What are the consequences of SPRUCE treatments on *Sphagnum* $CO_2$ exchange? 3) How does warming and $CO_2$ influence *Sphagnum*-associated microbial community composition, N-fixation, and thermal acclimation?

Previous work led by Rich Norby showed a decline in *Sphagnum* percent ground cover and NPP in response to warming (Section 2.1.5). Recent unpublished results show that $eCO_2$ may be influencing the NPP response to warming. We will continue our annual assessment of *Sphagnum* growth and cover and investigate if coming years will result in an $eCO_2$ by warming interaction on *Sphagnum* NPP.

Recent research has also shown that the *Sphagnum*-associated microbiome plays a key role in N-fixation and thermal acclimation (Petro et al. in press). To holistically link *Sphagnum* physiology and nutrient dynamics with associated microbes, we will deploy automated, closed-top chambers that will measure $CO_2$ exchange every half hour throughout the growing season. In addition, we will collect monthly samples for protist, bacteria, archaeal, and fungal community composition. This will be paired with N-fixation estimates ($^{15}N_2$ incubations) and corresponding metagenome analyses (JGI Community Sequencing Program) to infer plant and microbial metabolism. Furthermore, the inclusion of protists into the community analysis provides a unique perspective of how top-down bacterial predation influences *Sphagnum*–microbiome function.

*The dynamics and distribution of root growth throughout the peat profile at belowground processes at SPRUCE (Iversen, Childs, et al.)* – We will continue to monitor root growth in the SPRUCE experimental plots—both at the biweekly temporal scale to assess root phenology and rooting depth distribution using manual and AMRs, as well as at the annual temporal scale to quantify root biomass production and the chemistry of newly produced roots (see nutrient linkages in Theme 3). Thus far these data streams have allowed us to conclude that warming increases the growth of ericaceous shrub roots (Malhotra et al. 2020), extends the belowground growing season (Defrenne et al. 2021), and changes the balance of rhizosphere fungi (Defrenne et al. 2021). Continued collection of these data streams will allow us to address the following root-specific questions in response to long-term warming and $eCO_2$: (1) How does warming affect the phenology of root and fungal growth? (2) How is belowground phenology related to aboveground phenology, as well as edaphic and environmental conditions? (3) How does warming affect the distribution of fine roots throughout the peat profile?

The shallow distribution of woody fine roots above the average water table depth prior to initiation of the SPRUCE experimental manipulation (Iversen et al. 2018) led us to hypothesize that an observed drawdown of the water table level with warming will result in deeper rooting distributions in the bog. We are continuing to track this response in the root ingrowth cores and manual minirhizotron images. In addition, minirhizotron images are providing a novel glimpse at how the surrounding rhizosphere changes with peat depth. For example, we can observe whether each image is saturated (i.e., whether it is above or below the water table), something that we hypothesized would be possible at the onset of the project (Iversen et al. 2012). Preliminary comparison of saturated images with data from plot wells indicates that minirhizotron images may provide finer spatial-scale resolution of the effects of warming on the water table level. Furthermore, we have observed bubbles in minirhizotron images, especially at the water table interface, that may allow for investigation of the effects of warming on ebullition, and the gasses therein, in collaboration with other project partners (Ma et al. 2022).

*Net $CO_2$ and $CH_4$ efflux and isotopic tracer work (Hanson, Mayes, McFarlane et al.)* – Starting in 2022, we initiated the collection of net $CO_2$ and $CH_4$ flux observations from 2 automated, high-temporal resolution chambers per plot (Eosense Inc., eosAC-LT 50 cm diameter chambers) interfaced with field-deployable $CO_2$ and $CH_4$ analyzers (ABB Model GLA131-GGA analyzers). Four additional automated flux chambers are available for the characterization of heterotrophic-only flux in ambient bog locations.

In mid-summer 2025, active vegetation within the established automated chambers in each treatment plot will be removed for the assessment of treatment-specific, heterotroph-only contributions to $CO_2$ efflux.

In 2022 and 2023, comparative observations with manually obtained large collar flux data (Hanson et al. 2016; Hanson et al. 2020) will be collected to evaluate comparability of the two flux data sets.

Isotopic assessment of C released to the atmosphere in the form of $^{13}CO_2$, $^{14}CO_2$, $^{13}CH_4$, and $^{14}CH_4$ under subcontract by Karis McFarlane, Lawrence Livermore National Laboratory, provides the necessary measurement from which the source of released C can be determined (shallow and more recent vs. deep and older C sources).

*TOC concentrations and lateral outflow losses (Griffiths, Sebestyen)* – Weekly measurement of outflow volume and chemistry (TOC concentrations) from the outflow system will continue through 2025. TOC losses (fluxes) via outflow will be used in the estimation of ecosystem-scale C flux responses to warming and $eCO_2$. Outflow water samples will also be analyzed for nutrients, cations, anions, metals, pH, and specific conductivity to better understand the water chemistry and nutrient-budget responses to WEW and $eCO_2$ (Theme 3). The outflow data combined with inputs via precipitation and water table dynamics will be used to synthesize our understanding of the peatland hydrological responses to WEW and $eCO_2$ (see synthesis paper deliverable).

*Peat elevations (Hanson, Mayes)* – Changing peatland elevations will be evaluated annually (Hanson et al. 2018D) to characterize dynamic gains and losses of both water and C from the peat profile. Such data were previously used to test and verify the calculated C loss rates from plot-scale assessments of net C ecosystem budgets (Hanson et al. 2020).

*Isotopic assessments of vegetation and peat and peat profile sampling (McFarlane, Hanson)* – The application of our $eCO_2$ treatments from a defined source gas having unique $^{13}C$ and $^{14}C$ isotopic signatures provides the opportunity for independent evaluation of new C inputs into vegetation growth and storage pools as well as changing peat C stocks by depth. Increasing isotopic signatures of litterfall, and enhanced losses of $CO_2$ and $CH_4$ with warming (Section 2.1), support such changes. In 2025, we will subsample the vegetation in association with other destructive harvests and organize the collection of multiple peat cores for the assessment of a decade of change in isotopic signatures. At this time, we will also resample peat C, elements, and ash and bulk density as was done for pretreatment conditions and after 5 years of manipulation (in 2020). Peat characterizations as described in Tfaily et al. (2014) and Iversen et al. (2014D) will be repeated when isotopic signatures of input C stabilize (**Fig. E2**). Analysis of peat column changes will include both standard and equivalent ash methods (Grønlund et al. 2008, Rogiers et al. 2008, T. Schuur, *personal communication*).

#### 3.1.2.1 SPRUCE Post-Treatment Characterization of the Cumulative Decadal Responses

Key Personnel: Griffiths, Warren, Iversen, Mayes

Final assessments of shrub-layer vegetation and tree growth, including the subcontracted terrestrial lidar scans (Section 3.1.2), will be accomplished during the last year of treatments (i.e., 2025) to calculate aboveground contributions of shrub and tree NPP to plot-level C budgets.

Destructive harvests will be accomplished in 2026 to evaluate if warming and $eCO_2$ treatments have altered the allocation of C among foliage, branches, and boles of the respective species (Shrubs: *Rhododendron groenlandicum, Chamaedaphne calyculata, Vaccinium oxycoccos*; Trees: *Picea mariana, Larix laricina*). Destructively harvested tissue will also be used to assess hydraulic segmentation of root, stem, and branch/leaf xylem vulnerabilities to embolism. Prior to harvesting, lidar will be used on selected trees inside enclosures for validation of the lidar–leaf area models developed using destructive tree harvests from outside the enclosures.

Final leaf area for shrub-layer species will be derived from the destructive plot samples described previously, and for trees from the new allometric relationships. Leaf area is a key driver for photosynthetic C assimilation in model efforts described below.

Post-treatment peat cores will be extracted to examine changes in fine-root population biomass depth distribution and chemistry in response to experimental change. Larger peat blocks (0.5 X 0.5 m) will be sampled to a depth of 0.25 m to add characterization of coarse root biomass allometry for shrubs and trees.

Key synthesis papers for changes in the peatland C cycle because of warming with anticipated limited $eCO_2$ impacts will be led by Dr. Natalie A Griffiths following the methods outlined in Griffiths et al. (2017) and Hanson et al. (2020). We anticipate other synthesis paper on the decadal response to the warming by $eCO_2$ treatments in the following areas: peat elevation and C stocks (M. Mayes), altered phenology (A. Richardson), impacts on plant C and water relations (J. Warren), modified decomposition processes (N. Griffiths, R. Kolka), changes in ecosystem nutrient cycles (V. Salmon) and solute fluxes (N. Griffiths), hydrologic cycle changes (S. Sebestyen), and microbial community composition and function (C. Schadt and M. Mayes).

The ORNL SPRUCE group will also continue to interact with the ongoing work of a range of external collaborators who are expected to produce decadal syntheses of peatland response variables that impact C cycle processes (see page 193).

### 3.1.3 Changing Phenology and Physiological Processes (Task TH1.3)

Key Personnel: Warren, Gu, Richardson, Pearson

The primary questions driving Task TH1.3 are as follows:

1. *Are peatland ecosystems and their organisms vulnerable to atmospheric and climatic change?*
    a. *What changes are likely? To what degree will changes in plant and microbial physiology under $eCO_2$ impact a species' sensitivity to climate or competitive capacity within the community?*
2. *Do critical air and soil temperature thresholds exist for ecosystem processes and organisms? How does warming affect timing and rates of foliar, root, and fungal phenology?*

*Vegetation phenology (Richardson, Pearson, Hanson)* – Manual phenology observations (Heiderman et al. 2018D; Schädel et al. 2019D, 2020D, 2021D, 2022D) weekly during the active season and both plot- and shrub-level PhenoCam image collection and greenness analysis (Richardson et al. 2018, 2018Da, 2018Db) will continue to evaluate any long-term changes in the phenological responses of vegetation.

*Root and fungal phenology (Iversen, Childs, et al.)* – As described above, minirhizotron image collections will continue to be used to investigate the timing of root production, and associated fungal communities, throughout the growing season. An outstanding question remains as to whether belowground dynamics and an observed extension of the belowground growing season (Defrenne et al. 2021) matches the lengthening of the growing season observed aboveground in response to warming (Richardson et al. 2018). Furthermore, we will link these dynamics with changes over time in edaphic conditions, such as water table depth and soil temperature, and other environmental conditions assessed by the SPRUCE project team.

*Woody plant physiology (Warren, Gu)* – In addition to *Sphagnum,* woody vegetation responses to warming regulate energy, C, and water cycles through sensible and latent heat loss, NPP, and transpiration. These cycles are critical components of mechanistic models and thus knowledge of their sensitivities to WEW are key inputs to ELM-SPRUCE. We will continue exploring how the use of observed physiological responses to WEW impact model outputs, and then provide updated and new process data to address continued model uncertainties.

*Thermal acclimation of photosynthesis (Warren)* – As anatomical, morphological, and physiological acclimation to an altered environment can take multiple years, we plan to revisit joint foliar gas exchange and PAM fluorometry measurements after 10 years of warming. This campaign will assess several questions: 1) What is the degree of thermal acclimation of photosynthesis and respiration ($A_{max}$, $V_{cmax}$, $J_{max}$, $R_d$)? 2) What is the range of plasticity in thermal acclimation? 3) What are the thermal thresholds at which acclimation is no longer sufficient to maintain a positive C balance? 4) Do the $eCO_2$ treatments enhance physiological acclimation? Gas exchange responses will be assessed for the two tree species using LI-6800 systems at growth and common conditions (i.e., 25°C, 400 ppm $CO_2$) for comparison against similar measurements in 2016, 2017, 2019, and 2021. With participation of prior students, postdocs and collaborators, we will reassess photosynthetic responses over a range of temperature, $CO_2$ and VPD levels based on input from the modeling team.

While foliar temperature affects photosynthesis, net C uptake by woody vegetation is dependent on hydraulic feedbacks linked to plant water flux through the SPAC (new SPRUCE physiology work discussed in Theme 2). Woody respiration is also a topic of model interest and initial measurements will be conducted on branch material during summer 2023. Further work across both shrub and tree species will assess the relationship between woody tissue respiration and temperature. Respiration rates of woody root systems may also be conducted on samples collected outside the enclosures.

*Coupled measurements of SIF-EC (Gu)* – To complement gas exchange measurements, a coupled SIF-EC system has been deployed within an ambient plot at the shrub canopy level. The SIF component of the SIF-EC system is a second generation of FAME, which evolved from a prototype SIF system installed and tested at MOFLUX. To support the interpretation of the SIF dynamics observed by FAME and also the coupled modeling of photophysics, photochemistry, and biochemistry of photosynthesis (See Theme 2) at the SPRUCE site, we will install multi-probe Walz PAM fluorometry systems on *Sphagnum* and dominant shrubs. We will use the joint PAM-SIF-EC measurements to partition the measured net fluxes of $CO_2$ into GPP and respiration by applying the SIF-based partitioning approaches being developed in Theme 2. The partitioned shrub-level GPP and ecosystem respiration will be used to inform the ELM-SPRUCE model and complement other measurements of C uptake based on leaf-level gas exchange and sap flux.

### 3.1.4 Representing Peatland Ecosystem Response Processes within Mechanistic and Landscape Wetland Models (Task TH1.4)

Key Personnel: Shi, Mao, Xu, Luo, Ricciuto, Y. Wang

The primary question driving this MODEX task (Task TH1.4) is as follows*: Will ecosystem function at SPRUCE (e.g., hydrological and biogeochemical cycling) be compromised or enhanced by atmospheric and climatic change?* The Theme 1 modeling efforts propose to (1) project net C cycle changes with warming and $eCO_2$ consistent with experimental results and attributing changes to specific processes, (2) develop C allocation/phenology algorithms that include flexible C allocation coefficients as functions of environmental condition, (3) improve $CH_4$ simulated temperature and moisture responses and timeseries properties to capture how they are affected by microbial community changes, and (4) improve the simulated response of moss to warming. All efforts contribute to the completion of a fully functioning ELM-SPRUCE model with applications to wetland modeling at larger scales.

#### 3.1.4.1 SPRUCE Model Intercomparison Project (SPRUCEMIP) (Shi, Ricciuto)

SPRUCEMIP will evaluate the performance of multiple models against SPRUCE observations, and determine how model performance depends upon model structure, parameters, and assumptions. SPRUCE is a valuable testbed for the broader modeling community to improve the diagnosis and attribution of C fluxes in peatland ecosystems. The MIP activity addresses scientific questions aligned with Themes 1–4:

1. *What are the responses of net $CO_2$ and $CH_4$ fluxes from SPRUCE to warming and elevated $CO_2$, what are the contributions from ecosystem components, and how do these vary across models?*
2. *How do water availability and water cycle extremes interact with the treatments to regulate NEE and loss and energy balance?*
3. *How do warming and precipitation changes alter the distribution and dynamics of plant-available nutrients, and what are the implications for understanding and predicting ecosystem C fluxes?*
4. *What are the effects of plant and soil microbial community change to the treatments, and what are the implications for ecosystem C storage and $CO_2$ and $CH_4$ greenhouse gas fluxes?*

*SPRUCEMIP methods* – At least 10 peatland modeling groups will be participating in the SPRUCEMIP. In the first stage, all groups will use ambient plot atmospheric forcing data from 2015 to 2021 to drive a model spin-up simulation with pre-industrial conditions, and a transient simulation from 1850 to 2015. Measured plot-level meteorological forcing and $CO_2$ concentrations from the 10 treatment enclosures and the ambient plot will drive 11 simulations from 2015 to 2021 that can be compared against SPRUCE observations. A protocol is currently under development. As additional years of forcing and

SPRUCE observations are processed, we will extend the driver data set and interested modeling groups will be able update their simulations.

Modeling groups will provide standardized outputs and these results will be made available to the broader team for analysis. The SPRUCEMIP team will also use a matrix approach and traceability framework (Xia et al. 2013) for uncertainty quantification and attribution. We have already converted eight land C cycle models in a unified matrix form, and we will develop a numerical method to convert other participating peatland models in SPRUCEMIP into the matrix form by using model outputs. This will allow us to analytically determine sources of the across-model spread in land C dynamics. When all models were driven by the same GPP and environmental variables, the largest source of across-model variation was from inter-model differences in environmental scalars followed by the differences in baseline C residence time (Hou et al. accepted). Here we will consider model differences in vegetation productivity and coupling between above- and belowground processes including nutrient cycling.

Once the sources of the across-model spread are identified, we will apply a data assimilation technique to improve models with SPRUCE observations. Specifically, we will first use measured plant and ecosystem responses to five temperature and two $CO_2$ treatments to train the environmental scalars for plant and soil respiration. We expect that training of the environmental scalars will have the largest impacts on improving upscaling of model predictions as these scalars cause the largest spread across the models. We will also use data from measured various C and nutrient pool sizes (e.g., root biomass, tree and shrub biomass, soil C content together) with flux measurements to constrain residence times. We will also quantify acclimation and adaptation of ecosystem processes to warming and elevated $CO_2$.

The SPRUCEMIP timeline and next steps include 1) all the model groups are submitting the model outputs in 2023; 2) a virtual meeting in 2023 to present initial results and discuss possible papers; 3) plans for discussion and analysis of SPRUCEMIP results at a SPRUCE-focused international peatland workshop, mid-2024 time frame (Section 3.6) which will include both empirical and modeling participation. The MIP activity is also planning future simulations using downscaled ESM outputs (TH 5.2) and simulating additional treatments including water table drawdown simulation and nutrient addition.

#### 3.1.4.2 Modeling SPRUCE Response Mechanisms

Individual SPRUCE measurement tasks provide process-based quantitative regression algorithms for potential use within the higher-order modeling. The goal of process modeling improvement is to determine the nature of regressions between a given response variable and the sequence of warming treatments imposed by SPRUCE in the presence and absence of $eCO_2$ treatments. The primary modeling framework used here is ELM-SPRUCE, a site-scale version of ELM that includes peatland hydrology, PFTs and improved parameters (Shi et al. 2015, 2021). The current version updated to E3SMv2, is ELMv2-SPRUCE, but will transition into ELMv3-Peatlands to enable both site and regional modeling in coordination with TH5.2. ELMv3-Peatlands will include all previous version developments and it will enable further integration with FATES to predict vegetation dynamics. The mechanistic $CH_4$ model (Ricciuto et al. 2021, Yuan et al. 2021a) is currently only available in the initial version, ELMv0-SPRUCE, but will also be integrated into ELMv3-Peatlands. Ongoing Tasks include phenology characterization, $CH_4$ flux, growth and function of the *Sphagnum* PFT, hydrologic cycles and water stress, and plant growth and C allocation processes.

*Synchronized phenology and plant growth C allocation in ELM-SPRUCE (Mao, Wang, Walker)* – Two SPRUCE-experiment MODEX observations motivate a revision of ELM-SPRUCE vegetation C allocation and phenology (1) no significant plant growth response to $eCO_2$ has been observed at SPRUCE while ELM-SPRUCE predicts large growth responses to $eCO_2$ (Hanson et al. 2020), and (2) asynchronous leaf and root phenology (Defrenne et al. 2021). ELMv1-SPRUCE and ELMv2-SPRUCE development introduced more realistic environmental controls on spring leaf-out and autumn senescence and separated the leaf and root phenology of the seasonal deciduous and boreal evergreen trees (Meng L et al. 2021a, Wang and Mao et al. in review). We propose to improve model allocation and phenological processes by applying the Tethys-Chloris (TC) scheme to simulate environmental controls on C allocation coefficients (Fatichi et al. 2012; Fatichi 2010). We will use the integrated ELMv2-SPRUCE and ELMv3-Peatlands with FATES to develop the TC allocation scheme. The Plant Allocation and Extensible Hypotheses (PARTEH) module embedded within FATES is a general module that provides a flexible model structure in which specific allocation hypotheses can be developed. The TC scheme is suitable as a first step because it uses a C pool-based approach that is compatible with the existing biogeochemistry scheme of ELMv2-SPRUCE (Fatichi et al. 2012; Fatichi, 2010). The TC model calculates the allocation coefficients in each of its C pools depending on the phenological phase, soil moisture availability, light availability, and soil N availability. Compatible with FATES, the TC model implements allometric constraints to ensure the proportions of storage, root, and leaf C stay within realistic ranges.

The warming and $CO_2$ elevation experiments and drought occurrences at the SPRUCE site provide a natural test bed for implementing time-varying allocation coefficients in ELMv2-SPRUCE, due to the availability of observations under multiple levels of environmental stresses. We will first add code to calculate the allocation coefficients in ELMv2-SPRUCE as functions of soil water, light availability, and N limitation following the TC model. We will then conduct sensitivity analysis and model calibration on the selected allocation/phenology parameters of both the original and updated models. Optimized models will be evaluated against SPRUCE observations (e.g., PhenoCam's Green Chromatic Coordinate, root growth and mortality, biomass component), to determine the extent to which the new model structure improves predictions. MOFLUX and MA phenology data are also available to calibrate the models.

*Mechanistic $CH_4$ modeling (Xu, Ricciuto)* – We will integrate the Microbe functional-group based $CH_4$ module with microbially explicit mechanisms (Xu et al. 2015, Ricciuto et al. 2021, Yuan et al. 2021) from ELMv0-SPRUCE into the new ELMv3-Peatlands framework. The Microbe $CH_4$ module includes bacteria, fungi, and DOC in the soil biogeochemistry module, considers of the measured biomass and function of acetoclastic methanogens, hydrogenotrophic methanogens, aerobic methanotrophs, and anaerobic methanotrophs, and can simulate DOC and $CH_4$ cycling in response to warming and $eCO_2$. While ELMv0-SPRUCE is able to simulate $CH_4$ fluxes under ambient conditions, further refinement of microbial processes (TH4.1) and parameters is necessary to reproduce the strong treatment effects (Hanson et al. 2020). We will also evaluate the ability of the recently developed isotopic $CH_4$ module to simulate $^{13}C$ and $^{14}C$ fractionation of biogeochemical processes and $CH_4$ production and consumption.

Integrating Microbe into ELMv3-Peatlands will also allow for detailed study of the interactions between $CH_4$ cycling and hydrology (Theme 2), nutrient cycling (Theme 3) and facilitate evaluation of additional Microbe model developments in Theme 4. The 2021 drought impacts on $CH_4$ flux (i.e., cessation of net $CH_4$ efflux) will be parameterized and evaluated from available large-collar and autochamber flux data. Challenges remain in predicting water table height, especially in drought conditions. We will drive the model with observed water table heights to simulate the effects of drought at SPRUCE in 2021. To improve understanding of hydrologic feedbacks, we will also compare these simulations to a set of simulations forced with ambient water table height. Using observational data of vegetation physiology, thermal dynamic, DOC concentration, and $CH_4$ processes, ELMv3-Peatlands will be applied to address three questions: (1) how does water table drop affect microbial physiology and soil biogeochemistry?; (2) how do soil microbes adapt to reduced soil moisture and temperature change?; (3) how do microbial and physical mechanisms drive the $CH_4$ emission decline under drought?

*Further development of the Sphagnum PFT submodel (Shi, Ricciuto)* – The *Sphagnum* moss PFT was introduced into ELM to simulate peatland functional dynamics under changing environments (Shi et al. 2021). However, there are still uncertainties and biases in simulating *Sphagnum* productivity and the responses of *Sphagnum* to warming and $eCO_2$. To improve our model prediction capacity, we propose the following efforts:

- *Modeling peat layer dynamics and evaluating the water table depth* – The hydrologic cycle, especially water table depth, is a key factor that influences the seasonality of GPP in *Sphagnum* mosses (Lafleur et al. 2005, Riutta 2007, Sonnentag et al. 2010, Grant et al. 2012, Kuiper et al. 2014, Walker et al. 2017). With water table declines follow enhanced decomposition and subsidence of the peat layer which then repositions the peat surface closer to the water table. Peat layer elevation change has not been included in ELMv2-SPRUCE. We propose to implement dynamics of the peat layer to our model based on the peat depth calculation method of Integrating the McGill Wetland Model (MWM) (Shao et al. 2022) using the observed peat elevation data from SPRUCE to test our model.
- *Modeling plant growth and competition* – ELMv2-SPRUCE predicted increasing growth of shrubs with increased temperature and model sensitivity analysis indicated that parameters for the shrub PFT

had significant sensitivities to *Sphagnum* moss GPP. This indicates competition between the PFTs for resources. ELMv2-SPRUCE does not include light competition among multiple PFTs, and thus does not represent cross-PFT shading effects supported by ongoing work. We will introduce light competition to ELMv2-SPRUCE by adopting the same method as described in the PEATBOG model (Wu et al. 2013). Competition for photosynthetically active radiation is implemented through shading effects. The photosynthetically active radiation that reaches the moss layer is decreased by the stems and leaves of the shrubs. In parallel, we will test the capability of FATES in ELMv3-Peatlands, integrated with ELMv2-SPRUCE and Microbe (Task TH1.2).

- *Peat water status* – Water status of the peatland is critical for C sequestration in plants and soil. Peat of low water holding capacity (WHC) near saturation (Cai et al. 2010, Sulman et al. 2010) rapidly loses water with small water table drawdowns, while peat of high WHC near saturation retains large amounts of water with similar water table fluctuations (Parmentier et al. 2009). We propose to integrate our soil water content data and apply the soil water retention curves method from Dimitrov and Lafleur (2020) to ELMv2-SPRUCE.

### 3.1.4.3 Model–Data Integration using C Isotope Measurements (Yang, Ricciuto)

ELMv2-SPRUCE has been evaluated and improved using field-observed C, N, and P pools and fluxes. Measurements of C isotopes ($^{13}C$ and $^{14}C$) provide additional opportunity for model evaluation and identification of the areas for further model development. We have evaluated peatland C accumulation in ELMv2-SPRUCE by comparing the simulated $\Delta^{14}C$ vertical profile with the observed pretreatment $\Delta^{14}C$ vertical profile at SPRUCE site (McFarlane et al. 2019). Preliminary simulations with $\Delta^{14}C$ show that ELMv2-SPRUCE captured increasing depletion of $\Delta^{14}C$ with time under $eCO_2$, consistent with the observed $\Delta^{14}C$ in green leaves. We propose to take advantage of the comprehensive isotopic measurements from all treatment plots ($^{13}C$ and $^{14}C$ in plant tissues, peat, DOC, dissolved inorganic C and soil respiration) to model simulations to better understand the fate of C under $eCO_2$ and warming.

**Table 3.1. Deliverables for Theme 1 research. Post-SPRUCE syntheses are shown in green text.**

| Task | FY | Deliverable | Lead(s) |
|---|---|---|---|
| TH1.2 | 2024 | Paper: Net $CO_2$ and $CH_4$ flux in 2022–2023 contrasting new automated vs. older manual methods. | Mayes, Hanson, Krassovski |
| TH1.2 | 2024 | Paper: 5 year peat change 2016-2020 | Postdoc, Hanson |
| TH1.3 | 2024 | MODEX paper: Testing woody physiological $eCO_2$ and temperature responses | Warren, Ricciuto |
| TH1.1 | 2024 | Paper on outflow C and nutrient concentration responses | Griffiths |
| TH1.1 | 2024 | Paper on *Sphagnum* NEE, microbial food webs, and $N_2$-fixation | Weston, Gibert |
| Multiple | 2024 | International wetland meeting – what did we learn from SPRUCE and how do we extrapolate it beyond SPRUCE? | Mayes et al. |
| TH1.4 | 2025 | MODEX: Model intercomparison results to be published | Shi, Ricciuto |
| TH1.1 | 2026 | Sustain SPRUCE treatments and automated data collection through 31 December 2025 | Krassovski |
| TH1.2 | 2026 | Paper: Automated continuous measurements of $CO_2$ and $CH_4$ emissions from SPRUCE | Postdoc, Mayes, Hanson et al. |
| TH1.4 | 2026 | SPRUCE: Modeling of microbial activity and functions and comparison against measured microbial data | Xu, Ricciuto, Schadt, Mayes |
| TH1.3 | 2026 | SPRUCE: Synthesis paper on phenology changes | Richardson |
| TH1.4 | 2027 | SPRUCE: Modeling of microbial activity and functions and comparison against continuous measurements of $CO_2$/$CH_4$ emissions | Xu, Ricciuto, Schadt, Mayes |
| TH1.2 | 2027 | SPRUCE paper: Changing peatland vegetation composition responses to warming and elevated $CO_2$ | Weston |
| TH1.2 | 2027 | SPRUCE paper: Seven years of *Sphagnum* symbiont changes and consequences on host acclimation and $N_2$-fixation and $CH_4$-oxidation | Weston |
| TH1.4 | 2027 | SPRUCE paper: Improved *Sphagnum* and dynamic peat submodels | Shi, Ricciuto |
| TH1.4 | 2027 | SPRUCE paper: Improved schemes for phenology and plant growth C allocation | Mao, Wang, Walker |

| | | | |
|---|---|---|---|
| TH1.2 | 2028 | SPRUCE paper: Warming and $eCO_2$ effects on NEE of C and greenhouse gas emissions | Griffiths, Mayes |
| TH1.2 | 2028 | SPRUCE paper: Warming and $eCO_2$ effects on system hydrology | Sebestyen |

## 3.2 Theme 2: Ecosystem Water, Energy, and C Processes under Compounding Climatic Stressors

*How do water availability and water cycle extremes interact with climate change to regulate net ecosystem exchange and energy balance within temperate and boreal forests?*

Continuous availability of water is essential for ecosystems to function; yet sporadicity and unpredictability are the nature of precipitation and climate patterns that affect atmospheric demand for water. Water demand and supply are constantly out of balance for ecosystems ranging from the water limited at one end to the energy limited at another (Gu et al. 2016a, Denissen et al. 2022). This imbalance may become increasingly acute as the climate warms and some regions experience a progressively drier atmosphere, and precipitation regimes become dominated by more intense but less frequent precipitation events with increased drought or flood risk (Giorgi et al. 2014, Lee et al. 2021). State-of-the-art land surface models still cannot accurately predict the widespread ecological effects of persistent hydrologic imbalances (Liang et al. 2019) due to deficiencies in representing fundamental ecosystem energy, C, and water processes (Gu et al. 2016b; see also Theme 4).

Model deficiencies are rooted in incomplete understanding of major ecosystem processes. Energy is a major driver of ecosystem dynamics; yet we are not confident in our understanding of land surface energy components. A clear indication is that we cannot close the energy budget, and we don't know why (Wilson et al. 2002, Eshonkulov et al. 2019, Mauder et al. 2020). With respect to C processes, there is a lack of mechanistic, unbiased approaches to partitioning measurable net fluxes into unmeasurable component contributions — each of which is governed by different mechanisms and responds differently to environmental forcings. As a result, interpretations of current flux partitioning products may provide "right answers" but for wrong reasons (Wohlfahrt and Gu 2015). For water processes, we currently have inadequate quantitative understanding of regulations and controls of water flow along the SPAC, leading to treatment of plant and ecosystem water relations as a black box subject to empirical or modeled correlative input-output analyses. Ecosystem model performance cannot be improved unless we make concrete progress in understanding these fundamental processes.

Research at MOFLUX and SPRUCE together with our capabilities in modeling (e.g., ELM), global trait data gathering (e.g., FRED and LeafWeb), and focused observations (e.g., SIF, neutron imaging) offer an opportunity to advance our predictive understanding of fundamental ecosystem water, C, and energy processes under compounding climatic stressors. Here we research sensitive temperate and boreal forests from diurnal to decadal time scales. Key research activities under Theme 2 will be centered around assessing the following three interrelated hypotheses which are crucial to understanding and predicting land-atmosphere interactions in a changing climate.

1. **Resolving Energy Balance Processes.** This task has the ambitious goal of seeking a definitive answer to the recalcitrant problem of land surface energy closure by testing *the Missing Energy Hypothesis*: *At the time scales of seconds to hours, the transient (i.e., "missing" to observations and modeling) energy storages in photophysical, photochemical, and biochemical reactions of photosynthesis are sufficiently large such that observed net radiation cannot be balanced by latent and sensible heat fluxes and energy storages, and that land surface models cannot accurately predict surface temperature when only observable energy terms are accounted for.*
2. **Quantifying C Process Responses to Environmental Extremes**. The goal of this task is to develop mechanistic net flux partitioning approaches and apply them to test the general *Carbon Process Hypothesis*: *Ecosystem component fluxes (e.g., GPP, aboveground respiration, belowground respiration), modulated by plant traits and soil biogeochemical characteristics, differ in responsiveness and time constants in responses to prevailing temperature dynamics and the timing, magnitude, and frequency of precipitation events, leading to overestimation or underestimation of ecosystem responses to environmental extremes.*
3. **Quantifying Water Limitation Processes**. The general *Water Limitation Hypothesis to test under this task is that soil moisture availability, atmospheric water VPD, and physical and*

> *physiological constraints along the SPAC interact to shape plant and ecosystem water stress responses.* We will clarify how soil moisture and VPD collectively set the stage for the regulations of plant and ecosystem water use by stomatal conductance, plant hydraulics and soil–root connectivity, how their roles vary with antecedent and prevailing environmental conditions, including extreme weather events, and how C uptake and release dynamics are linked to constraints within the SPAC hydraulic pathway.

All knowledge generated from the mechanistic investigations outlined above will contribute to improved land surface models (Theme 5). Models are the only tool we can rely on to extend research findings from single sites like SPRUCE and MOFLUX to simulate future impacts on broader regions. Findings from testing the *Missing Energy Hypothesis* will improve land surface energy balance and C cycle modeling. Advances resulting from our detailed investigations of *Carbon Process Responses under Environmental Extremes* and *Water Limitation Processes* will lead to better constraints of C fluxes predicted by land surface models and provide data to improve water cycle modeling.

### 3.2.1 MOFLUX Operations and Support to DOE Programs and MA (Task TH2.1)

Key Personnel: Gu, Wood

MOFLUX, located at the University of Missouri's Baskett Forest in the Ozark Border Region of central Missouri, is situated within the geographically and ecologically distinct prairie-forest biome / precipitation transition in the central United States at the western edge of the vast temperate deciduous oak-hickory (*Quercus-Carya*) forest. MOFLUX is part of AmeriFlux and has been in continuous operation since 2004. Measurements at MOFLUX include integrated SIF-EC and meteorological observations, profiles of $CO_2$, water vapor, and temperature, leaf-level measurement of PAM fluorescence, gas exchange and predawn leaf water potential (Pallardy et al. 2018), ground-level measurements of auto- and heterotrophic respiration) and soil and litter decomposition experiments (see also Theme 4). Additional equipment will be deployed to MOFLUX as SPRUCE concludes in 2025 (see *Water Limitations Processes*). Finally, forest inventory, mortality, regeneration, and litterfall are routinely monitored along five transects spanning site hydrology. All measurements and instrument maintenance will continue over the next 5 years.

In addition to new and continuing process-level work at MOFLUX, new synergistic measurements are planned at MA to address key processes and above-belowground linkages across diverse species. MA's climate falls roughly halfway between SPRUCE and MOFLUX with both cold, prolonged winters and hot summers with periodic drought. MA has comprehensive automated and manual measurements of atmospheric and edaphic conditions, and focused measurements related to Themes 2 and 3. Data streams from SPRUCE, MOFLUX, focused process-level work at MA (TH2.3, TH3.2) and at ORNL's Spallation Neutron Source imaging beamlines (TH2.4), as well as the FRED and LeafWeb trait databases establish a solid foundation for testing hypotheses of Theme 2.

### 3.2.2 Resolving Energy Balance Processes (Task TH2.2)

Key Personnel: Gu, Kramer, Wood, B. Wang

Across flux sites around the world, the linear regression of the sum of sensible and latent heat fluxes ($H + L$) against the difference between net radiation and soil heat flux ($R_n - G$) has a slope statistically significantly less than 1, often less than 0.8 while the intercept can be either positive or negative (but more likely positive than negative). Also, the residual $R_n - G - H - L$ has a clear diurnal pattern with positive values during day and near zero (either positive or negative) during night (Wilson et al. 2002, Eshonkulov et al. 2019, Mauder et al. 2020). These patterns indicate some energy is "missing", at least at high-light conditions. MOFLUX data were the first used to systematically evaluate the dynamics of biomass heat and chemical bond energy storages (Gu et al. 2007). Nevertheless, such extra energy terms are not large enough to make up for the missing energy.

