SCIENCE PLAN AND PROGRESS REPORT FOR THE TERRESTRIAL ECOSYSTEM SCIENCE – SCIENTIFIC FOCUS AREA (TES SFA)

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

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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). Improved predictive knowledge of ecosystem dynamics is the long-term motivation for our research. Overarching science questions are:

1) How will atmospheric and climate change affect the structure and functioning of terrestrial ecosystems at spatial scales ranging from local to global and at temporal scales ranging from sub-annual to decades and centuries?
2) How do terrestrial ecosystem processes, and the interactions among them, control biogeochemical cycling of carbon and nutrients, the exchanges of water and energy, and the feedback to the atmosphere, now and in the future?

The proposed science includes manipulations, multi-disciplinary observations, database compilation, and fundamental process studies integrated and iterated with modeling activities. The centerpiece of our climate change manipulations is the Spruce and Peatland Responses Under Changing Environment (SPRUCE) experiment testing multiple levels of warming at ambient and elevated CO_2 on the vegetation response and biogeochemical feedbacks from a *Picea-Sphagnum* ecosystem. Other efforts aim to improve mechanistic representation of processes within terrestrial biosphere models by furthering our understanding of fundamental ecosystem functions and their response to environmental change. The TES SFA integrates experimental and observational studies with model building, parameter estimation, and evaluation to yield reliable model projections. This integrated model-experiment approach fosters an enhanced, interactive, and mutually beneficial engagement between models and experiments to further our predictive understanding of the terrestrial biosphere in the context of Earth system functions.

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*The TES SFA groups science tasks into the following broad organizational themes: large scale manipulations (Task 1), landscape observations (Tasks 2 and 6), multi-scale modeling (Tasks 3a, 3b, 3c and 3d), process-level studies (Tasks 4a, 4c and 5), and global trait databases (Tasks 4b, 7 and 8).

Executive Summary

The TES SFA supports research to understand and predict the interaction of Earth's terrestrial ecosystems and climate, and to assess vulnerability of terrestrial ecosystems to projected environmental change. The research focuses on how terrestrial ecosystems affect atmospheric CO_2 *and other greenhouse gases (e.g.,* CH_4*) and how the responsible ecosystem processes interact with climate and with anthropogenic forcing factors. Targeted experiments are conducted to quantify and predict ecosystem responses to warming and elevated* CO_2 *(e*CO_2*) and the feedbacks from ecosystems to the atmosphere and climate. Other process research aims to accurately quantify the exchange of* CO_2*, water vapor, and energy between the atmosphere and land ecosystems through processes such as photosynthesis, evapotranspiration, net production, storage pools, and autotrophic and heterotrophic respiration. TES SFA research also includes efforts to provide comprehensive databases, above- and belowground, to benefit the analytical needs of Earth System Models. Understanding achieved by TES SFA tasks on the fundamental functions and interactions of vegetation, microbial community and soil is used to improve mechanistic representation of ecosystem processes within terrestrial biosphere models.*

The TES SFA is developing capabilities for quantitative projection of future atmospheric greenhouse gas concentrations and ecological effects from environmental change, incorporating complex feedbacks and responses among terrestrial ecosystems, human activities, and Earth's climate system. Multiscale, multi-process studies of terrestrial ecosystem responses through integration of models, manipulative experiments, and observations (i.e., MODEX) will provide robust and fundamental scientific results, syntheses and analyses to advance predictive understanding. This advance in quantitative scientific understanding is used to improve the representation of terrestrial ecosystems in advanced Earth System Models (ESMs). The breadth and complexity of this undertaking require the scientific and technical expertise of multidisciplinary scientists from a range of institutions, who can deliver timely answers to questions of national and international importance. Quantitative, transparent and accessible science products produced by the TES SFA are available to decision-makers and stakeholders to evaluate and address climate change consequences. The TES SFA team's unique strengths in modeling, experimentation, and measurement are synergistically combined to answer pressing global change science questions. ORNL's powerful computation and informatics capabilities are available to support this vision of Earth System analysis. The TES SFA group focuses on interactions among the climate system, terrestrial ecosystems, biogeochemical dynamics, and land use change that are most suited to the team's current strengths and that have the potential for near and long-term impact.

Overarching Science Questions

The following overarching science questions and the subsequent description of key goals and milestones are focused on resolving uncertainties in terrestrial ecosystem response to atmospheric and climate change.

1) How will atmospheric and climate change affect the structure and functioning of terrestrial ecosystems at spatial scales ranging from local to global and at temporal scales ranging from sub-annual to decades and centuries?
2) How do terrestrial ecosystem processes, and the interactions among them, control biogeochemical cycling of carbon and nutrients, the exchanges of water and energy, and the feedback to the atmosphere, now and in the future?

Goals and Milestones

The TES SFA goals and long-term (5 to 10-year) milestones are summarized below. Details on progress and proposed work are documented in Sections 2 and 3, respectively.

Goal 1: Understand, quantify and model long-term ecosystem responses to the interactive effects of atmospheric and climatic change in an understudied but globally important ecosystem.

- *Long-term milestone:* Comprehensive predictive understanding of decadal peatland ecosystem responses to a range of technologically-advanced warming and elevated [CO_2] treatments in an ombrotrophic bog in northern Minnesota.

Goal 2: Understand drivers of ecosystem functions and interactions by integrating new process knowledge in the E3SM Land Model (ELM) and related models of varying complexity, and the use of state-of-the-art sensitivity analysis, uncertainty quantification, and model evaluation to obtain novel insights leading to new observations and experiments.

- *Long-term milestone:* Increased confidence in model projections based on improved mechanistic understanding and model representation of ecosystem processes, ranging from canopy photosynthesis to microbially-mediated decomposition, that govern responses to, and interactions with, environmental change.

Goal 3: Improve the understanding and model representation of the linkages among above- and belowground functional traits, their response to changing environmental conditions, and the resulting consequences for ecosystem biogeochemical cycling.

- *Long-term milestone:* Develop global ecological trait databases, available to the broader community of ecologists and terrestrial biosphere modelers, and use these databases to target novel observations and experimental manipulations that fill gaps in our mechanistic understanding and modeling of key ecological traits.

Goal 4: Improve process-based understanding of belowground biogeochemical cycling, including processes occurring at the root-soil interface, to support predictions of small- and large-scale belowground pools and fluxes in terrestrial biosphere models.

- *Long-term milestone:* Incorporate a flexible, comprehensive, and tested model of the belowground ecosystem into fully-coupled Earth System Models.

Goal 5: Achieve a predictive understanding of ecophysiological, biochemical and physical processes controlling the exchanges of carbon, water and energy between land and atmosphere with advanced observational and theoretical approaches.

- *Long-term milestone:* Develop and demonstrate a mechanistic model of photosynthesis involving light reactions for applications in ESMs, a light reactions-based approach for partitioning net ecosystem changes of carbon and water, and a reliable, easy-to-use sun-induced chlorophyll fluorescence (SIF) measurement system for flux communities around the world.

Research to accomplish these broad goals and objectives is organized as a series of tasks focused on terrestrial ecosystem responses to environmental and atmospheric change and to climate change forcing modifications driven by terrestrial carbon cycle (C-Cycle) processes or influenced by structural features. Completed, ongoing and new Tasks included in TES SFA efforts to date are listed below with parenthetical identification of their goals. The Task numbering scheme is used throughout this document and previous proposals and annual reports, enabling tracking of tasks through time.

Task 1: Spruce and Peatland Responses Under Changing Environments – SPRUCE (Goals 1,2,3,4,5)
Task 2: Synthesis of Walker Branch Watershed long-term monitoring – Completed
Task 3a: Improving process models with site-level observations and experimental data (Goals 1,2,3,4).
Task 3b: Regional and Global Land Ecosystem Modeling (Goals 1,2,3,4)
Task 3c: Functional Testing – Completed
Task 3d: Multi-Assumption Systems Modeling – New Effort (Goal 2,3,5)
Task 4a: Synthesis of the Partitioning in trees and soils studies – Completed
Task 4b: Root traits characterization (Goals 2,3,4)
Task 4c: Root function and modeling (Goals 2,3,4)
Task 5: Microbial processing of soil carbon (Goal 2,4)
Task 6: Coordinated ecophysiology, eddy covariance, sun-induced chlorophyll fluorescence studies – Refocused Effort (Goal 1, 2, 3, 4, 5)
Task 7: Implications of Fossil Emissions for Terrestrial Ecosystem Science – Completed
Task 8: LeafWeb data assimilation tool –New Task (Goal 3)

The TES SFA groups science tasks into the following broad organizational themes: large scale manipulations (Task 1), landscape observations (Tasks 2 and 6), multi-scale modeling (Tasks 3a, 3b, 3c and 3d), process-level studies (Tasks 4a, 4c and 5) and global trait databases (Tasks 4b, 7 and 8).