Energy balance research is high-risk because transient energy storage in photophysical, photochemical, and biochemical reactions of photosynthesis at multiple time and spatial scales has never been studied. It is high-payoff because energy drives all land surface processes and must be conserved. EC flux sites around the world cannot close their energy budget (i.e., the *Missing Energy Hypothesis*). If the problem is due to measurement bias, this would cast a dark cloud on the reliability of flux data critical to test land surface models; if failures are the result of inadequate energy-process understanding, one may question the fidelity of the state-of-the-art modeling. In a presentation to the flux community in March 2021, L. Gu first proposed the missing energy hypothesis and showed first-order calculations that suggest proton motive force (PMF, the electric and proton concentration gradients established across the thylakoid membrane due to photosynthetic electron transport) may have the right magnitude to be the missing energy (https://www.youtube.com/watch?v=hlhClCFpooo). If PMF is the confirmed missing energy, land surface models must be changed to represent the short-term dynamics of PMF to model land surface processes reliably. Although the *Missing Energy Hypothesis* is centered around energy, testing it requires an integrated C–water–energy modeling approach at both leaf and canopy levels because of the close coupling of these processes. Mid-cycle evaluation of our findings will determine our eventual research direction. We will either continue testing the *Missing Energy Hypothesis* at the canopy scale or switch to an alternative hypothesis focused on species energy-use strategies.

*Develop a PMF energy storage module* (FY 2024–FY 2025) – We will expand previously published simulations of the chloroplast PMF done at the Kramer Lab of Michigan State University (Cruz et al. 2001, Takizawa et al. 2007, Zaks et al. 2012, Davis et al. 2016, 2017) to estimate the total energy storage. These will be compared to spectroscopic measurements mimicking field conditions. These simulations will be used to guide the formulation of simplified representations of chloroplast bioenergetics to model PMF and the loss of free energy into heat along the ETC or around PSI reaction centers (Nelson and Cox 2017). Our goal is to develop a realistic PMF model that uses outputs of the CPPB model (see below). A proposed strategy is to predict PMF as a function of ATP production rate which in turn can be predicted from the CPPB model. The temporal change in the predicted PMF will be used as a component of the overall leaf energy budget equation.

*Coupled Photophysical, Photochemical, and Biochemical (CPPB) model of photosynthesis* (FY 2024–FY 2025) – During the previous funding period, we have successfully developed a model of photochemistry (Gu et al. 2023, detailed in **Appendix D**). This new photochemical model will be coupled with the photophysical model developed by Gu et al. (2019b) and the FvCB biochemical model (Farquhar et al. 1980) for complete modeling of photosynthesis. To complete the CPPB model, there are still two photosynthetic processes that remain to be represented (1) state transition, which refers to the movement of mobile light harvesting complex II between PSII and PSI in response to environmental changes, and (2) cyclic electron transport. The CPPB model will be tested against gas exchange and PAM fluorometry data collected by LeafWeb.

*Couple the PMF module with the CPPB model and a stomatal conductance ($g_s$) model* (FY 2026) – We will consider two candidate $g_s$ models. The first is the Medlyn $g_s$ model, which is an extension of the Ball-Berry model but incorporates ideas from the stomatal optimization theory (Medlyn et al. 2011). The second candidate is the Kromdijk $g_s$ model based on the redox state of plastoquinone (PQ; Kromdijk et al. 2019). The photochemical model of Gu et al. (2023) predicts the redox state of PQ, which can be used as an input to the Kromdijk model. The models will be assessed for their computational burden, which will be important for scaling our efforts to canopy scales and beyond.

*Parameterize and validate the PMF-CPPB-$g_s$ model with LeafWeb data* (FY 2026) – LeafWeb has collected a substantial amount of joint PAM fluorometry and gas exchange measurements from a large number of C3 and C4 species around the world during the past funding cycle (Section 2; Han et al. 2022d). These data allow parameterization and testing of the components of photophysics, photochemistry, biochemistry, and $g_s$ of the PMF-CPPB-$g_s$ model. We will parametrize the PMF module with typical parameter values found in the literature (e.g., Li et al. 2021; Nelson and Cox, 2017). We will use half of the LeafWeb joint PAM fluorometry and gas exchange data (hundreds of data sets from 30 species) to parameterize the PMF-CPPB-$g_s$ model and half of the data to test the model.

*Analyze leaf energy balance based on simulation with the PMF-CPPB-$g_s$ model* (decision point, FY 2026) – Once we have tested the PMF-CPPB-$g_s$ model, we will use it to simulate the partitioning of light energy absorbed by chlorophylls into different dissipation pathways (photochemical, non-photochemical, and SIF) and the partitioning of photochemical energy into the storage in PMF, the loss of free energy into heat, and the storage in chemical bonds of photosynthetic products. We will simulate a sunlit leaf at the very top of the MOFLUX forest and use the actual diurnal course of environmental variables measured by the flux tower to drive the PMF-CPPB-$g_s$ model. The simulation will be used to determine whether the transient dynamics of energy storage in PMF can play a significant role in affecting leaf energy balance and temperature. If the answer is no, we will consider an alternative energy use hypothesis.

*Scale up the PMF-CPPB model to the canopy level* (FY 2026–FY 2027) – If successful at the leaf level, we plan to scale up the PMF-CPPB model to the canopy level, which will require input of key photophysical, photochemical, and biochemical parameters and how they change within the canopy. We will leverage the LeafWeb database to estimate the vertical distributions of these photophysical and photochemical parameters based on their relationships with biochemical parameters.

*Implement and test the PMF-CPPB model in ELM* (FY 2027) – The implementation of the PMF-CPPB model in ELM will require changing the current code structure of ELM with respect to the calculations of photosynthesis, energy balance, and leaf temperature. New numerical algorithms will be developed to enable the modeling of PMF, photophysics, and photochemistry within the structure of stand-alone ELM for MOFLUX (Sun, Gu, and Dickinson 2012). We will test PMF-CPPB-ELM against measurements of $CO_2$, latent, and sensible heat fluxes at MOFLUX. If necessary, model parameters will be tuned so that the predicted and measured fluxes agree with each other.

*Analyze land surface energy balance based on simulation with PMF-CPPB-ELM and measurements at MOFLUX* (FY 2028) – We will use the PMF-CPPB-ELM to simulate the canopy-scale partitioning of light energy absorbed by chlorophylls into different dissipation pathways (photochemical, non-photochemical, and SIF) and the partitioning of photochemical energy into the storage in PMF, the loss of free energy into heat, and the storage in chemical bonds of photosynthetic products. A parallel analysis with corresponding MOFLUX flux measurements will also be conducted. The difference in the slope and intercept of the energy-balance equation between the PMF-CPPB-ELM and MOFLUX flux measurements will be analyzed to determine whether the transient energy storage in PMF can adequately explain the observed land surface energy imbalance or whether other processes (e.g., energy loss by horizontal advective fluxes not captured by the eddy covariance system) may also play a role under certain circumstances.

*Develop recommendations on how to analyze measurements at AmeriFlux and Fluxnet sites to test the Missing Energy Hypothesis* (FY 2028) – Given the constraints in resources and time, we don't expect to run the PMF-CPPB-ELM at other flux sites. However, based on the insights generated from MOFLUX, we will develop guidelines on the procedures and methods that can be adopted by other sites to analyze or reanalyze their flux measurements, aiming at confirming or falsifying the *Missing Energy Hypothesis*. We will report the guidelines to AmeriFlux and FLUXNET.

*The alternative Energy Use Hypothesis*. If the Missing Energy Hypothesis is rejected early at the leaf level, we will shift our research focus from PMF-centric to plant energy use strategies by testing the following hypothesis: The partitioning of light energy harvested by antenna complexes of photosystems among photochemical quenching, non-photochemical quenching, unregulated heat dissipation, and SIF emission depends on the developmental stage of water stress to plants, varies across species along the isohydric to anisohydric spectrum, and controls ecosystem GPP, and correlates with the magnitude of the observed land surface energy imbalance. A modeling framework similar to the testing of the Missing Energy Hypothesis will be developed and used.

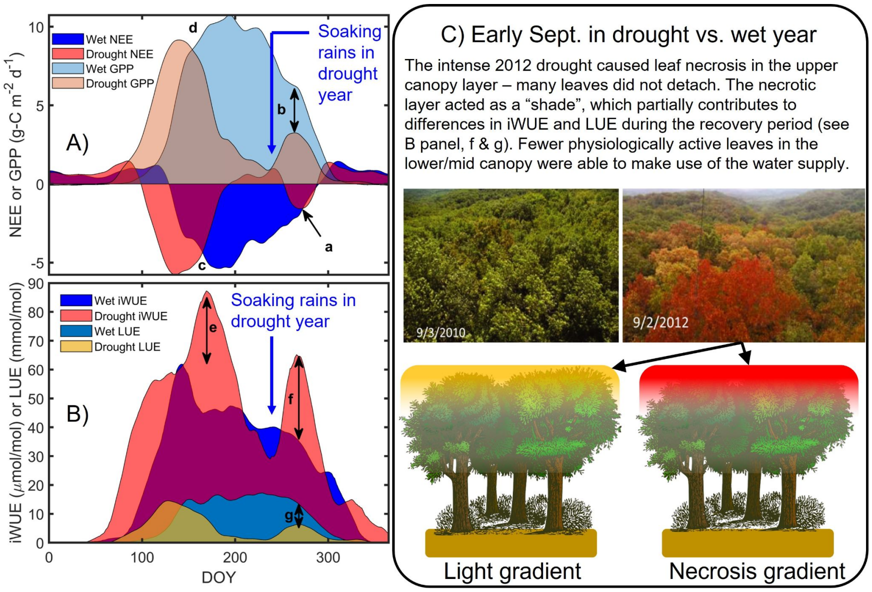
### 3.2.3 Quantifying C Process Responses to Environmental Extremes (Task TH2.3)

Key Personnel: Wood, Warren, Mayes, Gu

This task aims at mechanistic resolution in our understanding of individual C processes from point to ecosystem scale based on joint constraints of data and theory. Its execution will build upon measurements and the innovative net flux partitioning approaches that we have already developed (Kira et al. 2021; Liu et al. 2022), which will be refined further with our new theoretical advances in SIF and the photophysics, photochemistry, and biochemistry of photosynthesis (Gu et al. 2019a; Gu et al. 2022, 2023; Sun et al. 2023a and b).

Drought is a primary factor limiting global vegetation productivity (Gampe et al. 2021; Y. Liu et al. 2021; Madani et al. 2020; Stocker et al. 2019; Z. Zhang et al. in review). Drought, as a reduction in precipitation or an increase in atmospheric water demand (see Water Processes section below), is projected to increase in frequency and intensity during the twenty-first century (Novick et al. 2016; Zhao and Dai 2022) and the combination of drought and heat will amplify forest stress (McDowell et al. 2018; Hammond et al. 2022; Hartmann et al. 2022). Thus, unraveling the impacts of environmental extremes on ecosystem C cycling is urgently needed to benchmark and improve models of global environmental change.

Drought (soil and/or atmospheric), heat stress, and their combination elicit multiple physiological and structural responses that collectively modulate ecosystem NEE. In general, stomatal and non-stomatal responses to drought down regulate photosynthesis (e.g., **Fig. 3.1**), with downstream effects cascading through the ecosystem as the source of photosynthates is increasingly compromised. While long-term increases in growth temperature can lead to morphological, anatomical, or biochemical acclimation over time (e.g., increasing the thermal optima of photosynthesis, Theme 1), plant responses to short-term acute heat stress are more abrupt and can reach a mortality threshold quickly. Thus, new knowledge of ecosystem responses to changes in temperature over long (Theme 1) and short (e.g., heat waves; Themes 1 and 2) time scales is needed.



The intense 2012 drought caused leaf necrosis in the upper canopy layer – many leaves did not detach. The necrotic layer acted as a "shade", which partially contributes to differences in iWUE and LUE during the recovery period (see B panel, f & g). Fewer physiologically active leaves in the lower/mid canopy were able to make use of the water supply.

**Fig. 3.1. Smoothed seasonal cycles for an intense drought year (2012) and a wet year (2008) at MOFLUX for (A) NEE and GPP, and (B) mid-day ecosystem light use efficiency (LUE) and intrinsic water use efficiency (iWUE). (C) The intense drought caused leaf necrosis in the upper layer, which had important implications on ecosystem function after re-wetting. In the drought year, (panel A, 'a') NEE recovered to values similar to the wet year after re-wetting but there was limited recovery of (b) GPP and (c) maximal net $CO_2$ uptake was higher despite (d) lower peak gross $CO_2$ uptake; (panel B, 'e') before ecosystem wilting, there was amplified iWUE when VPD was very high; (f) during recovery iWUE greatly exceeded values in the wet year, while (g) LUE remained well below wet reference conditions. GPP was taken as the difference between measured soil respiration and NEE.**

In addition to assessing impacts of drought development on C processes, there is a paired need to assess their resilience and recovery following drought. Recovery involves rehydration and reactivation of multiple metabolic pathways and functions. In the absence of catastrophic hydraulic failure (see Water Limitation section, below), rehydration can occur within hours or days (Gu et al. 2016a), with photosynthesis and other processes lagging behind (Galle et al. 2007; Miyashita et al. 2005; Wood et al. 2023). At MOFLUX, we observed differential recovery in NEE, GPP, intrinsic water use efficiency (iWUE), and light use efficiency (LUE) following drought-ending rains in 2012 (Wood et al. 2023) (Fig

3.1). The degree to which recovery occurs depends on not only the magnitude of re-wetting, but also the intensity and duration of antecedent water stress, degree of concurrent heat stress, and whether there was permanent damage to tissues or organs—in some situations, there is a legacy that lasts for several years (Warren et al. 2011; Kannenberg et al. 2019, 2020; Yu et al. 2022).

We seek to enhance the predictive understanding of drought and heat stress response and recovery on above- and belowground forest function, and net and component C exchange from daily to decadal time scales. We will leverage coordinated measurements of C, water, and energy processes across spatial scales, ranging from point scales to integrated tower-based measurements that include both long-term data records (MOFLUX) and new data streams (MA). Belowground, autotrophic ($R_A$) and heterotrophic ($R_H$) respiration exhibit differential responses to drought stress and depend on microbial populations, root production and exudates, and root traits (Atkin et al. 2000; J. Zhang et al. 2021). Limited studies have separated root and soil respiration rates by individual species (e.g., Hanson et al. 2000, Reich et al. 2008; Roumet et al. 2016), yet these data are needed to include species or PFT-dependent root processes in models (Warren et al. 2015; McCormack et al. 2017). Databases such as FRED (Iversen et al. 2021) provide important resources for modelers, but root physiology data are sorely underrepresented. The overall Carbon Process Hypothesis will be tested by evaluating the following two more specific sub-hypotheses:

- *Carbon Flux – Ecosystem photosynthesis is more responsive to rewetting and better able to recover from drought and heat stress compared to aboveground and belowground respiratory fluxes, all of which have differential environmental sensitivities.*
- *Drought Legacy – Drought intensity, duration, and timing regulate shifts in C allocation and growth dynamics such that GPP, leaf production, and radial stem growth are reduced following drought, with increased allocation to root growth.*

*Evaluation of the C Flux Sub-Hypothesis* – Here we focus on the forest C flux responses and recovery from drought and heat stress at diel to seasonal time scales. Analyses will be conducted to exploit the high-temporal resolution of automated data streams at MOFLUX and detailed belowground respiration components at MA. Furthermore, at MOFLUX, we will extend our innovative 3-way partitioning that separates NEE into GPP, as well as above- ($R_{\text{above}}$) and belowground ($R_{\text{below}}$) respiration (X. Liu et al. 2022) to further partition $R_{\text{below}}$ (i.e., soil respiration) into autotrophic ($R_{\text{below,A}}$) and heterotrophic ($R_{\text{below,H}}$). In the present funding cycle, we will explore a more mechanistic SIF model, derived from fundamental photophysical, photochemical, and biochemical principles of photosynthesis (Sun et al. 2023a), for SIF-based NEE partitioning. Specifically, the evaluation of the *Carbon Flux Sub-Hypothesis* will take the following steps:

(1) We will first analyze data collected at MOFLUX since 2017 and for which we have direct constraints on $R_{\text{below,A}}$ and $R_{\text{below,H}}$. This will involve a combination of ML (Yu et al. 2022, Yuan et al. 2022) and wavelet (Grinsted et al. 2004) techniques to identify and quantify environmental responses of the different C fluxes. In assessing GPP dynamics, we aim to assess whether stress-induced decreases in fluxes are caused by physiological or structural factors (Yu et al. 2022) and to study resource use efficiency dynamics in greater detail. This will be achieved by developing different ML models trained using different data features to evaluate differences in model outputs (Stocker et al. 2018; Yu et al. 2022). One of the reasons for conducting these analyses first is to construct models that can be used to predict $R_{\text{below,A}}$ and $R_{\text{below,H}}$ for our complete data record to apply in conjunction with the 3-way partitioning. In this way we can constrain these four C fluxes for the entire data record and for subsequent analyses under the *Carbon Flux Sub-Hypothesis* as well as under the *Drought Legacy Sub-Hypothesis*.

(2) To assess time constants of flux responses to drought and rewetting, we will analyze the results of 4-way partitioning (GPP, $R_{\text{above}}$, $R_{\text{below,A}}$ and $R_{\text{below,H}}$) extended to the entire data record in Step 1. We will investigate the temporal dynamics of daily C fluxes in response to rainfall. Here, we will use predawn leaf water potential as an indicator of ecosystem water status and to stratify data according to stress-level and rainfall event magnitude. We will then model the temporal responses to rainfall by testing different functions because we anticipate responses to differ in terms of the magnitude of the effect, and direction. For instance, the direction of the response of GPP or belowground fluxes will depend on antecedent water stress, with rainfall-induced increases and decreases in soil $CO_2$ efflux when the forest is suffering from drought stress and when it is well-watered, respectively (X. Liu et al. 2020). For GPP, we also expect

differential responses depending on antecedent water stress, with the strongest and fastest responses under intermediate levels of water stress.

(3) At MA, we will continue our focus on separating belowground root, mycorrhizal, and soil heterotrophic respiration ($R_A$, $R_M$, $R_H$) to provide species-specific respiration data on a diverse set of deciduous / evergreen and arbuscular / ectomycorrhizal species. To better link those respiration dynamics to prevailing atmospheric and edaphic conditions, we plan to install new soil water potential sensors to create soil water retention curves in six of the intensively measured tree stands. Similar to the partitioning work at MOFLUX, we will assess time constants of component flux responses to drying and rewetting to assess sensitivity of component resilience. Data will be used to develop predictive relationships to quantify the responses of these three components of belowground respiration to drought or heat stress, which will be complementary to other ongoing nutrient–C feedback research at MA (Theme 3).

*Evaluation of the Drought Legacy Sub-Hypothesis* – To assess impacts of drought legacies we will leverage novel data sets at MOFLUX, particularly the longest running predawn leaf water potential data set in the world (at weekly to biweekly time steps). We will build upon an approach similar to Yu et al. (2022) who developed ML models to assess drought legacies on GPP derived from EC and radial growth. This approach has several advantages: (1) characterization of seasonal variations in legacy effects, (2) separation of the effects of meteorology and drought legacy during the recovery period, and (3) estimation of model uncertainties to enable more robust interpretation of legacy effects. We aim to extend the Yu et al. approach beyond GPP and radial growth. We will consider all component fluxes obtained by completing the *Carbon Flux Sub-Hypothesis*, and additional measurements such as foliar and reproductive productivity. We also plan to expand bottom-up, process-based measurements of hydraulic limitations through the plants (see 3.2.4). Together, these analyses will provide a holistic understanding of drought legacies on above- and belowground ecosystem processes.

We will leverage the longer record of growth contained in the tree-ring records and conduct a separate analysis of the whole chronology to gain insights into longer-term patterns of drought response and recovery over the past century that was characterized by a broader range of drought conditions than has been experienced in the EC record at MOFLUX. We will make use of Missouri Division 3 climate data for these analyses. Prior to conducting the analysis, we will validate the climate data against MOFLUX observations, and develop site-specific corrections as needed. We will then conduct traditional climate response analyses (Zang and Biondi 2015) as well as the newer ML algorithms described by Yu et al. (2022).

### 3.2.4 Quantifying Water Limitation Processes (Task TH2.4)

Key Personnel: Warren, Wood, Weston, Gu

This research will provide detailed mechanistic understanding of how spatial patterns of water availability, atmospheric demand, and transport throughout the SPAC control plant physiological stress. Considerable effort has been directed toward determining how these components modulate ecosystem C and water fluxes, as well as light- and water- use efficiencies at eddy flux tower sites (Grossiord et al. 2020; Lansu et al. 2020; L. Liu et al. 2020; Novick et al. 2016; Stocker et al. 2018; Q. Zhang et al. 2019). Such studies have underscored the significance of both soil water deficit and VPD in determining ecosystem drought responses—and furthermore, that VPD limitation can exceed that of soil water deficit due to hydraulic resistances through the SPAC (e.g., Fu et al. 2022). Under severe air or soil water supply limitation, ecosystem-scale wilting can occur, which elicits a breakdown in ecosystem water vapor and $CO_2$ exchanges (Wood et al. 2023). Quantification of component mechanisms underlying ecosystem response to drought remains limited due to gaps in spatial or temporal observations of soil-plant water status, lack of knowledge of the location of breakdown in the SPAC (e.g., rhizosphere, xylem), and limitations to scaling organ/tissue response up to whole ecosystems.

At SPRUCE, observations and measurements have shown elevated $CO_2$ to have only a limited hydraulic benefit to the plants. Instead, plant responses have been dominated by temperature and temperature-driven increases in hydraulic stress (Warren et al. 2021; Peters et al., under review). Some hydraulic failure has been observed with warming, despite available soil water. This indicates that plant hydraulic capacity may not be sufficient to satisfy the increased atmospheric demand for water induced by warming treatments – especially the temperature-driven increase in VPD or an increase in boundary layer conductance due to imposed turbulence. Hydraulic failure may also reflect a consequence of inadequate rooting depth (Iversen et al. 2018) or root-specific conductance limitations (Warren et al. 2021). At MOFLUX, precipitation patterns and soil water availability control integrated water stress at the species and community level impacting ecosystem C flux and evapotranspiration, and with time, tree mortality (Gu et al. 2015; Gu et al. 2016a and b; Wood et al. 2018). We propose studies to assess a) impact of WEW and $eCO_2$ on boreal tree hydraulics, b) plant and ecosystem water use efficiencies in response to precipitation and atmospheric aridity, c) influence of plant water stress on photosynthetic acclimation to temperature, d) drought impacts on the soil–root hydraulic pathway, and e) influence of plant microbial symbiont diversity on plant response to drought or temperature.

*Impact of WEW and elevated $CO_2$ on boreal tree hydraulics* – At SPRUCE, whole tree water use and relative stress in response to treatments have been measured by sap flow and leaf water potential (Warren et al. 2021). These measurements will continue through summer 2025. We plan to assess relative resistance through the SPAC pathway (roots, wood, leaves) of two tree species (*L. laricina and P. mariana*) to characterize hydraulic bottlenecks that limit water availability to foliage (Johnson et al. 2016). Data are essential for modeling efforts that partition hydraulic resistance through the SPAC (e.g., Sperry et al. 1998; Venturas et al. 2018; Carminati and Javaux 2020; Koven et al. 2020).

*Plant and ecosystem water use efficiencies in response to precipitation and atmospheric aridity* – In 2026 post-SPRUCE treatment efforts, we will develop more comprehensive plant and soil water relations assessments at MOFLUX. These will include soil water potential, tree sap flow and branch xylem water potential (stem psychrometers) and midday leaf water. These data will quantify diel and seasonal patterns of whole tree hydraulic conductance, capacitance, and sensitivity to changing abiotic conditions, and are needed to link tree- with (flux-based) ecosystem-scale NEE. Hydraulic measurements through the SPAC will provide insight into the mechanisms underlying the community-level ecosystem wilting point, and there will be a particular focus on response to compounding stressors, such as simultaneous or sequential drought and extreme heat events. MOFLUX data will be used for modeling via the FATES-HYDRO model (Koven et al. 2020; Chitra-Tarak et al. 2021). To further bolster our efforts, we will encourage and guide potential collaborator and student opportunities (e.g., LU, an HBCU) for additional targeted destructive measurements of species-specific plant hydraulics.

*Influence of plant water stress on photosynthetic acclimation to temperature* – Drought (Theme 2) and warming (Theme 1) cooccur to reduce photosynthesis more so than when applied alone (Rivero et al. 2022). Atmospheric $CO_2$ concentration further regulates stomatal conductance and together with heat and drought provides a complex multi-stressor physiological syndrome that is experienced at both SPRUCE and MOFLUX. We will shift focus and resources to MOFLUX in FY 2026–FY 2028 to intensify bottom-up ecophysiological measurements to assess how soil (and plant) water availability may interact with temperature to mediate photosynthesis. We will assess foliar photosynthetic and respiratory temperature response curves across dominant Missouri tree species, and opportunistically leverage natural heat waves and droughts to collect associated leaf level data (e.g., gas exchange/PAM fluorometry, water potentials). Data are needed to model ecophysiological impacts of compounding climate extremes (temperature and heat) in ELM.

*Drought impacts on the soil–root hydraulic pathway* – While we can measure hydraulic failure in bulk soil and in different plant organs, investigation of hydraulic failure at the rhizosphere, or soil–root interface has been limited. One of the most promising techniques to address this is neutron imaging, which can resolve soil water in situ at resolutions <50 µm. Prior work at the two ORNL neutron source facilities has yielded significant insight into rhizosphere hydration and root-trait dependent water uptake dynamics (e.g., Warren et al. 2013, Dhiman et al. 2018, Warren et al., being revised). Beginning in FY 2024, we will leverage the Spallation Neutron Source's new advanced VENUS Imaging beamline (Bilheux et al. 2015) planned for initial operation in summer 2025, with an initial focus on soil–root gap formation and its impact on water uptake under drying conditions (Ahmed et al. 2018). We will also explore the potential to use cutting-edge neutron beamlines to identify or assess exchanges of C or nutrients within the rhizosphere.

*Influence of plant microbial symbiont diversity on plant response to drought or temperature* – In addition to the direct effects of multi-stressor scenarios on plant physiology and production, we have shown that SPRUCE treatments alter the community composition of plant-associated symbionts such as cyanobacteria (Carrell et al. 2021 and 2022b). Furthermore, this change in *Sphagnum* symbionts indirectly influences $N_2$-fixation and the host plant's ability to acclimate to laboratory-imposed heat wave conditions (Carrell et al. 2022a). These results bring to question the importance of symbiont community composition on plant resilience or acclimation to abiotic stressors such as drought or heat. As part of the photosynthetic temperature response curve measurements at MOFLUX, we will test if species that maintain the greatest symbiont diversity will be more resilient to additional environmental stressors (e.g., Voolstra and Ziegler 2022). 16S and internal transcribed spacer (ITS) amplicon sequencing will be used to determine microbial symbiont diversity matrices in leaves and roots from the intensively measured trees. Although it may be difficult for plant-associated microbial diversity indices to be widely applicable to ELM parameterization, the inclusion of microbes in soil-related modeling is gaining interest (Theme 4) and this Task will determine if such efforts should be developed for plant models.

### 3.2.5 LeafWeb (Task TH2.5)

Key Personnel: Gu

LeafWeb aspires to become a comprehensive automated online tool to support cutting-edge environmental photosynthesis research and monitoring both for the global community and for the TES SFA. The next 5 years will be critical for LeafWeb to materialize this aspiration as LeafWeb expands its services from a single functionality of analyzing leaf gas exchange measurements (e.g., $A/C_i$ curves) with the FvCB biochemical model of Farquhar et al. (1980) and Sharkey (1985) to joint analyses of PAM fluorometry and gas exchange measurements with the CPPB model of photosynthesis. An important factor to consider during the LeafWeb functionality expansion is to avoid potential disruption to the research of LeafWeb users. The CPPB model of photosynthesis is the future direction as the currently widely applied FvCB model is incomplete (Farquhar et al. 2001), cannot take full advantage of available leaf photosynthesis measurements to improve C cycle modeling, and has limited applications in providing guidance for genetic improvement of photosynthesis via bioengineering and for remotely sensing photosynthesis with SIF. However, it will take time for photosynthesis researchers to accept and become familiar with the photophysical and photochemical models of Gu et al. (2019b, 2022, and 2023), and to apply these new models in their research. Thus, for the foreseeable future, a lot of LeafWeb users will likely continue to only have a dominant demand for $A/C_i$ curve analysis. For these considerations, we will make both the old and expanded LeafWeb available during the new funding cycle (FY 2024–FY 2028). New developmental activities for LeafWeb are as follows:

*Integrate and test the codes of photophysical and photochemical models of photosynthesis into the existing code structure of LeafWeb* (FY 2024–FY 2026) – We plan to leverage our successful photophysical, photochemical and biochemical models (Gu et al. 2019a, 2022, 2023; Han et al. 2022a, b, and c; Sun et al. 2023a) for application to LeafWeb analyses. We have already started the integration and testing of the codes for these new models in the background processing code structure of LeafWeb in offline modes. The integration and testing will continue in the new funding cycle. This is a massive effort, given the number of new photosynthetic processes involved and the amount of coding required. We will take a step-by-step approach. All new codes will be thoroughly tested for stability, consistency, cost function and parameter convergence, and processing time in the LeafWeb environment with three combinations of data type: actual PAM fluorometry data alone, gas exchange data alone, and joint PAM fluorometry and gas exchange measurements. We will use data files from different LeafWeb users in different countries to test the capability of the new LeafWeb in processing highly diverse data sets.

*Implement and test the state-of-the-art C4 photosynthesis model in LeafWeb* (FY 2026–FY 2027) – The C3 and C4 photosynthesis share the same photophysics and photochemistry but differ in biochemistry. We will continue the ongoing effort of replacing the simple empirical C4 model of Collatz et al. (1992) with the more realistic biochemical model of Yin and Struik (2021) and von Caemmerer (2021). The new C4 biochemical model and its coupling with the photophysical and photochemical models of Gu et al. (2019a, 2022, 2023) will be tested in the code structure of LeafWeb with C4 photosynthesis data that are collected by LeafWeb.

<u>*Increase flexibility in data submission for LeafWeb automated analyses*</u> (FY 2024) – We will onboard a smart data reading program to minimize the preparation time of input data by LeafWeb users. The smart reading program will eliminate the need to follow strict data formats, facilitating the conversion of the output data from instrument (e.g., Licor, Walz) formats to input files readable by LeafWeb.

<u>*Launch the new LeafWeb*</u> (FY 2028) – Once we have completed the development and test of the new LeafWeb, we will invite seasoned photosynthesis researchers from different countries to test it and ask them to give feedbacks which will be used to further improve LeafWeb. After this period of test run, we will formally launch the new LeafWeb to the global photosynthesis research community.

<u>*Train users for new LeafWeb*</u> (FY 2028) – We will provide detailed guidance on how to prepare data for new LeafWeb analyses and on how to interpret LeafWeb outputs. Easy-to-use, spreadsheet- based tools will be developed for users to freely download from LeafWeb and explore components of the coupled model of photophysics, photochemistry, and biochemistry of photosynthesis. The graphic functions of LeafWeb will be enhanced so that users can graph variables of their choice.

<u>*Full LeafWeb data release and syntheses*</u> (FY 2026–FY 2028) – LeafWeb collects hundreds to thousands of data files per year online. Often data files are also sent directly to TES SFA LeafWeb researchers for offline analyses. Due to limited funding support, only a small fraction of the collected data files has been quality-checked and publicly released on an irregular basis (https://www.leafweb.org/information/data-publications/). We will hire a postdoctoral photosynthesis researcher to quality-check each historical file individually for accuracy of photosynthetic data as well as any associated metadata for all data collected. The owner of each historical file will be contacted for correction, updates, and willingness to publicly release data. Variable names and data formats will be corrected to the current LeafWeb standard. All historical input data files will be re-analyzed with the current LeafWeb optimization code to ensure consistency of analysis across users and files. We will then release all input and output data collected by LeafWeb and agreed upon by all data owners. The postdoctoral scientist will represent LeafWeb in publications and meetings, train users on using LeafWeb, and develop questions and answers for LeafWeb users. The postdoc will also synthesize LeafWeb data for interspecies variations and commonalities in key photosynthetic parameters. This postdoctoral scientist will also participate in other research activities that require the use of LeafWeb data.

**Table 3.2. Deliverables for Theme 2 research. Post-SPRUCE syntheses are shown in green text.**

| Task | FY | Deliverable | Lead(s) |
|---|---|---|---|
| TH2.2 | 2024 | Publish papers on Testing the Missing Energy Hypothesis | Gu |
| TH2.3 | 2024 | MOFLUX: Publish paper on long-term radial tree growth climate responses, and correlations with NPP when data overlap | Wood |
| TH2.4 | 2024 | SPRUCE: Sap flow synthesis paper | Warren |
| TH2.4 | 2024 | Neutron-based rhizosphere hydration dynamics – Paper | Warren |
| TH2.4 | 2024 | MOFLUX: Publish ecosystem scale hydraulics paper | Wood |
| TH2.2 | 2025 | Model paper: Coupled photophysical, photochemical, and biochemical processes | Gu |
| TH2.3 | 2025 | MA: Publication of root, mycorrhizal and soil respiration dynamics across diverse species | Warren, McCormack |
| TH2.3 & 2.4 | 2025 | MOFLUX: Develop ML model frameworks for analyzing flux and biometric time series for testing C and water sub-hypotheses | Wood, Gu, Mayes |
| TH2.4 | 2025 | MOFLUX: Publish paper on soil respiration spatial variation | Mayes, Wood |
| TH2.4 | 2025 | MOFLUX: Publish paper on influence of rainfall dynamics on daily cycle climate | Wood |
| TH2.2 | 2026 | Complete leaf energy balance simulation with the PMF-CPPB-gs model; Make decision regarding continuation of the primary or alternative hypothesis | Gu |
| TH2.4 | 2026 | MOFLUX: Publish paper on species and community dehydration-rehydration dynamics | Wood, Gu |
| TH2.2 | 2027 | Implementation of the leaf model in a canopy model with (primary hypothesis) or without (alternative hypothesis) the PMF module | Gu, B. Wang |

| | | | |
|---|---|---|---|
| TH2.3 | 2027 | MOFLUX: Publish paper on C flux sub-hypothesis | Wood, Gu, Mayes |
| TH2.3 | 2027 | MOFLUX: Data analysis for testing drought legacy sub-hypothesis | Wood, Gu |
| TH2.4 | 2027 | SPRUCE: Moss water by temp by microbiome paper | Weston |
| TH2.4 | 2027 | MOFLUX: Publish paper on ecosystem water-use efficiency responses | Wood, Gu, Warren |
| TH2.5 | 2027 | **LeafWeb**: C4 code operational | Gu |
| TH2.5 | 2027 | **LeafWeb** data release:  historical and PAM efforts | Postdoc |
| TH2.2 | 2028 | Paper on land surface energy balance or energy dissipation pathways under different climate conditions | Gu, Wood |
| TH2.3 | 2028 | MOFLUX: publish paper on drought legacy sub-hypothesis | Wood, Gu |
| TH2.4 | 2028 | SPRUCE – Leaf gas exchange/physiological acclimation ELM MODEX – paper | Warren, Ricciuto |
| TH2.4 | 2028 | MOFLUX – whole plant hydraulic conductivity – Paper | Wood, Warren |
| TH2.4 | 2028 | MOFLUX water by temp by microbiome paper | Weston |
| TH2.5 | 2028 | **LeafWeb** paper: Synthesis of assembled data | Postdoc |

### 3.3 Theme 3: Nutrient C Feedbacks

*How does environmental change alter nutrient distribution and dynamics, and what are the implications for understanding and predicting ecosystem C fluxes?*

A key theme for the evaluation of ecosystem responses to future environmental change is the interactive role nutrients play in determining both ecosystem function and plant and microbial community functional composition. Nutrient limitation can determine the response of the ecosystem C balance to climate drivers (Reich et al. 2006, Fernández-Martínez et al. 2014, Wieder et al. 2015, Zhou et al. 2022), nutrient losses can shape the new equilibrium of an ecosystem recovering from disturbance (Rastetter et al. 2020), and nutrient acquisition by plants and microbes can alter long-term ecosystem stoichiometry and storage of C (LeBauer and Treseder 2008, Averill et al. 2019).

Despite the critical role nutrients play in shaping ecosystem function and composition, the level of mechanistic detail with which ESMs represent nutrient cycles varies widely, causing large differences in model responses to simulated perturbations (Davies-Barnard et al. 2020). In CMIP6, there was a smaller C-climate feedback in ESMs that were nutrient-enabled vs. C-only models at $-30 \pm 22$ Pg C °C$^{-1}$ and $-64 \pm 71$ Pg C °C$^{-1}$ respectively (Arora et al. 2020). Some model studies suggest a substantial indirect fertilization effect on C uptake (Thornton et al. 2007, 2009, Sokolov et al. 2008), while others suggest that changes in vegetation C:N offset the indirect fertilization effect and lead to lower C gain (Zaehle et al. 2010). These modeling studies highlight the importance of nutrient-C interactions in making projections of terrestrial ecosystem C balance in a warmer world, as well as the high uncertainty surrounding them.

Recent syntheses and model comparisons have identified three knowledge gaps that present significant obstacles to improving the mechanistic representation of nutrient-C feedbacks in ESMs. These include (1) the need for more empirical ecosystem nutrient budgets that include inputs, losses, and nutrient-use efficiency (NUE; Davies-Barnard et al. 2020), (2) quantification of changing plant C allocation in response to nutrient availability (Thomas et al. 2015;, Wieder et al. 2015, Terrer et al. 2018), and (3) decomposition frameworks that explicitly consider microbial demand for C vs. nutrients (Soong et al. 2020). We will leverage the unique research capacity at SPRUCE to test the effects of warming-induced increases in nutrient availability in a C-rich, nutrient-limited northern ecosystem under a range of warming and elevated $CO_2$ scenarios.

Results from the first 6 years of the experimental treatments at SPRUCE indicate that though some metrics of nutrient availability have increased with warming, plant C stocks have not been stimulated, indicating that indirect nutrient fertilization did not offset increased C losses via decomposition (Hanson et al. 2020, Iversen et al. 2023, Section 2.1.3). These results suggests that some ESM assumptions could be overestimating the impact of indirect nutrient fertilization in peatlands. Nitrogen and P released from *Sphagnum*-derived litter, altered plant litter inputs, and altered decomposition could be taken up by roots, immobilized by microbes, protected by physiochemical soil properties, or lost from plant-accessible peat horizons by moving deeper into the profile or through lateral outflow. Therefore, assessing the spatial and temporal availability of these nutrients will be crucial for understanding the peatland ecosystem response to changing N and P dynamics. The role phenology and fungal partnerships play in shaping the resource acquisition strategies can be addressed with comprehensive vegetation nutrient budgets and destructive belowground harvests at SPRUCE as well as by expanding existing root-, leaf-, and stem phenological measurements at MA (Theme 1; also Theme 2 – belowground respiration) to include measurements of resin-available nutrients in these mono-specific plots.

Investigating the environmental change impacts on nutrient distribution and dynamics across a broad range of ecosystems requires a diverse set of study sites and tools. Expanding nutrient observations and modeling at MOFLUX will add another dimension to our understanding and model predictive capacity, as the site has strongly coupled C and water dynamics at the opposite end of a water gradient from the saturated S1 Bog. Extreme dry events reduce plant and microbial N immobilization and interrupt plant N conservation processes which can lead to a buildup of inorganic soil N that is susceptible to leaching in subsequent rain events (Leitner et al. 2020). Oscillation between extreme wet and dry events can also increase C, N and P losses via erosion (Berhe et al. 2018). The diverse array of field sites at SPRUCE, MA, and MOFLUX, along with tools like FRED that encompass plant nutrient acquisition traits from around the world (Iversen et al. 2017) will allow us to place our findings into the important global context that ESMs require. Under Theme 3, we will address the following hypotheses:

1. *Warming-induced changes to the vegetation and peat stocks will accelerate ecosystem nutrient cycling by altering the magnitude, timing, and location of nutrient pools and fluxes, but these nutrients may not be immediately accessible to plants to support increased productivity in part because of increased nutrient immobilization in plants and microbes under e*$CO_2$.
2. *The response of plants with different nutrient acquisition strategies to climate drivers is shaped by shifting relationships between belowground phenology timing, fungal partners, and nutrient availability.*
3. *Intensifying hydroclimatic variability in drought-prone sites like MOFLUX will increase ecosystem nutrient demand, contributing to declines in forest productivity. The nature of this ecosystem response will depend on how the magnitude, frequency, and timing of wet vs. dry events affects the balance of plant, microbial, and abiotic nutrient cycling processes.*

Work to address these three hypotheses is divided into three research tasks that will utilize field sites at SPRUCE, and MOFLUX, and MA, laboratory soil incubations, modeling tools (ELM-SPRUCE, ELM-TAM, and MAAT), and curation and expansion of a global root-trait database (FRED).

### 3.3.1 Nutrient Dynamics of Organic Matter Decomposition (Task TH3.1)

Key Personnel: Salmon, Yang, Griffiths, Kolka, Sebestyen

The SPRUCE experiment presents an opportunity to address Hypothesis 1 due to the observed decline of *Sphagnum* moss and peat elevation that have been associated with increased inorganic N and P availability in soils (Norby et al. 2019, Hanson et al. 2020, Iversen et al. 2023, Petro et al. in press) but not in porewater or lateral outflow from the plots. Prior to SPRUCE treatment initiation, *Sphagnum* biomass represented roughly half of plant biomass N and P pools (Salmon et al. 2021) so the near-total loss of this PFT in the warmest plots represents a significant input to the decomposing near-surface acrotelm. The loss of peat elevation and accelerated decomposition in the acrotelm and catotelm (Hanson et al. 2020, Wilson et al. 2021, Ofiti et al. 2022) associated with SPRUCE warming treatments also indicate that turnover of C, N, and P has shifted. The total impact of SPRUCE treatments on peat N and P decomposition will be characterized empirically and modeled with ELM-SPRUCE while high temporal and spatial resolution measurements of N and P in porewater, and lateral outflow at the site will capture the ecosystem-scale impacts of shifting nutrient interactions at SPRUCE (Task TH1.2).

*SPRUCE peat N and P processes (Salmon)* – Empirical measurements include a long-term soil incubation of acrotelm peat to characterize 6 years of experimental treatments at SPRUCE on N and P pool sizes and turnover rates. This experiment utilizes warm temperatures (30°C) and moist conditions (field capacity) to accelerate mineralization of C, N, and P so that quickly and slowly cycling pools can be discerned using a two-pool kinetic model fit to cumulative losses of each element. This methodology follows the approach of Updegraff et al. (1995) and Bridgham et al. (1998) and will implement the MAAT framework for MCMC parameter fitting. Gaseous losses of $CO_2$, $CH_4$, and $N_2O$ are measured using a Picarro G2508 and dissolved losses are measured as inorganic N and P in 0.01M $CaCl_2$ leachate. Initial and final sorbed P will be measured with dilute acid fluoride extracts (Kuo, 1996). This soil incubation will generate data on potential net mineralization rates, pool sizes, and turnover rates for quick vs. slow cycling N and P within the acrotelm. Differences in these metrics between treatments will yield insight into how litter inputs as well as environmental conditions have altered N and P decomposition at SPRUCE.

We also propose measuring gross N mineralization and nitrification using $^{15}N$ isotope pool dilution (IDP) techniques in 2025 (Davidson et al. 1991, Hart et al. 1994). Isotope pool dilution will be applied to discrete depth intervals of soil homogenized from soil cores in a 24 h period following collection (Braun et al. 2018). Isotope pool dilution measurements will provide insight into in situ production rates of mineral N prior to uptake by plant roots or the immobilization/protection via microbial processes, complementing the net effect of past decomposition on mineralization dynamics from the long-term incubation experiment.

*SPRUCE Sphagnum decomposition (Griffiths, Kolka)* – In addition to peat N and P mineralization rates, the decomposition rates of two predominant *Sphagnum* species (*S. angustifolium*, *S. divinum*) are being assessed as part of a 10-year multi-species decomposition experiment (see also Theme 4). The final set of *Sphagnum* litterbags will be collected in 2025 for estimation of decomposition rate, and changes in C, N, and P content over time.

*SPRUCE nutrients in leaf litter (Salmon, Griffiths)* – The decline of *Sphagnum* with warming at SPRUCE represents a significant nutrient input to residual surface peat, but aboveground litter production is another flux that must be considered. As such, we propose to conduct annual measurements of leaf litter C, N, and P content for the dominant plant species at SPRUCE. Collections for these measurements will primarily be made post senescence in October and samples will be sorted, dried, and ground prior to analysis of %C, N, and P. Comparisons with peak season leaf chemistry and specific leaf area measurements will allow nutrient resorption to be tracked annually, yielding insight into nutrient recycling of individual plant species.

*SPRUCE depth-specific porewater and lateral outflow N and P concentrations (Griffiths, Sebestyen)* Measurement of nutrient concentrations in porewater and lateral outflow at SPRUCE will continue through 2025. Porewater samples will be collected bimonthly from 6 depth-specific piezometers (−0, −0.3, −0.5, −1, −2, and −3 m depths) per enclosure. Flow-weighted, composited water samples will be collected weekly from the lateral outflow system (as described in Theme 1). Porewater and lateral outflow samples will be analyzed for inorganic (nitrate, ammonium, phosphate) and total (N, P) nutrient concentrations. Fluxes of N and P from lateral outflow will also be calculated for inclusion in ecosystem-level N and P budget assessments.

*Improved representation of organic matter decomposition and N and P mineralization in ELM-SPRUCE (Yang)* – Measurements of C, N, P dynamics from *Sphagnum* decomposition at SPRUCE and peat incubation experiments provides valuable information for improving model representation of decomposition of dead *Sphagnum* and N and P mineralization. In the current version of ELM-SPRUCE, the specific biochemical properties of *Sphagnum* (decay inhibitive phenolic compounds) are represented with a “lignin-like” approach that assigns *Sphagnum* litter a high lignin content to ensure a long turnover time. Although this “lignin-like” approach helped improve model simulations by effectively slowing the litter decomposition rate, evaluations using $^{14}C$ soil profile still shows that ELM-SPRUCE simulated surface peat (dead *Sphagnum*) is decaying too fast. We propose to improve the representation of *Sphagnum* decomposition by explicitly considering the inhibitive effects of special biochemical compounds in our model. The better representation of *Sphagnum* decomposition is critical for accurate prediction of N and P mineralization fluxes. We will use measurements from *Sphagnum* litter decomposition bags for model parameterization and the incubation data will be used for model evaluation. Model–data discrepancies will provide directions for further model development. We will also evaluate the new approach using *Sphagnum* decomposition data at other peatland sites in Canada and Europe (Moore et al. 2007; Theme 5 Task TH5.1).

Iversen et al. (2023) showed that compared with observed resin N and P availability, the simulated magnitude of warming-induced N and P availability in ELM-SPRUCE is much lower. Resin nutrient data also show increasing warming responses with depth while ELM-SPRUCE simulations showed decreasing nutrient mineralization with depth. One possible reason for the discrepancies could be that organic matter (C, N, and P) leaching downward is not captured in ELM-SPRUCE. We propose to have dissolved organic matter transport included in ELM-SPRUCE. Porewater nutrient concentration will be critical for model parameterization and evaluation. The explicit representation of dissolved organic matter will also help provide a better estimate of C, N, and P export via lateral outflow in E3SM, and dissolved organic matter is also needed for some microbial models (Theme 4).

Nutrient resorption during leaf senescence is assumed constant in the current version of ELM-SPRUCE based on the SPRUCE pretreatment leaf and leaf litter nutrient concentration measurements. However, it could change depending on environmental conditions, soil nutrient availability, and vegetation nutrient status. We will evaluate the litter chemistry data collected in Task TH3.1 to improve the parameterization or representation of nutrient resorption for each PFT at the site.

### 3.3.2 Nutrient Acquisition by Plants (Task TH3.2)

Key Personnel: Salmon, McCormack, Iversen, Yang, B. Wang

Hypothesis 2 will be addressed using data from SPRUCE and MA sites, and integration of ELM-SPRUCE with ELM TAM (Section 2.7.1). At SPRUCE, the growth response of understory plants and canopy trees to warming treatments, $eCO_2$, and *Sphagnum* represents an opportunity to compile an empirical, climate-relevant N and P budget for parameterization and benchmarking. Such budgets will require nutrient-focused measurements during destructive harvests at the end of SPRUCE experimental manipulations. Model development around fine root processes and the vertical distribution of plant nutrient access will rely on belowground traits in FRED as well as expanded measurements at MA that add resin-available N and P to collaborator's ongoing physiological data sets and preliminary ecosystem-level N budgets forestry plots at these monospecific plots.

*SPRUCE annual observations of vegetation nutrient stoichiometry (Salmon)* – Collections of aboveground leaves and stems are currently made for all species in the SPRUCE plots as part of the $^{13}C$, $^{14}C$, and $^{15}N$ isotope analysis (Theme 1). We propose supplemental annual %C, N, and P measurements to this so that the nutrient stoichiometry of all plant species at SPRUCE is continuously monitored. Adding this analysis to the isotope samples is an efficient and productive way to utilize sample materials and ensure consistent monitoring of C, N, and P so that the ratio of these elements (stoichiometry) can be tracked and used to inform PFT-specific parameters in ELM-SPRUCE. In addition to measuring the nutrient stoichiometry of aboveground plant tissues, we will also analyze %C, N, and P of fine-root tissues from in-growth cores (Theme 1).

*SPRUCE destructive N and P observations at the end of experimental manipulations (Salmon et al.)* – The end of the SPRUCE experimental treatments in 2025 will involve destructive measurements that were not possible in previous years of the experiment, and can support important insights into belowground C and nutrient cycling in long-term experimental manipulations (e.g., Iversen et al. 2012). We will leverage this opportunity to gain insight into the N and P nutrient acquisition by plants as well as free-living and mycorrhizal microbes. Peat sampling for depth-resolved N and P stocks will be conducted and ash-corrected profiles will be compared to take into account the impact of potential subsidence or compaction (von Haden et al. 2020).

*Increasing global coverage of root trait data for model development (McCormack, Iversen)* – FRED leverages existing and emerging data sources to increase the amount of data available to parameterize and constrain model processes as well as enable novel empirical studies that identify robust relationships among root and plant traits that can inform further model improvements. We will develop and disseminate FRED with ongoing extraction and incorporation of existing data from publicly available sources, and the incorporation of data submitted directly by researchers. We will target incorporation of traits that are needed to parameterize and implement model routines associated with high parameter and model uncertainty, with a particular emphasis on fine-root traits related to the amount and timing of nutrient acquisition, including fine-root physiology (respiration (TH2.4), nutrient and water uptake-related parameters) and fine-root dynamics (e.g., lifespan and phenology).

*MA resin collections (McCormack)* – Similar to the monthly resin measurements that have historically taken place at SPRUCE, high-resolution spatial and temporal coverage of nutrient dynamics in soil at MA will be conducted to link species-specific root growth to spatial and temporal availability of nutrients under an array of mono-specific tree species that will inform PFT-specific plant-soil mechanistic understanding and model representation. The measurements will begin following SPRUCE efforts so that the analytical load is distributed across the funding period. Resins will be deployed in 10 of the most heavily instrumented MA plots in 2025. Resin access tubes will be installed at three replicate locations per plot (n=30 access locations) and each access location will have tubes at −10 and −30 cm depths to span the depth interval over which root production and phenology is measured. Monthly resin deployments will start in 2026 so that soil layers disturbed by the installation process will have time to recover. Extraction and analysis protocols will follow the SPRUCE methods followed for resin deployments from 2013-2023 (Iversen et al. 2023).

Resin collections at MA are complemented by additional data streams that characterize the spatial and temporal patterns of fine-root growth and are further integrated with data characterizing whole-tree and ecosystem-level measures of growth and activity over time (e.g., partitioned root, mycorrhizal, and heterotrophic respiration, tree sap flow, leaf canopy phenology, stem expansion phenology). Measurements of fine-root, stem, and leaf phenology are carried out in a total of 23 monospecific plots while other measurements, including resin collections, are strategically deployed to subsets of plots to maximize functional and phylogenetic diversity needed for model parameterizations of PFTs.

*Improve representation of fine-root nutrient uptake (Yang, B. Wang)* – The current version of ELMv2-SPRUCE can reproduce observed NPP for each PFT, but the model failed to capture the observed increased productivity of shrubs in response to warming at SPRUCE. Malhotra et al. (2020) hypothesized that the strong increases in fine-root length in response to warming by the ericaceous shrubs could lead to much greater nutrient acquisition and therefore increased productivity. Our modeling experiments showed that if we allow shrubs to have access to more soil volume and increase their nutrient uptake in response to warming, their productivity will be increased consistent with experimental data. To capture the observed fine-root responses, we will introduce root traits into the model and link root traits with nutrient uptake. We propose to introduce ELM-TAM, the newly developed 3-pool fine root structure, into the model to improve the representation of nutrient uptake (Wang et al. in press). Measurements of fine-root traits and responses to treatments will be used to improve model representation and parameterization. FRED root trait data, along with PFT-specific parameters from MA, will be used when SPRUCE observations are not available.

*Improved representation of fine-root vertical profiles for nutrient uptake (Yang)* – Accurate estimates of nutrient uptake also require realistic representation of fine-root profiles in the model. The original fine-root profile for nutrient uptake in ELM-SPRUCE is based on Jackson et al. (1996). Iversen et al. (2018) showed that fine-root growth at SPRUCE sites is shallowly distributed in nutrient-limited surface peat layers above the average summer water table level. We've modified the fine-root profile based on the pretreatment measurements. We propose to further improve the fine-root vertical profile by introducing the dynamic allocation of fine roots across soil depths. We will start from the dynamic rooting depth algorithm developed for upland ecosystems in E3SM (Drewniak 2019) and modify the formulation and/or parameterization utilizing dynamic rooting depth distribution from minirhizotron measurements at SPRUCE (Theme 1; Defrenne et al. 2021).

We will integrate the new developments/improvements on nutrient cycling in ELMv2-SPRUCE with ELMv3-Peatlands including FATES (TH1.4 and TH5.2). We will evaluate the simulated ecosystem N and P budget against empirically based N and P budgets at SPRUCE. We will also evaluate model performance at other peatland sites that have measurements of N and P (see also Theme 5). We will perform simulations to explore the impacts of these model improvements on simulated peatland ecosystem responses to warming and $eCO_2$. We expect that with more realistic representation of fine-root profile and fine-root nutrient acquisition, we will be able to better capture the observed responses at SPRUCE and improve our predictive capability for peatland ecosystems in the future.

### 3.3.3 Ecosystem N Responses to Hydroclimate Variability (Task TH3.3)

Key Personnel: Craig, Mayes, Wood, Griffiths, Walker

Proposed N and P measurements at MOFLUX aim to complement ongoing data sets. MOFLUX is a site with low N availability (Pallardy et al. 1988), so we will focus measurements on N—developing a site-level budget—but we will also monitor P, which can limit ecosystem processes in unglaciated temperate soils (Hou et al. 2020). These nutrient data sets will enable evaluation of Hypothesis 3 in a temperate forest system that experiences high precipitation variability and frequent drought. Though global change research in drought-prone regions has typically focused on water and C interactions, recent work highlights the critical role that nutrients can play in mediating ecosystem responses to moisture variability (Gessler et al. 2017). For example, in response to drought, inhibition of N uptake by both plants and microbes may lead to a buildup of available soil N. This accumulated N could contribute to post-drought recovery or could leach away and contribute to the gradual degradation of ecosystem functioning (Krüger et al. 2021, Müller and Bahn 2022). Such responses depend on the balance of the plant, microbial, and abiotic processes that govern nutrient cycling, and these processes are likely to depend on the type, magnitude, frequency, and timing of climatic perturbations. These efforts are efficiently pursued at MOFLUX site due to 1) the high density of unique empirical data at the site, 2) existing ELM site-specific parameterization (MOFLUX) that can provide modeled variables for MAAT inputs (Liang et al. 2019), and 3) the presence of well-studied mineral soils that are appropriate for microbially explicit, soil C modeling in Theme 4 (Singh et al. 2021).

In this task, we seek to improve model representation of nutrient cycling responses to moisture perturbations. We will assemble a seasonal N budget with companion P dynamics for MOFLUX, repeating measurements across multiple years to capture nutrient dynamics across seasons and extreme events. We will use these data in coordination with water and C flux data (Theme 2), and microbial and soil C data (Theme 4) to develop, calibrate, and benchmark a multi-assumption nutrient-explicit soil decomposition model (using MAAT) and an ecosystem model (ELM-FATES). This effort will result in an improved predictive understanding of the environmental drivers of soil nutrient cycling and the role of nutrient cycling in ecosystem responses to potential hydroclimatic futures.

Ongoing empirical observations at MOFLUX will be complemented by a suite of new observations. A limited set of new observations (e.g., plant and soil nutrient pools) will begin in FY 2024 and the remainder will begin in FY2026 following the end of SPRUCE experimental manipulations. New inputs to the ecosystem in the form of wet N deposition have been monitored at a nearby NADP site located ~1 km from MOFLUX since 1981 (https://nadp.slh.wisc.edu/sites/ntn-MO03/).

*Plant and soil nutrient pools (Craig, Mayes, Wood)* – We will monitor ecosystem N pools using plant tissues and soils collected on a quarterly basis as a part of Theme 4. We will supplement Theme 4 measurements—total soil N (0–15 cm), leaf litter, coarse woody debris, and roots–with measurements of leaf N and soil inorganic N pools ($NH_4$ and $NO_3$). We will additionally collect data on soil available and plant P pools using Bray extracts (Bray and Kurtz, 1945) and microwave digestions, respectively.

*Soil N transformations (Craig, Mayes, Wood)* – To capture intra-annual variability in internal soil N transformations at MOFLUX, we will also quantify net N mineralization and nitrification quarterly. We will quantify ammonium and nitrate before and after static incubations at field conditions. We will supplement these seasonal measurements with *ad hoc* assays during and immediately following extreme events (e.g., during severe droughts and subsequent wet-ups). Anion and cation binding resins will be deployed at 5-cm depth to obtain an integrated measure of plant-available $NH_4$ and $NO_3$ across each growing season. We will use resin access tubes as in TH3.2. Tension lysimeters will be installed to 50 cm depth (when possible) to sample porewater quarterly. Weekly growing season measurements and monthly winter measurements of soil $N_2O$ and $CH_4$ fluxes are being initiated in 2023 by the University of Missouri using a portable Fourier-transform infrared–based system and we propose continuing these measurements for 2–3 years to capture IAV in these fluxes.

*Nutrients in ephemeral streams (Griffiths, Wood)* – The outlet of the watershed in which the MOFLUX footprint resides will be instrumented for measurement of streamflow and water chemistry (yellow dot on **Fig. 3.2**). A stream flume will be installed in the stream channel and high-frequency (e.g., 15-min) data collected by a water-level sensor will be used to calculate stream flow. Due to the ephemeral nature of stream flow in this area, an autosampler, triggered by the initiation of flow, will be set up to collect samples for nutrient analyses. These samples will be retrieved weekly and analyzed for inorganic (nitrate, ammonium, phosphate) and total (N, P) nutrient concentrations, and N and P fluxes will be calculated.

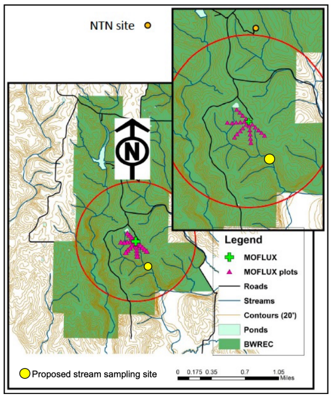


**Fig. 3.2. Footprint of the MOFLUX site (red circle), with the location of the eddy covariance tower (green cross), soil plots (pink triangles), and proposed location for measurements of stream flow and water chemistry (yellow circle).**

_Nutrients in sediments (Griffiths, Wood)_ – Erosion rates in drainages down to ephemeral streams in the MOFLUX tower footprint will be monitored with erosion pins that have been shown effective in complex, vegetated hillslopes (Myers et al. 2019). These point-measurements of erosion will be complemented by measurements of sediment-associated N and P export via stream sampling. Water samples will be collected for suspended sediment analysis using gravimetric approaches. The samples will then be analyzed for percentage of N on an elemental analyzer and for percentage of P using Kjeldahl digests followed by $PO_4$ analysis on a Lachat autoanalyzer at ORNL and sediment-associated N and P fluxes will be calculated.

_Nutrient-explicit C modeling (Craig, Mayes, Walker)_ – Soil nutrients limit microbial activity and, in turn, soil microbes mediate nutrient processes that are critical to ecosystem functioning. It is therefore important to accurately represent microbe-nutrient interactions in soil models. Though most soil microbial models focus on C, several models now explicitly include coupled C and N cycles (e.g., Sulman et al. 2017, Kyker-Snowman et al. 2020, Wang et al. 2021, Zhang et al. 2021). The models represent different assumptions about important dimensions of N cycling such as microbial limitation, mineralization pathways, and stoichiometry (Manzoni and Porporato 2009). Because the implications of these different model structures are not fully understood, we implemented several C-only soil microbial models in MAAT and uncovered substantial structural uncertainty driven by key microbial processes (Section 2.4). We hypothesize that alternative representations of microbial nutrient cycling processes are driving uncertainty among existing coupled C-N soil microbial models.

We will add N dynamics and C-N coupling to the generalized multi-assumption soil decomposition model that has been developed in MAAT. Many of the development groups for the C models in MAAT have gone on to add an N component in recent years (Sulman et al. 2017, Wang et al. 2021, Kyker-Snowman et al. 2020). Our plan is to assimilate these nutrient explicit models in MAAT and compare their simulated responses to global change drivers (altered moisture, N deposition, and temperature). The model assumptions affecting C and N coupling that we will test include flexible vs. rigid stoichiometry; partitioning between microbial and plant uptake; allocation of limited nutrients to enzyme production, biomass growth, and respiration. Parametric and process-level sensitivity analyses from MAAT will be paired with newly collected MOFLUX N budget data, ongoing C flux observations, and laboratory incubations, to evaluate alternative soil C-N model configurations and parameterize selected models. The resulting ensemble of MOFLUX-optimized soil C-N models will be used to simulate C and N cycling responses to future hydroclimatic scenarios. We will also evaluate the extent to which N and P dynamics mediate C and nutrient cycling responses to hydroclimate variability at the ecosystem level using the nutrient-enabled version of ELM (ELM-FATES). The new nutrient budget data in combination with existing data streams on forest demography and ecosystem fluxes will be ideal for establishing an ELM-FATES test bed at MOFLUX.

**Table 3.4. Deliverables for Theme 3 research. Post-SPRUCE syntheses are shown in green text.**

| Task | FY | Deliverable | Lead(s) |
|---|---|---|---|
| TH3.1 | 2024 | Paper: SPRUCE surface peat incubation NP dynamics analysis | Salmon et al. |
| TH3.1 | 2025 | SPRUCE paper: $^{15}N$ isotope dilution for gross N mineralization and nitrification | Salmon et al. |
| TH3.2 | 2025 | FRED Release of v4.0 | Iversen, McCormack |
| TH3.3 | 2025 | MOFLUX paper: MAAT Develop nutrient-explicit soil decomposition model | Craig, Walker |
| TH3.1 | 2026 | MODEX paper: representation of N and P dynamics in ELM-SPRUCE | Yang, Salmon, et al. |
| TH3.3 | 2026 | Initiate annual MOFLUX measurements of N in plant tissue and soil N transformations, and stream instrumentation | Wood, Craig, Mayes, Griffiths et al. |
| TH3.2 | 2027 | FRED Release of v5.0 with emphasis on fine-root nutrient acquisition | Iversen, McCormack |
| TH3.3 | 2027 | MOFLUX paper: nutrient-explicit decomposition model | Craig, Mayes et al. |
| TH3.3 | 2027 | MOFLUX paper: empirical N budget | Craig et al. |
| TH3.2 | 2028 | SPRUCE: MODEX Empirical NP budget paper | Salmon, Yang et al. |
| TH3.2 | 2028 | Paper on the representation of fine root processes in ELM-SPRUCE | Yang, B. Wang, Salmon |
| TH3.3 | 2028 | MOFLUX paper: Nutrient-enabled FATES at MOFLUX | Walker |

### 3.4 Theme 4: Soil C Cycling and Microbial Processes

*How do temperature, water availability, and plant inputs affect soil C and microbial functions, and what are the implications for ecosystem C storage and greenhouse gas fluxes?*

Soil and microbial processes control short and long-term cycling of C within both organic and mineral soils. Providing improved data and algorithms for soil C cycle models that include measurable soil pools and the roles of microbial community structure and activity is key to resolving the current and future trajectory of soil C and climate change. In the past 4 years, the TES SFA has found that soil moisture, texture, the forms of C present, and microbial activity differentially affect greenhouse gas emissions and soil C turnover rates (Section 2.6). In this new proposal, we further dissect these interactions as part of MOFLUX and SPRUCE because of their positions on opposing ends of eastern US moisture regimes and their ability to provide insight into the role of these edaphic factors on greenhouse gas emissions, microbial functions, and soil C storage.

Temperature manipulations at the SPRUCE site demonstrate that the millennia-old C pools and their resident microbial populations deep in the peat profile are slow to respond to the experimental warming treatments (Wilson et al. 2016, Kluber et al. 2020, Wilson et al. 2021ab). Contrastingly, *ex-situ* incubation studies (Hopple et al. 2020) and recent in situ studies of DOC and surface flux patterns (Hopple et al. 2020, Wilson et al. 2021a, Washburn et al., in preparation) show that shallower, less-decomposed peat in the acrotelm, and DOC pools in the porewater are responding to imposed temperature treatments and, are likely fueling the exponential increases in surface $CH_4$ flux that have been observed at SPRUCE (Hopple et al. 2020, Hanson et al. unpublished observational data). These observations are partially supported by modeling efforts customized for northern peatlands that also largely agree with observed trends (Ricciuto et al. 2019, Yuan et al. 2021a, 2021b). Nevertheless, the observed stronger impact of warming on $CH_4$ emissions are somewhat underestimated by the ELM-SPRUCE model. The sustained duration of manipulated temperature at SPRUCE, superimposed on natural seasonal variations, likely alters the ebb and flow of different microbial functional groups, such as aerobes, methanogens, and methanotrophs, as a function of time and treatment intensity, and potentially affects the resultant emissions. One of the challenges in modeling soil microbes is explicitly representing short-term acclimation and long-term adaptation to climate warming and $eCO_2$ by considering microbial community structure and physiology. For example, a theoretical modeling study found that warming reduced C use efficiency (CUE) and limited microbial biomass, thus mitigating $CO_2$ emissions. Additionally, the study pointed out that microbial adaptation or a change in microbial community composition could accelerate the $CO_2$ loss (Allison et al. 2010). How microbial acclimation and adaptation respond to warming and elevated $CO_2$ remain a big unknown at SPRUCE. Connecting functional outcomes–e.g., greenhouse gas emissions–with microbial biomass and functional groups will greatly advance the understanding of complex microbial community activities at SPRUCE and beyond, enabling predictive modeling of climate futures in wetland ecosystems.

At MOFLUX, periodic droughts are an important ecosystem stressor (Section 2.2). Field, modeling, and laboratory studies demonstrate the importance of this stressor for soil C dynamics but have yielded distinct findings about the direction and magnitude of effects. Analysis of long-term field data shows that hot and wet conditions promote $CO_2$ emissions at MOFLUX, compared to cool and dry conditions (Section 2.6). A modeling study using the MEND model (Wang et al. 2015) predicted a nonlinear response of SOC decomposition to soil moisture changes at MOFLUX, where decreased decomposition by microbes under drying was not compensated for by increased decomposition under wetting conditions (Liang et al. 2021). The net result for frequent and high-intensity droughts was decreased greenhouse gas emissions and increased SOC. In a lab incubation study, greater emissions were observed for non-steady-state vs. steady-state conditions because aggregation and microbial activity were differentially affected by the frequency and severity of drying and rewetting (Singh et al. 2021, 2023). Thus, the timing, frequency, and severity of drought and rewetting conditions can affect greenhouse gas emissions as well as SOC, yet the nature of these interactive effects requires further study.

Additionally, there is a trajectory of changing litter inputs at MOFLUX that have not yet been considered. A strong drought in summer 2012 affected leaf production and litterfall for 3 subsequent years, and a late 2007 spring frost stunted leaf and flower production, likely reducing inputs (Section 2.23). Predicting relationships between changing plant productivity and belowground C storage is essential to our ability to predict the trajectory of SOC at MOFLUX or at any upland site experiencing periodic droughts, freezing events, and other climatic changes. The newest generation of soil C models—which include microbial and mineral processes—make dramatically different predictions about how soil C stores will respond to alterations of either the rate or chemistry of plant inputs (Sulman et al. 2018). In prior TES SFA work, we identified key processes that lead to divergence among model predictions when represented differently in soil C models, such as microbial biomass growth and turnover (Craig et al. 2020) and decay kinetics of the mineral-associated C pool (Section 2.4). Yet, at present, we lack the experimental and observational data sets necessary to rigorously evaluate those processes that govern microbial responses to both moisture extremes and changes in plant inputs. Microbial processes can impart considerable nonlinearities upon C cycling through priming, microbially mediated SOC formation, microbial physiological acclimation, and microbial adaptation. Nonlinear processes are not captured by first-order kinetic models in Century or in most ESMs, including ELM. Continued climate change is expected to cause more abrupt changes in temperature and precipitation, and microbial models provide greater capability to predict realistic, nonlinear responses. This is particularly important at transition sites like MOFLUX, which is located at the forest–prairie ecotone, where precipitation and soil moisture exert considerable control over ecosystem functions. Primary hypotheses being addressed in Theme 4 are:

1. *Continued warming and drying at SPRUCE will result in progressive changes to microbial community and function that will alter greenhouse gas emissions and decrease soil C stores.*
2. *Intensifying magnitude and frequency of seasonal drying and wetting, with concomitant forest decline at MOFLUX will decrease soil C inputs, stocks, and respiratory losses.*

The following tasks combine experimental and modeling approaches to resolve the two hypotheses listed above. The first task focuses on SPRUCE, and the second task focuses on MOFLUX.

### 3.4.1 Subsurface Microbial Observations and Modeling at SPRUCE (Task TH4.1)

Key Personnel: Schadt, Griffiths, Mayes, Xu, Kolka

<u>*Microbial community assessments*</u> – To explore hypothesis 1, we will utilize ongoing SPRUCE experimental efforts and new sample collections to predict the effects of continued warming and drying on the microbial biomass, community structure, activities, and ecosystem-level functions of greenhouse gas emissions and peat C stores. Microbial community assessments by metagenomic sequencing in

collaboration with JGI have been completed for annual peat core samples from 2015, 2016, and 2018, are being prepared from 2022 samples, and are planned for final harvest in 2025. These have resulted in the assembly of a catalog of over 600 unique microbial genomes. While data to date have observed only relatively subtle and slow changes, these final assessments will be important as we wrap up the 10-year lifespan of the SPRUCE experiment. Microbial genomes recovered from peat are also planned to be supplemented and complemented by new work on porewater communities and detailed DOC/SOC characterization using metabolomic approaches in collaboration with Georgia Tech, Florida State, and the Environmental Molecular Sciences Laboratory (EMSL). We will continue our ongoing measurements of C, N, P, dynamics in the peat profiles. In the past 2 years, these have also been supplemented by measures of microbial biomass C and N using chloroform fumigation as well as qPCR for ratios of fungi, bacteria, and archaea. In the coming cycle we will expand the qPCR assessments to understand the microbial dynamics among methanogens, methanotrophs, and acetogens three times per year (May, July, October) from acrotelm samples as well as continued annual measurements of the deep catotelm peat. The qPCR approaches we employ for 16S (bacteria, archaea and fungi) and methanogens have been described in prior work at the SPRUCE site (Wilson et al. 2016). We will add similar assessments of acetogens targeting formyltetrahydrofolate synthetase (FTFHS) gene primer sets from Xu et al. (2009) and methanotrophs targeting pmoA gene primers from Kolb et al. (2003). We will also complete the series of metagenomic analyses at SPRUCE with samples taken this past summer (2022) and planned for the final year of the experiment (2025) to add to the time series of metagenomic data from 2015, 2016, and 2018 that were completed in collaboration with JGI (Wilson et al. 2021b, Roth et al., in preparation).