TES SFA activities interact with Earth System Modeling activities at Oak Ridge National Laboratory (ORNL) to improve the representation of terrestrial ecosystem processes and biogeochemical cycles required to reduce uncertainty in ESM predictions of future climate and terrestrial response.

Data systems and informatics are not a separate focus area, but an integral part of the TES SFA and are incorporated within each of the above Tasks. ORNL is developing and deploying data and information management, and integration capabilities needed for the collection, storage, processing, discovery, access, and delivery of data, including experiment and model results. These capabilities and systems are designed to facilitate uncertainty characterization and quantification. Systems will be developed for assimilating available measurements, synthetic analysis results, model forcing and boundary condition data sets, and model results. Such an information system facilitates model-data integration and provides accessibility to model output and benchmark data for analysis, visualization, and synthesis activities.

Approach

Advancing process representation and reducing uncertainty through identifying and improving structural deficiencies in terrestrial biosphere models are accomplished through organized interactions among data collection, experimental manipulation, and model development across a range of temporal and spatial scales. Experiments and field observations are employed to better understand organismal responses to environmental and atmospheric changes from molecular- through whole-plant responses to the integrated function of entire ecosystems. Our efforts focus on unresolved ecosystem processes and understudied ecosystems subject to greater rates of change under projected climate futures. When necessary, new technologies are invented or developed to enable such studies. We use model-data assimilation and multivariate model benchmark evaluation in all aspects of the TES SFA's research program. The SFA uses a multi-model approach in all analyses to allow rich and robust interpretation of experimental results and orderly model improvement. Products of the TES SFA include primary research publications, synthesis activities (e.g., critical review papers, model-data intercomparisons, and international workshops), archived experimental and modeling data sets, and multi-scale model-data assimilation systems delivering analyses of climate change forcing and terrestrial ecosystem responses appropriate for local-to-global analyses.

Highlights for the period March 2015 through September 2018

- We have produced 166 published, accepted or in press papers since March 2015 (Appendix A). Papers include publications in *Science*, *Nature*, *Proceedings of the National Academy of Sciences, Nature Communications*, *Nature Climate Change* and *Eos* among others. *Twenty-one* additional manuscripts are being actively reviewed as of the submission of this report.
- SPRUCE – We have sustained whole-ecosystem warming (WEW) treatments continuously within target expectations since August 2015. Elevated CO_2 treatments on half of the SPRUCE WEW plots were initiated on 15 June 2016 and have been maintained during daylight hours throughout the active growing season (~April through October) in all years. Hanson *et al.* (2017) fully describes the SPRUCE experimental system.
- SPRUCE – A major paper summarizing responses to deep peat heating was published in *Nature Communications* (Wilson *et al.* 2016) showing the initial resilience of ancient peat to warming responses.
- SPRUCE – A number of pretreatment analysis and characterization papers for SPRUCE were published over the reporting period (Jensen *et al.* 2015, Griffiths and Sebestyen 2016, Hanson *et al.* 2016, Hobbie *et al.* 2017, Iversen *et al.* 2018, McFarlane *et al.* 2018).
- SPRUCE – Xu *et al.* (2016) published a major review on past and current methane modeling approaches.
- SPRUCE – A paper describing temporal and spatial variation in peatland carbon cycling parameters (Griffiths *et al.* 2017) has fully defined uncertainty for our peatland study.

- SPRUCE – Anthony Walker published a paper on *Sphagnum* species net and gross photosynthetic capacity (Walker *et al.* 2017) that represents the empirical basis for modeling *Sphagnum* vegetation layers within the land surface component of ecosystem and Earth System models.
- SPRUCE – A high-impact paper in *Nature* (Richardson *et al.* 2018) describes phenology responses of SPRUCE vegetation to the first two years of warming. Notable and surprising is the warming-induced extension of the fall growing season normally considered to be under day length control.
- SPRUCE – After two years of whole-ecosystem warming, lateral water fluxes (i.e., stream flow) decreased with warming likely due to increased evapotranspiration. Total organic carbon and cation (i.e., potassium, calcium) concentrations in stream water and porewater are higher in warmer enclosures, possibly reflecting increased mineralization. However, there were no measurable changes in nutrient (N and P) concentrations in porewater, likely because any nutrients that are mineralized are rapidly taken up by biota in this nutrient-poor ecosystem.
- SPRUCE – Warming has increased the amount of plant-available nutrients, especially in deeper peat.
- Walker Branch – As part of wrap-up activities for Walker Branch research, multiple papers were published describing in-stream biogeochemical dynamics (Griffiths and Tiegs 2016, Brooks *et al.* 2017, Hill and Griffiths 2017, Griffiths and Johnson 2018). Data from Walker Branch were also included in three papers that examined global patterns in stream biogeochemical dynamics (Follstad Shah *et al.* 2017, Norman *et al.* 2017, Tank *et al.* 2018).
- Modeling – Jiafu Mao published a paper in *Nature Climate Change* (Mao *et al.* 2016a) that attributes long-term trends in leaf area index in the northern extratropical latitudes to human activity using satellite data and coupled Earth system models.
- Modeling – A series of publications have been produced following active MODEX activities involving SPRUCE empirical data sets and ecosystem models (Huang *et al.* 2017, Jiang *et al.* 2018a, Ma *et al.* 2017).
- Modeling –A calibration approach was successfully implemented using surrogate modeling to improve E3SM land model predictions as the Missouri flux site using observations.
- Modeling –A new detection and attribution capability for offline land model simulations for determining the causes of changes in runoff in the continental US was developed and applied.
- Modeling – ELM-SPRUCE was integrated into E3SM version 1, improving predictions of nutrient cycling at the site.
- Modeling – Multi-Assumption Architecture and Testbed (MAAT) v1.0 code was published open source on GitHub https://github.com/walkeranthonyp/MAAT.
- Root Traits – Colleen Iversen initiated the Fine Root Ecology Database (FRED; https://roots.ornl.gov; Iversen *et al.* 2017), which has been downloaded hundreds of times across five continents, for use by modelers and empiricists alike. Version 2 of FRED was released to the public in early June 2018 from an updated web platform (McCormack *et al.* 2018). There was considerable interest in this release from the broader community of root and rhizosphere ecologists; the project was liked or re-tweeted hundreds of times on Twitter.
- Root Function – Warren *et al.* (2015) published a Tansley review on the incorporation of root structure and function in models that was noted as an ISI Web of Science highly cited paper.
- Root Function – Following poor performance of hydraulic models to simulate a well characterized plant-soil system using parameters derived from root-free soil, Jeff Warren is funding an MS student to assess how roots or fungal hyphae impact soil hydraulic properties and results will be used to estimate model sensitivity to improvement of hydraulic parameters.
- MEND – Melanie Mayes and team showed that the future trajectory of soil organic carbon stocks may be more responsive to changes in soil moisture than to temperature, particularly in tropical and subtropical environments (Wang *et al.* 2019). Application of their microbial model to the long-term Harvard forest warming experiment found that carbon use efficiency was decreased

while microbial turnover was increased and that warming increased the sensitivity of both parameters, resulting in a small net gain of soil C stocks (Li *et al.* 2018).