*Decomposition experiments* – We will complete multiple, long-term organic matter decomposition experiments in 2025 at SPRUCE. The final set of litterbags from the multi-species litter decomposition experiment and the final set of peat decomposition ladders will be retrieved from the enclosures in autumn 2025 (years 10 and 8 of the incubations, respectively). Samples will be analyzed for mass loss, and C, N, and P content, and collection of subsamples from the litterbags and peat ladders is planned for amplicon-based assessment of microbial communities (bacteria/archaea 16S rRNA genes + fungal internal tracer spacer (ITS) rRNA genes). We will continue our biannual measurements of cotton strip decomposition in years 8, 9, and 10 of SPRUCE, as the cotton strips, which are 95% cellulose, have provided evidence that labile C decomposition is responsive to warming treatments except in the near-surface peat, where moisture limitations appear to play a much stronger role on decomposition.

*Incubations* – Lab-scale incubations will provide companion data to separately examine the effects of warming and drying, which are currently not resolvable at the field scale. The cotton-strip decomposition experiments described above tend to show little temperature effects at shallow peat depths (<30 cm), but strong temperature effects >30 cm. The 2021 drought showed that decomposition in the near-surface peats (<30 cm) was sensitive to moisture content, suggesting that the lack of response to warming in the shallow acrotelm is related to low soil moisture. We propose a set of long-term incubations using soils from the S1 Bog that separately interrogate moisture and temperature effects, using a range of temperatures and moistures present at SPRUCE. $^{13}C$-depleted *Sphagnum* and other litter will be collected from inside the elevated $CO_2$ SPRUCE enclosures to provide a tracer for litter decomposition and separate the decomposition responses of litter and peat. We will measure $CO_2$ emissions, trace the fate of the depleted $^{13}C$ signature, and will analyze the microbial community using the same methods as in the decomposition experiments, over 4 destructive harvests, for up to a year.

*Microbial modeling* – The ELM-SPRUCE model will be integrated with observational data to address microbial acclimation and adaptation under warming and $eCO_2$ to answer three questions: 1) how does microbial physiology (CUE and metabolic activity) change under warming and $eCO_2$? 2) how does microbial community structure (bacteria vs. fungi) shift in response to warming and $eCO_2$? 3) how do microbial acclimation and adaptation affect soil C cycling via necromass production and microbial respiration? The incubation and decomposition experiments will also provide additional insights to explore how changes in soil moisture interact to control emissions and microbial activities. To address the first question, we will 1) improve the model representation of microbial dependences on temperature to allow microbes to acclimate to changing environments and rapidly recover upon return to normal conditions, and 2) incorporate long-term microbial adaptation (permanent changes in metabolic activity) to mimic microbial behaviors when environmental stresses persist (i.e., long-term droughts). To address the second question, we will explicitly incorporate bacterial-fungal competition for mineral N and DOC (Maynard et al. 2019) and their different responses to warming and substrate (mainly DOC) availability. The modeling efforts and model improvement in the first two tasks will enable the model to address the third question. We will examine the bacterial and fungal dynamics in consideration of their differentiation in driving the soil biogeochemistry cascade. Our recent modeling study highlighted the different roles that bacteria and fungi play in driving C mineralization and necromass formation across the United States (He et al. being revised); we will apply the modeling approach to examine how bacteria and fungi drive necromass formation and microbial respiration under warming and $eCO_2$ at the SPRUCE site. This modeling activity will assimilate data from microbial community structure assessments, decomposition experiments, and incubation experiments to address a fundamental issue in microbial C cycling.

### 3.4.2 Microbial and Soil C Trajectory at MOFLUX (Task TH4.2)

Key Personnel: Craig, Mayes, Schadt, Wood, Gu

*Field activities* – To explore hypothesis 2, we will continue and expand our ongoing efforts at MOFLUX to determine the trajectory of soil C stocks with concomitant forest decline (see Theme 2) and forms in the future. Since 2017, on a quarterly basis we have collected soil cores from MOFLUX and analyzed them for pH, C and N content, texture, moisture content, DOC and dissolved organic N, microbial biomass C and N, and root length and density. Also in 2017, we initiated a trenching experiment to isolate the heterotrophic respiration component of total $R_{\text{soil}}$ in 4 of the 12 total automated soil flux chambers (see also Theme 2). These past and continuing measurements in the new proposal, along with long-term EC, SIF, and meteorology datastreams at MOFLUX, will enable a comprehensive modeling activity focused on connections between aboveground and belowground activities and functions in this new phase of the SFA. In this proposal, we will add analyses of P pools and N fluxes (described in Theme 3), and new qPCR analyses of the microbial community to segregate seasonal trends in soil fungi, bacteria, and archaea from total microbial biomass assessments as part of continued the quarterly sampling. We will also add determination of particulate- and mineral-associated organic C and N, which are relevant to microbial activity and the long-term fate of soil C (Lavallee et al. 2019; Whalen et al. 2022). Beginning in 2026, we will work with Theme 2 to deploy 12 automated Eosense flux chambers and ABB gas analyzers – currently deployed at SPRUCE – to continuously measure emissions of $CO_2$ and $CH_4$, of which approximately half will be deployed on trenched pedons for the isolation of heterotrophic respiration.

*Litter collection and field-scale decomposition experiments* – To determine inputs, leaf litter and coarse woody debris are regularly collected at MOFLUX (since 2003). In this proposal, we will add analyses of C, N, P, and lignin content in both leaf and root samples (in collaboration with Themes 2 and 3) to evaluate how both the rate and quality of organic inputs change in response to environmental stressors. We have also recently initiated a series of root decomposition experiments (September 2022) at 15 and 40 cm depth, to be collected at 6 months and yearly thereafter for the next 5 years. We will initiate a second set of field-scale decomposition experiments (November 2023) involving leaf litter with collections on the same time frames. We will repeatedly deploy short-term (i.e., 1–2 years) leaf and root decomposition experiments each fall to capture the effects of IAV and extreme moisture conditions on the early stages of the decay processes. In 2024, we will establish root-ingrowth cores to quantify belowground productivity over this entire new proposal cycle.

*Incubation experiments* – New incubations will be used to determine how microbial functioning and community composition respond and acclimate to altered moisture regimes and plant inputs. In the warming literature, the response of key microbial growth parameters, such as CUE, has been quantified and implemented in models (Allison 2014, Li et al. 2014). Methodological constraints have so far precluded an equivalent understanding of how these growth parameters respond to moisture extremes. Here, we will employ a novel method using incorporation of $^{18}O$ from water vapor to enable the quantification of microbial growth, turnover, and CUE in both wet and dry soils without confounding effects from soil rewetting (Canarini et al. 2020). To determine how the growth and turnover of the microbial biomass responds to soil moisture, we will incubate composite surface soil samples (0–10 cm depth) at four steady-state soil moisture levels: average WHC, dry (−50% WHC), wet (+50% WHC), and saturated (100% WHC). In a fifth treatment, we will simulate three dry-wet cycles (10%–100% WHC) as in Singh et al. (2023) to examine how microbial processes acclimate to altered moisture regimes. The resulting experimental microcosms (including 3 replicates of each moisture treatment) will include sufficient replication for destructive harvesting (3 times for steady state, 6 times for transient) to determine microbial biomass via chloroform fumigation; and growth, turnover, and CUE via the $^{18}$O water vapor method. To monitor microbial respiration, $CO_2$ efflux will be measured weekly. Incubations will continue for 90 days, which should allow treatments to reach steady-state or transient equilibria (Singh et al. 2023).

In a second incubation experiment, we will explore the effects of altered plant inputs on microbial and soil C dynamics. We will test alternative hypotheses about microbial and mineral processes that we have found to be leading contributors to model structural uncertainty in the context of altered inputs: microbial biomass dynamics and mineral-associated decay kinetics. Specifically, we will quantify the response of microbial growth and turnover along a gradient of input rates and qualities, using $^{13}$C-labeled substrate incorporation into microbial biomass, and mineral-associated soil C to concurrently track microbial growth and turnover; mineral-associated soil C formation; and soil C priming effects. We will vary input chemistry in terms of C quality (glucose vs. cellulose) and N availability (aspartic acid vs. succinic acid) as in Chari and Taylor (2022). Inputs will be applied continuously at 4 different rates (including zero-addition controls) under wet (65% WHC) and dry (−50% WHC) conditions to plot the functional response of microbial and mineral processes to altered inputs under normal and dry conditions. During the 30 day incubations, we will monitor $CO_2$ efflux and its $^{13}$C signature and include sufficient replication to monitor $^{13}$C dynamics of the microbial biomass in sequential destructive harvests. After 30 days, some replicates will be collected for soil C tracing, while the glucose incubations will continue with unlabeled substrates for another 180 days. The purpose of the longer-term incubation is to track the decay kinetics of the newly formed mineral-associated C. During this time, we will continue to monitor $CO_2$ efflux and $^{13}$C dynamics through headspace and destructive harvests.

*Microbial modeling* – Accurate and predictive microbial soil C models remain elusive, with substantial structural differences among existing models often leading to widely diverging results and predictions (Sulman et al. 2018). We will initiate a new modeling activity using MAAT, which has incorporated several different microbial models, including MEND, MIMICS, CORPSE, and Millennial (https://github.com/walkeranthonyp/MAAT) to help understand the underlying differences between model structures. For our work under this proposal, parameterization will be aided by recent modeling studies using ELM (Liang et al. 2019) and MEND (Liang et al. 2021, Jian et al. 2020), and transient and steady-state incubations using MOFLUX soils (Singh et al. 2021, Singh et al. 2023, Kluber et al. 2020) for model set up and calibration. Finally, using MAAT, we will leverage results from the incubation experiments as well as existing data on different soil and plant types (e.g., Singh et al. 2021, Li et al. 2018) to evaluate current and newly developed process representations for microbial functions in upland soils. The newly refined models representing microbial acclimation to moisture conditions and plant inputs will be calibrated using our field data collected at MOFLUX and soil $CO_2$ from Theme 2 to investigate how potential future moisture regimes and plant input trajectories will affect soil C cycling in the drought-prone prairie-forest ecotone.

**Table 3.5. Deliverables for Theme 4 research. Post-SPRUCE syntheses are shown in green text.**

| Task | FY | Deliverable | Lead(s) |
|---|---|---|---|
| TH4.2 | 2024 | MODEX paper: trends and controls of autotrophic and heterotrophic respiration at MOFLUX 2017–2022 | Mayes, Wood, Gu, Craig |
| TH4.1 | 2025 | SPRUCE: Separating the effects of warming and drying of peat in lab incubations | Mayes, Schadt, Griffiths, Kolka |
| TH4.2 | 2026 | MOFLUX incubation paper: Microbial CUE responses to moisture extremes along a precipitation gradient | Craig, Mayes |
| TH4.1 | 2026 | SPRUCE paper: Synthesis paper on microbial communities | Schadt, Mayes et al. |
| TH4.2 | 2027 | MODEX paper: Optimizing microbial soil C models for representing effects of altered plant inputs at MOFLUX | Craig, Mayes, TBD |
| TH4.1 | 2027 | SPRUCE: Synthesis paper: Organic-matter decomposition responses to warming and $eCO_2$ | Griffiths, Kolka, Schadt |

| | | | |
|---|---|---|---|
| TH4.2 | 2028 | Short- and long-term root and leaf decomposition at MOFLUX | Mayes, Wood, Craig, Schadt |
| TH4.2 | 2028 | Synthesis article including demonstrated model improvements using MAAT at MOFLUX | Craig, Mayes, TBD |
| TH4.1 | 2028 | SPRUCE: How temperature, e$CO_2$, and warming affect microbial functions and emissions | Xu, Mayes, Schadt |
| TH4.2 | 2028 | MOFLUX paper: Soil and microbial function: Trends 2022–2027 | Mayes, Schadt, Craig |

### 3.5 Theme 5: Regional Integration and Extrapolation

*Are the humid, high-C ecosystems of North America more vulnerable to changing climate and disturbance regimes than predicted by CMIP6? How does the collective knowledge gained from the TES SFA affect our understanding of the C feedbacks in the region?*

The state-of-the-art for predicting terrestrial C feedbacks to atmospheric $CO_2$ increase are the various ensemble simulations in the CMIP6 DECK (Arora et al. 2020, Canadell et al. 2021, Eyring et al. 2016). Under all Shared Socioeconomic Pathways (SSPs), the CMIP6 ensemble predicts an increase in C across the boreal and temperate region (Canadell et al. 2021). This C increase is driven by a positive C concentration ($CO_2$ fertilization) feedback of ~0.01 kgC $m^{-2}$ $ppm^{-1}$ with strong model agreement and a close to neutral C–climate feedback but with a dipole (positive feedback in the boreal, negative in the temperate) and little model agreement (Arora et al. 2020, Canadell et al. 2021). The low model agreement in the magnitude and sign of the C–climate feedback is indicative of the fact that many models do not represent the processes controlling C–climate feedbacks in as much mechanistic detail as the physiology of $CO_2$ fertilization. For example, the vulnerability of belowground C stores to climatic perturbations depends on chemical and physical protection mechanisms that are often missing from ESMs (see Theme 4). Furthermore, there are significant feedback processes missing in CMIP6 models, such as peat formation and loss, demographic biome shifts, and responses to extremes and disturbance.

In the region of the SPRUCE experiment, the CMIP6 ensemble predicts a C–climate feedback of about −0.5 kgC $m^{-2}$ $°C^{-1}$ while the SPRUCE experiment indicates a C–climate feedback of −2.2 kgC $m^{-2}$ $°C^{-1}$. Although there is a scale mismatch in this comparison, site-level ELM simulations of the SPRUCE experiment cannot reproduce the observed feedback without incorporating peatland processes and PFTs in ELMv2-SPRUCE (Shi et al. 2021) and substantial further calibration efforts (Section 2.1). At MOFLUX, ELM was not able to predict how a strong drought and a late spring freeze affected litterfall, LAI, and GPP (Liang et al. 2019), with potential consequences for predicting C-climate feedbacks. Thus, TES SFA experiments and modeling indicate that the state-of-the-art CMIP6 ensemble, including ELM, may not accurately predict feedbacks in temperate and boreal regions.

These uncertainties are compounded by poor understanding of vegetation dynamics. Studies of observed boreal C-climate relationships and climate change suggest a loss of boreal C from southern range contraction only partially compensated for with northern range expansion (Koven, 2013), indicating that vegetation dynamics might be important. However, only 3 of the 11 CMIP6 models used to calculate C feedbacks included vegetation dynamics.

Finally, weather extremes such as early spring freeze events and early summer heat waves in the presence of cold soils at SPRUCE (Appendix E) resulted in dramatic canopy damage, especially in the warmer treatment plots. Weather extremes are currently much more intense than projected by models, such as, the heatwave in the Pacific northwest in 2021, which may have an outsized impact on C–climate feedbacks. High-resolution, empirically downscaled climate projections are likely to better represent potential climate extremes (Rastogi et al. 2022, Nicholas and Battisti 2012).

To quantify the impacts of our model improvements on these C-climate feedbacks, we will develop a regional testbed for high-resolution simulations that includes high-C temperate and boreal ecosystems represented by our core and secondary sites (SPRUCE, MOFLUX, MA, Walker Branch). This region will be simulated at 4km resolution using an updated version of ELM informed by Themes 1–4, and it will include southern Boreal ecosystems and eastern humid temperate forests. This domain includes key C stores over a large range of potentially vulnerable temperate and boreal ecosystems and incorporates much of the currently humid eastern-side of the strong continental gradient in aridity index (**Fig. 3.3**). The sub-continental scale of the domain makes high-resolution model ensembles computationally feasible. We will mask agricultural areas from the simulations as they are outside the scope of our study. Coastal interfaces (including the Great Lakes) and areas with greater than 10% permafrost (**Fig. 3.3a & c**) will also be masked. In addition to the regional simulations, we will also perform global simulations at 0.5°x 0.5° resolution to understand the impacts of our model developments on the global C cycle and to compare with other global modeling efforts. Simulations at both scales will be informed by identifying vulnerable areas through compound indicators, and by extensive site-level calibration and validation.

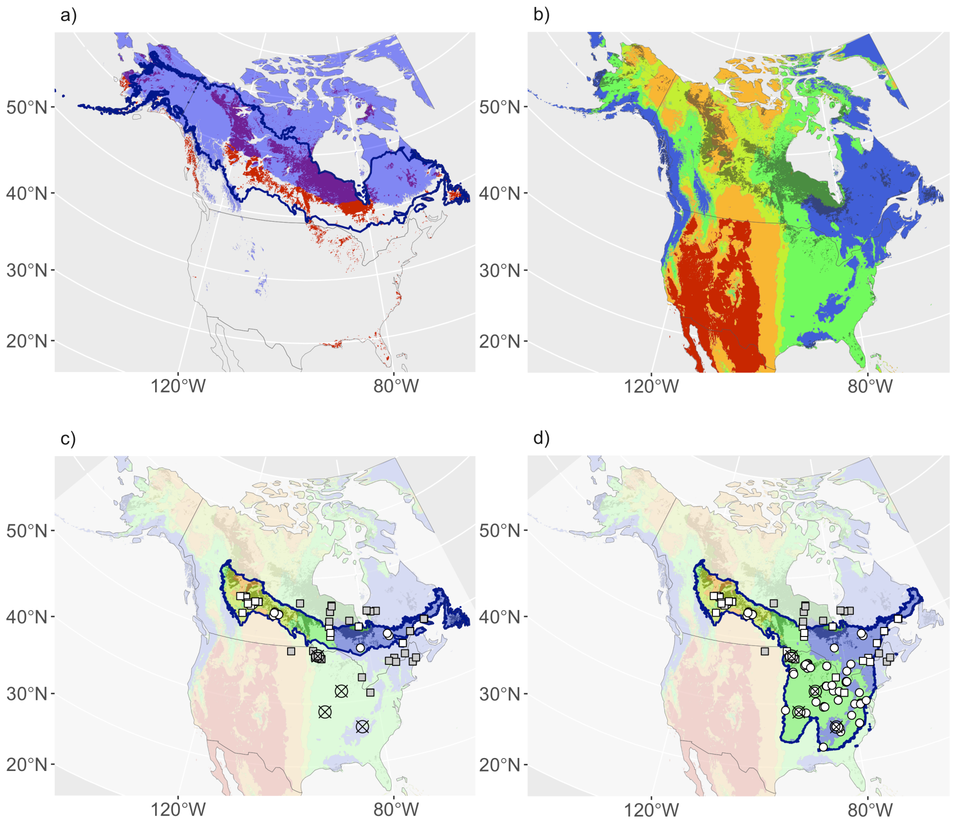


**Fig. 3.3. Development of regional North American modeling domain for Theme 5. a) Boreal zone (outlined in dark blue, Brandt et al. 2009) with permafrost >10% (blue, Gruber et al., 2009) and peatlands >20 % (red, Hugelius et al., 2020), purple areas show overlap. b) Peatlands (dark) overlain on Aridity Index (AI, precipitation/potential evapotranspiration, Zomer et al. 2022) zones based on World Atlas of Desertification and (Lugo et al. 2009): desert (AI 0.0-0.25, red), semi-arid (AI 0.25-0.5, orange), dry-subhumid (AI 0.5-0.65, yellow-green), subhumid (AI 0.65-1.0), and humid (AI >1). c) Non-permafrost Boreal zone (dark blue outline) overlain on AI zones and area outside of the domain faded. d) the high-resolution modeling domain composed of non-permafrost Boreal zone as in c and adding eastern continental subhumid and humid AI zones. Also shown (on c and d) are our core and secondary study sites (circles with an x), wetland sites (white squares in domain, grey squares outside domain), and > 50 AmeriFlux and 12 ForestGEO sites (white circles with black borders) to be used for site-scale model evaluation and calibration (TH5.1).**

This theme will address the following three hypotheses through three related tasks:

1. *Key uncertainties for both boreal and temperate C–climate feedback projections are associated with processes and parameters related to hydrology, nutrient cycling, productivity, and decomposition among plant functional types under changing environmental conditions.*
2. *The CMIP6 ensemble and E3SM under-predict boreal and temperate C–climate feedbacks due to missing peatlands, missing plant demographics, and coarse spatial resolution (i.e., underestimates the vulnerability of ecosystem C).*
3. *The most vulnerable C stores of boreal and temperate ecosystems are those in vegetation or organic soils located near ecological boundaries (e.g., boreal/temperate, forest/prairie). These stores are sensitive to processes like decomposition and mortality, likely to be exposed to multivariate climate change, and likely to occur near to ecosystem tipping points.*

We address these three hypotheses using multi-site model uncertainty quantification, calibration, and evaluation (Task TH5.1); an ensemble of high-resolution (4 km) ELM simulations across a study domain representative of North American humid and high-C ecosystems (Task TH5.2); and a compound ecosystem vulnerability analysis across North American boreal and temperate ecosystems that incorporates high-resolution remotely sensed data, high-resolution meteorological observations and projections, other high-resolution ecosystem data sets, and model results (Task TH5.3). Each Task also informs the others within the theme, leverages model advances and data sets developed in Themes 1–4, and uses existing DOE and broader scientific community data, such as AmeriFlux and ForestGEO. Theme 5 integrates site-scale, process-scale, and trait database results with ELM at regional scales.

### 3.5.1 Model Uncertainty Quantification, Calibration, and Evaluation (Task TH5.1)

Key Personnel: Ricciuto, Shi, Yang, Y. Wang

This task will address hypothesis 1**.** Our current site-level model ELMv2-SPRUCE integrates the default version of ELMv2 included in E3SM with developments from previous phases of the SFA. ELMv2-SPRUCE also retains the functionality of the default version of ELMv2 to simulate non-peatland sites like MOFLUX. To quantify drivers of uncertainty in model predictions, we will perform ensembles of ELMv2-SPRUCE at multiple sites with varying input parameters. These ensembles will be used to train surrogate models, which will then enable efficient parameter sensitivity analysis and site-level calibration using observations from our study sites. The site level calibrations will inform parameters in the proposed ELMv3-Peatlands (TH5.2) that will have both site and regional modeling capabilities. Proposed model developments in Themes 1-4 will then be incorporated into ELMv4-Peatlands (TH5.2). We will repeat the proposed calibration workflow for ELMv4-Peatlands in site simulation mode.

*Study sites* – Sensitivity analysis and calibration will be performed at SPRUCE, MOFLUX, MA, Walker Branch and approximately 100 additional sites (**Fig. 3.3d**). Prior DOE-funded work on Walker Branch Watershed in eastern Tennessee provides further site-specific data for the evaluation of drought driven changes in ecosystem processes (Hanson and Weltzin 2000; Hanson et al. 2004; Hanson and Wullschleger 2003). Additional sites will be chosen to be representative of variability in ecosystems within our study region (see Task TH5.2), helping to avoid over-fitting in model calibration and enable robust regional simulations. These sites will include EC sites, forest inventory sites, and vulnerable grid cells identified by the analysis in Task TH5.3. We will focus on sites within the region to be simulated in Task TH5.2; we will select EC sites from the AmeriFlux and National Ecological Observatory Network (NEON) networks including wetland sites as a priority, and temperate deciduous, boreal evergreen and grassland sites. Forest inventory sites will be selected from the ForestGEO network.

Based on our criteria, over 90 sites are available in our high-resolution domain; those especially relevant include wetland sites Mer Bleue (Moore et al. 2011), Bog Lake Fen (Feng et al. 2020); site clusters like the Chequamegon Heterogenous Ecosystem Energy-balance Study network (Desai et al. 2022); and temperate sites including Morgan Monroe State Forest (Roman et al. 2015) and University of Michigan Biological Station (Gough et al. 2008). Additional North American and Eurasian wetland sites (e.g., Helbig et al. 2022) and forest EC sites outside of the regional domain (e.g., Bergeron et al. 2006) will be selected to improve the parameterizations for these systems. We will also include sites with ecosystem manipulation studies including FACE (Free-air Carbon Enrichment) that have well established model intercomparison protocols (e.g., Walker et al. 2014). We will extend the existing capability for the Offline Land Model Testbed (OLMT) to support the execution of ensemble simulations, sensitivity analysis, and calibration of model parameters using information from multiple sites simultaneously.

*Sensitivity analysis using surrogate models* – We will use global sensitivity analysis to determine which parameters most influence model output quantities of interest (QoIs). Relevant QoIs include components of NEE (e.g., NPP, heterotrophic respiration, net $CH_4$ flux), the responses of these quantities to changing climate (e.g., the difference in NPP between an SSP scenario and present-day conditions), and key ecosystem response variables identified in TH5.3.

We will select 50–100 uncertain ELM parameters covering a broad range of ecosystem processes, expanding upon previous work (Ricciuto et al. 2018) to include $CH_4$ cycling (Ricciuto et al. 2021, Yuan et al. 2021), improved phenology (Meng L et al. 2021a), nutrient cycling, decomposition, and forest demography-related parameters. Parameter ranges or distributions will be informed by FRED (Task TH3.2), LeafWeb (Task TH2.6), TRY (Kattge et al. 2011) and expert opinion. Based on previous work (Ricciuto et al. 2018), we anticipate a required ensemble size of around 2500 members. Each ensemble simulation includes model spin-up to achieve steady-state C and nutrient pools under pre-industrial conditions; transient simulation from 1850 to present, including time-varying $CO_2$, climate, nutrient deposition and land-use; and environmental manipulation where applicable.

Global sensitivity analysis requires an even larger number of model evaluations using different parameter combinations, which may be accomplished using surrogate models (Sargsyan et al. 2014). A surrogate model predicts the response of a model QoI as a function of the model input parameters, and it is fit to the ensemble of training simulations from the original model. Here we train a surrogate model with a neural network for each QoI; when the number of QoIs is large, training becomes cumbersome, and we apply singular value decomposition to reduce the dimensionality of the outputs while retaining surrogate accuracy (Lu et al. 2019). The ELM ensembles and generation of neural-network-based surrogate models are already automated for individual sites in OLMT; we will extend OLMT to allow for multiple sites simultaneously, to automate dimension-reduction methods, and to allow additional environmental manipulations to support incorporating additional experimental data.

We then sample from the surrogate model and calculate sensitivities using the Sobol method (Sobol, 1993), a variance-based decomposition approach that calculates indices related to first order, second order (interactions), and total sensitivity to the uncertain parameters. These sensitivity indices will be shared across themes to assist in prioritization of data synthesis and sampling, experimentation, and model development. Down-selection of parameters for calibration is challenging given the potentially large number of QoIs to be used in an optimization and differences in sensitive parameters among those QoIs. Sensitivities for a given QoI are likely to vary as a function of ecosystem type (Ricciuto et al. 2018), time of year (Safta et al. 2015), and with changes in climate (Hanson et al. 2020). We will determine the 20–30 most influential parameters for model calibration by adding their rankings across all relevant QoIs.

*Calibration and PFT parameterization* – Model calibration will be performed using the MCMC Metropolis–Hastings algorithm (Metropolis et al. 1953, Hastings 1970) to sample from the surrogate models. MCMC is a Bayesian method capable of estimating posterior probability density functions for both model parameters and QoIs given observations, their associated uncertainties, and prior parameter distributions. As with the sensitivity analysis, it is more computationally efficient to perform MCMC using surrogate models of ELM given the large number of required model evaluations. This technique has been successfully applied at MOFLUX (Lu et al. 2018) and will be extended to include observations from multiple locations. Surrogate models for calibration require predicting the original model responses with greater accuracy than for sensitivity analysis, and they may prove difficult to train for some sites given the complex behavior of many interacting processes. We will test the feasibility of a phased approach by first developing surrogate models for leaf and photosynthesis parameters with the simpler satellite phenology version of ELMv2-SPRUCE (Shi et al. 2015, 2021) and performing calibration of those parameters that can then be used as inputs for the full version of ELMv2-SPRUCE. We will also leverage work underway in the E3SM project to replace costly model processes (e.g., spin-up) with surrogate representations, potentially increasing the ensemble size for training our QoI surrogate models.

QoIs for model calibration include biomass, soil C stocks, EC $CH_4$, NEE, GPP and latent heat fluxes, SIF, soil temperature and moisture, forest size-distributions, PFT co-existence, and basal area proportions (Li et al. 2023). We will also explore calibration using relationships in ecosystem functional space (Gu et al. 2016), which may better test the model's ability to represent key mechanisms (for example, the linear relationship between precipitation and GPP). Multiple types of observations (e.g., NEE and biomass) will simultaneously constrain model parameters using an aggregated multi-objective cost function; this approach will also allow for an assessment of which data streams have the most value in constraining model parameters and predictions (Keenan et al. 2013). OLMT already supports single-site calibration using multiple constraints, and it will be extended to support multi-site calibration and to support including the ecosystem functional space relationships. We will also include additional optimization methods including the DiffeRential Evolution Adaptive Metropolis algorithm (Vrugt et al. 2008) that may improve MCMC performance when we have many parameters to optimize.

For the selected sites (see below), we will use OLMT to first optimize each site individually. We will perform a cluster analysis on the optimized parameters to determine whether the default categorization of PFTs in ELM is appropriate for our region of interest, or whether additional types are necessary. Sites will then be aggregated accordingly, and a multi-site calibration will be performed to obtain optimized model parameters for each PFT. These calibrated parameters will serve as the inputs for the regional simulations in Task TH5.2.

### 3.5.2 Regional High-Resolution Modeling (Task TH5.2)

Key Personnel: Ricciuto, Shi, Walker, Wang

This task will address hypothesis 2. We will also evaluate the companion hypothesis that due to the forementioned missing processes as well as poor representation of plant allocation, that the C-concentration physiological feedback may be over-predicted. To evaluate, we will run an ensemble of offline ELM simulations across our study domain that include standard CMIP configurations, higher-resolution configurations, and richer process representations developed by the TES SFA (and other projects).

*Model configuration and development* – To enable these regional simulations, we must develop ELM to incorporate complex landscapes including uplands and peatlands. ELMv2-SPRUCE enabled the simulation of the S1 Bog (and site-scale simulation of other bogs) by (1) introducing hummock-hollow microtopography with hydrology including lateral flows and a perched water table, (2) incorporating *Sphagnum* physiology, and (3) adjustments to other PFT and soil parameters (Shi et al. 2015, 2021). An initial regional scaling exercise will take a simple approach of running ELMv2-SPRUCE at 0.5° resolution. Building on ELMv2-SPRUCE and targeting successive releases of ELM, we will develop ELM-Peatlands, a version of ELM capable of both site and regional simulations over the proposed domain (**Fig. 3.3d**).

Targeting integration with ELMv3 to be released by the E3SM project in 2024, for ELMv3-Peatlands we will develop a new subgrid structure that allows the representation of multiple types of wetlands and their lateral connections to each other and to upland systems (**Fig. 3.4**). This will be facilitated by building lateral connections among topographic units in the sub-grid scheme developed in ELMv2 (Hao et al. 2022). This development will be further informed by the planned Peatlands Workshop (Section 3.6.2) focused on how results from the SPRUCE experiment inform peatland responses to climate change beyond the S1 Bog. A key goal of that meeting will be to develop plans for how to represent peatlands

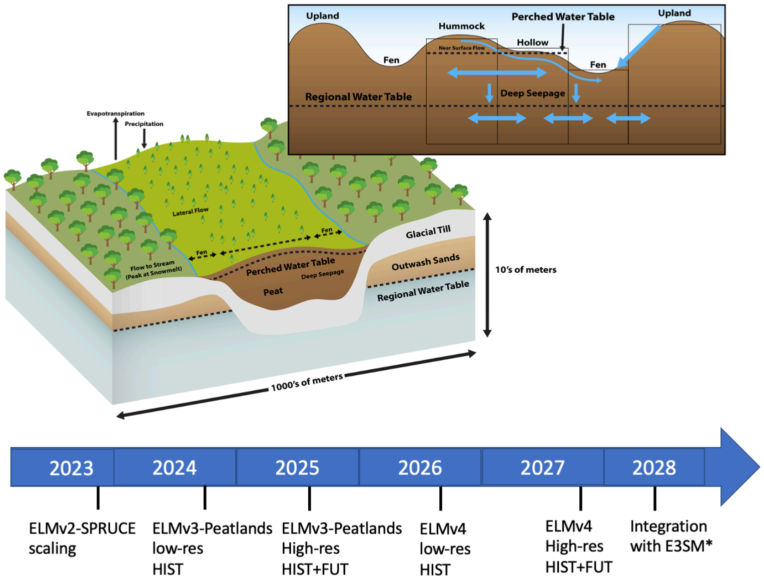


**Fig. 3.4. ELM-Peatlands sub-grid structure to be used in versions 3 and 4 and timeline for the model simulations using this framework. The two-column approach in Shi et al. (2015, 2021) is extended to four columns with fens and uplands and considers lateral interactions, allowing generalization of ELMv2-SPRUCE for regional domains. We begin with low-resolution historical (HIST) simulations, extending to high-resolution future simulations (FUT) in our regional domain with versions 3 and 4. We will maintain ELM-Peatlands as a branch of E3SM, integrating developments as appropriate for offline ELM testing and fully integrating in 2028 to allow fully coupled simulations.**

across our study region at high resolution and evaluate how to inform ELMv3-Peatlands by generalizing structure, processes, and parameters in ELMv2-SPRUCE. ELMv3-Peatlands will integrate existing SFA developments, such as the Microbe module (Xu et al. 2015) and will be parametrized based on effort in TH5.1. We will also include initial testing of the FATES-enabled version of the model to simulate vegetation dynamics. ELM-FATES uses the same decomposition and hydrology sub-models as ELM, so FATES can be readily connected to the proposed sub-grid structure of ELMv3-Peatlands.

ELMv4-Peatlands will incorporate model developments proposed in Themes 1-4: the Microbe module (Themes 1 and 4), improved nutrient cycling and root function (Theme 3), and improved phenology and allocation (Theme 1), as well as further developments to integrate FATES (e.g., vegetation parameterizations for *Sphagnum* in FATES in TH1.3). TH5.1 will calibrate ELMv4-Peatlands for coexistence of the 4 major PFTs at SPRUCE and other PFT combinations at TH5.1 sites. A key advantage of FATES is the ability to simulate dynamic vegetation with mechanistic mortality, providing predictions of how ecotones and vegetation may shift with changing climate. ELMv4-Peatlands will also include improved model parameterizations from final sampling and destructive harvesting at SPRUCE.

As well as PFT parameterization, model evaluation and calibration in Task TH5.1 will provide an estimate of model accuracy. The site-based model MCMC ensembles provide an estimate of the uncertainty in the predictions from the posterior parameter distributions. We will scale these site-level estimates of uncertainty using regional representativeness analysis to estimate the uncertainty associated with each ensemble member.

*High-resolution meteorological data* – For these high-resolution (4 x 4 km) simulations, we will develop a high-resolution, empirically downscaled climate data set including historical reanalysis and future projections. High-resolution, empirically downscaled climate projections will provide greater spatial accuracy of the projections and greater accuracy in the representation of variability statistics (Rastogi et al. 2021, Nicholas and Battisti 2012). These high-resolution data sets will be derived from CMIP6 model projections with daily precipitation, temperature maximum, temperature minimum, and directional wind outputs available, needed for spatial downscaling. Spatial downscaling will use the 1 km DAYMET (Thornton et al. 2020) data set to empirically bias-correct and downscale model projections to 1/24° (~4 km) using the method of Rastogi et al. (2022). These data will be temporally downscaled to every 3 h using the Global Soil Wetness Project Version 3 data set (Kao et al. 2022).

Climate driving data will incorporate scenarios relevant to the Paris Agreement and subsequent COP negotiations—SSPs designed to result in mean global heating of approximately 1.9°C, 2.6°C, and 4.5℃ by 2100 (SSP1-1.9, SSP1-2.6, SSP2-4.5) as well as the more extreme scenario resulting in 8.5 ℃ (SSP5-8.5). We will also downscale the simulated climate data from the idealized 1% increase in $CO_2$ concentration per year scenarios: 1pct$CO_2$-RAD (radiatively coupled) and 1pct$CO_2$-BGC (biogeochemically coupled) for direct comparison to these feedback estimates in the Intergovernmental Panel on Climate Change (IPCC) AR6 report (Arora et al. 2020, Canadell et al. 2021).