- MOFLUX – At the Missouri eddy covariance site, and over the 2005–2015 time period, growing season net ecosystem productivity (NEP) and (R_s) were largely controlled by plant water stress and correlated to a significant linear relationship with community predawn leaf water potential integrals (Gu *et al.* 2015; 2016a,c).
- MOFLUX – MOFLUX scientists contributed to the evaluation of NASA OCO-2 SIF products, resulting in a high-profile paper in *Science*. The Fluorescence Auto-Measurement Equipment developed by MOFLUX scientists has been in successful operation at MOFLUX since Sept 2016 (Gu *et al.* 2018). Data obtained so far reveal highly asymmetrical seasonal and diurnal patterns of SIF emission. These patterns suggest strong dependence of SIF emission on long-term changes in canopy photosynthetic capacity and short-term variations in canopy microstructure, plant physiological stress and non-photochemical quenching.
- LeafWeb – The LeafWeb data portal has been redone and redeployed on a user-friendly server to enable its use by a wider researcher group. LeafWeb – Parameter estimation for C4 photosynthesis models has been enabled in LeafWeb.

Terrestrial Ecosystem Science SFA and USDA Forest Service Funded Participants for the period from March 2015 through September 2018.

Robert J. Andres	ORNL Senior Research Staff Member
Deanne J. Brice	ORNL Technician
Joanne Childs	ORNL Master Technician
Natalie A. Griffiths	ORNL R & D Staff
Lianhong Gu	ORNL Distinguished Research Staff
Paul J. Hanson	ORNL Corporate Fellow
Leslie A. Hook	ORNL R & D Staff
Colleen M. Iversen	ORNL Senior R & D Staff
Anthony W. King	ORNL R & D Staff
Laurel A. Kluber	ORNL Postdoctoral Research Associate
Randall K. Kolka	USDA Forest Service Researcher
Misha B. Krassovski	ORNL R & D Staff
John Latimer	ORNL SPRUCE Part-time field technician (2014 to present)
Junyi Liang	ORNL Postdoctoral Research Associate
Dan Lu	ORNL R & D Associate
Avni Malhotra	ORNL Postdoctoral Researcher
Jiafu Mao	ORNL R & D Staff
Melanie A. Mayes	ORNL Senior R & D Staff
Karis J. McFarlane	Lawrence Livermore National Laboratory - Scientist
William Robert Nettles	ORNL SPRUCE Site Manager and Technical Staff
Richard J. Norby	ORNL Corporate Fellow
Keith Oleheiser	XCEL Engineering SPRUCE Full-time field & lab technician (2015 to present)
Jana R. Phillips	ORNL Senior Technician
Daniel M. Ricciuto	ORNL R & D Staff
Christopher W. Schadt	ORNL Senior R & D Staff
Stephen D. Sebestyen	USDA Forest Service Researcher
Xiaoying Shi	ORNL R & D Staff
Anthony Walker	ORNL R & D Staff
Dali Wang	ORNL Senior R & D Staff
Gangsheng Wang	ORNL R & D Associate
Eric J. Ward	ORNL Postdoctoral Researcher
Jeffrey M. Warren	ORNL R & D Staff
David J. Weston	ORNL Senior R & D Staff
Jeffrey D. Wood	Assistant Research Professor, University of Missouri – Columbia
Stan D. Wullschleger	ORNL Corporate Fellow

Xiaojuan Yang	ORNL R & D Staff

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Narrative (Sections 1 Through 7)

1. BACKGROUND AND PROGRAM OVERVIEW

Oak Ridge National Laboratory's (ORNL) Terrestrial Ecosystem Science Scientific Focus Area (TES SFA) conducts fundamental research in support of the DOE BER Climate and Environmental Sciences Division (CESD) Strategic Plan (US DOE 2018). The TES SFA addresses all five CESD grand challenges by integrating data and models to understand and predict Earth System drivers and biogeochemical cycling, especially in critical ecosystems such as high-latitude regions. The TES SFA strives to expand fundamental knowledge of terrestrial systems and translate that knowledge into mechanistic Earth System Models (ESMs), in particular the Energy Exascale Earth System Model (E3SM). The TES SFA also addresses grand challenges identified in the 2017 BERAC Grand Challenges Report (BERAC 2017) by advancing our understanding of the interactions among key players of the Earth System (e.g., microbial communities, vegetation, and humans) with a systems science approach. The TES SFA emphasizes information translation through levels of ecosystem organization connecting complex fine-scale biological processes with large-scale biosphere-climate feedbacks. Data management and access activities are an integral part of TES SFA efforts to share not only scientific progress but also data products with the broader scientific communities.

1.1 ORNL TES SFA Vision

Improved integrative understanding of terrestrial ecosystem processes to advance Earth System predictions through experiment-model-observation synergy

Predictive understanding of ecological processes developed from observations, as well as laboratory and field experiments improves model process conceptualization and parameterization. In turn, sensitivities, uncertainties and identified weaknesses of model predictions inform new observations and experiments, and the development of new ecosystem process understanding. TES SFA research integrates insights from process models with data obtained using a diverse array of approaches across a range of scales, including observations from field sites and remote sensing, and community-assisted collection of ecological trait data from across the globe. This integration is realized through the development and application of empirically or theoretically-driven process models, model-data fusion and intercomparison, model performance benchmarking, and uncertainty characterization and quantification. This model-experiment synergy (MODEX) occurs within the framework of predictive Earth System modeling and simulation using high-performance, leadership-class computing.

1.2 TES SFA Philosophy and Research Overview

TES SFA research is an iterative process (Fig. 1.1) translating mechanisms to terrestrial biosphere models with a quantitative understanding of model uncertainties, which in turn informs priorities for future measurements. Our paradigm is to identify and target critical uncertainties in coupled climate and terrestrial ecosystem processes and feedbacks, prioritized by their influence over global change

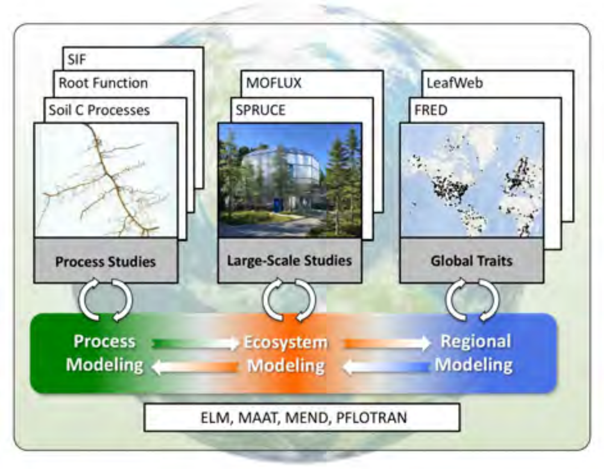


Fig. 1.1. Diagram of the TES SFA research philosophy and activity flow illustrating an iterative exchange between model projections, question or hypothesis development and the execution of observations and experiments to better understand impacts of multi-factor environmental changes on ecosystems and their contribution to Earth System functions. SIF = solar induced fluorescence; MOFLUX = Missouri flux site; SPRUCE = Spruce and Peatland Responses Under Changing Environments experiment; LeafWeb = photosynthetic trait archive; FRED = Fine Root Ecology Database; ELM, MAAT, MEND, PFLOTRAN are all models.

predictions on decadal timescales. New measurements and experiments are employed to obtain new knowledge required to characterize, quantify, and reduce these uncertainties.

Terrestrial ecosystem research aims at the deep integrative understanding of biophysical, biochemical, physiological, and ecological processes. Terrestrial biosphere models codify this understanding in a hypothesis-driven, mechanistically consistent framework to simulate the coupled operation of the carbon, nutrient, and hydrological cycles and energy fluxes at sub-hourly to multi-annual timescales and at ecosystem to landscape spatial scales. These models are built upon, validated by, and constrained by historical and contemporary observations and experiments. Nevertheless, the future trajectory of terrestrial ecosystems remains highly uncertain. Further integration of models and experimental manipulations are required to enable reliable projections of ecosystem responses and feedbacks to future climate and other atmospheric forcing.

ORNL's current large-scale environmental change study, the Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment focuses on the response of a *P. mariana–Sphagnum* peat bog in northern Minnesota to multiple levels of warming at ambient or elevated CO_2. The experiment offers a platform for testing mechanisms controlling vulnerability of organisms and ecosystem processes to important climate change variables and provides data for model development.

The TES SFA also supports smaller-scale, process-level manipulations of ecosystem processes ranging from photosynthesis to root function to mechanistic studies of soil carbon cycling, as well as long-term monitoring of landscape flux and sun-induced chlorophyll fluorescence (SIF) measurements at the Missouri flux (MOFLUX) site.

Data from large- and small-scale TES SFA observations and experiments are integrated into models to identify and reduce terrestrial process and parameter uncertainties in the global Earth system. The Multi-Assumption Architecture & Testbed (MAAT) and Energy Exascale Earth System Model (E3SM) provide frameworks for this model-data integration and uncertainty quantification. Model predictions are improved through parameterization, calibration, and the development of new process-based submodels focused on key aspects of wetland, boreal and temperate forest systems, for example the Microbial Enzyme Decomposition (MEND) model.

Given the opportunities for serendipity in scientific research, the TES SFA has built-in mechanisms within its overall planned and organized research tasks to allow timely exploration of emerging scientific issues that are unplanned but nevertheless important to the TES SFA Vision and relevant to the CESD Strategic Plan. These mechanisms facilitate the formation of novel ideas and new research frontiers, as well as the growth of early career staff.

TES SFA research is ambitious in its scope, effort, and resource requirements. It undertakes the challenge of fully utilizing, testing and extending the broad interdisciplinary facilities of a DOE National Laboratory. ORNL's SFA research plans and philosophy attempt to eliminate an artificial distinction between experimental or observational studies and modeling so that the science can be advanced efficiently and effectively.

1.3 Overarching Questions, Goals and Deliverables

The following overarching science questions and the subsequent description of key goals and milestones focus on improving our understanding and model representation of significant uncertainties in terrestrial ecosystem responses to atmospheric and climate change. These questions have been updated from their original form to reflect advances and changes in emphasis of TES SFA research.

1. **How will atmospheric and climate change affect the structure and functioning of terrestrial ecosystems at spatial scales ranging from local to global and at temporal scales ranging from sub-annual to decades and centuries?**
2. **How do terrestrial ecosystem processes, and the interactions among them, control biogeochemical cycling of carbon and nutrients, the exchanges of water and energy, and the feedback to the atmosphere, now and in the future?**

The TES SFA goals and long-term (5- to 10-year) milestones are briefly summarized below.

Goal 1: Understand, quantify and model long-term ecosystem responses to the interactive effects of atmospheric and climatic change in an understudied but globally important ecosystem.

- *Long-term milestone:* Comprehensive predictive understanding of decadal peatland ecosystem responses to a range of technologically-advanced warming and elevated [CO_2] treatments in an ombrotrophic bog in northern Minnesota.

Goal 2: Understand drivers of ecosystem functions and interactions by integrating new process knowledge in the E3SM Land Model (ELM) and related models of varying complexity, and the use of state-of-the-art sensitivity analysis, uncertainty quantification, and model evaluation to obtain novel insights leading to new observations and experiments.

- *Long-term milestone:* Increase confidence in model projections based on improved mechanistic understanding and model representation of ecosystem processes, ranging from canopy photosynthesis to microbially-mediated decomposition, that govern responses to and interactions with environmental change.

Goal 3: Improve the understanding and model representation of the linkages among above- and belowground functional traits, their response to changing environmental conditions, and the resulting consequences for ecosystem biogeochemical cycling.

- *Long-term milestone:* Develop global ecological trait databases, available to the broader community of ecologists and terrestrial biosphere modelers, and use these databases to target novel observations and experimental manipulations that fill gaps in our mechanistic understanding and modeling of key ecological traits.

Goal 4: Improve process-based understanding of belowground biogeochemical cycling, including processes occurring at the root-soil interface, to support predictions of small- and large-scale belowground pools and fluxes in terrestrial biosphere models.

- *Long-term milestone:* Incorporate a flexible, comprehensive, and tested model of the belowground ecosystem into fully-coupled Earth System Models.

Goal 5: Achieve a predictive understanding of ecophysiological, biochemical and physical processes controlling the exchanges of carbon, water and energy between land and atmosphere with advanced observational and theoretical approaches.

- *Long-term milestone:* Develop and demonstrate a mechanistic model of photosynthesis involving light reactions for applications in ESMs, a light reactions-based approach for partitioning net ecosystem changes of carbon and water, and a reliable, easy-to-use SIF measurement system for flux communities around the world.

Details on progress are documented in Section 2. Near term (1-3 year) milestones are described in the Research Plans of Section 3. Deliverables for the TES SFA were originally described and justified in the earlier SFA plans (http://tes-sfa.ornl.gov/node/17) and were revised in the first triennial review (January 2012). They have been updated to reflect progress over time. The following material is annotated and tracked by Task number so that it can be consistently compared with past review documents and annual progress reports. Parenthetical identification of the goals addressed by each task are presented in the following list.

Task 1: Spruce and Peatland Responses Under Changing Environments – SPRUCE (Goals 1,2,3,4,5)
Task 2: Synthesis of Walker Branch Watershed long-term monitoring (Prior goal)
Task 3abc: Mechanistic terrestrial biosphere modeling (Goals 1,2,3,4)
Task 3d: Multi-Assumption Systems Modeling (Goals 2,3,5)
Task 4a: Synthesis of the Partitioning in trees and soils studies (Prior goals and 2,4)
Task 4bc: Root Traits (FRED), Root Function and Modeling – New Tasks (Goals 2,3,4)
Task 5: Microbial processing of soil carbon (Goals 2,4)
Task 6: Terrestrial impacts and feedbacks of climate variability, events, and disturbances: MOFLUX(Goals 1,2,3,4,5)
Task 7: Implications of Fossil Emissions for Terrestrial Ecosystem Science (Prior goal)
Task 8: LeafWeb – (Goal 2,3,5)

The TES SFA groups science tasks into the following broad organizational themes: large-scale manipulations (Task 1), landscape observations (Tasks 2 and 6), multi-scale modeling (Tasks 3a, 3b, 3c and 3d), process-level studies (Tasks 4a, 4c and 5) and global trait databases (Tasks 4b, 7 and 8). These theme areas are highlighted in the text and Table of Contents to help the reader navigate to Sections of the proposal that are of most interest to the reader.

2. PROGRESS MARCH 2015 THROUGH SEPTEMBER 2018

This summarizes TES SFA activities accomplished since the 2015 review. We have published 166 peer-reviewed papers in leading national and international scientific journals, sustained the SPRUCE infrastructure, improved process-based predictive models from local- to regional- to global scales, developed publicly available datasets of global importance, and provided leadership in national and international ecological and climate change-related workshops and meetings, and in our interactions with the public. 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.

A full listing of TES SFA publications is provided in Appendix A, data sets produced by each task are listed in Appendix B, and tables summarizing progress on deliverables established in 2015 are presented in Appendix C.

LARGE-SCALE MANIPULATIONS AND LANDSCAPE OBSERVATIONS*

2.1 SPRUCE Experiment (Task 1)

The SPRUCE experiment (Hanson *et al.* 2017) is the first **whole-ecosystem**, forest-scale experiment to increase temperatures from deep soils throughout tree canopies in combination with increased atmospheric CO_2 concentrations. The decade-long experiment initiated in August 2015 is being carried out in an ombrotrophic bog peatland ecosystem of northern Minnesota dominated by trees *Picea mariana* (black spruce, henceforth *P. mariana*), *Larix laricina* (larch, henceforth *L. laricina*), ericaceous shrubs *Rhododendron groenlandicum* (Labrador tea, henceforth *R. groenlandicum*) and *Chamaedaphne calyculata* (leatherleaf, henceforth *C. calyculata*), 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 following text provides succinct descriptions of SPRUCE infrastructure operations and science accomplishments since March 2015. Published works are described and recent results are highlighted, and reference to publicly-available data sets are made to provide more methodological detail. Prior descriptions of SPRUCE are also available at http://mnspruce.ornl.gov/content/spruce-project-documents.

2.1.1 SPRUCE Infrastructure and Operations

SPRUCE warming treatments at + 0, 2.25, 4.5, 6.75 and +9 °C (Fig. 2.1) have been running continuously since August 2015, only interrupted by associated 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 whole-ecosystem warming 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.