*Model initialization and parameterization* – High-resolution simulations also require high-resolution model initialization data sets. For initialization of soil properties, we will regrid the 30 arc-second (~0.9 km) *Harmonized World Soils Database v1.2* (https://www.fao.org/soils-portal/data-hub/soil-maps-and-databases/harmonized-world-soil-database-v12/en/) to 4 km, leveraging parallel efforts by the ORNL team on the E3SM project. We will also use this database for topographical terrain classification of the hydrological sub-grid units (**Fig. 3.4**). We will test multiple datasets as inputs for peatland area including Peat-ML (Melton et al. 2022) and PEATMAP (Xu et al. 2018). For static PFT distributions and dynamic future land use change, we will use the 1 km database developed by (Chen et al. 2022) to be consistent with the SSP scenarios.

*Model simulations and execution* – We will run an ensemble of six scenarios (SSP1-1.9, SSP1-2.6, SSP2-4.5, SSP5-8.5, 1pct$CO_2$ RAD, and 1pct$CO_2$ BCG), at two resolutions (0.5° and 1/24°, ~4 km), and five model configurations (ELMv2-SPRUCE (low-res only), ELMv3-Peatlands, ELMv3-FATES-Peatlands (low-res only), ELMv4-Peatlands, and ELMv4-FATES-Peatlands). The total number of ensemble members is 48. At the 4 km resolution of the downscaled CMIP6 climate projections, each simulation over the study domain will consist of around 0.28 million grid cells. These will be run on the ORNL Climate Change Science Institute (CCSI) Compute and Data Environment for Science (CADES) cluster using CPU parallelization and numerical spin-up. At the 0.5° global resolution of the CMIP6 climate projections, each simulation over the study domain will consist of around 62,000 grid cells.

Model analysis – We will use the International Land Model Benchmarking (ILAMB) software to assess model performance (Collier et al. 2018). To calculate the C–climate and C concentration feedbacks, analysis will follow the method of Arora et al. (2020). Our analysis will partition the feedbacks into GPP, CUE, and vegetation and soil turnover time responses (Arora et al. 2020, Hajima et al. 2014, Walker et al. 2015). These metrics will be calculated and compared among the feedback simulations of various resolutions and model configurations. For the SSP scenarios, the differences in C changes among the three scenarios will be compared to assess the impacts of various policy scenarios on ecosystem C stocks, as well as other metrics of ecosystem structure and function. The impacts of resolution and the various model configurations will be examined and the causes of difference identified.

### 3.5.3 Quantification of Boreal and Temperate Ecosystem Vulnerabilities and Their Model Uncertainties (Task TH5.3)

Key Personnel: Mao, Wang, Jin, Craig, Chen

To address hypothesis 3, we will (1) develop a set of Compound Indicators for Vulnerable Ecosystems (CIVE) that can identify where and in which season the greatest vulnerability is expected under climate change, informing model calibration (e.g., site selection in Task TH5.1) and ecosystem experiments, (2) compare the results of applying the framework on historical observations and historical and future model simulations (e.g., CMIP6 simulations at 0.5°–1°, ELM simulations at 4 km from Task TH5.2) to determine the historical-future changes and model biases and uncertainty, and (3) reduce the biases and uncertainty in model-projected future ecosystem vulnerability using a machine-learning based emergent constraint framework.

Vulnerability of boreal and temperate ecosystems – Ecosystem vulnerability has three components: exposure, sensitivity, and adaptive capacity (Weißhuhn et al. 2018). Exposure means the probability of occurrence of a hazard, disturbance, or stress; sensitivity means the susceptibility to the hazard; and adaptive capacity means the ability to cope with the hazard and its consequences (Weißhuhn et al. 2018). In boreal and temperate ecosystems, well-known environmental stressors include high temperature and VPD, extreme events (heat waves, droughts, floods, ice-storms), and wildfires. These drivers have been demonstrated to regulate essential function and structure of ecosystems (e.g., photosynthesis, respiration, mortality, growing season length, vegetation community — Kirpotin et al. 2021, Mao et al. 2016a, Sizov et al. 2021). Because of such diversity in stressors and response variables, comprehensive assessment of ecosystem vulnerability requires integrating information across various inputs. This can be achieved by averaging output or using dimensionality reduction techniques to derive compound indicators of vulnerability (Balaganesh et al. 2020, Dossou et al. 2021).

Development of CIVE – The CIVE will include estimates of exposure, sensitivity, and adaptability. To measure the ecosystem exposure to each stressor, we will create bins in one (e.g., for temperature) or two dimensions (e.g., intensity and frequency of extreme events and wildfires) and sum up the values in each bin (Wu et al. 2019). To calculate the sensitivity of each ecosystem variable to each stressor, we will use partial correlation and more sophisticated regression methods (Wu et al. 2019). To estimate adaptive capacity, we will use ecological and engineering resilience metrics, which quantify the ability of ecosystems to remain stable in face of disturbances from a global and local point of view (Dakos and Kéfi 2022, Baumbach et al. 2017, Tang et al. 2021, Wang and Mao et al. in review). For stressors, we will focus on annual mean temperature, heat waves, droughts, floods, ice-storms, and wildfires. For ecosystem variables, we will include GPP, ecosystem respiration, aboveground and belowground biomass C, SOC, and fraction of PFTs.

After calculating the 3 CIVE subindices for all the combinations of stressors and ecosystem variables, we will normalize them and use absolute values when necessary to make the results comparable in space and across different combinations. Then, we will average the exposure, sensitivity, and adaptive capacity to derive a single vulnerability value for each spatial location and combination of driver and ecosystem variable. Finally, we will pass the resulting matrix of vulnerability indices (spatial points x combination of variables) to dimensionality reduction methods (e.g., Hoffman et al. 2013) to obtain a single CIVE value for each spatial point. The results of dimensionality reduction will not only enable identifying the "hot spots" (i.e., where the CIVE is the largest) but also reveal the spatial patterns of correlation or mutual cancellation between different aspects of ecosystem vulnerability (i.e., different combinations of stressors and ecosystem variables). The CIVE can be applied separately for each season of the year to enable identifying the "hot moments".

*Observed and modeled CIVE* – The application of CIVE to historical observations, will focus on high-resolution, high-quality data sets including (1) MODIS-based GPP (500 m), (2) irrecoverable C data set of Noon et al. (2021), (3) DAYMET meteorological data sets (1 km) (Thornton et al. 2020), (4) MODIS and VIIRS Active Fire Products (1 km and 375 m, respectively), (5) ESA CCI land cover maps (300m; which shows vegetation types), and (6) Soil Heterotrophic Respiration Database (Stell et al. 2021). To test our hypothesis that organic soils are particularly susceptible to multivariate climate change, we will leverage recent mapping of soil C stored in organic vs. mineral-associated forms (Georgiou et al. 2022). We will augment the CIVE analysis with a synthesis of global change experiments to determine whether mineral protection of C mediates the response of soil C to multiple climate and atmospheric stressors.

For the application of CIVE to model simulations, we will download historical and future simulations from the CMIP6 repository and use the historical and future simulations by the improved and optimized ELM at 4 km produced by Task TH5.2. If site observations proposed in Task TH5.1 are long enough to allow statistically robust calculation of exposure, sensitivity, and adaptive capacity, we will also include the site observations and the site simulations of the un-optimized and optimized ELM.

*CIVE-based model uncertainty quantification and constraint* – For the historical (e.g., 2000–2022) and future period (e.g., 2040–2060), we will calculate the CIVE using observations and model simulations and examine spatial patterns and seasonal variations. The identified hot spots and hot moments can be used to inform further site selection in Task TH5.1 or the design of new ecosystem experiments for the scientific community. We will compare the CIVE between the observations and historical model simulations to determine how well the updated ELM from other Themes (e.g., Theme 1) can reproduce historical ecosystem vulnerability, and how much uncertainty exists across different model parameterizations and structures. We will compare the CIVE between the historical and future model simulations to determine the effects of environmental change. The historical and future CIVE are expected to differ because the exposure to stressors will change, and because the response of vegetation to climatic drivers is nonlinear (Li et al. 2022), making it possible for future sensitivity and adaptive capacity to exceed present-day bounds. Finally, we will apply the previously developed machine-learning based emergent constraint method (Yu and Mao et al. 2022) onto the CIVE and the individual indicators for each combination of stressor and ecosystem variable and determine how well the constraining framework can reduce the model biases and projection uncertainties. This procedure will use both the historical observations (e.g., observed CIVE and environmental variables highly related to CIVE) and the historical and future model ensemble simulations (e.g., CMIP6 SSPs outputs, OLMT simulations from Task TH5.2) per the necessity of the emergent constraint method.

**Table 3.7. Deliverables for Theme 5 research. Post-SPRUCE syntheses are shown in green text.**

| Task | FY | Deliverable | Lead(s) |
|---|---|---|---|
| TH5.1 | 2025 | Complete muti-site optimization framework in OLMT | Ricciuto |
| TH5.1 | 2025 | Optimize PFT-level parameters for use in ELMv3-Peatlands | Ricciuto |
| TH5.2 | 2025 | Implement 4-column peatland regional modeling framework | Ricciuto |
| TH5.2 | 2025 | Finish preparing high-resolution downscaled climate driver data | Walker |
| TH5.3 | 2025 | MODEX paper: Global investigation of how soil C traits mediate ecosystem responses to multivariate environmental change | Craig |
| TH5.3 | 2025 | Development of Compound Indicators for Vulnerable Ecosystems (CIVE) | Mao |
| TH5.1 | 2026 | Optimize parameters for Microbe and FATES enabled versions of ELMv3-Peatlands | Ricciuto |

| | | | |
|---|---|---|---|
| TH5.2 | 2026 | Complete 0.5 and 1/24 degree simulations using ELMv3-Peatlands | Shi |
| TH5.3 | 2026 | Calculation and analysis of observed and modeled CIVE for the historical and future periods | Mao |
| TH5.1 | 2027 | Produce calibrated PFT-level parameterizations for ELMv4-Peatlands | Ricciuto |
| TH5.2 | 2027 | Paper on C feedbacks | Walker, Shi, Ricciuto |
| TH5.3 | 2027 | CIVE-based ELM and CMIP6 uncertainty quantification | Mao |
| TH5.2 | 2028 | 0.5 and 1/24 degree simulations using ELMv4-Peatlands | Shi |
| TH5.2 | 2028 | Synthesis of warming response mechanisms to global peatlands. | Shi, Ricciuto, Walker |
| TH5.3 | 2028 | CIVE-based ELM and CMIP6 projection constraint | Mao |

## 3.6 Other TES SFA Supported Activities

### 3.6.1 Support for Independently Funded Collaborators

External and independently funded collaborations on the SPRUCE project (https://mnspruce.ornl.gov/node/667) will continue to be supported as a core effort through the maintenance of the SPRUCE treatments, enabling site access, the coordination of their participation in annual peat coring efforts, and the engagement of project staff on discipline-specific publications and broader syntheses.

### 3.6.2 International Wetland/Peatland Meeting

Dr. Melanie Mayes is taking the lead in planning a multi-institution international meeting on peatlands and other wetlands, along with Drs. Dan Ricciuto, Natalie Griffiths, and David Weston of ORNL, Dr. Nigel Roulet of McGill University (who also serves on the SPRUCE Advisory Board and co-leads the Peatland Carbon Study at the Mer Bleue peat bog), and Drs. Randy Kolka and Stephen Sebestyen of the USDA Forest Service. This activity was planned for earlier in the project but delayed due to the COVID-19 pandemic. The workshop is tentatively scheduled for the week of 10 June 2024 in northern Minnesota and will include field trips to SPRUCE and potentially other wetlands. We will invite participation of the Wetland Society, the wetlands sections of the Soil Science Society of America, the USDA-Forest Service, the Ecological Society of America, and DOE's Next Generation Ecosystem Experiments (NGEE) Arctic and COMPASS projects. A planning committee of ORNL and non-ORNL participants (those listed above and others) will define the scope of the meeting likely to include a combination of empirical observations, manipulative studies, and comparative modeling sessions associated with the fate of peatlands and other wetland ecosystems facing unprecedented environmental and atmospheric changes. An inclusive budget of $100K in FY 2024 is being set aside for this effort.

The team will also submit a proposal to *New Phytologist* for partial support ($8,000–10,000 EUR) for travel for European participants, and as such, will target *New Phytologist* for a summary publication. This meeting will comply with DOE's Statement of Commitment regarding conference participation (https://science.osti.gov/hep/Funding-Opportunities/Physics-Research-University-Program-Guidelines/Conference-Guidelines). Similar to our Promoting Inclusive and Equitable Research (PIER) plan (Section 6), the conference organizers will ensure a professional and safe environment for all attendees regardless of race, ethnicity, gender, gender identity or expression, sexual orientation, physical ability, nationality, age, socioeconomic status, and religious, political or personal beliefs. The meeting will adhere to the TES SFA's Code of Conduct (Section 6) which will address discrimination, harassment, and assault (including but not limited to sexual harassment and assault). The Code will be shared with everyone in advance of the meeting and will provide a mechanism for reporting complaints. The Code will include a plan for recruitment of speakers and attendees from diverse (in terms of gender representation, seniority, race, and so on) and underrepresented populations, and will address barriers for attendees including childcare and physical accessibility.

## 4. MANAGEMENT AND TEAM INTEGRATION

### 4.1 Organizational Structure and Key Personnel

The TES SFA includes science and management tasks and broad organizational themes to guide and direct research activities. The organization chart for the TES SFA beginning in FY2024 is shown in **Fig. 4.1**.

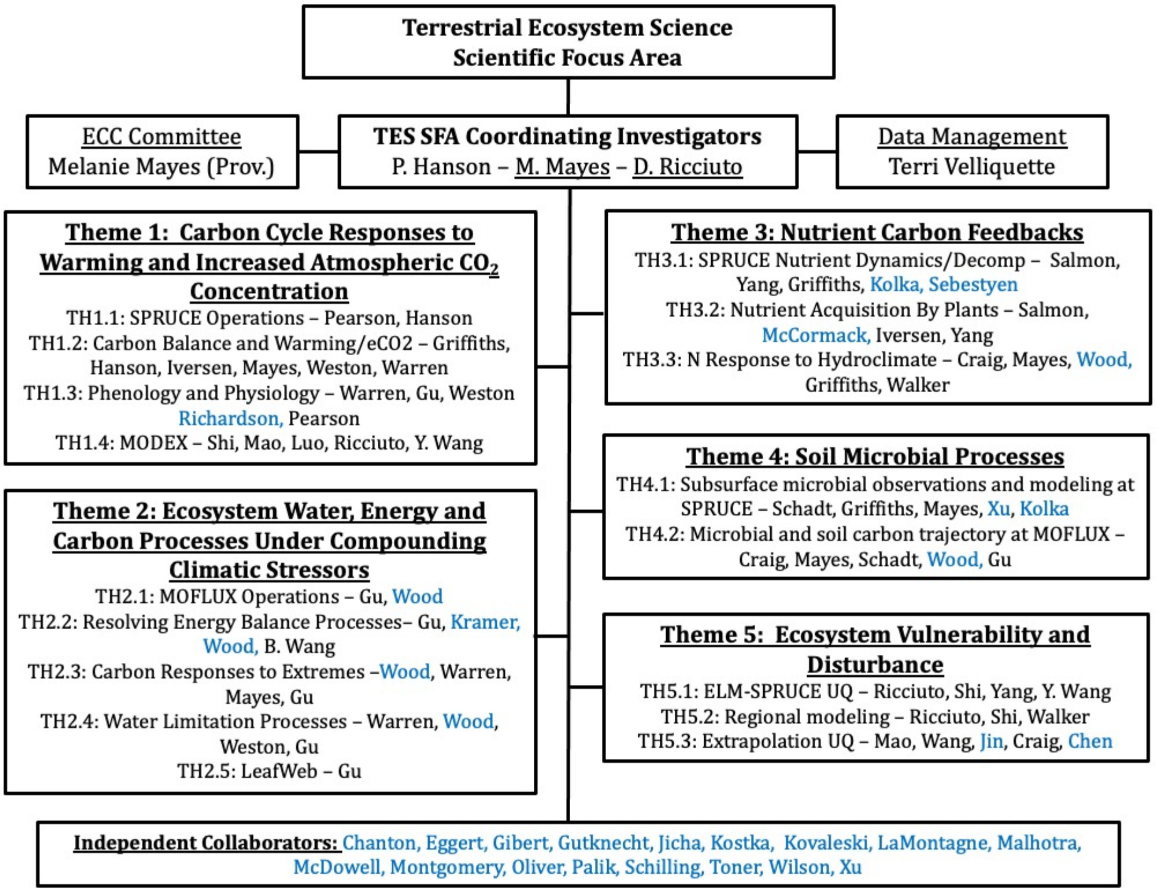


**Fig. 4.1 – Organizational chart for the TES SFA effective October 2023. Persons presented in blue text are non-ORNL participants in the ORNL TES SFA.**

Dr. Paul J. Hanson transitions from his role as lead Co-Principal Investigator for the TES SFA to that of a science advisor and Theme 1 participant in FY2024 until his planned retirement. Dr. Melanie A. Mayes and Dr. Daniel M. Ricciuto take over as the co-PI for empirical and modeling-focused tasks, respectively, which are integrated across the TES SFA. Theme Leads and Task leads described in **Fig. 4.1** and Section 7 are given independent science and financial responsibility to achieve the goals of their respective Themes and Tasks. Within ORNL, the responsibility for the TES SFA resides within the Biological and Environmental Sciences Directorate and is aligned with associated and related activities of the CCSI. The Executive Committee consists of the project Co-PIs, leads from each Theme, data management, and a representative from the Early Career Community (Section 6).

### 4.2 Project Planning and Execution

Periodic (typically monthly) teleconferences are held between the TES SFA PIs and DOE BER with the selective inclusion of project staff to cover topical items of interest. As described in Section 6, the Executive Committee meets regularly to discuss project personnel, equity, science objectives, and progress. Each Theme meets periodically to evaluate program integration and ensure progress on research tasks.

Annual budget planning for the TES SFA's proposed expenditures is a cooperative activity between the Co-PIs and ORNL accounting staff. When new annual funds are received from DOE BER they are distributed among the TES SFA Theme and Task Leads according to the funding schedule laid out in Table B3. Theme and Task Leads are expected to manage their funds throughout the fiscal year without exceeding planned funding levels. If Theme overages do occur the Coordinating PIs will cover any cost over runs from sequestered contingency carry-over funding from prior fiscal years. If such funds are insufficient, the Co-PIs consults withThemes or Tasks having excess funds within a fiscal year to balance the overall TES SFA budget.

As outlined in the following budget documents for FY 2026 through FY 2028, contingency funding accumulated since the inception of the ORNL TES SFA in the $2 million range is intended to be applied to anticipated costs associated with the phased decommissioning of the SPRUCE experiment following the completion of manipulations at the end of 2025.

### 4.3 Collaborative Research Activities

A variety of collaborations, both within the TES SFA and externally, have been and will continue to be fostered to provide necessary expertise or effort in areas critical to the completion of research tasks (see page 193). ORNL subcontract collaborations are detailed in the description of budget details. We continue to encourage key external groups to develop complementary research tasks for the benefit of TES SFA research tasks.

## 5. DATA MANAGEMENT, ESS-DIVE, COLLABORATION

The TES SFA continues to recognize the importance of the open sharing of DOE-supported scientific data products with the scientific community as well as the community at large. The TES SFA, Data Management Team (DMT) will continue its support of the research team archiving data, assigning DOIs, and making their data publicly accessible. These data sets will be freely available in a timely manner on the TES SFA and SPRUCE websites, mirrored at the DOE long-term repository at ESS-DIVE, and further distributed from ESS-DIVE into the larger repository network at DataONE (https://search.dataone.org/data). Data sets contributed to the project archive will be held to the TES SFA Data Management Plan (Appendix C) to reflect DOE and project-specific policies plus the expectations of the ESS-DIVE repository. The TES SFA Data Management Plan follows the DOE Office of Science, Statement on Digital Data Management (https://science.osti.gov/Funding-Opportunities/Digital-Data-Management) providing the data life cycle guidelines for the management of data within a project.

The DMT is responsible for developing the Data Management Plan; collaborating with staff at the ESS-DIVE repository; facilitating website function; and maintaining communication with the project team members regarding questions on data submission workflow, requirements, policies, formatting, and standards. In preparation for the SPRUCE experiment close-out, the DMT will develop a close-out timeline for data set submissions and work with researchers to ensure the delivery of data sets to ESS-DIVE.

### 5.1 Data Submission and Publication

All project-supported datasets are submitted to the respective SPRUCE or TES SFA data archive at ORNL or other DOE data type specific repository (e.g., AmeriFlux, JGI, EMSL) in a timely manner set forth in the Data Policy (see Appendix C). TES SFA research will be made publicly available concurrent with a manuscript publication if not before. All data are freely available for public access and users of these data products are recommended to follow the Creative Commons Attribution 4.0 data usage rights (CC BY 4.0) https://creativecommons.org/licenses/by/4.0/. Proper attribution of data is expected from all team members along with contacting other team members for collaboration opportunities when using their data. See the project's Data Fair Use Policy (Appendix C) for more details. In addition, project publications should contain the full data set citation in the publication reference section including the registered DOI. While data sets can be noted in the Acknowledgements or in Supporting Information, it should not be in exclusion of the Reference section.

For tracking the ingest of datasets and other tasks such as website issues, the collaborative work management tool Trello has proven useful and will continue to be used for its efficiency and tracking of deliverables. The DMT will work with the project team to develop a dataset backlog spreadsheet to assist the DMT work planning.

The DMT will have continuous reviews of the data ingest workflow looking for and incorporating improvements in assigning DOIs, developing more FAIR data products, improving data access, and incorporating the tools at the ESS-DIVE repository. The DMT will continue to populate a table for tracking team member ORCID IDs and incorporating these unique identifiers for researchers into the data sets and DOI records which is beneficial for the researcher in tracking and connecting their works.

### 5.2 Websites

The DMT is responsible for making data available to project team members and to the public on the respective SPRUCE or TES SFA websites and to post the latest data policies. The websites will be reviewed and updated as needed to reflect the current proposal research. The DMT team abides by ORNL requirements to ensure that stored data and information are protected from loss by using routine and tested backup protocols.

With the close-out of the SPRUCE experiment, the DMT will develop a plan for archiving important materials and incorporating information into the TES SFA website and the ESS-DIVE project data portal.

### 5.3 Code and Software Sharing

The DMT will encourage modelers and researchers to provide open-source products and assist in assigning DOIs to code and software products using DOECODE.

Public releases of the SPRUCE-specific E3SM code will continue to be managed by the E3SM project and subject to E3SM policies and licensing (https://e3sm.org/resources/policies/). Development branches of the E3SM code for research purposes are available through https://github.com/E3SM-Project/E3SM/. Future releases (version 3 and beyond) will be released through DOECODE with a 3-Clause BSD license. The Multi-Assumption Architecture and Testbed (MAAT) is open source and available at https://github.com/walkeranthonyp/MAAT.

### 5.4 ESS-DIVE Repository

The permanent TES SFA data archive is the ESS-DIVE repository (https://ess-dive.lbl.gov/). The TES SFA project existed prior to the stand-up of the ESS-DIVE repository with an established project archive and a well-established process for the archiving and sharing of project data products with the public. While this workflow has served the project well, the project will begin taking full advantage of the ESS-DIVE repository tools and functions. The TES SFA will be reviewing, modifying, and improving our workflow to incorporate ESS-DIVE more fully. With the increase of data products being mirrored and eventually transferred to the ESS-DIVE repository, the DMT will have more engagement with the ESS-DIVE staff on dataset submissions and with OSTI staff on DOI record transition (see Appendix C).

### 5.5 Collaboration

The DMT will have a presence at the annual ESS PI meeting to interact with the ESS community especially with other DMTs. Through additional opportunities, the DMT will build relationships with colleagues both within DOE and externally through interactions with the ESS Community, Earth Science Information Partners (ESIP), DOE OSTI, ORNL Distributed Active Archive Center (DAAC), Atmospheric Radiation Measurement user facility, ESS-DIVE, and so on. From these interactions, the TES SFA can stay current with community archiving expectations, maintain awareness of data management best practices, and can discuss project challenges and seek improvements. Terri Velliquette will continue to serve on the ESS-DIVE Archive Partnership Board learning of upcoming improvements to the repository and bringing project concerns to the board. She will also continue to serve as the Data Management Co-lead on the DOE ESS Cyberinfrastructure Working Group hosting quarterly meetings and assisting in the organization of the annual meeting.

## 6. PROMOTING INCLUSIVE AND EQUITABLE RESEARCH (PIER) PLAN

The ORNL TES SFA will create and maintain an equitable, inclusive, encouraging, and supportive research environment through the following four objectives: (1) maintain a management structure and develop a Code of Conduct to support project equity, (2) include a diverse group of individuals in the project and provide career advancement opportunities, (3) develop strong mentoring skills and cultural awareness among the entire team, and (4) seek the involvement of people historically underrepresented in the research community in the project.

*Management structure and Code of Conduct.* The goal of the TES SFA is to provide a professional and safe environment for all people regardless of race, ethnicity, gender, gender identity or expression, sexual orientation, physical ability, nationality, age, socioeconomic status, and religious, political, or personal beliefs. The TES SFA expects ethical behavior and scientific integrity from the entire team, such as full acknowledgement and attribution of contributions in papers, presentations, data publications, etc. Harassment, bullying, and discrimination of any kind will not be tolerated. The overall SFA Science Management Team consists of the SFA Coordinating Investigators, Theme Leads, all Task Leads, and the Data Manager. The Science Management Team, and all SFA participants, will meet monthly to discuss science progress and continually update project planning. The Executive Committee includes the SFA Coordinating Investigators, the Data Manager, the Theme Leads, and an Early Career Community representative (see below). The Executive Committee will meet regularly to discuss logistics, personnel development, and inclusion and equity within the group. Early Career Community representation on the Executive Committee will enable open communications between junior staff and project leaders, and thereby improve the ability to address any ethical, mentoring, or safety problems at the highest level.

The concept for an Early Career Community is designed to facilitate leadership and peer mentoring among students, technicians, and postdoctoral research participants. The Community will hold regular Microsoft Teams meetings to provide opportunities for developing multi-institutional collaborative research, troubleshooting problems with equipment and models, sharing science findings, conducting dry runs of science posters and presentations, and planning for longer-term career goals. Here, the more advanced community members (postdocs and technicians) can directly mentor the less experienced members (graduate and undergraduate students). This arrangement will benefit the junior researchers by promoting specific opportunities for engagement, and for demonstrating how the shape of career paths develop in science over time. More senior researchers will gain experience in mentoring junior researchers, and these interactions will make everyone more marketable for academic and research positions. Program funds will be requested from ORNL Environmental Sciences Division to support Early Career leadership roles.

The SFA will continue to follow ORNL's Research Code of Conduct (https://www.ornl.gov/content/research-integrity), which addresses research activities, communicating and proposing research, interpersonal interactions, and research misconduct. The Executive Committee will lead the development of a Code of Conduct in the first year of the SFA renewal, following examples available from sister DOE projects, such as NGEE Arctic and NGEE Tropics; and using concepts developed more broadly in the scientific community, e.g., https://science.osti.gov/SW-DEI/Community-Resources and https://serc.carleton.edu/advancegeo/resources/codes_conduct.html. The Code will also set expectations for behavior at meetings organized by the TES SFA (e.g., Section 3.6.2). Following these resources, our Code of Conduct will include these recommended components:

1. Identifies and defines appropriate and inappropriate behaviors
2. Goes beyond ethical treatment of data to include ethical treatment of people
3. Clearly specifies reporting and investigative procedures
4. Outlines disciplinary action for conduct violations
5. Includes protection against retaliation
6. Has built in mechanism for continued reevaluation of its effectiveness and for its revision

In the project, we will focus on both physical and emotional safety in the lab, field, and the office. Some ongoing programs are already available through ORNL's Environmental Sciences Division. One example: group leaders, traveling workers, and health/safety staff conduct a pre-travel briefing to address issues of physical and emotional safety ahead of any field work trip. Regarding concerns, we will devise a mechanism so that all participants can provide direct or anonymous feedback to anyone on the Executive Committee. This mechanism will also be available for complaints and issues observed during meetings sponsored by the TES SFA. Any feedback will be thoroughly evaluated, investigated, and remedied, while maintaining confidentiality during the investigation to the extent possible. Additionally, ORNL has an Employee Concerns Program that operates as a safety net within the Laboratory, providing an objective and independent avenue for staff to express concerns and have them constructively addressed.

*Project diversity and career advancement.* The Executive Committee includes Theme/Task Leads and the Data Manager. Nearly half of the Executive Committee members is anticipated to be women and will include at least one early career researcher (PhD within the last 10 years). There are five Themes, and each Theme has multiple hypotheses that translate to Tasks within each Theme. Task leadership includes early career researchers to distribute leadership among the SFA team. Leadership activities will position early career researchers to respond competitively to anticipated future Early Career Award opportunities, as well as other opportunities for research leadership. The TES SFA succession plan (Section 7) considers hiring plans and explicit succession proposals for the future of the TES SFA.

There are likely to be several positions which may be recruited during the project duration within the project, or as part of the broader BESSD organization, that will join the TES SFA team. Each position opening will be treated as an opportunity to increase the diversity of the research community at ORNL consistent with the goals of the ORNL DEI workforce initiatives (https://diversity.ornl.gov/goals/). We will directly contact our colleagues at Historically Black Colleges and Universities (HBCUs), Hispanic Serving Institutes, and Minority Serving Institutes (MSIs) – many of these institutions are in the southeastern US or are near our two major field sites. In particular, ORNL has strong collaborations with North Carolina A&T, Tennessee State, Florida A&M, Howard, and Fisk universities. Direct outreach to known colleagues is likely to be the most successful approach. We will direct job advertisements to national programs like Women in Engineering, Society of Women Engineers, Society of Hispanic Professional Engineers, National Society of Black Engineers, and Society for Advancement of Chicanos/Hispanics and Native Americans in Science. Our interview panels will seek to have an equitable gender balance, and as much other kinds of diversity as possible within the project and organization, while being mindful of over-burdening individuals from under-represented groups. We will include an awareness of unconscious bias during candidate screening, evaluation, interviews, and offers. Once onboarded to ORNL, staff evaluations are conducted at the Group level, and then compared at the Section level according to staff position on the pay ladder, i.e., Research and Development (R&D) staff are compared against R&D staff of their same level. A similar leveling process occurs at the Division and then the Directorate level to avoid bias in pay and to maintain equity.

Provisions in the *Management structure and Code of Conduct* section above aim to create an inclusive and welcoming social environment for a diverse SFA staff. We will also provide equitable support for individuals where personal circumstances make access to the norms of a scientific career more difficult. For example, under ORNL policies, many new parents return to work after 6-11 weeks. But young babies need regular care, which can make travel to scientific meetings especially hard. To the extent possible, we will work with conference organizers to provide daycare and scholarships for travel for accompanying caregivers, because this is not currently allowable under Federal travel rules. We will seek to find other ways to equitably support travel and other norms of a research career for people with different family and personal circumstances. One idea we are investigating would involve ORNL benefits providing this kind of coverage.

ORNL has deployed resources to make diverse groups more at home in the community. There are four updated private lactation rooms (with sinks, refrigerators, and storage lockers) including in the main Environmental and Biological Sciences building, and in the building that hosts the Climate Change Science Institute. The main Environmental and Biological Sciences building also has two gender-neutral restrooms, and ORNL is making more additions. ORNL has many Employee Resource Groups (https://diversity.ornl.gov/ergs/): African-American Resource Council, Asian Pacific American Club, Future Leaders Network, Hispanic and Latino Organization for Leadership and Awareness, PRISM for LGBTQIA+ and Allies, THRIVE for All Abilities and Allies, Women's Alliance Council, and a Veterans group for current and former armed forces, families, and communities. These groups are introduced to new staff during on-boarding and each Employee Research Group holds events each year.

At ORNL, an active postdoctoral association (https://ornlpostdoc.wordpress.com/) provides opportunities for leadership, self-governance, and mentoring. There are training opportunities for postdocs for proposal writing, presentations and communication skills, leadership coaching, interviews skills, and academic packet development. ORNL's Environmental Sciences Division Director Dr. Eric Pierce holds a Postdoc Roundtable in which he establishes a community of postdocs, provides career development activities such as seminars, CV preparation, job applications, referencing, and so on. Additionally, he holds regular individual meetings with postdocs. Each postdoc or student in this project is mentored by one or more staff in their research area, and if they are located at ORNL, they will also be mentored by a Group Leader.

We will seek out additional enrichment programs for postdocs, undergraduate, and graduate students, that involve CV preparation, job interviews, and career advice, such as Michigan Engineering's annual NextProf workshops (https://nextprof.engin.umich.edu/). Junior researchers will be provided opportunities to serve as session organizers with established SFA researchers in conferences. ORNL has additional training resources such as the Center for Creative Leadership, 7 Habits of Highly Effective Leaders, and several courses focusing on communication in English for non-native speakers.

*Mentoring skills and cultural awareness.* We will implement yearly voluntary training for SFA project staff using science-based curricula from the Center for the Improvement of Mentored Experiences in Research (CIMER) (https://cimerproject.org/). CIMER is a partner in NSF's Inclusive Graduate Education Network (IGEN) alliance. Since at least 2021, CIMER has focused on training Facilitators from the National Laboratories. Theme Leads Mayes and Salmon are currently Trained Facilitators in the CIMER curricula, and more SFA participants will be recruited in the future if possible. There are also additional Facilitators at ORNL who may be able to assist. The curriculum involves 8 sessions conducted in small groups that are led by the Trained Facilitators. Scenario analysis, group discussions, and personal reflections are tools designed to foster understanding, build sensitivity to the needs of diverse mentees, and develop mentoring skills. Following the implementation of this learning curricula in FY 2024, the Executive Committee and the Early Career Community will work together to draft a two-way mentoring agreement that will outline expected conduct, communications protocols, and delivery of research outcomes specific to different mentoring relationships in the SFA (mentor and postdoc, mentor and graduate student, mentor and post-bachelors, mentor and undergraduate student). Following NGEE Arctic and NGEE Tropics, we will partner with ADVANCEGeo (https://serc.carleton.edu/advancegeo/index.html) to host yearly sessions on bystander intervention education.

Managers in ORNL's Biological and Environmental Sciences Directorate are currently engaging in a year-long learning activity through Linked-in Learning called "Allies and Advocates: Leaning into the Discomfort" which is designed to engage leaders to foster and promote inclusive behaviors across the organization. These lessons are being shared by Group Leaders with all division staff. Allyship, unconscious bias, authentic communication, anti-racism, and bystander training are addressed, and a new directorate-wide effort is focused on parenting.

*Increasing the involvement of underrepresented groups.* Participants in this project have a long-standing relationship with Tennessee State University (TSU), an HBCU. In the past, the SFA has funded the work of a TSU PhD student, and currently, there are two DOE Research and Development Partnership Pilot projects at TSU, "Simulating Greenhouse Gas Emissions of a Peatland Ecosystem Under Global Warming and Elevated $CO_2$ at the SPRUCE Experimental Site" and "On Improvement of Soil Organic Carbon Modeling and Simulation via Integrated Deep Learning and Data Assimilation Approaches" (https://www.energy.gov/science/articles/department-energy-announces-47-million-research-and-development-partnership-pilots). The SPRUCE-oriented project is tied to Themes 1 and 5 of the TES SFA and the soil C-oriented project is tied to Theme 4 of the TES SFA. These investigators and their students will be invited into project and Theme meetings to facilitate their understanding of and involvement in the SFA. TSU is also applying for a DOE Climate Resilience Center (https://science.osti.gov/grants/FOAs/FOAs/2023/DE-FOA-0002915) that will further encourage engagement between ORNL and TSU. ORNL Environmental Sciences Division is also having discussions with two other institutions with successful Research and Development Partnership Pilot awardees (University of Minnesota at Duluth [an MSI] and Central Michigan University) – their relative proximity to the SPRUCE site could facilitate their involvement.