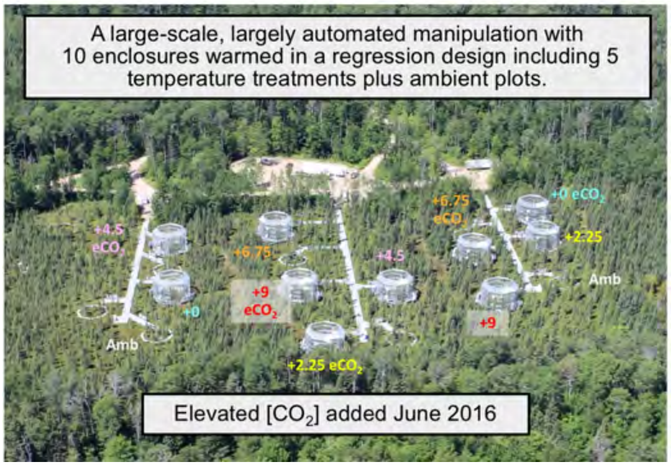


Fig. 2.1 The SPRUCE experimental site at the beginning of whole-ecosystem warming.

Appendix F provides details on achieved whole-ecosystem warming and eCO_2 treatments for the 2016, 2017 and 2018 calendar years (Table F1). The treatment data are archived in Hanson *et al.* (2016D).

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 ∂ ‰ for ^{13}C and -520 Δ ‰ for ^{14}C (Appendix F). Through two full active seasons of eCO_2 exposures, new plant tissue growth under eCO_2 continues to show isotopic changes suggesting that the combined current and storage reserves contributing to new tissue development had not yet achieved a new equilibrium after two full years of exposure.

<u>*Subsurface Hydrology*</u> – 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).

2.1.2 Peat Characterization of the S1 Bog

A key publication on historical peatland accumulation rates for the S1 Bog (McFarlane *et al.* 2018) was completed. We found that the bog has been accumulating carbon 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.

<u>*Bog elevation measurements*</u> – Because warming and eCO_2 treatments are hypothesized to have dramatic effects on peat C stocks, we have been tracking plot elevation over time. Since the initiation of whole-ecosystem warming (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).

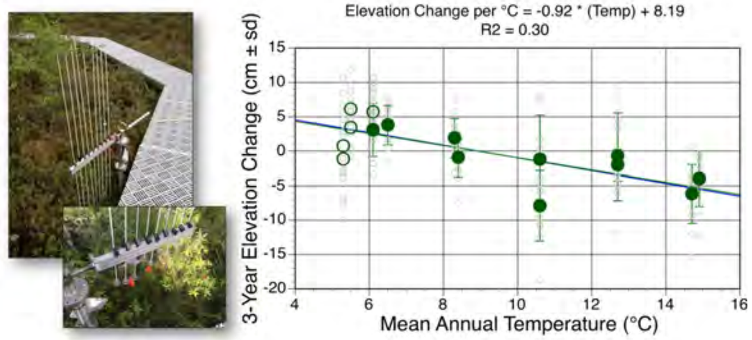


Fig. 2.2 Cumulative change in peat elevation by treatment temperature throughout the period from 2016 through 2018. The 3-year mean annual temperature plotted is the average of data at +2 m air and -2 soil temperatures.

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, collapse of the *Sphagnum* layer (see next section), or from 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 about 1.4 kg C per m^2.

2.1.3 Vegetation Phenology and Aboveground Production

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 (http://phenocam.sr.unh.edu/webcam/). Richardson *et al.* (2018) published the first two years of phenology results in *Nature,* which reported that WEW linearly correlated with an unexpected delay in autumn greendown and an expected advance in spring greenup of the dominant woody species.

Aboveground production for woody vegetation and forbs – After two years of warming, a significant pattern of reduced tree growth is evident (Fig. 2.3 left graph) driven primarily by declines in *P. mariana* growth. Opposite the patterns for trees, the shrub-layer growth showed an increasing trend with warming (Fig. 2.3 right). No apparent growth changes driven by eCO_2 treatments for trees or shrubs have yet developed. Within the shrub layer some species show either increases, decreases or no change with warming.

Sphagnum production - Pretreatment measurements of *Sphagnum* production in 2015 identified multiple problems with the standard growth protocols (including use of crank wires, brush wires, and bundles), especially for quantifying growth throughout an entire growing season. Thus in 2016, we developed and established a new method in which *Sphagnum* is collected *in situ*, measured, placed into mesh cylinders at their native stem densities, and replaced into the intact *Sphagnum* community to be retrieved 1 year later for quantification of new growth. Measurements of growth (dry matter increment) were subsequently coupled with measurements of *Sphagnum* community composition across three transects in each enclosure. These methods are fully described in Norby and Childs (2018D). There was no *Sphagnum* growth response to warming or eCO_2 treatments 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. Warming had a profound effect on *Sphagnum* percent cover, where declines began

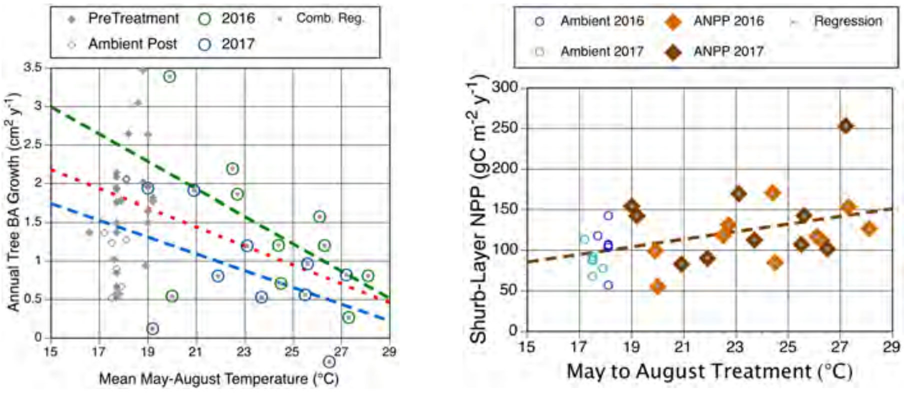


Fig. 2.3 Combined tree growth for *Picea mariana* and *Larix laricina* (left) and net primary production (NPP) for non-tree, shrub-layer vegetation (right) in 2016 and 2017 under whole-ecosystem warming.

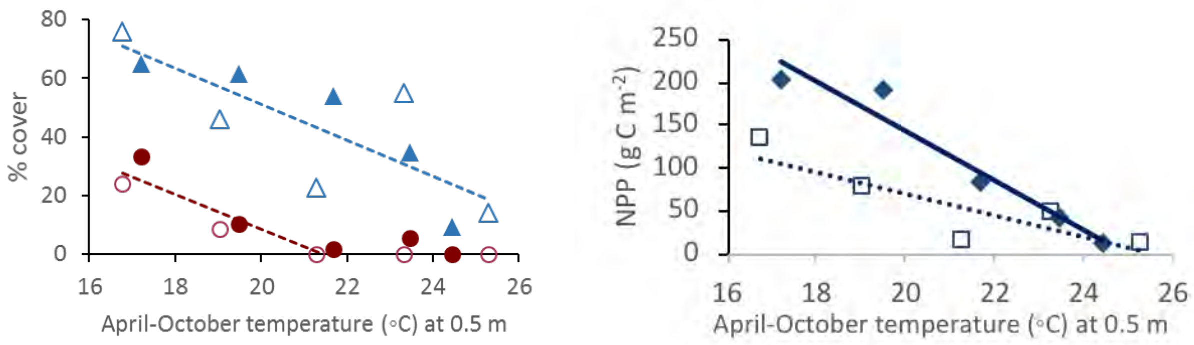


Fig. 2.4 (Left) Fractional cover of *S. angustifolium/fallax* (blue) and *S. magellanicum* (red) in 2018; closed symbols: ambient CO_2; open symbols: eCO_2. (Right) Net primary production of *Sphagnum* in 2018 in ambient CO_2 (closed symbols) and eCO_2 (open symbols.

in 2016 and increased through 2017 and 2018, increasing the area of ground with no live *Sphagnum* cover (Fig. 2.4 left). Net primary production (NPP) of *Sphagnum*, calculated as dry matter increment times fractional cover and converted to C units, declined with increasing temperature in 2017 and 2018, and was less in eCO_2 plots in 2018 (Fig. 2.4 right). The response to temperature is related to drying of the hummocks, and the response is likely an indirect response to eCO_2 increased shrub cover in warmer enclosures. 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.