The TES SFA team and the University of Missouri host a successful DOE Reaching a New Energy Sciences Workforce (RENEW) project (https://science.osti.gov/-/media/funding/pdf/Awards-Lists/FY22-BER-RENEW.pdf) at the HBCU Missouri Lincoln University, which is only 30 minutes from the MOFLUX site. In this project, Lincoln students will collect data and maintain instrumentation deployed to monitor energy, water, and C budgets using an experimental watershed approach involving a network of microclimate monitoring stations and a stream depth gauging station at the outlet of a watershed in the footprint of MOFLUX. Thus, their work will contribute directly to Theme 2 and they will be involved with meetings and field and modeling activities. Different cohorts of 5 undergraduates and 1 graduate student from Lincoln will spend an intensive week at ORNL each summer for the next three years, learning about eddy covariance, data science, and Earth system modeling specifically in a workshop environment. Students from the University of Missouri will also participate. They will learn about ORNL history, science opportunities, and will meet with scientists in a variety of venues (e.g., lunch, seminars, tours, informal conversations). ORNL scientists will also help lead an overnight trip to the Great Smoky Mountains National Park, which is an International Biosphere Reserve. Some of them will be sponsored to attend NEON's 2-week Fluxcourse (https://www.neonscience.org/get-involved/events/flux-course) to learn very specialized skills in calculating fluxes from eddy covariance data.

Undergraduate students, particularly from the schools we have engagements with, will be encouraged to apply for undergraduate and graduate internship programs at ORNL. Undergraduates can apply to the SULI and the Minority Serving Institution Partnership Program, both of which enable students to work directly with mentors from ORNL while receiving stipends and living expenses. ORNL also offers additional paid programs for both undergraduate and graduate students (see https://education.ornl.gov/), as well as longer-term subcontracting opportunities to the Strata-G Corporation or directly to universities. As a part of the SFA, we will conduct outreach to Native American educational institutions in Minnesota to attract undergraduate technical participants to SPRUCE field work in the summers of 2024, 2025, and 2026. We expect some flexibility in funds through carryover and small changes in scope to enable funding of these positions. Doctoral students are eligible to apply to the DOE Office of Science Graduate Student Research program, which involves developing an in-depth proposal to conduct research, for 6 months to 1.5 years, in association with the National Laboratories. Their research proposal undergoes a panel review to determine the awardees, who will receive a stipend and living expenses during their appointment. Additionally, ORNL staff regularly recruit PhD students from the Graduate Degrees for Minorities in Engineering Fellowship program (https://education.ornl.gov/gem/), which is a prestigious program aimed at high-achieving minority students. Students from all of our collaborating institutions – which extends well beyond those listed in the PIER plan – will be encouraged to consider related topics for senior theses and advanced degrees. In most themes, we have set aside funds for student researchers to enable student growth and staff mentoring skills. For example, in Themes 1 and 4, two PhD students will be funded at San Diego State University (a Hispanic Serving Institute). Students will have the opportunity to be co-mentored by faculty, staff, postdocs, and technicians from the collaborating institutions, and thereby gain an understanding of the many diverse career pathways in science. Faculty and staff interactions will foster personal relationships that will translate into longer-term opportunities and networks for the students and enable their success in science.

## 7. PERSONNEL

The TES SFA is supported by more than 40 dedicated scientific and technical staff with a record of research, publication, and leadership in climate change research. The original team (established in 2009) has undergone numerous staff changes over time but has been supplemented by developing staff in both the modeling and experimental areas and by acquisition of key technical support personnel.

- Dr. Paul J. Hanson is the TES SFA Coordinating Investigator. He provides integrated leadership across tasks and coordinates financial management. Dr. Hanson has 37 years of experience as a plant physiologist and environmental ecologist. He previously served as an ORNL Group Leader from 2006 through 2020 managing a 29-member Ecosystem Science Group within the Environmental Sciences Division at ORNL. He was a Subject Editor for *Global Change Biology* for 18 years and is the coordinating investigator for the SPRUCE task of the TES SFA.
- Dr. Daniel M. Ricciuto is the coordinating investigator for all terrestrial C-cycle modeling aspects of the TES SFA. Dr. Ricciuto is group leader of the Earth Systems Modeling group in the CCSI within the Environmental Sciences Division at ORNL. His research expertise covers the application of data assimilation techniques that confront terrestrial C-cycle models with observations, and in the quantification of prediction uncertainty and parameter sensitivity in land surface models. Dr. Ricciuto's efforts are focused on improving model parameterization and predictive skill at spatial scales ranging from individual research and observation sites to the entire globe.
- Dr. Melanie A. Mayes has 20 years of experience in soil biogeochemistry and serves as the ORNL Biogeochemical Dynamics Group Leader in the Environmental Sciences Division. She is an Associate Editor for the journal *Biogeochemistry* and has previously edited for *Soil Science Society of America Journal*. She was a lead science editor for the Global Change Research Program's 2018 State of the Carbon Cycle Report. She is a co-lead of Theme 4 in this version of the TES SFA.
- Ms. Terri Velliquette serves as the Data Management Coordinator on two projects bringing her expertise and technical skills for data policy and archive management. She also serves on the ESS-DIVE Archive Partnership Board and is the Data Management co-lead on the DOE ESS Cyberinfrastructure Working Group.
- Mr. Thomas Ruggles is on the DMT ingesting data sets including developing metadata and reviewing data files plus maintains the TES SFA and SPRUCE web sites with project information, resources, and public data access.

*Personnel Actions Since 2019* – Key staffing changes since FY2019 provide an understanding of overall turnover experienced within the TES SFA during the COVID-19 pandemic. Dr. Richard J. Norby retired and then participated under subcontract. His prior responsibilities for a SPRUCE Task on *Sphagnum* have been transferred to Dr. David Weston.

Dr. Colleen Iversen has recently taken on new roles in the DOE NGEE Arctic program with reduced time dedicated to her TES SFA tasks. However, she retains her oversight role for SPRUCE belowground root tasks and will play a role in long-term interpretation and syntheses of results. Dr. Iversen's past responsibilities on nutrient cycling have been transitioned to Dr. Verity Salmon.

Data management organization and support activities were transitioned form Dr. Les Hook to Ms. Terri Velliquette and Mr. Thomas Ruggles since 2021.

Responsibilities for on-site SPRUCE operations and technical management in Minnesota have transferred from Mr. W. Robert Nettles to Mr. Kyle Pearson who is now supported by a full-time technician: Mr. Mark Guilliams.

Postdoctoral positions held by Drs. Camille Defrenne, Jennifer Peters, and Spencer Roth have been completed. Drs. Bin Wang and Soren Weber are the currently active postdoctoral researchers supported by the TES SFA. A new postdoctoral researcher is onboarding for the SPRUCE project.

Dr. Matt Craig who worked on MAAT in a postdoctoral position has since been hired as an Associate R & D Staff Scientist at ORNL. In addition, a SULI intern, Ms. Abigail Johnson, has started a PhD in mathematical biology at North Carolina State University as a part of a Provost Doctoral Fellowship.

Technical staff retirements and transitions within ORNL have also led to the hiring of Mr. Geoff Schwaner and other full-time senior and entry level technicians.

<u>*Succession Planning and Recent and Anticipated 2026 Transitions*</u> – We use various methods to replace TES SFA staff to ensure project continuity and productivity through time. New TES SFA staff are often hired through postdoctoral research associate positions and their performance and contributions to task activities are tracked. Our postdocs are vetted for potential future roles as task leads. Where an identified disciplinary need is established (and for which adequate funding is available) the TES SFA may hire established staff persons directly into a task leadership role. When such a need is identified, but TES SFA funding is not sufficient to initiate a hire, ORNL internal funds may be requested through a strategic hire program.

Within the TES SFA, budget management is executed as proposed by the Coordinating Investigators with feedback from Theme and Task leads when variations from the proposed expenditures arise. Individual Task leads (or other more specific sub-task leads) are given the responsibility to track scientific progress and for managing their fiscal resources within an annual cycle. Training to allow new staff to understand ORNL procedures, accounting systems, and managerial activities is provided. Such training, in addition to side-by-side transitional mentoring with established staff, provides developing staff with the information and skill sets required to transition into leadership roles. ORNL also has formal programs for mentoring high-potential early career staff, and we use informal mentoring to enable career development.

**Dr. Paul J. Hanson plans to retire from ORNL following an appropriate transiton period.** This transition will allow Melanie A. Mayes to step into the management roles for the TES SFA and others to take on SPRUCE operations and post-SPRUCE experimental work. His retirement and the associated completion of SPRUCE active treatments at the end of 2025 frees up substantial funding within the TES SFA to enable existing staff and newly hired personnel to devote more time to SPRUCE final measurements, data archiving, post-SPRUCE analysis, modeling, syntheses and decommissioning efforts.

Dr. Melanie Mayes will begin transitions to overall TES SFA management roles in FY2024. Mr. Kyle Pearson will continue to manage post-SPRUCE on-site operations in FY2026 through FY2028. SPRUCE synthesis activities will be led by various staff as described in the Theme-specific personnel summaries below.

The following proposed individual Theme and sub-task leads take responsibility for their respective initiatives.

**Theme 1 Carbon Cycle Responses to Warming and Increased Atmospheric $CO_2$ Concentration**

**Task TH1.l** Paul J. Hanson leads the management and operations of the SPRUCE project with direct support of the onsite Project Manager, Kyle Pearson. Kyle Pearson is located fulltime in Grand Rapids, Minnesota. He maintains SPRUCE operations with the support of a single full-time technical support person (Mark Guilliams). Misha Krassovski (Technical Professional systems engineer) designed and maintains site communication equipment, and he works with Kyle and Mark to sustain operations of the automated data acquisition system for SPRUCE (both environmental and biological monitoring systems). A coordinating panel consisting of the SPRUCE coordinating investigator (Hanson initially), the local USDA Forest Service contact (Kolka), the Theme and sub-task leaders for all SPRUCE activities, and members from the scientific community make up the experimental advisory panel. This group serves as the decision-making body for major SPRUCE experiment operational considerations and is the decision-making body for vetting requests for new research initiatives to be conducted at SPRUCE.

**Task TH1.2** Natalie Griffiths, Paul J. Hanson, Colleen Iversen, David Weston, Melanie Mayes, Steve Sebestyen, and postdoctoral research staff are splitting efforts in this area.

Paul Hanson will transition his lead on tree and shrub growth and vegetation phenology to Natalie A. Griffiths and Technical staff. David Weston leads characterization of growth and community dynamics of the diverse *Sphagnum* communities occupying the bog surface beneath the higher plants. Colleen Iversen, with technical assistance from Joanne Childs and John Latimer (subcontractor) follow belowground root and fungal growth. Jonathan Stelling has agreed to join the TES SFA as a post-doc beginning in May 2023. He will be based in Grand Rapids, Minnesota (supervised David Weston and Melanie Mayes). Community compositional changes are being led by Brian Palik (USDA Forest Service) and Rebecca Montgomery (University of Minnesota). Work on hydrologic cycling is led by Steve Sebestyen (USDA Forest Service) and Natalie Griffiths (ORNL).

**Task TH1.3** Lianhong Gu, Jeff Warren, Andrew Richardson, and Kyle Pearson work on this task. Characterization of plant physiological responses are led by Jeff Warren, past and planned postdoctoral staff, and independently funded external collaborators. We are actively encouraging additional external participation in the observations of physiological processes including gas exchange, carbohydrate dynamics, C partitioning, hydraulic conductivity, and woody respiration assessments. Through an external subcontract, Andrew Richardson interprets automated tree and shrub canopy phonologic patterns assisted by Kyle Pearson who collects biweekly on-the-ground observations of changing vegetation conditions.

**Task TH1.4** Key modelers include Xiaoying Shi, Jiafu Mao, Xiaojuan Yang, Daniel Ricciuto, and Yaoping Wang at ORNL with external subcontracted efforts led by Xiaofeng Xu and Yiqi Luo. Dr. Shi will lead SPRUCEMIP with contributions from Dr. Ricciuto and Dr. Wang. Dr. Shi and Dr. Ricciuto will further improve the *Sphagnum* submodel as well. Dr. Luo will also work with SPRUCEMIP outputs to create a traceability framework. Dr. Mao will lead efforts to improve phenology and allocation modeling in ELM-SPRUCE along with Dr. Wang. Dr. Yang will work in improving the representation of isotopes in ELM-SPRUCE, as well as nutrient cycling. Dr. Xu and Dr. Ricciuto will further improve the representation of methane cycling. All personnel will be involved in working with empiricists in Theme 1 to validate and calibrate ELM-SPRUCE with past and proposed observations.

**Theme 2 Ecosystem Water, Energy, and C Processes under Compounding Climatic Stressors**

Jeff Warren (ORNL) leads plant hydraulic and water relations work along the SPAC, including neutron imaging of root-rhizosphere dynamics and collaborates with Luke McCormack (MA) on soil respiration at MA. Melanie Mayes (ORNL) leads soil C flux activities at MOFLUX. Jeff Wood (University of Missouri) leads onsite activities at MOFLUX, including analysis of ecosystem responses to drought. Lianhong Gu (ORNL) leads activities in measuring and analyzing fluxes of trace gases, water vapor, energy and SIF, and leads LeafWeb. David Kramer (Michigan State University) contributes to detailed investigation of PMF bioenergetics. David Weston leads investigations of microbial-plant interactions.

**Theme 3 Nutrient Carbon Feedbacks**

Verity Salmon will lead the empirical measurements of N and P mineralization, vegetation nutrient stoichiometry, and the SPRUCE destructive N and P observations at the end of experimental manipulations. Verity Salmon will also work with Natalie Griffiths on measuring leaf litter nutrient concentration. Griffiths, along with Steve Sebestyen (USDA Forest Service) and Keith Oleheiser (ORNL) will lead efforts on measuring depth-specific nutrient concentration in porewater and lateral outflow, and C, N, P dynamics during *Sphagnum* decomposition. Luke McCormack will collect measurements of nutrient cycling and nutrient uptake at MA. Xiaojuan Yang will lead the efforts in integrating the measurements at SPRUCE and MA into ELM-SPRUCE to improve the model representation of nutrient cycling dynamics and nutrient uptake. Matt Craig and Melanie Mayes will lead the measurements of nutrient pools and fluxes at MOFLUX. Matt Craig, Melanie Mayes, and Anthony Walker will develop nutrient-enabled MAAT framework and evaluate and improve MAAT and ELM-FATES using measurements at MOFLUX.

Luke McCormack and Colleen Iversen will further develop and expand FRED to include more fine root traits relevant to nutrient uptake and increase the global coverage.

**Theme 4 Soil Carbon Cycling and Microbial Processes**

**Task TH4.1** Chris Schadt and technician Alyssa Carrell, along with SPRUCE technical staff, will complete the sampling and analysis of SPRUCE microbial communities. Funding limitations in FY 2024–2025 mean that the analyses will be performed in FY 2026 and beyond. Natalie Griffiths and Randy Kolka lead the field-scale decomposition tasks, with assistance from Chris, Alyssa, and SPRUCE technical staff for analyses. Melanie Mayes will lead the SPRUCE incubation experiments, with assistance from Natalie, Chris, and SPRUCE technical staff. Xiaofeng Xu of San Diego State University will lead the microbial modeling portion.

**Task TH4.2** Jeff Wood at the University of Missouri will collect MOFLUX samples and ship them to Melanie Mayes for analyses by SPRUCE technical staff. Field-scale litter decomposition experiments will be assembled by Jeff Wood, Melanie Mayes, and Matt Craig, and analyses of the microbial community will be performed by Chris Schadt and technician Alyssa Carrell, along with SPRUCE technical staff. Matt Craig will lead the incubation experiments with assistance from Melanie Mayes and SPRUCE technical staff. Matt Craig and a new R&D staff hire will lead the MOFLUX soil C and microbial modeling activities using the MAAT framework.

**Theme 5 Regional Integration and Extrapolation**

**Task TH5.1** Daniel Ricciuto will lead model-data calibration efforts using OLMT. Xiaoying Shi and Xiaojuan Yang will help to integrate the model developments from themes 1-4 into the site-level versions of ELM-SPRUCE and ELM-Peatlands to be used. Anthony Walker will help to test and develop FATES within the ELM-Peatlands framework.

**Task TH5.2** Anthony Walker will lead the regional modeling efforts and work with Daniel Ricciuto and Xiaoying Shi to perform the simulations. Deeksha Rastogi and Shih-Chieh Kao will assist in providing downscaled meteorological drivers for the high-resolution simulations. Dali Wang will provide other input datasets and the high-performance computing infrastructure to perform the high-resolution simulations.

**Task TH5.3** Key modelers include Jiafu Mao, Yaoping Wang, and Matthew Craig at ORNL with external subcontracted efforts led by Mingzhou Jin and Anping Chen. Dr. Mao will lead efforts to develop the CIVE and identify where and in which season the greatest vulnerability is expected along with Dr. Wang and Dr. Craig. Dr. Jin will compare the modeled and observed CIVE to quantify model uncertainties. Dr. Chen will apply the emergent constraint framework to reduce uncertainties in model-projected CIVE. All personnel will work together and be involved in working with modelers in TH5.1 and TH5.2, evaluating and constraining CIVE simulations across scales.

Person-specific annual effort is summarized for periods of ongoing SPRUCE operations (FY2024 and FY2025; Table 7.1), and for post-SPRUCE research efforts (Table 7.2).

**Table 7.1 – Anticipated FY 2024–FY 2025 average annual person hours by TES SFA Task (160 hours = 1 person month).**

| Personnel Contributing to Tasks | TES SFA Mgmt | SPRUCE Operations | Theme 1 | Theme 2 | Theme 3 | Theme 4 | Theme 5 |
|---|---|---|---|---|---|---|---|
| **Scientific Staff** | | | | | | | |
| Craig M | -- | -- | -- | -- | 320 | 300 | 160 |
| Griffiths N | -- | -- | 100 | -- | 250 | 250 | -- |
| Gu L | -- | -- | 560 | 820 | -- | -- | -- |
| Hanson P | 180 | 160 | 1280 | -- | -- | -- | -- |
| Iversen C | -- | -- | 140 | -- | 100 | -- | -- |
| Mao J | -- | -- | 310 | -- | -- | -- | 560 |
| Mayes M | -- | -- | -- | -- | -- | 650 | -- |
| Ricciuto D | -- | -- | 360 | -- | -- | -- | 355 |
| Salmon V | -- | -- | -- | -- | 700 | -- | -- |
| Schadt C | -- | -- | -- | -- | -- | 530 | -- |
| Shi X | -- | -- | 340 | -- | -- | -- | 340 |
| Walker A | -- | -- | -- | -- | 300 | -- | 340 |
| Wang D | -- | -- | -- | -- | -- | -- | 440 |
| Warren J | -- | -- | 850 | 320 | -- | -- | -- |
| Weston D | -- | -- | 455 | -- | -- | -- | -- |
| Yang X | -- | -- | 160 | -- | 340 | -- | 160 |
| Other Science Staff | -- | -- | 175 | 100 | 372 | 270 | 305 |
| USDA Forest Service In Kind – Science** | -- | -- | -- | -- | 440 | 440 | -- |
| **Postdoctoral Staff** | | | | | | | |
| Stelling, Weber | -- | -- | 1872 | -- | -- | 480 | -- |
| **Technical Professional** | | | | | | | |
| Krassovski M | 450 | 450 | -- | -- | -- | -- | -- |
| Ruggles T | 450 | -- | -- | -- | -- | -- | -- |
| Velliquette T | 450 | -- | -- | -- | -- | -- | -- |
| **Technical Staff** | | | | | | | |
| Schwaner G (ORNL) | 1300 | -- | -- | -- | -- | -- | -- |
| Childs J (ORNL) | 1500 | -- | -- | -- | -- | -- | -- |
| Pearson K (ORNL-MN) | -- | 1872 | -- | -- | -- | -- | -- |
| Guilliams M (ORNL-MN) | -- | 1872 | -- | -- | -- | -- | -- |
| Oleheiser K (ORNL-MN) | -- | -- | -- | -- | 1872 | -- | -- |
| Other Technical (ORNL) | 1500 | -- | 468 | 200 | -- | 120 | -- |
| Wood (Univ. of Missouri) | -- | -- | -- | 468 | -- | -- | -- |
| **Estimated Annual Person Hours By Task** | 5830 | 4354 | 7070 | 1908 | 4694 | 3040 | 2660 |

*Some hours for support staff shown under Task 1 apply across the TES SFA.

**Unfunded in-kind effort estimated by Randall K. Kolka USDA Forest Service, Northern Research Station.

**Table 7.2 – Anticipated FY 2026–FY 2028 average annual person hours by TES SFA Task (160 hours = 1 person month).**

| Personnel Contributing to Tasks | TES SFA Mgmt | SPRUCE Operations | Theme 1 | Theme 2 | Theme 3 | Theme 4 | Theme 5 |
|---|---|---|---|---|---|---|---|
| **Scientific Staff** | | | | | | | |
| Craig M | -- | -- | -- | -- | 320 | 500 | 116 |
| Griffiths N | -- | -- | 100 | -- | 250 | 250 | -- |
| Gu L | -- | -- | 400 | 960 | -- | -- | -- |
| Hanson P | 27 | 53 | -- | -- | -- | -- | -- |
| Iversen C | -- | -- | 267 | -- | 200 | -- | -- |
| Mao J | -- | -- | 375 | -- | -- | -- | 625 |
| Mayes M | 200 | -- | -- | 240 | -- | 600 | -- |
| Ricciuto D | -- | -- | 375 | -- | -- | -- | 375 |
| Salmon V | -- | -- | -- | -- | 781 | -- | -- |
| Schadt C | -- | -- | -- | -- | -- | 587 | -- |
| Shi X | -- | -- | 375 | -- | -- | -- | 375 |
| Walker A | -- | -- | -- | -- | 300 | -- | 355 |
| Wang D | -- | -- | -- | -- | -- | -- | 468 |
| Warren J | -- | -- | 600 | 627 | -- | -- | -- |
| Weston D | -- | -- | 470 | 465 | -- | -- | -- |
| Yang X | -- | -- | 185 | -- | 360 | -- | 185 |
| Other Science Staff | -- | -- | 702 | 320 | 828 | 500 | 1400 |
| USDA Forest Service In Kind – Science** | -- | -- | -- | -- | 400 | 400 | -- |
| **Postdoctoral Staff** | | | | | | | |
| Stelling, TBD | -- | -- | 1610 | 1558 | 1868 | -- | -- |
| **Technical Professional** | | | | | | | |
| Krassovski M | 450 | 450 | -- | -- | -- | -- | -- |
| Ruggles T | 500 | -- | -- | -- | -- | -- | -- |
| Velliquette T | 500 | -- | -- | -- | -- | -- | -- |
| **Technical Staff** | | | | | | | |
| Schwaner G (ORNL) | 1500 | -- | -- | -- | -- | -- | -- |
| Childs J (ORNL) | 1500 | -- | -- | -- | -- | -- | -- |
| Pearson K (ORNL-MN) | -- | 1872 | -- | -- | -- | -- | -- |
| Guilliams M (ORNL-MN) | -- | 1872 | -- | -- | -- | -- | -- |
| Oleheiser K (ORNL-MN) | -- | -- | -- | -- | 1872 | -- | -- |
| Other Technical (ORNL) | 1500 | -- | 0 | 467 | 120 | 267 | -- |
| Wood (Univ. of Missouri) | -- | -- | -- | 468 | -- | -- | -- |
| **Estimated Annual Person Hours By Task** | 6177 | 4247 | 5469 | 5105 | 7299 | 3104 | 3899 |

*Some hours for support staff shown under Task 1 apply across the TES SFA.

**Unfunded in-kind effort estimated by Randall K. Kolka USDA Forest Service, Northern Research Station.

## 8. FACILITIES AND RESOURCES

ORNL has made substantial investments in climate change modeling, the development of innovative large-scale experimental infrastructures through the Laboratory Directed Research and Development program (LDRD), and in the construction of other critical infrastructure, including a field support building (Building 1521), greenhouses, the Joint Institute for Biological Sciences, and renovations in support of molecular ecology. Other internal funding is allocated annually from the division or directorate based on need and general utility to the acquisition of multi-user instrumentation that will benefit multiple users and projects. Greenhouses, incubation chambers and walk in growth chambers (including an extreme chamber; -10 to +55 °C) are available.

ORNL's Environmental Sciences Division hosts instruments for measuring soil and water chemistry and greenhouse gasses. In the lab, the Environmental Sciences Division has a Picarro G2508 analyzer that can continuously measure $CO_2$, $CH_4$, $NH_4$, $N_2O$, and water vapor in incubation experiments. A Columbus Instruments Micro-Oxymax Respirometer is available for continuous measurements of lab-scale incubations (up to 24 channels) and is capable of detecting $CO_2$, $CH_4$, $H_2S$, $H_2$, and $O_2$. A Shimadzu GC-2014 with AOC autosampler is designed to detect $CO_2$, $CH_4$, $N_2O$, $O_2$, and CO in gaseous or liquid headspace samples in the laboratory. A Picarro water isotope analyzer available for analysis of natural abundance stable isotopes of water. Two Shimadzu TOC-L/TNM-L combustion analyzers can determine DOC and dissolved organic N in liquid samples. A Smartchem 200 Discrete Analyzer, Seal AutoAnalyzer 3 HR, and a Lachat Quickchem 8500 are used for automated determination of $NH_4$, $NO_3$ and $PO_4$ concentrations of liquid samples. An Elementar CN analyzer is available for determination of C and N in solid phase samples. ORNL also has an EA coupled to an isotope ratio mass spectrometer for measuring the $\delta^{13}C$ and $\delta^{15}N$ signature of solid samples (Thermo Fisher Delta V Advantage Mass Spectrometer, Conflo IV, and EA Flash Isolink). An Ethos-Up microwave digester is available for digestion of soil and rock materials. Two high performance liquid ion chromatography are available for determination of anions and organic acids (Agilent G5668A, Thermo (Dionex) ISC-5000+ DC/EG/DP). There are two inductively-coupled plasma mass spectrometry instruments (PerkinElmer NexION 2000) for elemental isotopic analysis. A variety of shakers, centrifuges and ultracentrifuges, and incubators are available for batch and microbial work. A large glovebag is available in the soils lab for anaerobic incubations and analyses. The plant and soils labs are outfitted with equipment to perform drying, sorting, sieving, grinding, and storage of plant and soil materials.

The TES SFA is supported by world-class computing capabilities. The National Leadership Computing Facility provides an open, unclassified resource that we use to enable breakthroughs in climate prediction. It houses the largest unclassified computing capability available to climate change researchers in the world. Personnel within the Atmospheric Radiation Measurement Program data system and the NASA Distributed Active Archive Center for Biogeochemical Dynamics provide additional expertise in the area of data management. ORNL established CADES to meet the need for integrated computing and data capabilities in an efficient and cost-effective manner. CADES offers the following data and infrastructure resources: a multi-petabyte parallel file system and computing cluster in a CADES open research environment. The CADES Kernel system coming online in 2023 features an 18,000-core computing cluster available to all users at ORNL with 140 128-core AMD 7713 processors. 20 additional nodes have been purchased for exclusive use by the ORNL CCSI, including this project. Data may be archived from CADES directly to the High-Performance Storage System, a 132 PB system managed by the ORNL Leadership Computing Facility consisting of tape and disk storage components with Linux servers and storage software.

The High Flux Isotope Reactor and the Spallation Neutron Source at ORNL are used to understand physical, chemical, and biological complexity in plant and soil processes. The Versatile Neutron Imaging Beam line at the Spallation Neutron Source (VENUS) comes online in 2024. Other external facilities to be used include the LLNL – Center for Accelerator Mass Spectrometry provides large volume, high precision $^{14}C$ measurements. Pacific Northwest National Laboratory's Environmental Molecular Science Laboratory combines advanced instrumentation such as high-throughput mass spectrometry, advanced microscopy instruments, and nuclear magnetic resonance instruments with high performance computing.

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# Listing of External Collaborations

## TES SFA FUNDED EXTERNAL COLLABORATIONS

The following individuals or groups are being subcontracted to facilitate the execution of TES SFA task science. Subcontract budget details are provided in the Section G.5.

**Theme 1:** Funding will be provided for 1) onsite SPRUCE maintenance, 2) sustained support for operation of the AMR systems, 3) support for $^{14}C$ analysis of air, peat, and plant material and their interpretation with Karis McFarlane at Lawrence Livermore National Laboratory, 4) terrestrial lidar scanning including focused allometry-based model assessment of tree LAI through time with Nancy Glenn at Boise State University, and 5) automated phenology observations and their interpretation by Andrew Richardson at Northern Arizona University. Other funding will be allocated to fund manual minirhizotron data collection under subcontract (John Latimer), and support for on-site operations (Pokegama Electric).

**Themes 1, 2, and 5:** We will contract with Dr. Xiaofeng Xu at San Diego State University to continue incorporating his microbial decomposition and methane module into CLM, and to parameterize and evaluate this model with SPRUCE observations. A second subcontract is planned to Dr. Yiqi Luo (Cornell University) for software development and development of data assimilation techniques at the SPRUCE and MOFLUX sites for ecological forecasting.

**Theme 2:** We contract with Dr. Jeffrey D. Wood and a full-time technician (Mr. Brian Widmer, supervised by Dr. Wood) at the University of Missouri for full management and support of the operation of the MOFLUX tower site. Dr. Wood is also a key contributor to various science objectives related to C, water, and energy tasks as outlined in the description of Theme 2 in Section 3.2.

We contract with Dr. David Kramer and a graduate student (Mr. Josh Temple, supervised by Dr. Kramer) at the Michigan State University to conduct mechanistic simulations of the dynamics of chloroplast PMF, and estimate the total energy storage including contributions from the trans-thylakoid electric field, proton concentration and ion gradients.

We contract with Mr. James Kolpack at Kolpack Software Engineering to manage the LeafWeb user interface (www.leafweb.org) and develop graphic and data searching capabilities for LeafWeb.

**Theme 3:** Luke McCormack will be subcontracted to support 1) management and field data collection at The Morton Arboretum as well as 2) curation, development, and release FRED. These efforts directly contribute to execution of research objectives in Theme 3 (3.3.2, Nutrient acquisition by plants) and Theme 2 (3.2.4, Quantifying C process responses to environmental extremes).

**Theme 4:** Dr. Xiaofeng Xu at San Diego State University will integrate high spatial resolution metagenomic and microbial data from the SPRUCE site to understand how different microbial functional groups and soil physical and chemical properties contribute to emissions of $CO_2$ and $CH_4$.

## INVESTIGATOR-INITIATED SPRUCE COLLABORATIONS

SPRUCE has generated significant interest in the scientific community, and we have strived to actively attract and engage a range of collaborators to address disciplines and science questions not covered by ORNL and USDA Forest Service researchers. We have hosted more than 25 projects representing 21 universities, Lawrence Livermore National Laboratory, the USDA Forest Service (Minnesota and Oregon), the US Environmental Protection Agency (EPA; Duluth, Minnesota) and the DOE Joint Genome Institute. More than 100 persons are on our distribution listing for these funded projects and routinely participate in monthly teleconferences on SPRUCE science and project operational details.

The following list of current research projects were initiated and developed by the listed investigators and institutions to take advantage of SPRUCE research and infrastructures. Their funding is independent from the TES SFA budget, but their efforts are coordinated with overall SPRUCE project activities through monthly discussions and organized campaign-based sampling activities.

1. **Uncovering the microbial networks that degrade plant-derived phenolic compounds and their role in peatland soil carbon sequestration: revisiting the 'enzyme latch' hypothesis.** PIs: Joel E.

Kostka, Georgia Institute of Technology and Jeffrey P. Chanton, Florida State University. Source of Support: U.S. Department of Energy (2022 – 2025).

2. **CAREER Grant: Integrating a Microbial Data System with an Earth System Model for Evaluating Microbial Biogeochemistry.** PI: Xiaofeng Xu, San Diego State University (2022 – 2027).
3. **Effects of whole ecosystem warming on chill accumulation and cold hardiness of woody perennials**. PI: Al Kovaleski, University of Wisconsin, Source of support: McIntire-Stennis Formula Grant (2021 – 2024).
4. **Using nutrient cycling to understand ecosystem function and response to climate change.** PI: Terri M. Jicha, US Environmental Protection Agency (2014 – present).
5. **Black spruce and Eastern tamarack cone production and cone characteristics.** PI: Jalene M. LaMontagne, DePaul University (2017 – present).
6. **Root trait responses to peatland warming**. PIs: Avni Malhotra and Tiia Määttä, University of Zürich (2022 – present)
7. **Soil fauna biodiversity sampling at SPRUCE**. PI: Zoë Lindo, University of Western Ontario (2015 – present).
8. **Mercury and sulfur dynamics in the spruce experiment.** PIs: Brandy Toner, University of Minnesota and Randy Kolka and Steve Sebestyen, USDA Forest Service MN. Source of Support: USDA Forest Service Northern Research Station, Department of Energy (ORNL), Congressional Directive (2013 – present).
9. **Wood decomposition rates and functional types in a shifting climate.** PIs: Jonathan Schilling and Jason Oliver, University of Minnesota, and Randy Kolka, US Forest Service. Source of Support: USDA Forest Service Northern Research Station, University of Minnesota, (2015 – present).
10. **Microbial growth and carbon and nutrient use partitioning under peatland warming and elevated $CO_2$.** PI: Jessica Gutknecht, University of Minnesota. Source of Support: Sea Grant, USDA Forest Service Northern Research Station (2016 – present).
11. **The net impact of rising $CO_2$ versus vapor pressure deficit on plant mortality.** PI: Nathan McDowell, Pacific Northwest National Laboratory. Source of Support: National Science Foundation.

# APPENDIX A: ORNL TES SFA Publications

Published, accepted and in press articles completed since the last triennial review (i.e., March 2019 through September 2022). We have published 178 unique papers over this 4-year period which equals 44.5 publications per year, or on average 6.8 Publications FTE$^{-1}$ where an FTE is a full-time equivalent research professional.

Participants since March 2019 included in the count of 26 FTEs: Iversen, Griffiths, Gu, Hanson, Johnston, King, Krassovski, Liang, Liu, Lu, Malhotra, Mao, Mayes, Norby, Ricciuto, Salmon, Schadt, Shi, Yang, Walker, Wang G, Ward, Warren, Weston, Wood and Xu.

## ORNL TES SFA Publications March 2019 through February 2022

1. Albert, LP, Restrepo-Coupe N, Smith MN, Wu J, Chavana-Bryant C, Prohaska N, Taylor TC, Martins GA, Ciais P, Mao JF, Arain MA, Li W, Shi XY, Ricciuto DM, Huxman TE, McMahon SM, Saleska SR (2019) Cryptic phenology in plants: Case studies, implications, and recommendations. *Global Change Biology* 25:3591-3608. doi:10.1111/gcb.14759.
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3. Bastos A, O'Sullivan M, Ciais P, Makowski D, Sitch S, Friedlingstein P, Chevallier F, Rödenbeck C, Pongratz J, Luijkx IT, Patra PK, Peylin P, Canadell JG, Lauerwald R, Li W, Smith NE, Peters W, Goll DS, Jain AK, Kato E, Lienert S, Lombardozzi DL, Haverd V, Nabel JEMS, Poulter B, Tian H, Walker AP, Zaehle S (2020) Sources of Uncertainty in Regional and Global Terrestrial $CO_2$ Exchange Estimates. *Global Biogeochemical Cycles* 34: e2019GB006393. doi:10.1029/2019GB006393
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9. Caplan JS, Meiners SJ, Flores-Moreno H, McCormack ML (2019) Fine-root traits are linked to species dynamics in a successional plant community. *Ecology* 100:e02588. https://doi.org/10.1002/ecy.2588
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## APPENDIX B: ORNL TES SFA Data Sets and Software

The TES SFA data products are served to the public with CC BY 4.0 data usage rights license and accessible on the SPRUCE (https://mnspruce.ornl.gov) and TES SFA (https://tes-sfa.ornl.gov) websites with some available at the ESS-DIVE repository (https://data.ess-dive.lbl.gov/data). Researchers are encouraged to publish the federally funded scientific data in a timely manner. While all metadata records are available to the public, researchers may request that some data collections be accessible only to the project team typically while awaiting associated manuscript publication. Data users should include the full data set citation with the DOI in the reference section of any published paper.

These datasets include regularly updated time-series of SPRUCE environmental data, peat analyses, modeling archives, code releases, results of laboratory incubations, links to genomic products at JGI, "supporting validation data" for specific publications (e.g., organic matter characterization), web-based tools (e.g., LeafWeb), historical Walker Branch data, literature compilations (e.g., FRED 3.0), and characterization of SPRUCE plots (e.g., elevation).