2.1.4 Belowground Production – Fine Roots

Fine roots contribute to ecosystem C, water, and nutrient fluxes and we aimed to determine how the amount and timing of fine-root growth in the forested, ombrotrophic S1 Bog varied across gradients of vegetation density, peat microtopography, and changes in environmental conditions. Iversen *et al.* (2018) found that the fine roots of trees and shrubs were concentrated in raised hummock microtopography, with more tree roots associated with greater tree densities and a unimodal peak in shrub roots at intermediate tree densities. Fine-root growth tended to be seasonally dynamic, but shallowly distributed, in a thin layer of nutrient-poor, aerobic peat above the growing season water table.

Through the first four growing seasons under WEW we gathered ~100,000 manual minirhizotron images from across 48 tubes (4 per plot; ~110 images per tube per week), and ~78 million automated minirhizotron images from novel, automated minirhizotron (AMR) technology that facilitates high-resolution (100×) measurements of root-fungal dynamics (1 per plot; 35,000 images per tube per week).

These images show that the belowground growing season in the warmed plots is extended well past when the surface peat is frozen in plots receiving less warming. Full analysis of productivity, mortality and fine-root standing crop in quantitative length or mass units from the minirhizotrons is dependent on an extremely labor-intensive digitization process and will be a key milestone for the coming years (see section 3.1). Along with images from the pre-treatment experiment, these images have been compiled into an accessible data set that will be updated annually (Childs *et al.* 2019D).

We used root ingrowth cores to evaluate the fine-root growth response of peatland plants to warming. Between 2014 and 2016, warming significantly increased fine-root growth on an ecosystem scale, but a mixed-effects model including soil moisture and temperature suggested that the increase in root growth was driven by drying rather than warming. Shoulder sampling periods (October to June) had negligible growth before WEW was initiated, however in 2016 this sampling period shows fine-root growth increased with warming. Across all sampling periods, fine roots growing in hollows had a greater growth response than hummocks, primarily driven by reduced moisture content and perhaps more available nutrients. The faster-growing shrub and *L. laricina* fine roots showed greater growth increases with warming than *Picea*, which may be partially due to less relative C availability in spruce (see Vegetation Physiology section below). Our results suggest that warming will continue to increase fine-root growth and that this response will be especially large in the previously water-saturated hollows that are becoming increasing aerobic due to drying.

2.1.5 Vegetation Physiology

Woody Plant Physiology – Beginning in 2015 we established long-term automated measurements of sap flow and stem diameter in trees and soil water content within the hummock hollow complex in the 12 SPRUCE measurement plots. The sap flow measurements and complementary gas exchange and water potential data 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 occurred in *L. laricina* water use with temperature (Fig 2.5). 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. As a result, in the warmest plots there has been some tree mortality, including top dieback and branch tip damage in both species. Ongoing work is focused on assessing the trade-offs between growth and defense, and consequences of each strategy by assessing gas exchange, fluorescence, water-use efficiency, non-structural carbohydrates, water potential, pigments and sap flow. The sap flow system has also indicated a strong temperature effect (but not CO_2) on spring phenology by increasing initiation of sap flow by between 1 and 3 days (or more) per degree warming and extending sap flow into the fall by ~1 day per degree warming for *L. laricina* or more than 3 days per degree 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) and sap flow will continue to be monitored to maximize our ability to track and measure this critical response. We have also developed a technique to deploy soil moisture sensors inside peat-packed mesh cylinders to determine soil moisture responses in the highly variable bulk density peat hummocks and hollows. Results indicate progressive soil drying with warming.

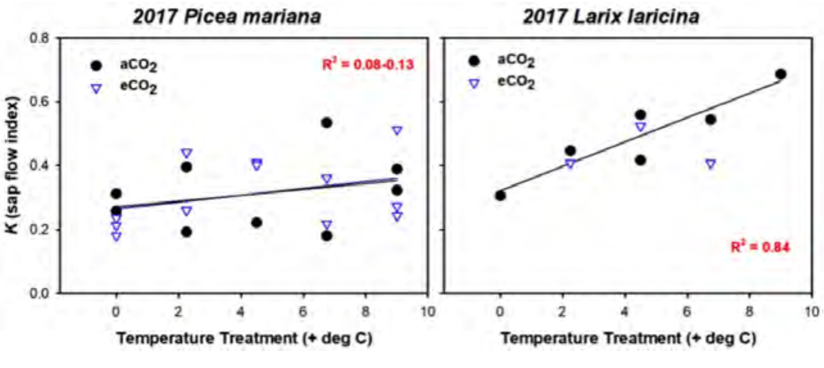


Fig. 2.5 Differential tree water use in response to temperature, but not CO_2 at the SPRUCE site illustrates different hydraulic strategies by *Picea* and *Larix*. *Picea* reduced stomatal aperture, maintained safe leaf water potentials, and stable water use. *Larix* kept stomata open, increased water stress, and increased water use.

Initial responses of foliar gas exchange after the first year of WEW indicated species-specific shifts in thermal acclimation of both photosynthesis and respiration, and corresponding shifts in nitrogen (N) content, but no effect of eCO_2. Based on these results and feedback from the SPRUCE science advisory board, we initiated an intensive, 2-week long combination of field and laboratory campaigns in collaboration with the University of Western Ontario and the University of Minnesota to thoroughly assess thermal and CO_2 acclimation of the key photosynthetic and respiratory parameters essential to process-based modeling. This work included collecting iterative daily predawn clippings from each of the four primary woody species, *P. mariana, L. laricina, R. groenlandicum and C. calyculata* and transporting them to the UMN growth-chamber facilities for gas exchange assessments. The campaign involved more than 15 people, 13 gas exchange machines, 6-8 growth chambers and yielded 1000+ photosynthesis-CO_2 temperature response (A-Ci) and foliar (dark) respiration temperature response curves ranging from ~10 to 45+ °C. Data are being organized, analyzed and processed through LeafWeb to generate the required $V_{c,max}$ and J_{max} photosynthetic parameters to assess photosynthetic acclimation. Data will build upon pretreatment C physiology analysis and modeling (Jensen *et al.* 2015a, 2015b, 2018, *in press*) We also have collected some initial stem respiration temperature response curves that indicate woody respiration increases up to 55 °C but then declines at temperatures above 55-60 °C. Data from the foliar, stem and root respiration assessment will be used to explore theoretical and novel respiratory-temperature response equation frameworks that will be later incorporated into ELM. There have also been increases in foliar non-structural carbohydrates with eCO_2 treatment, which complement pretreatment data (Furze *et al.* 2018). Initial branch and leaf morphological analyses suggest reduced leaf mass per area for most species, denser foliar display for *L. laricina* but less dense for *P. mariana*, and reductions in the Huber value (sapwood area: leaf area) for the trees – this latter point suggesting increased hydraulic limitations. Along with ongoing allometry and LIDAR work to assess changes in leaf area or biomass, results will be used to test and improve foliar, shoot or hydraulic trait acclimation in the model.

Sphagnum Physiology – S1 Bog vegetation is dominated by peat mosses (*Sphagnum* spp.) that contribute substantially to bog NPP (~43%; Griffiths *et al.* 2017), peat accrual, and together with their associated microbiome contribute to ecosystem C and N cycling. Pretreatment measurements from clear-top LiCOR 8100 soil respiration chambers sampling *Sphagnum* communities in the hollows identified considerable uncertainly in CO_2 flux predictions throughout the growing season. Using hourly measurements of CO_2 flux throughout the growing season, we identified the seasonal cycle of hollow *Sphagnum* GPP that peaked in late summer, well after the peak in photosynthetically active radiation. Our analysis showed that water table height was the key driver variation in *Sphagnum* GPP in the early summer and that temperature was the primary driver of GPP in the late summer and autumn. Modeling activities using these data resulted in a function to describe the interaction of SAI (stem area index) with water table as the primary driver of seasonality in *Sphagnum* GPP (Fig. 2.6; Walker *et al.* 2017).

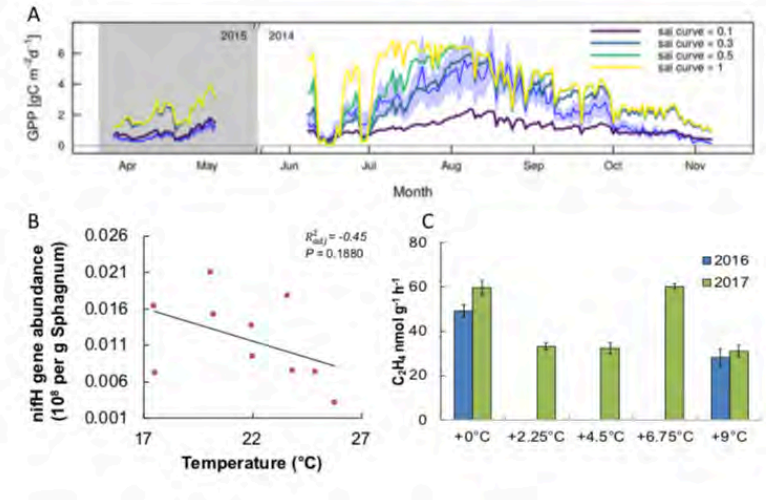


Fig. 2.6. Contribution of *Sphagnum* and its associated microbes to C and N cycling. Modeling results describing the interaction of *Sphagnum* photosynthesizing tissue (stem area index; SAI) with water table as the primary driver of seasonality in *Sphagnum* GPP (A). Absolute abundance of the *nifH* N-fixation marker gene in relation to temperature (B), and resulting N-fixation activity estimated from acetylene reduction assay in 2016 and 2017 (C).

While this ombrotrophic bog is by definition low in nutrients, *Sphagnum* production estimates (Section 2.1.3) suggest that less than 25% of the N needed to support the observed production could be accounted for by N deposition, which implies an additional exogenous source of N to this system, i.e., bacterial N fixation. Using DNA extracted from *Sphagnum*, we assessed the abundance of the N_2-fixing marker gene, *nifH,* which shows a negative correlation with increasing temperature (Fig. 2.6b). The T-induced reduction in N_2-fixing bacteria was also reflected by less N_2-fixation at elevated temperatures based on acetylene reduction (Carrell *et al.* 2019). These results show that *Sphagnum*-associated N_2-fixation is decreasing with temperature, but the reasons why, consequences to production, and the long-term trends in this response remain to be determined. Note that these reductions in surface *Sphagnum* N_2

fixation with increased temperature might be offset by increased N mineralization in the peat (see next section).

2.1.6 Rhizosphere Processes

Plant-available nutrients – We used ion-exchange resins to assess if WEW and eCO_2 increase plant-available nutrients within hummock-hollow microtopography and throughout the peat profile. In 2017, after two full years of WEW, resin-available nutrients increased with warming, with average available NH_4-N five times greater in surface peat and 20 times greater in deeper peat in the +9°C treatment compared with the +0 °C treatment (Fig. 2.7). The greater magnitude of the increase below the rooting zone was likely because of increased nutrient uptake by the vegetation or microbes from surface peat layers (i.e., greater competition for nutrients). Interestingly, the same warming response was not apparent in porewater at a comparable depth increment in the hollows (Section 2.1.9). Thus, ion-exchange resins can be conceptualized as a 'plant root', competing for nutrients with plants and microbes and accumulating those nutrients over time, while porewater chemistry represents the pool of residual nutrients that were not immobilized by plants or microbes.

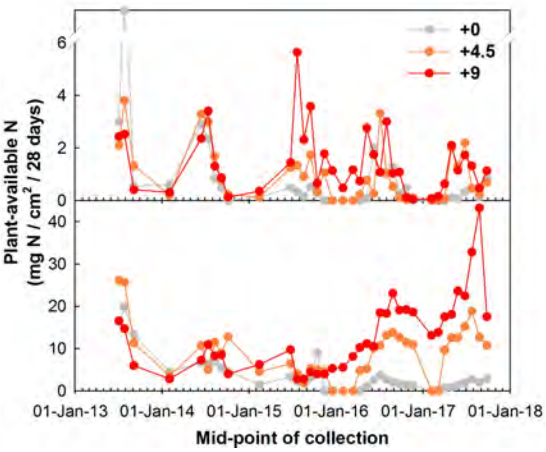


Fig. 2.7 Changes in the resin-availability of NH_4-N over time from 2013 to 2017 in the hummocks, at a 10-cm depth from the surface of the peat (a) or 60-cm depth from the surface (b). At each depth, each data point is averaged over the two resin arrays in each experimental plot, and also averaged across the two experimental plots per experimental treatment shown (i.e., averaged across ambient and elevated [CO_2]; there is thus far no obvious effect of elevated [CO_2] on nutrient availability).

Response of microbial communities and processes to Deep Peat Heating and WEW – Warming is expected to lead change microbial communities both due to the direct effects of warming and indirect effects such as drying that may alter biogeochemical processes such as methane production and oxidation rates, N- fixation rates, or interactions between plant productivity, priming and decomposition, all of which are mediated by microbial communities. During the first 2 years of warming under deep peat heating and WEW very limited responses of peat microbial communities have been observed. Using combined molecular and biochemical characterization we were able to show with rRNA QPCR and amplicon sequencing that, while microbial communities are strongly depth stratified (Tfaily *et al.* 2012, Lin *et al.* 2014a&b, Steinweg *et al.* 2018), responses to the treatments during this phase were very limited, especially in the deep peat (Wilson *et al.* 2016). Follow-on incubation experiments suggest this response is not limited by P or N as had been suggested previously (Kluber *et al. in revision*). Indeed, temperature and pH do seem to limit CH_4 production from the deep peat such that overall responses were slow to develop during even the ideal conditions provided by the 70-day incubations. This suggests that *in situ* responses of these recalcitrant deep peat communities may develop over time.

2.1.7 Decomposition and Flux of CO_2 and CH_4

Decomposition – Using six common litter types (i.e., *P. mariana* needles, shrub leaves, fine roots, *Sphagnum*) we found no clear effect of warming on the decomposition of aboveground litter types after 2 years. However, decomposition rates of fine roots (*P. mariana* and *R. groenlandicum*) tended to increase with warming. There may be several explanations for the differences in above- vs belowground litter decomposition, including differences in chemistry, biology (i.e., different decomposers), and methodology (i.e., different mesh sizes, deployment depths). A second decomposition experiment with mixed species bags found that breakdown of *P. mariana* needles and *R. groenlandicum* leaves was faster when mixed with *Sphagnum* than without. This finding is opposite our hypothesis of a slower breakdown rate due to the known inhibitory effect of *Sphagnum* (and its secondary chemistry) on decomposition rates. The faster decomposition may be due to the ability of *Sphagnum* to hold moisture. Given that aboveground litter decomposes within a *Sphagnum* matrix, it is likely mixed species litterbags result in more representative decomposition rates in the bog. A third experiment revealed that labile C decomposition (cotton strips = 99% cellulose) increased with warming, but there was no clear pattern with depth. Given that labile C decomposition responded to warming, but aboveground litter types did not, this suggests that litter chemistry may be limiting decomposition more so than temperature at least in the initial stages of litter breakdown. Lastly, we are collaborating on a study led by R. Kolka of the USFS that was initiated in October 2017 to measure the decomposition of peat at different depths (0, 10, 20, 30 cm) in the SPRUCE enclosures using decomposition ladders. These measurements were initiated in response to comments during the previous ORNL TES SFA review.

Net CO_2/CH_4 efflux – After two full growing seasons under experimental warming and eCO_2 we have observed limited effects of eCO_2, and differential responses of CO_2 and CH_4 fluxes in response to warming. CO_2 efflux appears to increase with warming with a slight "acclimation" in higher temperature treatments (perhaps a drying effect). CH_4 fluxes also increase with warming, and this response appears to be particularly strong in the higher temperature treatments. When you combine these treatment trends with *in situ* temperatures throughout an annual cycle, we estimate that the +9 °C treatments show a 19 and 194 % increase in fluxes of CO_2 and CH_4, respectively (Fig. 2.8).

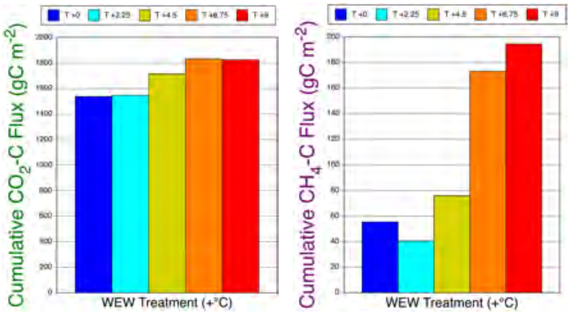


Fig. 2.8 Estimated annual CO_2 (left) and CH_4 (right) flux for the SPRUCE study site for 2017.