**TES SFA Software:**

1. MAAT v1.3.1 is now open source and is available at https://github.com/walkeranthonyp/MAAT.
2. IMACSS, the software that controls FAME, has been licensed to Campbell Scientific Inc.

**SPRUCE Public Data Sets (**New or Upgraded since February 2019):**

1. **Baysinger MR, Wilson RM, Hanson PJ, Kostka JE, Chanton JP (2021D). **SPRUCE Compositional Stability of Peat in Ecosystem-Scale Warming Mesocosms, 2014 and 2019**. Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.25581/spruce.093/1820162
2. **Childs J, Defrenne CE, Brice DJ, Woodward J, Holbrook KN, Nettles WR, Taggart M, Iversen CM (2020D) **SPRUCE High-Resolution Minirhizotrons in an Experimentally-Warmed Peatland Provide an Unprecedented Glimpse at Fine Roots and their Fungal Partners: Supporting Data**. Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.25581/spruce.081/1637336
3. **Dusenge ME, Ward EJ, Warren JM, McLennan DA, Stinziano JR, Murphy BK, King AW, Childs J, Brice DJ, Phillips JR, Stefanski A, Villanueva R, Wullschleger SD, Cruz M, Reich PB, Way DA (2020D) **SPRUCE Photosynthesis and Respiration of *Picea mariana* and *Larix laricina* in SPRUCE Experimental Plots, 2016-2017**. Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.25581/spruce.056/1455138
4. Dusenge ME, Stinziano RJ, Warren JM, Ward EJ, Wullschleger SD, Hanson PJ, Way DA (2018D) **SPRUCE Whole Ecosystem Warming (WEW) Photosynthesis and Respiration of *Picea* and *Larix* in Experimental Plots, 2016.** Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.25581/spruce.056/1455138
5. Fernandez CW, Heckman K, Kolka R, Kennedy PG (2019D) **SPRUCE Fungal Necromass Litter Bag Decomposition Study in SPRUCE Experimental Plots, 2016-2018.** Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.25581/spruce.063/1503589
6. Finzi AF, Giasson MA, Gill AL (2016D) **SPRUCE Autochamber $CO_2$ and $CH_4$ Flux Data for the SPRUCE Experimental Plots.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, US Department of Energy, Oak Ridge, Tennessee. http://dx.doi.org/10.3334/CDIAC/SPRUCE.016
7. Furze ME, Jensen AM, Warren JM, Richardson AD (2018D) **SPRUCE S1 Bog Seasonal Patterns of Nonstructural Carbohydrates in Larix, Picea, Rhododendron, and Chamaedaphne, 2013.** Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.25581/spruce.037/1473917

8. **Graham JD, Glenn NF, Spaete LP (2019Da) **SPRUCE Terrestrial Laser Scanning of Experimental Plots Beginning in 2015.** Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.25581/spruce.067/1515552
9. Graham JD, Glenn NF, Spaete LP (2019Db) **SPRUCE Microtopography of Experimental Plots Derived from Terrestrial Laser Scans Beginning in 2016.** Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.25581/spruce.068/1515553
10. Griffiths NA, Hook LA, Hanson PJ (2016Da) **SPRUCE S1 Bog and SPRUCE Experiment Location Survey Results, 2015 and 2020.** Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.3334/CDIAC/spruce.015
11. Griffiths NA, Sebestyen SD (2016Db) **SPRUCE S1 Bog Porewater, Groundwater, and Stream Chemistry Data: 2011-2013.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, US Department of Energy, Oak Ridge, Tennessee. http://dx.doi.org/10.3334/CDIAC/spruce.018
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94. Furman OS, Tfaily MM, Nicholas SL, Wasik JC, Sebestyen SD, Kolka RK, Nater EA, Toner BM (2016D) **SPRUCE Peat Mercury, Methylmercury and Sulfur Concentrations from Experimental Plot Cores, 2012.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, US Department of Energy, Oak Ridge, Tennessee. http://dx.doi.org/10.3334/CDIAC/spruce.027
95. Heiderman RR, Nettles WR, Ontl TA, Latimer JM, Richardson AD, Hanson PJ (2018D) **SPRUCE Manual Phenology Observations and Photographs Beginning in 2010**. Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.25581/spruce.054/1444106
96. **Krassovski MB, Hanson PJ (2020D) **SPRUCE Experimental Plot Top View Aerial Photographs beginning June 2019.** Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee. https://doi.org/10.25581/spruce.076/1604061
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29. **Tool for Evaluating Mesophyll Impact on Predicting Photosynthesis (TEMIPP).** TEMIPP is a Microsoft Excel spreadsheet-based tool used for demonstrating the impact of lacking an explicit representation of mesophyll diffusion in a photosynthetic model on the predicted response of photosynthesis to the increase in $CO_2$ partial pressures. TEMIPP is provided as a supplement to the recent publication: Sun Y, Gu L, Dickinson RE, Norby RJ, Pallardy SG, Hoffman FM (2014) Impact of mesophyll diffusion on estimated global land $CO_2$ fertilization. *Proceedings of the National Academy of Sciences of the United States of America* 15774–15779, doi: 10.1073/pnas.1418075111. Download TEMIPP at http://TES SFA.ornl.gov/node/80.
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# APPENDIX C: ORNL TES SFA Data Management Plan

The open sharing of all data and results from TES SFA experiments, research, and modeling tasks among researchers, the broader scientific community, and the public is critical to advancing the mission of DOE's TES program. Active data sharing facilitates delivery of SFA products to our stakeholders and the broader community. This Data Management Plan. and data use policy mirrors the DOE policies provided below and will be updated, if needed, following any new policy releases.

- DOE Office of Science https://science.osti.gov/Funding-Opportunities/Digital-Data-Management
- Biological and Environmental Research Program https://science.osti.gov/ber/Funding-Opportunities/Digital-Data-Management
- DOE Public Access Plan (https://www.energy.gov/sites/default/files/2014/08/f18/DOE_Public_Access%20Plan_FINAL.pdf)

ESS-DIVE is the permanent data archive for Earth and environmental science data. ESS-DIVE is funded by the Data Management program within the Climate and Environmental Science Division under the DOE's Office of Biological and Environmental Research program (BER) and is maintained by the Lawrence Berkeley National Laboratory. The TES SFA is working in collaboration with ESS-DIVE to mirror archived data products produced by the TES SFA to this final repository. The TES SFA Data Management Team (DMT) will evaluate the current archive process to better incorporate and utilize the repository in the archive workflow since ESS-DIVE has made major improvements in functionality that now facilitates our project workflow. These evaluations and improvements are noted throughout the data management plan.

The TES SFA has a DMT of two staff members responsible for metadata and data ingest and archive; to develop the Data Management Plan and Data Policies; to facilitate website function and content update by working with ORNL Drupal team; and to provide access to public and private data packages on the project websites and at ESS-DIVE. The DMT team attends regular staff meetings and all-hands meetings to provide updates on the latest data released, to encourage team members to attend ESS-DIVE webinars/workshops, to answer questions, and to hear about data in development. The team also works closely with staff at ESS-DIVE and OSTI plus maintains involvement with other groups to learn about how standards are being developed and implemented (e.g., Earth Science Information Partners, ORNL DAAC).

In preparation for the SPRUCE experiment close-out, the DMT will develop a close-out timeline for dataset submissions and work with researchers to ensure the delivery of datasets to ESS-DIVE. The DMT will maintain an open collaboration and regular meetings with ESS-DIVE and OSTI during the wrap-up and transfer of ownership for data packages and DOIs. Access of the SPRUCE data packages will continue to be available through the ESS-DIVE repository.

## Data Types and Sources

TES SFA research data will be incoming from observations and platforms through the ecosystem manipulation at the SPRUCE experiment, a landscape-scale observation site at MOFLUX, and process-level observations at MA; plus, laboratory soil incubations; models; and curation and expansion of a global root-trait database (FRED); and support of improvements to the web-based analytical archive tool LeafWeb. At SPRUCE specifically, data collection will continue for automated data collection, new destructive sampling during the decommissioning, and synthesis products. The SPRUCE experiment will continue until 2025 with a ramping down of data collection with all SPRUCE data products transferred to ESS-DIVE by the end of FY2028.

For more details about the research data to be collected, methods, and deliverables, see the individual themes in Section 3 Research Plans and Appendix E.

## Content and Format

The project leverages existing tools and expertise to provide data management support to the project by adopting standards-based, open-source approaches to ensure interoperability with current and future DOE BER systems and other projects.

Currently, the TES SFA registers DOIs for all data products using the OSTI E-Link System. Comprehensive metadata can be entered that will facilitate the transfer of metadata, documentation, and data to the ESS-DIVE repository. Moving into the new proposal, the data ingest and archive workflow is being modified for improvement to implement ESS-DIVE as the starting point eliminating the need for transfer of the metadata from OSTI to ESS-DIVE. DOIs will then be assigned with ESS-DIVE as the intermediary with OSTI.

Data sets will follow the metadata and data requirements of ESS-DIVE https://ess-dive.lbl.gov/archive/. Metadata captures information about the investigators, the specific task, parameters, keywords, time periods, quality assurance, and locations associated with the data. Users may provide data products plus additional documentation such as user guide or readme file, images, data files, model code, and so on. The DMT maintains an iterative approach to reviewing the metadata and data with the researcher to ensure requirements are met including recommendations on format, content, and keywords. The preferred non-proprietary file format for public sharing of tabular data products is the comma separated value format. For geospatial spatial products, GeoTIFF and NetCDF are the preferred formats for raster data and ESRI shapefiles for vector products.

New incoming data will have a minimal set of ESS-DIVE Reporting Formats https://ess-dive.lbl.gov/data-reporting-formats/ applied (CSV, FLMD, and Model Products) while encouraging team members to implement additional reporting formats if they exist for their data type. Reporting formats aim for a level of data harmonization for the diverse, multidisciplinary environmental data types generated by the earth science community to create more Findable, Accessible, Interoperable, and Reusable (FAIR) data packages. The ESS community developed formats include instructions on creating and submitting data dictionaries; providing file-level metadata; controlled vocabularies for certain data types; and contents for model data product submissions.

## Sharing and Preservation

The sharing of data that supports publications following the standards and reporting formats provided by ESS-DIVE in a publicly accessible data portal allows access to the information and data thus providing for the transparency and validation of the publication results. The Data Management Plan and the Data policy is posted on both the TES SFA and SPRUCE website.

Currently, all results of laboratory experiments and sample analyses, synthesis of information, genomics analyses, and model products (inputs, codes, outputs) developed in support of TES SFA tasks and collected specifically at the SPRUCE experiment facility, are submitted to the respective SPRUCE or TES SFA data archive at ORNL or other data type specific repository (e.g., AmeriFlux, JGI, EMSL) in a timely manner set forth in the Data Policy. The ORNL TES SFA agrees to the ESS-DIVE data contributor license and specifies that research data is served to the public with Creative Commons Attribution 4.0 data usage rights (CC BY 4.0) https://creativecommons.org/licenses/by/4.0/ and that metadata will always be available under a Creative Commons Public Domain (CC0 1.0) https://creativecommons.org/publicdomain/zero/1.0/.

Data will be available for access in multiple locations: the SPRUCE (https://mnspruce.ornl.gov) and TES SFA (https://TES SFA.ornl.gov) websites; ESS-DIVE Search; customized ESS-DIVE project data portals for both TES SFA and SPRUCE (https://data.ess-dive.lbl.gov/portals/SPRUCE_Experiment ); and the DataONE Search. DataONE is a network of repositories for earth observational data and ESS-DIVE is a contributing member thereby making the project data more broadly available for public access.

## Code Sharing

Public release of SPRUCE-specific E3SM code will be managed by the E3SM project and subject to E3SM policies and licensing (https://e3sm.org/resources/policies/). Development branches of the E3SM code for research purposes will also be available through https://github.com/E3SM-Project/E3SM/. Code developments will be discussed and agreed upon by the TES SFA modeling team, with the understanding that our goal as a group is to make the developments here available to the larger community as soon as possible and assign a DOI through DOECODE. For reproducibility, publications using model output will include information about the specific version used in the simulations. Public release removes the 'rights' of code developers to be automatically considered for co-authorship. However, we encourage users of the released model to consider informing or including those developers to the extent it would benefit the users' analyses.

The Multi-Assumption Architecture and Testbed (MAAT) will continue to be open source and available at https://github.com/walkeranthonyp/MAAT. 'Git tags' will be used to version according to a) major developments, b) moderate developments, and c) minor developments and bug fixes (MAAT version a.b.c). Each version of code associated with a manuscript is also tagged for reproducibility (MAAT version a.b.c_<first author><year>) and associated model outputs are archived as a dataset.

## Timeline

The diverse set measurements vary greatly in their temporal measurement frequency, ranging from, for example, 30 min averages of 1 min air temperature measurements, lengthy soil incubations, to annual aboveground vegetation measurements. The complexity of measurement methods varies widely, from an instantaneous reading to an extensive extraction process and genetic sequencing. The amount of processing and analysis effort and time needed to create a given product varies accordingly.

For sharing among SPRUCE participants: Automated environmental measurements are now available within hours of collection through the data visualization and download tool (Vista Data Vision); annual survey and seasonal measurement data are available within 120 days from the completion of the measurements; results of laboratory analyses of vegetation tissues, soils, isotopic composition, and so on are generally available within 60 days from completion of analyses.

For sharing with the public: Environmental measurements are provided as annual updates; annual surveys and seasonal measurement results are available with publication of analysis papers. Similarly, results of laboratory analyses are made available concurrently with publication of papers.

## Quality Checks

Related to the timeline for data sharing are the quality checks to be performed prior to data sharing among participants (Quality Level 1) and then prior to public access (Quality Level 2). Guidelines for defining data quality levels:

*Quality Level 1* indicates an internally consistent data product that has been subjected to quality checks and data management procedures including, for example: site documentation has been reviewed for completeness; procedures and protocols were reviewed for compliance; calibrations and quality control samples have been evaluated and necessary corrections made; the data have been adjusted for "zero drift" (continuous measurements), or for "blank bias" (lab analyses) as appropriate; consistency checks have been performed with other measurements within the same data file. These internal consistency checks might include diurnal analyses to look for expected patterns, or time series analyses to detect outliers, extreme values, or time periods with too little or too much variation.

*Quality Level 2* indicates a complete, externally consistent data product that has undergone interpretative and diagnostic analysis by the SPRUCE participants, for example, in addition to Level 1 procedures the data have been closely examined by the data manager and/or data users for external consistency when compared to other related data. External checks might include correlation by scattergram, comparison of data with other similar data for the same time period, and comparison of a measurement made by two different methods. If comparisons were not within the precision of the measurements, then measurement records and other information have been reviewed. When data products have been updated because of additional quality checks or discovery of errors, the data should be resubmitted to the archive and the quality level documentation changed (e.g., to Level 2

For completeness, *Quality Level 0* data are products of unspecified quality that have been subjected to minimal processing in the field and/or in the laboratory—raw data, data sheets, scanned data sheets, notebooks, and so on. Raw data is accepted in the archive.

## TES SFA Data and Modeling Products in Publications:

Research data and modeling research products presented in publications resulting from the proposed TES SFA research will be made available to the public concurrent with publication of the paper. This includes data used to generate charts, figures, images, and so on. Model and data products can be archived prior to a paper publication or independent of one. The metadata should include information about any special tools, software, or accessibility requirements for the data. Research data, in this context, is defined as the data required to validate the published results. For modeling products, this includes model codes, inputs, and output for transparency and reproducibility of results. Data users should include the full data set citation with the DOI in the reference section of any published paper. Data sets can also be noted in the Acknowledgements or in Supporting Information but not in exclusion of the Reference section. When possible, the data team will utilize available database fields at OSTI and ESS-DIVE to cross-connect data sets to their associated publications. These research data products will be accessible through the TES SFA data archive and ESS-DIVE repository.

**Data Fair Use Policy:**

The data provided for public access are freely available and were furnished by the TES SFA and SPRUCE research teams who encourage their use. Users of these data products and project information should do the following as recommended by the project and the CC BY 4.0 attribution terms:

- Inform (via email) the scientist(s) of your use of the archived data and of any publications that result from your use of the data. Contact information is provided on the project website and, when mirrored/transferred, the data package at ESS-DIVE.
- Frequently check the publicly accessible data archive to ensure that you are using the latest version of the data.
- Acknowledge (1) data products, including model simulations, as a citation with corresponding data DOIs, as provided in the data archive documentation or from the landing page at ESS-DIVE (when product is available), (2) website information downloads as a bibliographic web citation, or (3) general project information as an acknowledgement or personal communication. No other citation form is applicable.
- Acknowledge the agency or organization that supported the collection of the original data when publishing original analyses and results using these data.
- Include these terms as publication keywords as applicable:
    - TES SFA: ORNL, ORNL TES SFA, DOE Office of Science
    - SPRUCE: SPRUCE Experiment, ORNL, ORNL TES SFA, DOE Office of Science, Marcell Experimental Forest, Northern Research Station, USDA Forest Service.
- Provide an electronic reprint of your independent work to the TES SFA so that all publications resulting from these data may be tracked, recorded, and referenced.

**Transfer of Research Data to DOE ESS-DIVE Archive**

ESS-DIVE is the DOE-sponsored repository for "research funded by or related to the DOE's Office of Science Biological and Environmental Research program (BER) under its Subsurface Biogeochemical Research (SBR) and Terrestrial Ecosystem Science (TES) Programs in the Environmental Systems Science (ESS) activity" (https://ess-dive.lbl.gov/about/). The TES SFA began managing a data archive prior to the creation of the ESS-DIVE repository; however, the final archive for all the project datasets and model products will be the ESS-DIVE repository. The DMT initiated the process of mirroring TES SFA public data products to the repository in the previous proposal period and this effort will continue. An improved workflow will be developed to implement ESS-DIVE as the starting point of the archive process. Ultimately, all metadata and data from the TES SFA will be at the ESS-DIVE repository unless it is archived elsewhere in an approved discipline-specific repository (e.g., AmeriFlux) and ESS-DIVE will have the long-term archive responsibility.

**Protection**

TES SFA will not store personally identifiable or sensitive environmental information in its data system. If any are discovered, it will be removed. Intellectual property rights of investigators (for digital data) are protected by data system enforced access restrictions and promoted through data citation guidance and DOIs. Researchers are more often being connected with products using their ORCID identifiers and this is being implemented within the TES SFA metadata through fields available at OSTI and ESS-DIVE. Stored data at ORNL are protected from loss due to system failures or inadvertent deletion by routine and tested backup protocols. Metadata and data mirrored and ultimately fully transferred to ESS-DIVE will ensure an additional backup in the short-term and follow the ESS-DIVE backup protocols in the long-term.

**Rationale/Justification**

The rapid, open sharing of all data and results from TES SFA research and modeling tasks to researchers, the broader scientific community, and the public is critical to advancing the mission of DOE's TES program. Active data sharing facilitates delivery of federally funded SFA products to our stakeholders providing data transparency and research validation. TES SFA team members continue to develop, deploy, and manage the data systems, repositories, tools, and integration capabilities needed for the collection, quality assurance, storage, processing, sharing, analysis, and archiving of data and model products.

These capabilities facilitate model–data integration and provide accessibility to model output and benchmark data for analysis, visualization, and synthesis activities in support of the TES SFA Vision. The TES SFA data management plan complies with the DOE Office of Science's Statement on Digital Management:

> *Sharing and preserving data are central to protecting the integrity of science by facilitating validation of results and to advancing science by broadening the value of research data to disciplines other than the originating one and to society at large. To the greatest extent and with the fewest constraints possible, and consistent with the requirements and other principles of this Statement, data sharing should make digital research data available to and useful for the scientific community, industry, and the public.*

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## APPENDIX D: Supplement for Section 2's Progress-to-Date Materials

The following text and figures provide additional details of Section 2 progress to date material for the as it relates in Dr. Lianhong Gu's improvements to photosynthesis models.

***<u>Bellows theory of granal thylakoid structure and function of higher plants</u>*** – The bellows theory (Gu et al. 2022) was developed by accident during our quest for a photochemical model of photosynthesis. During this effort we discovered that light-induced thylakoid swelling/shrinking is important for modeling photosynthetic linear electron transport (see progress 6.3). This provided a clue on why higher plants have grana stacks (Gu et al. 2022). In higher plants, PSII and PSI are found in grana stacks and unstacked stroma lamellae, respectively. To connect them, electron carriers negotiate multi-media tortuous paths, subject to macromolecular blocking. Why does evolution select an apparently unnecessary, inefficient bipartition? Here we systematically explain this perplexing phenomenon. We propose that grana stacks, acting like bellows in accordions, expand the volume of ultrastructural control on photosynthesis through thylakoid swelling/shrinking induced by osmotic water fluxes. This control coordinates with varying stomatal conductance and turgor of guard cells which act like accordions' air buttons. The thylakoid ultrastructural dynamics regulates macromolecular blocking/collision probability, direct diffusional pathlength, duty division of cytochrome $b_6f$ complex, luminal pH via osmotic water fluxes, and separation of pH dynamics between granal and lamellar lumens in response to environmental variations. With the two functionally asymmetrical photosystems distantly located from each other, the ultrastructural control, non-photochemical quenching, and C reaction feedbacks maximally cooperate to balance electron transport with gas exchange, provide homeostasis in fluctuating light environments, and protect photosystems in drought. Grana stacks represent dry/high irradiance adaptation of photosynthetic machinery to improve fitness in challenging land environments. Our theory unifies many well-known but seemingly unconnected phenomena of thylakoid structure and function of higher plants. It also suggests that it was not coincidental that higher plants were evolved from Charophyta which is a fresh water green algae and happens to be the only algae group that has grana stacks.

***<u>A broadly applicable photochemical model of photosynthesis</u>*** – Redox reactions control photosynthetic electron transport (PET). This control is key to understanding PET regulation and linkage between light and C reactions and is at the center of photochemical modeling of photosynthesis. Currently we lack a steady-state model of redox control of PET and are unable to determine redox conditions of key electron carriers and enzymes of PET in natural environments. To overcome this deficiency, we used two levels of structural complexity to represent redox reactions along the ETC, allowing us to gauge how much detail and depth are needed to adequately model PET. The simpler representation, denoted "OC", follows the dichotomy of typical PAM fluorometry. A reaction center is considered open (O) if the primary quinone acceptor (a tightly bound plastoquinone, $Q_A$) is in its normal (ground, i.e., oxidized) state and capable of accepting electron for photoreduction whereas a reaction center is considered closed (C) if $Q_A$ is already reduced and thus unable to accept new electron and perform photochemistry. The OC representation is depicted in **Fig. D1**.

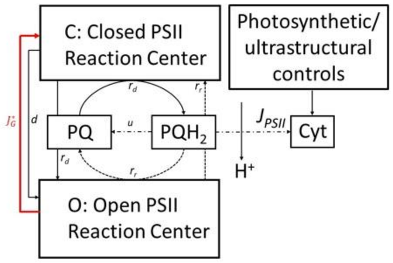


**Fig. D1. The movement of electrons through PSII to the cytochrome $b_6f$ complex (Cyt) as represented by the Open (O) – Closed (C) redox reaction model. A functionally active reaction center can be either in the open state** (i.e., **the acceptor is in the natural, ground, or re-reduced**

**state) or closed state** (i.e., **the acceptor is reduced). PQ denotes free plastoquinone whereas PQH$_2$ denotes plastoquinol. Excitation energy ($J_G^*$) is needed for the transition from the open to closed PSII state whose back transition is described by the first-order rate constant *d*. $J_G^*$ is controlled by the light availability and regulated by non-photochemical quenching (NPQ). $r_d$ and $r_r$ are the second-order rate constants for the electron transfer from the closed reaction center to plastoquinone to form PQH$_2$ and for the reverse reaction, respectively. *u* is the second-order rate constant for the oxidation of PQH$_2$ by the RieskeFeS protein of Cyt and the accompanying transport of proton from the stroma to lumen. The activities of Cyt are regulated by photosynthetic and ultrastructural controls which reflect the feedforward and feedback regulation of ETC and form the boundary condition to close the system of redox equations.**

The more complex representation divided the PSII reaction centers based on the redox conditions of Q$_A$ and the loosely bound plastoquinone (Q$_B$). We denote this representation as 'Q$_A$Q$_B$'. Q$_A$ can be either in the ground state or singly reduced whereas Q$_B$ can be either in the ground state, singly, or doubly reduced state, resulting in six possible redox state combinations. Any combination that has Q$_A$ in the ground state is considered open; otherwise, it is closed. The diagram for the Q$_A$Q$_B$ model is shown in **Fig. D2**.

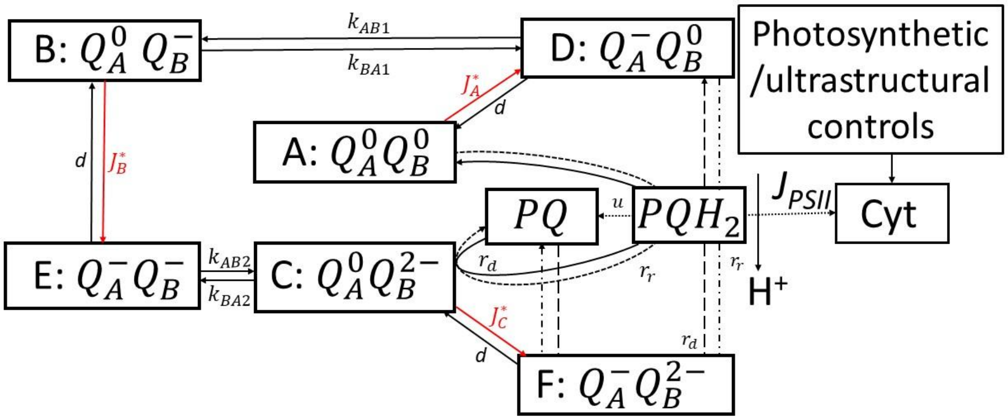


**Fig. D2. The movement of electrons through PSII to the cytochrome b$_6$f complex (Cyt) as represented by the Q$_A$Q$_B$ redox reaction model. The tightly bound plastoquinone (Q$_A$) can be either in the ground state ($Q_A^0$) or reduced state ($Q_A^-$) whereas the loosely bound plastoquinone (Q$_B$) can be either in the ground state ($Q_B^0$), singly reduced state ($Q_B^-$), or doubly reduced state ($Q_B^{2-}$). The resultant six PSII states are denoted by A, B, C, D, E, and F, respectively. Excitation energy is consumed in three scenarios when Q$_A$ accepts an electron and changes the redox state from $Q_A^0$ to $Q_A^-$ as indicated by $J_A^*$, $J_B^*$, and $J_C^*$, respectively. The gross excitation energy flux $J_G^* = J_A^* + J_B^* + J_C^*$ is controlled by the light availability and regulated by non-photochemical quenching (NPQ). $k_{AB1}$ and $k_{AB2}$ are the first-order rate constant for the transfer of electron from the reduced Q$_A$ to the ground and singly reduced Q$_B$ to form the states of $Q_AQ_B^-$ and $Q_AQ_B^{2-}$, respectively while $k_{BA1}$ and $k_{BA2}$ are the first-order rate constants for the corresponding reverse transfer of electron. $r_d$ and $r_r$ are the second-order rate constant for the electron transfer from $Q_B^{2-}$ to PQH$_2$ and for the reverse reaction, respectively. *u* is the second-order rate constant for the oxidation of PQH$_2$ by the RieskeFeS protein of Cyt and the accompanying transport of proton from the stroma to lumen. While the same labels *u*, $r_d$, and $r_r$ are used in the OC and Q$_A$Q$_B$ model, they may have different values in the two models because the reactants are different. The activities of Cyt are regulated by photosynthetic and ultrastructural controls which reflect the feedforward and feedback regulation of ETC and form the boundary condition to close the system of redox equations.**

For both the OC and Q$_A$Q$_B$ models, we applied the Marcus theory of electron transfer in proteins to model the dependence of redox reactions on temperature. We modeled the thylakoid swelling/shrinking (Kirchhoff et al. 2011; Kirchhoff, 2014; Li et al. 2020) as a function of light intensity, which is used to modulate the fraction of the cytochrome $b_6f$ complex available for linear electron transport. According to the OC model, the relationship between the linear electron transport rate ($J_{II}$) and the fraction of open PSII reaction centers ($q$) under either the lake or puddle model connectivity of photosynthetic units is governed by the following equation:

$$J_{II} = \frac{2Uf_Tf_sf_q(q_r-q)q}{(R_1+2R_2f_sf_q-1)q+q_r}. \tag{E.1}$$

Here $U = uN_{cyt_T}N_{PQ_T}$ with $u$ the second-order rate constant for the oxidation of plastoquinol ($PQH_2$) by the RieskeFeS protein of Cyt and the accompanying transport of proton from the stroma to the lumen, $N_{cyt_T}$the foliar concentration of Cyt for linear electron transport, and $N_{PQ_T}$ the total foliar concentration of mobile plastoquinone (oxidized and reduced) for linear electron transport. $R_1 = r_r/r_d$ with $r_d$ and $r_r$ being the second-order rate constant for the electron transfer from the reduced acceptor to plastoquinone to form $PQH_2$ and for the reverse reaction, respectively. $R_2 = \frac{u}{r_d}\frac{N_{cyt_T}}{N_{PSII}}$ with $N_{PSII}$ the foliar concentration of PSII reaction centers whose functional reversible fraction is denoted by $q_r$. $f_q = \frac{1+a_q}{1+a_q\times q}$ quantifies the redox poise balance between PSII and Cyt such that the fraction of Cyt available for linear electron transport $q_{cyt} = f_q \times q$. $a_q$ is a PSII – Cyt stoichiometry parameter. $f_T$ is the standardized temperature response function for the rate constants of redox reactions. It is derived from the Marcus theory of electron transfer in proteins and given by $\sqrt{\frac{T_0}{T}}e^{E_T\left(\frac{1}{T_0}-\frac{1}{T}\right)}$. $E_T$ is the temperature ($T$) sensitivity parameter related to the Gibbs free energy of activation, and $T_0$ is the reference temperature. The light-induced thylakoid swelling/shrinking function, denoted by $f_s$, is given by: $f_s = \frac{V}{V_{max}} = \frac{1}{1+c_se^{-b_s\times I}}$. Here $V$ is the total volume of thylakoid at a given level of absorbed photosynthetically active radiation $I$, and $V_{max}$ is the maximum thylakoid volume when it is fully swollen. $b_s$ and $c_s$ are two empirical coefficients with $b_s$ controlling how fast the thylakoid expands and $c_s$ setting the maximum impact of macromolecular crowding on the diffusion of PQ and PC.

For the $Q_AQ_B$ model, the steady-state $J_{PSII} – q$ relationship is obtained by solving the following cubic equation:

$$J_{PSII}^3 + a_2J_{PSII}^2 + a_1J_{PSII} + a_0 = 0. \tag{E.2}$$

Here,

$$a_2 = \frac{(2R_2f_sf_q-k_2)(R_1+2R_2f_sf_q)q+\frac{2Uf_sf_q(R_1-1-k_{AB})}{k_{PSII}}q+\left[\frac{2Uf_sf_q(1+k_{AB})}{k_{PSII}}q+k_1R_1q-k_1q-2q+2q_r\right](R_1+2R_2f_sf_q-1)}{(R_1+2R_2f_sf_q-1)(R_1-1-k_{AB})/(k_{PSII}f_T)}. \tag{29}$$

$$a_1 = \frac{\left(k_1R_1+k_2R_1+2k_2R_2f_sf_q+\frac{2Uf_sf_q(1+k_{AB})}{k_{PSII}}\right)q^2+(k_1q+2q-2q_r)(R_1+2R_2f_sf_q-2)q}{(R_1+2R_2f_sf_q-1)(R_1-1-k_{AB})/(2Uf_T^2f_sf_qk_{PSII})}. \tag{E.3}$$

$$a_0 = \frac{4U^2f_T^3f_s^2f_q^2k_{PSII}(k_1q+2q-2q_r)q^2}{(R_1+2R_2f_sf_q-1)(R_1-1-k_{AB})}. \tag{E.4}$$

The $Q_AQ_B$ model has four new parameters in addition to those that appear in the OC model. They are $k_1$, $k_2$, $k_{AB}$, and $k_{PSII}$. $k_1 = \frac{k_{BA1}}{k_{AB1}}$, $k_2 = \frac{k_{BA2}}{k_{AB2}}$, $k_{AB} = \frac{k_{AB1}}{k_{AB2}}$, $k_{PSII} = k_{AB1}N_{PSII}$. $k_{AB1}$ and $k_{AB2}$ are the first-order rate constant ($s^{-1}$) for the transfer of electron from the reduced $Q_A$ to the ground and singly reduced $Q_B$ to form the states of $Q_AQ_B^-$ and $Q_AQ_B^{2-}$, respectively while $k_{BA1}$ and $k_{BA2}$ are the first-order rate constant ($s^{-1}$) for the corresponding reverse transfer of electron. The same $f_T$, $f_q$, and $f_s$ apply to the $Q_AQ_B$ model as in the OC model.

For both the OC and $Q_AQ_B$ models, the redox state of the Cyt pool can be described by the fraction of Cyt available for linear electron transport ($q_{cyt}$):

$$q_{cyt} = \frac{(1+a_q)q}{1+a_q\times q}. \tag{E.5}$$

The redox state of the PQ pool for the OC model is given by

$$q_{PQH_2} = \frac{q_r-q}{(R_1+2R_2f_sf_q-1)q+q_r}. \tag{E.6}$$

The corresponding expression for the $Q_AQ_B$ model is given by

$$q_{PQH_2} = \frac{J_{PSII}}{2Uf_Tf_sf_qq}. \tag{E.7}$$

These equations are all derived for the first time. They are all valid regardless of the connectivity of photosynthetic units because they govern the post-charge separation electron transport along the ETC while photosynthetic unit connectivity concerns whether and how excitation energy can be shared among different photosynthetic units, which occurs prior to charge separation. All parameters of the redox model can be estimated by fitting Eq 6.1 or 6.2 to PAM fluorometry measurements.

We used measurements of PAM fluorometry of light, $CO_2$, $O_2$, and temperature responses from 23 C3 and four C4 species in Canada, China, Finland, The Netherlands, and USA to evaluate the derived OC and $Q_AQ_B$ models. These measurements were collected from different users of LeafWeb. The species include three lianas, three shrubs, two boreal deciduous trees, one boreal evergreen needle-leaf tree, three temperate deciduous trees, four tropical deciduous trees, three tropical evergreen trees, one C3 grass, three C4 grasses, and five crop varieties. **Figs. D3** and **D4** show examples of evaluation for the OC and $Q_AQ_B$ models, respectively.

***Testing the predictions of the bellows theory*** – Among oxygenic photosynthetic organisms, higher plants are unique. Their thylakoids have stacked grana and unstacked stroma lamellae with photosystems and ATP synthases unevenly distributed between them. The bellows theory suggests this bipartite architecture coupled with stomata allows photosynthetic machinery to adapt to dry and high irradiance conditions in fluctuating land environments. Like bellows, grana stacks increase the degree of ultrastructural control on redox reactions and diffusion of electron carriers through thylakoid swelling/shrinking induced by osmotic water fluxes in coordination with guard cell turgor to avoid overreducing the ETC, and to balance electron transport with gas diffusion through stomata. This theory predicts thylakoid swelling occurs simultaneously with stomatal opening, and the development of non-photochemical quenching (NPQ) is positively correlated with thylakoid swelling, and faster after thylakoid is fully swollen. We tested these predictions by inferring the light-induced thylakoid swelling function from measurements on numerous C3 and C4 species. We found for all species measured, stomatal conductance (**Fig. D5**) and NPQ (**Figs. D6** and **D7**) increase as thylakoid swells, and NPQ has the maximal sensitivity at the light intensity at which thylakoid is fully swollen. These findings support the bellows theory and identify new research directions in plant water and energy use strategies and photosynthesis modeling.

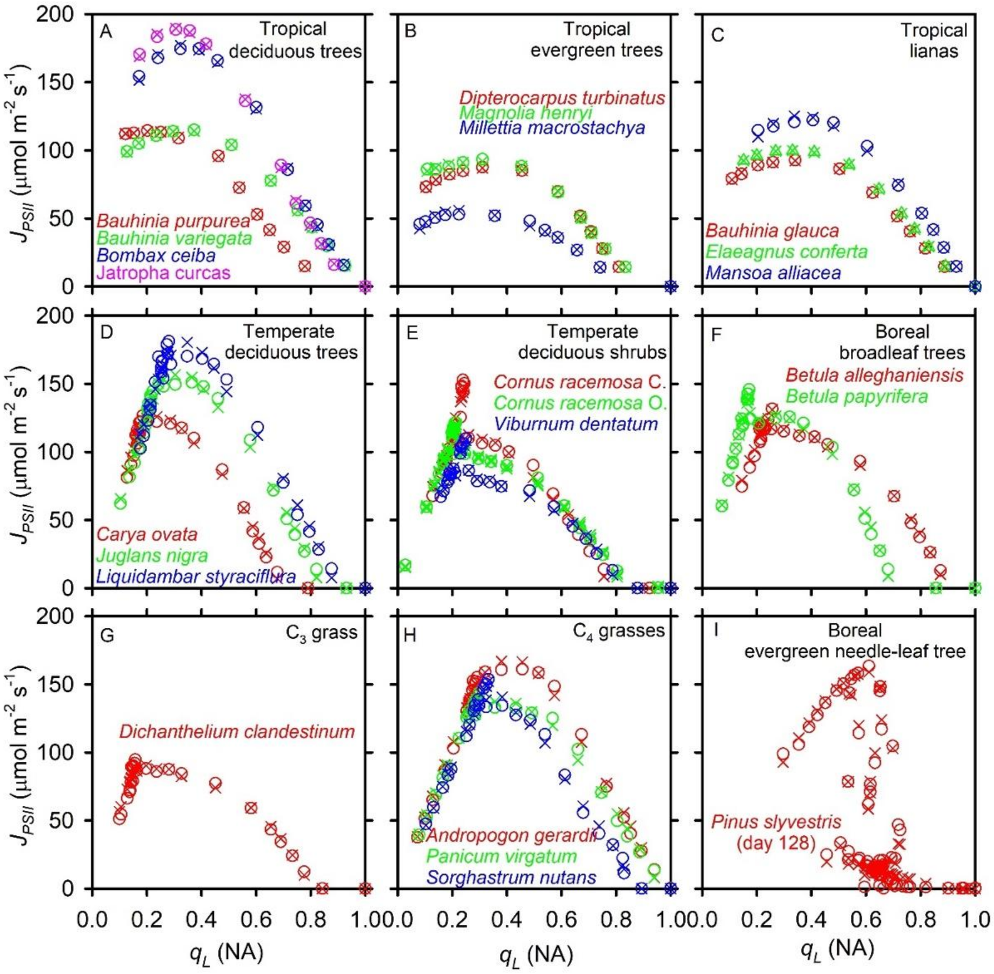


**Fig. D3. Examples demonstrating the performance of the OC model for predicting the linear electron transport rate ($J_{PSII}$) as a function of fraction of open PSII reaction centers ($q_L$) with the lake connectivity of photosynthetic units for a variety of non-crop species. The thylakoid swelling is enabled. Measurements are either from light response only—systematic variation of light intensity at a fixed ambient CO$_2$ concentration (A, B, and C)—or light response in conjunction with CO$_2$ response—systematic variation of ambient CO$_2$ concentration at a fixed light intensity (D, E, F, G, and H), or natural diurnal environmental variations (I). $J_{PSII}$ and $q$ generally vary in the opposite direction for light response but in the same direction for CO$_2$ response. Colors, circles, and × denote species, measurements, and model fits, respectively. All model fits have $r^2 > 0.97$ and $P < 0.001$.**

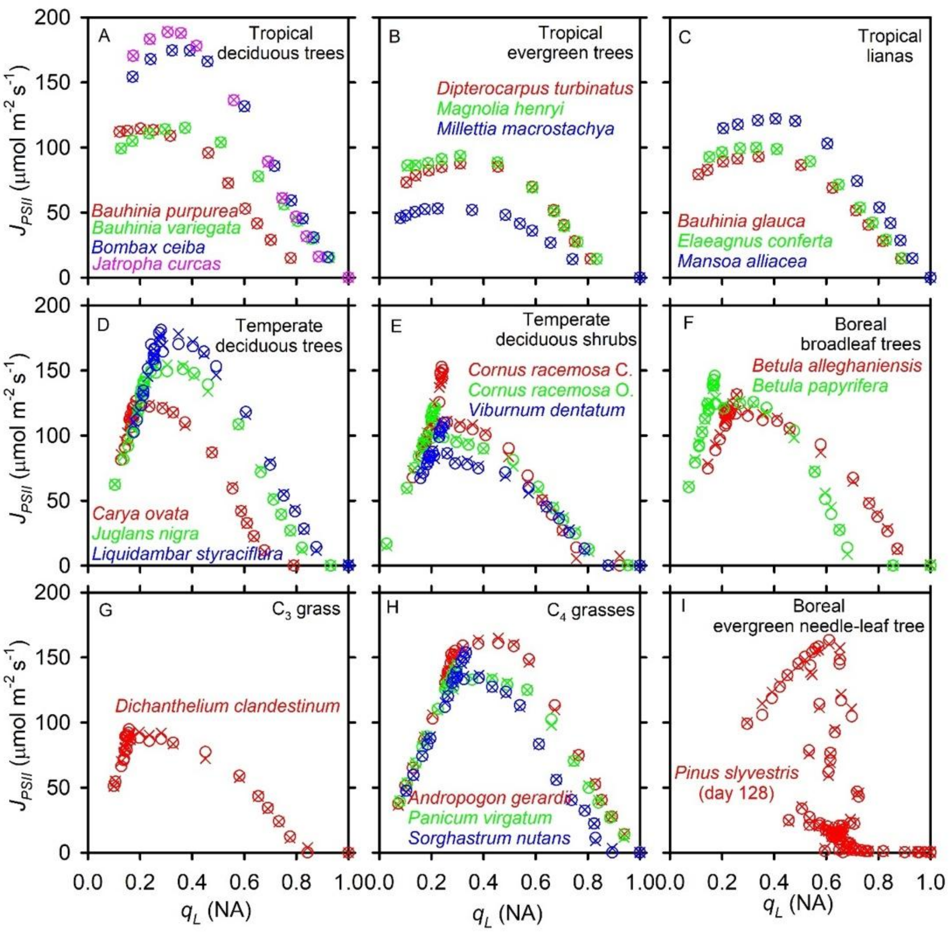


**Fig. D4. Examples demonstrating the performance of the $Q_AQ_B$ model for predicting the linear electron transport rate ($J_{PSII}$) as a function of fraction of open PSII reaction centers ($q_L$) with the lake connectivity of photosynthetic units for a variety of non-crop species. The thylakoid swelling is enabled. Measurements are either from light response only—systematic variation of light intensity at a fixed ambient $CO_2$ concentration (A, B, and C)—or light response in conjunction with $CO_2$ response—systematic variation of ambient $CO_2$ concentration at a fixed light intensity (D, E, F, G, and H), or natural diurnal environmental variations (I). $J_{PSII}$ and $q$ generally vary in the opposite direction for light response but in the same direction for $CO_2$ response. Colors, circles, and × denote species, measurements, and model fits, respectively. All model fits have $r^2 > 0.98$ and $P < 0.001$.**

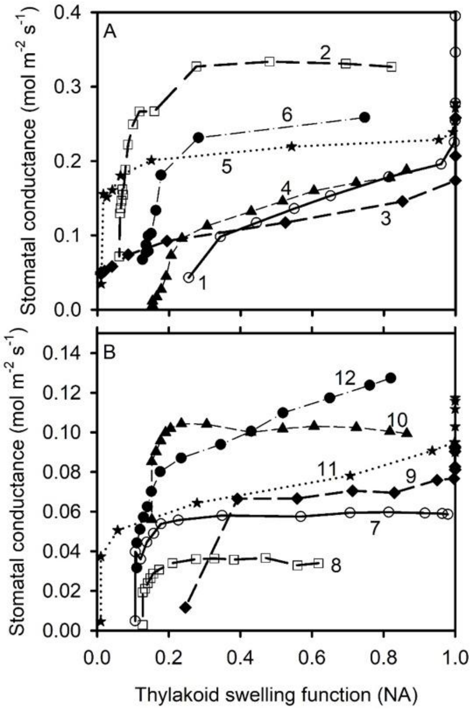


**Fig. D5. Examples of variations of stomatal conductance with thylakoid swelling function inferred from PAM fluorometry measurements using the OC model. . Each curve is marked with a number in A and B and represents a species/cultivar: 1, *Bauhinia glauca*; 2, *Solanum lycopersicum*, tomato Basket Vee; 3 *Solanum lycopersicum*, tomato Growdena; 4, *Zea mays*; 5, *Bauhinia purpurea*; 6, *Oryza sativa*, rice IR64; 7, *Cornus racemosa* 'Ottzam'; 8, *Betula alleghaniensis*; 9, *Magnolia henryi*; 10, *Juglans nigra*; 11, *Dichanthelium clandestinum*; 12, *Sorghastrum nutans*.**

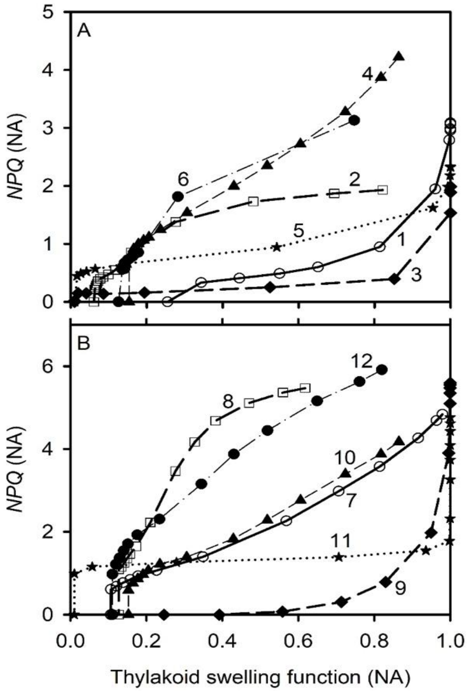


**Fig. D6. Examples of variations of nonphotochemical quenching (NPQ) with thylakoid swelling function inferred from PAM fluorometry measurements using the OC model. Each curve is marked with a number in A and B and represents the species/cultivar as in Fig. D5.**

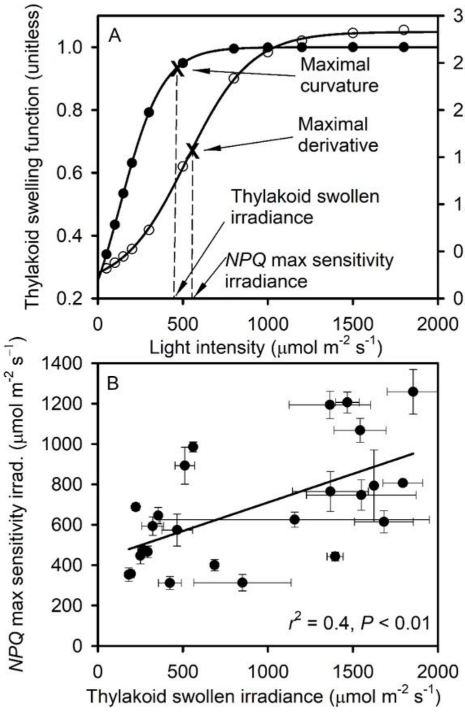


**Fig. D7. Variations of the nonphotochemical quenching (*NPQ*) maximal sensitivity irradiance with the thylakoid swollen irradiance across species inferred from PAM fluorometry measurements using the OC model. As illustrated in A, the *NPQ* maximal sensitivity irradiance is the light intensity at which the *NPQ* light response (A, right axis) has the maximal derivative which is calculated from a sigmoid fitting to the measurements. The thylakoid swollen irradiance is the light intensity at which the thylakoid swelling function (A, left axis) has the maximal curvature before leveling off. In B, the vertical and horizontal bars represent one standard error averaged across the replicas of the same species. To avoid unreliable extrapolation, Plot B includes only response curves for which the maximal curvature of the thylakoid swelling function falls within the range of light intensity used in the measurements.**

# APPENDIX E: SPRUCE Treatment Performance Data

## SPRUCE Infrastructure and Operations

SPRUCE warming treatments at +0, +2.25°C, +4.5°C, +6.75°C, and +9°C (**Fig. E1**) have now been running through 7 full annual cycles since August 2015. Continuous operations have only rarely been interrupted by limited equipment failures and maintenance activities. Warming treatments are maintained day and night throughout the year. Elevated $CO_2$ exposures ($eCO_2$, ~+500 ppm) are applied only during daytime hours during the active growing season (April through November). Hanson et al. (2017) provides a full description of the SPRUCE WEW and $eCO_2$ treatments and their performance for pre- and post-treatment periods, while Krassovski et al. (2015) and (2018) describe the data acquisition and communication systems needed to operate SPRUCE.

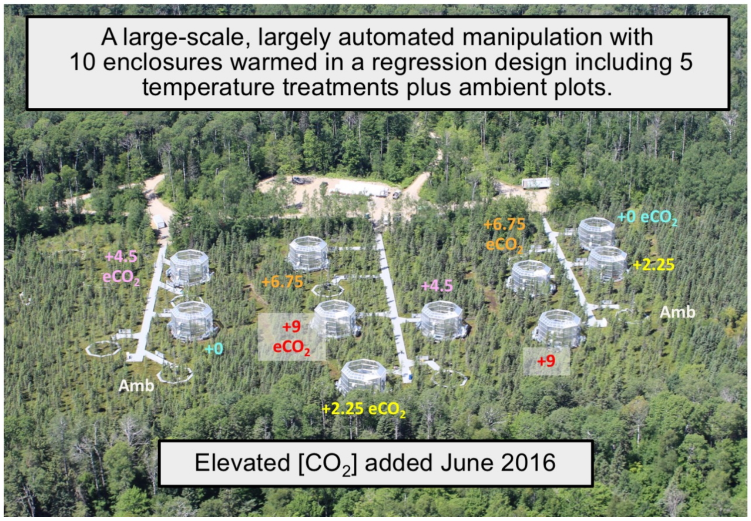


**Fig. E1. The SPRUCE experimental site at the beginning of WEW.**

**Table F1** shows the achieved WEW treatments and $eCO_2$ treatments for 2016, 2017, 2018, 2019, 2020, 2021, and 2022 calendar years. Treatment data are archived in the Hanson et al. (2016D) data set.

**Table F.1. Mean annual air and soil temperatures and $CO_2$ concentrations by SPRUCE plots and all years of WEW and the percent of time that temperature (0.5 h data) or $CO_2$ target differentials (6 min data) are achieved. At longer averaging times (e.g., hours, days) or for greater deviations from targets the performance approaches 100% for all variables.**

| **Plots** | **Target temperature differential** | **Mean annual air temperature at +2 m and [% of days within 0.5°C of target differential for 0.5 h data]** | **Mean annual soil temperature at −2 m and [% of days within 0.5°C of target differential for 0.5 h data]** | **Ambient daylight mean growing season [$aCO_2$] [% of 6 min intervals within 10% of target differential]** | **Elevated daylight mean growing season [$eCO_2$]* [% of 6 min intervals within 10% of target differential]** |
|---|---|---|---|---|---|
| **2016** | (D°C) | (°C) [%] | (°C) [%] | ppm [%] | ppm [%] |
| Plots 7 & 21 | Ambient | 6.0 [100], 7.0 [100] | 5.5 [100], 6.1 [100] | 397 [100], 402 [100] | — |
| Plots 6 & 19 | +0 | 8.2 [100], 7.9 [100] | 5.0 [100], 6.1 [100] | 403 [100] | 862 [90] |
| Plots 11 & 20 | +2.25 | 10.6 [96], 10.6 [86] | 7.4 [ 84], 7.4 [ 88] | 401 [100] | 855 [84] |
| Plots 4 & 13 | +4.5 | 12.7 [98], 12.6 [96] | 9.6 [ 98], 9.8 [100] | 406 [100] | 854 [90] |
| Plots 8 & 16 | +6.75 | 14.7 [85], 14.7 [88] | 11.8 [99], 11.8 [100] | 397 [100] | 887 [92] |
| Plots 10 & 17 | +9.0 | 17.0 [69], 16.8 [80] | 14.0 [98], 13.8 [56] | 414 [100] | 858 [77] |

| | | | | | |
|---|---|---|---|---|---|
| **2017** | (Delta °C) | (°C) | (°C) | ppm | ppm |
| Plots 7 & 21 | Ambient | 5.0 [100], 6.7 [100] | 5.9 [100], 6.4 [100] | 401[100] | — |
| Plots 6 & 19 | +0 | 6.9 [100], 6.6 [100] | 5.1 [100], 6.5 [100] | 404 [100] | 826 [90] |
| Plots 11 & 20 | +2.25 | 9.4 [ 80], 9.7[93] | 7.5 [ 68], 7.5 [ 71] | 403 [100] | 829 [81] |
| Plots 4 & 13 | +4.5 | 11.7 [97], 11.6 [96] | 9.6 [ 93], 9.8 [ 99] | 407 [100] | 835 [65] |
| Plots 8 & 16 | +6.75 | 13.7 [94], 13.7 [96] | 11.8 [100], 11.8 [96] | 408 [100] | 887 [95] |
| Plots 10 & 17 | +9.0 | 15.8 [92], 15.9 [91] | 14.0 [100], 13.8 [100] | 411 [100] | 888 [79] |
| | | | | | |
| **2018** | (Delta °C) | (°C) | (°C) | ppm | ppm |
| Plots 7 & 21 | Ambient | 4.0 [100], 4.4 [100] | 5.6 [100], 6.0 [100] | 402 [100] | — |
| Plots 6 & 19 | +0 | 6.4 [100], 6.0 [100] | 4.4 [100], 6.0 [100] | 404 [100] | 821 [94] |
| Plots 11 & 20 | +2.25 | 8.3 [89], 8.4 [90] | 6.9 [71], 7.0 [73] | 407 [100] | 819 [88] |
| Plots 4 & 13 | +4.5 | 10.8 [93], 10.9 [93] | 9.1 [61], 9.2 [83] | 407 [100] | 845 [92] |
| Plots 8 & 16 | +6.75 | 13.0 [86], 12.9 [87] | 11.2 [99], 11.3 [76] | 410 [100] | 915 [72] |
| Plots 10 & 17 | +9.0 | 15.1 [89], 15.0 [86] | 13.3 [96], 13.2 [99] | 415 [100] | 957 [52] |
| | | | | | |
| **2019** | (Delta °C) | (°C) | (°C) | ppm | ppm |
| Plots 7 & 21 | Ambient | 3.8 [100], 3.7 [100] | 5.4 [100], 5.9 [100] | 412 [100] | — |
| Plots 6 & 19 | +0 | 5.6 [100], 5.0 [100] | 4.2 [100], 5.9 [100] | 418 [100] | 843 [77] |
| Plots 11 & 20 | +2.25 | 7.7 [94], 7.6 [84] | 6.6 [85], 6.8 [68] | 411 [100] | 846 [79] |
| Plots 4 & 13 | +4.5 | 10.0 [97], 10.2 [98] | 8.9 [84], 9.0 [80] | 420 [100] | 859 [85] |
| Plots 8 & 16 | +6.75 | 12.3 [99], 12.2 [97] | 11.0 [99], 11.0 [90] | 422 [100] | 936 [64] |
| Plots 10 & 17 | +9.0 | 14.3 [88], 14.3 [92] | 13.1 [87]. 13.0 [91] | 422 [100] | 946 [58] |
| | | | | | |
| **2020** | (Delta °C) | (°C) | (°C) | ppm | ppm |
| Plots 7 & 21 | Ambient | 5.5 [100], 5.2 [100] | 5.5 [100], 6.2 [100] | 402 [100] | — |
| Plots 6 & 19 | +0 | 7.1 [100], 6.3 [100] | 4.6 [100], 6.1 [100] | 409 [100] | 816 [68] |
| Plots 11 & 20 | +2.25 | 9.1 [91], 9.1 [85] | 7.0 [77], 7.0 [74] | 409 [100] | 817 [70] |
| Plots 4 & 13 | +4.5 | 11.5 [99], 11.6 [96] | 9.2 [87], 9.3 [81] | 407 [100] | 860 [82] |
| Plots 8 & 16 | +6.75 | 13.9 [98], 13.7 [95] | 11.4 [98], 11.4 [91] | 411 [100] | 897 [86] |
| Plots 10 & 17 | +9.0 | 15.9 [97], 15.8 [95] | 13.5 [92], 13.4 [88] | 416 [100] | 892 [82] |
| | | | | | |
| **2021** | (Delta °C) | (°C) | (°C) | ppm | ppm |
| Plots 7 & 21 | Ambient | 5.9 [100], 6.4 [100] | 5.0 [100], 5.9 [100] | 414 [100] | — |
| Plots 6 & 19 | +0 | 7.7 [100], 7.8 [100] | 4.2 [100], 5.7 [100] | 424 [100] | 862 [60] |
| Plots 11 & 20 | +2.25 | 9.9 [94], 10.0 [99] | 6.7 [81], 6.9 [69] | 417 [100] | 869 [56] |
| Plots 4 & 13 | +4.5 | 12.1 [98], 12.3 [99] | 8.8 [89], 8.9 [87] | 421 [100] | 862 [49] |
| Plots 8 & 16 | +6.75 | 14.5 [99], 14.4 [98] | 11.0 [99], 11.0 [95] | 423 [100] | 909 [87] |
| Plots 10 & 17 | +9.0 | 16.4 [88], 16.5 [92] | 13.2 [85], 13.0 [88] | 426 [100] | 871 [55] |
| | | | | | |
| **2022** | (Delta °C) | (°C) | (°C) | ppm | ppm |
| Plots 7 & 21 | Ambient | 3.7 [100], 4.2 [100] | 5.7 [100], 6.3 [100] | 421 [100] | — |
| Plots 6 & 19 | +0 | 5.4 [100], 5.4 [100] | 4.6 [100], 5.9 [100] | 427 [100] | 809 [61] |
| Plots 11 & 20 | +2.25 | 7.3 [78], 7.6 [88] | 7.1 [75], 7.2 [61] | 422 [100] | 827 [68] |
| Plots 4 & 13 | +4.5 | 9.7 [90], 10.0 [95] | 9.3 [87], 9.3 [85] | 421 [100] | 828 [54] |
| Plots 8 & 16 | +6.75 | 12.2 [97], 11.7 [85] | 11.4 [98], 11.4 [84] | 430 [100] | 877 [67] |
| Plots 10 & 17 | +9.0 | 14.3 [95], 13.6 [79] | 13.6 [83], 13.4 [87] | 432 [100] | 847 [52] |

*Growing seasons were DOY 168 to 321 for 2016; DOY 98 to 312 for 2017; DOY 93 to 309 for 2018; DOY 91 to 312 for 2019; DOY 92 to 295 for 2020; DOY 111 to 307 for 2021; DOY 119 to 311 for 2022. Daylight hours were 0800 through 1800.

*Subsurface Hydrology* – A subsurface corral system to measure water flow and collect water samples from the outflow of each experimental chamber was installed beneath each enclosure and has been described (Sebestyen and Griffiths 2016) data are available for aqueous outflows and available nutrients (Sebestyen et al. 2021D).

*Tissue isotopic Change* – The eCO$_2$ treatments are provided with pure CO$_2$ from an ammonium fertilizer plant and yield unique $^{13}$C- and $^{14}$C-CO$_2$ signatures once they are diluted in the enclosures. The unique isotopic signatures of the added CO$_2$ treatments were in the range of −27 to −28 ∂ ‰ for $^{13}$C and −540 D ‰ for $^{14}$C. Through 5 full active seasons of eCO$_2$ exposures new tissue growth under eCO$_2$ has stabilizing at an alternate isotopic signatures commensurate with the experimental exposures to eCO$_2$. Tissue $^{13}$C and $^{14}$C signatures for *Sphagnum* and *Maianthemum* plants are different that for the taller plant species because they reincorporate respired forms of [CO$_2$] from the peat profile (**Fig. E2**).

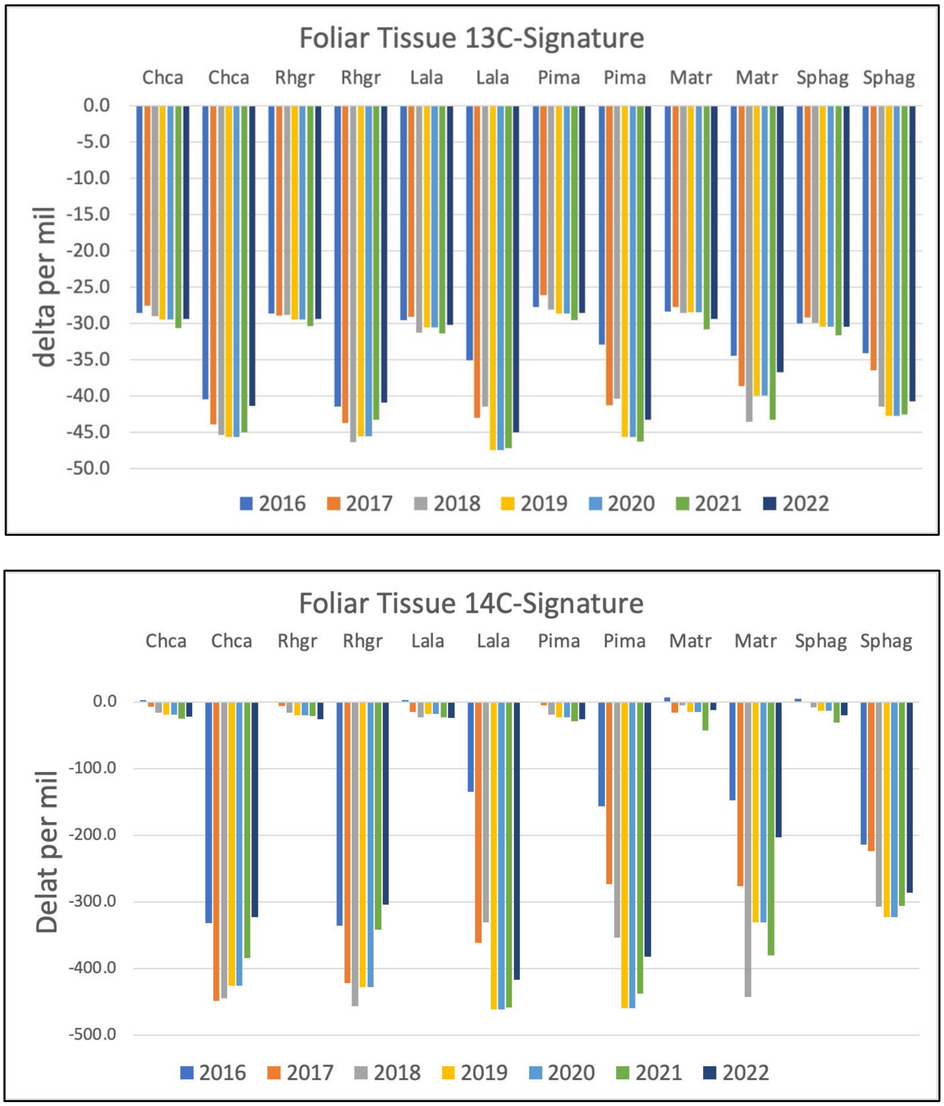


**Fig. E2. Isotopic signatures for $^{14}$C (upper) and $^{13}$C (lower) new aboveground foliar tissue growth across plots and eCO$_2$ treatments.**

*The 2016 Spring Freeze Event* – In the spring of 2016, a late season cold snap impacted the SPRUCE experiment and was described by Richardson et al. (2018). This event led to foliar tissue damage for *Larix* and *Picea* trees that were leafing out in the +9°C treatment plots. The damage led to some mortality and changes in crown appearance for some trees of each species.

*The 2021 Drought* – In summer of 2021, the research site experienced an “extreme drought” as characterized by the Drought Monitor product developed and distributed by NOAA scientists (https://droughtmonitor.unl.edu/Maps/MapArchive.aspx). The driest year and lower water tables for the

Marcell Experiment Forest were recorded in 1976, a year with only 412 mm of precipitation representing 52% of the annual average precipitation inputs. Precipitation in 2021 was 663 mm. In the warmest plots, the water table depths approached those of the historic 1976 drought (see red points in **Fig. E3**).

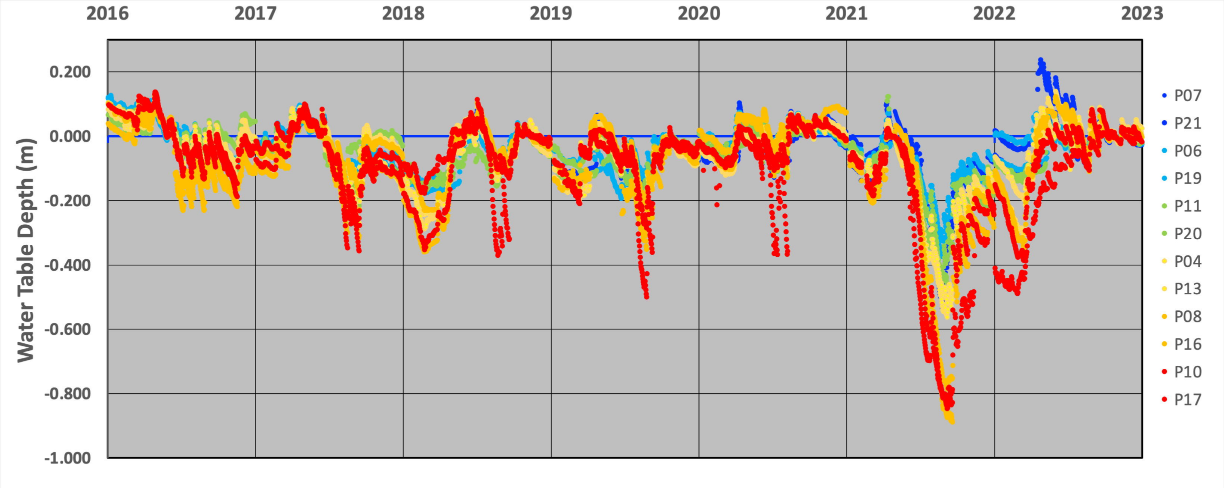


**Fig. E3. Normalized water table depths for all plots and warming treatments from 2016 through.**

*Extreme Event: Dramatic Spring Warming Tree Foliar Tissue Damage in 2022* –
On 19 and 20 June 2022, midday air temperatures in Plot 10 reached 46°C–48°C, PhenoCam images document a dramatic transition during this period of healthy *Picea* foliage to necrotic tissues (**Fig. E4**; red brown foliage). Prior to this event the only similar transition occurred following the spring freeze event of April 2016.

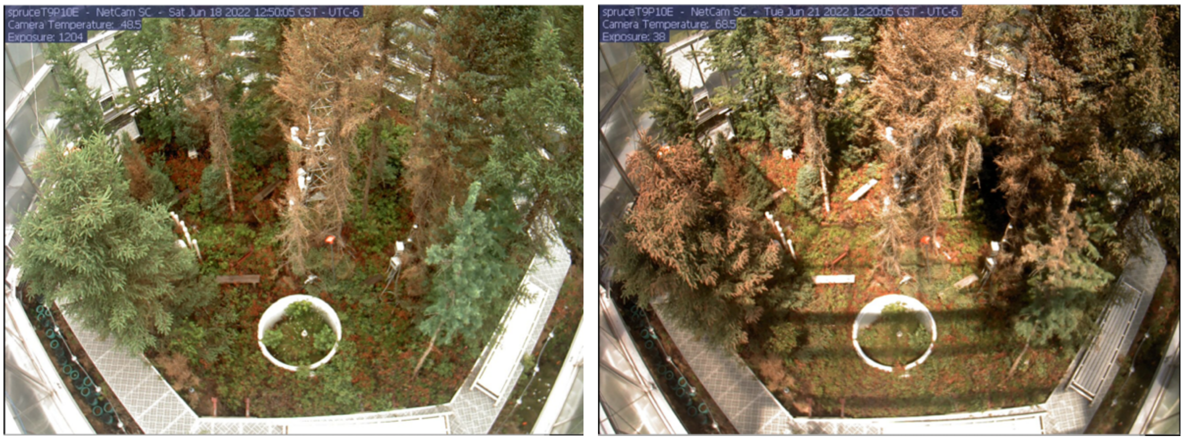


**Fig. E4. Before 18 June 2022 (left Image) and post-heat wave (right image) PhenoCam images for the +9°C treatment Plot 17.**

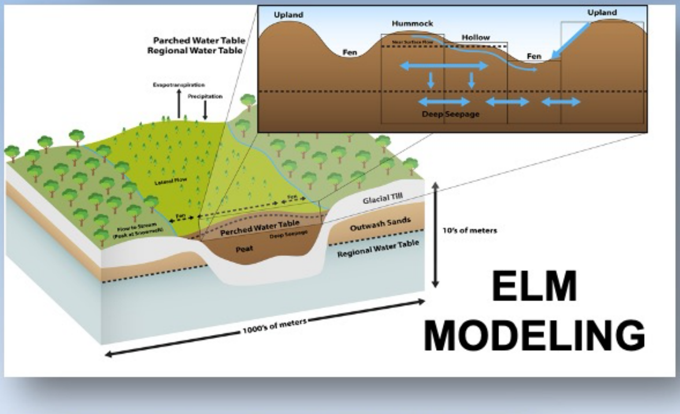
*Disruption of Treatments* – Normal SPRUCE operations have produced only minor interruptions of warming and $eCO_2$ treatments for maintenance issues since the treatments were initiated. However, on Friday, 16 June 2022 at 1700 CST when the propane vaporizer serving Transect #3 and warming plots 16, 17, and 20 failed. The cause of the failure is unknown and was unobserved. The resulting "burn" of equipment and small amounts of adjacent surface litter and foliage has been recorded and a safety review was completed. Replacement hardware has been acquired and installed and various operational procedures adjusted following the recommendations of an ORNL-level review. Environmental monitoring in the affected plots continued uninterrupted and the quantitative record of the temperature treatments for those plots remains intact. Independent belowground warming using electrical resistance heating continues.

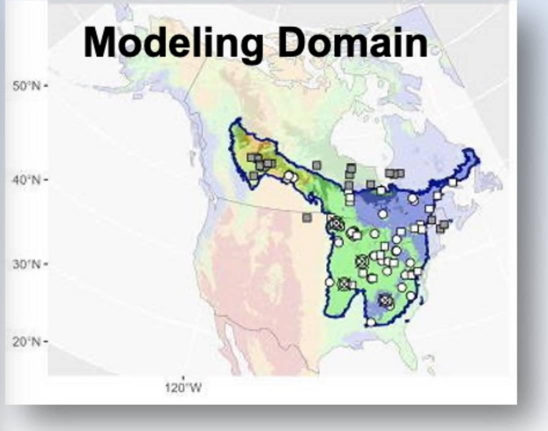
<u>*SPRUCE Data Issues*</u> – The SPRUCE field site received an improved fiber optic gigabit internet connection that facilitated better access to data logger controls, soil flux chamber instruments, real-time PhenoCam images, the EC flux system, and a mobile integrated EC/SIF system. This enabled a near-real-time transfer of the automated plot environmental monitoring data from the SPRUCE site in Minnesota to ORNL where it is available for project access and visualization. Data acquisition and real time display of SPRUCE experimental plot monitoring data are fully implemented (http://sprucedata.ornl.gov). More than 1,100 sensors were deployed across 16 instrumented plots. Real-time visual displays of selected monitoring and infrastructure operational control parameters are provided using Campbell Scientific's Real-Time Monitor and Control software. Vista Data Vision software were implemented for performance monitoring, data visualization, and data review by the SPRUCE Team.

## Back Cover

ORNL TES SFA Illustrations from the top and left to right:

- Image from the SPRUCE Experiment in northern Minnesota.
- Representation of the E3SM Land model (ELM) being improved and used with ORNL TES SFA tasks.
- Logo for the DOE Office of Science Earth System Science program.
- Schematic representation and image of the MOFLUX eddy covariance site operated by ORNL in conjunction with the University of Missouri located on the forest-praire boarder region of central Missouri.
- Map representing the domain region being studied by tasks of the ORNL TES SFA showing embedded research sites available for model-experiment learning and interpretation.
- Logo for the primary sponsor of the ORNL TES SFA DOE Office of Science.





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