2.1.8 Carbon Budget for the S1 Bog and Bog Net Primary Production

Griffiths *et al.* (2017) combined data from numerous SPRUCE measurement tasks to produce a comprehensive synthesis of error propagation and uncertainty analysis for the S1 Bog C cycle (Fig. 2.9).

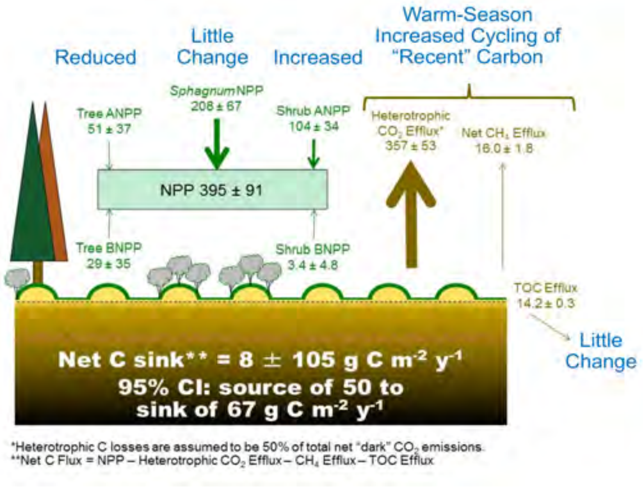


Fig. 2.9 Full uncertainty analysis of the S1 Bog C cycle (Griffiths *et al.* 2017) showing an average net sink of C with very large error bars. Directions of change for key fluxes inferred from first-year whole ecosystem warming results for the extreme of +9 °C are shown in blue text.

The results showed a very small net gain of C of 8 g C m^{-2} y^{-1} prior to the initiation of WEW. However, the combined error terms from this analysis do not allow us to conclude whether the bog is currently a net sink or source of C to the atmosphere. Unless changes in response to the experimental treatments are very large, conclusions on whole-ecosystem C cycle responses to warming and eCO_2 will need to employ isotopic tracer or discrimination techniques to resolve the direction and magnitude of change in ecosystem C balance.

Carbon Cycle Assessments for the S1 Bog – Assessments of vegetation growth were combined with large-collar flux data to produce initial estimates of the response of the ecosystem C balance of the SPRUCE peatland to warming (Fig. 2.10). Based on this analysis, in both 2016 and 2017 the bog appears to be an increasing C source with warming, but there is no clear effect of eCO_2. Overall, we estimate C loss per °C of warming to be 20 g C m^{-2} y^{-1}. Declining bog elevation data assessments confirm a pattern of C loss with warming (Section 2.1.2).

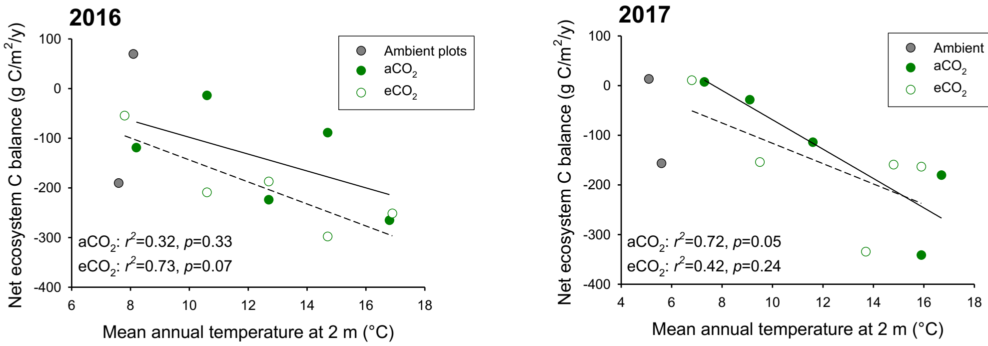


Fig. 2.10 Change in peatland C balance for 2016 and 2017 as a function of treatment temperatures.

2.1.9 Hydrology and Porewater Chemistry

Hydrological fluxes out of the SPRUCE chambers, along with porewater chemistry measurements, have been used to: (1) establish baseline conditions in the S1 Bog, (2) quantify variation among depth profiles across local peatland ecosystems (S1 Bog, S2-Bog, Bog Lake Fen), (3) assess initial responses to deep-peat heating (in 2014), and (4) track WEW treatment responses (2015 onward).

Hydrology and Water Chemistry – Lateral water fluxes (i.e., stream flow) from SPRUCE enclosures are quantified through a combination of isolation of individual plots using the belowground corrals and state-of-the art sump systems (Sebestyen and Griffiths 2016). Lateral water fluxes decreased with warming (Fig. 2.11) likely due to increased evapotranspiration caused by the increasing atmospheric vapor pressure deficit with warming. Further, there was a general pattern of higher total organic carbon (TOC) and cation (i.e., calcium) concentrations in outflow from the warmer plots likely due to increased mineralization and leaching of recently produced organic matter. Despite the higher TOC concentrations in outflow from warmer enclosures, the TOC fluxes from warmer enclosures were lower in 2016 and 2017 (Fig. 2.11) because stream flow was the predominant driver of TOC fluxes. However, in 2018, TOC fluxes from the warmest plots were as high or higher than the TOC fluxes from the cooler plots, reflecting both the higher TOC concentrations and lower stream flow (Fig. 2.11).

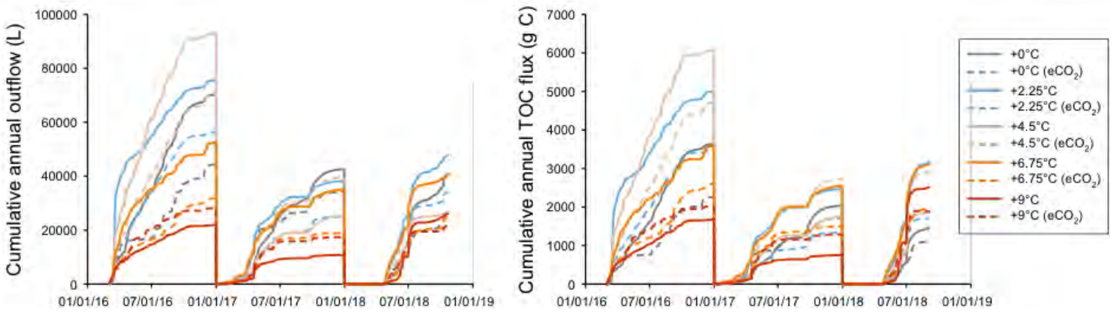


Fig. 2.11 Cumulative annual stream flow/lateral outflow (left figure) and cumulative annual total organic carbon (TOC) fluxes (right figure) from SPRUCE enclosures and responses to warming over three years

(2016, 2017, 2018). Outflow from enclosures in 2016 was complicated by residual effects of installation and leaks (enclosures 8, 13, & 20). Leaks were fixed in summer 2016.

Porewater – Depth-specific piezometer wells were installed in all SPRUCE experimental plots in 2013 to allow for periodic manual porewater sampling. TOC and cation concentrations increased in shallow porewater (0, 30 cm depths) with warming, consistent with the outflow observations (described above), but there were no changes in nutrient concentrations (e.g., ammonium or nitrate) at these depths, which indicates that the enhanced nutrient availability based on ion-exchange resins in the upper soil was rapidly sequestered by roots and microbes in this nutrient-limited ecosystem. No changes were observed in deeper porewater (>50 cm) for any measure of chemistry. As described above, increased TOC concentrations may reflect increased mineralization in response to warming. A manuscript detailing pre-treatment variation in porewater chemistry in the S1 Bog was completed (Griffiths and Sebestyen 2016), and a second manuscript describing variation in porewater chemistry among peatlands (bogs to fens) in the Marcell Experimental Forest is in progress. Porewater TOC responses to deep peat heating were reported in Wilson *et al.* (2016).

2.1.10 SPRUCE Collaborations

The SPRUCE project 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 are hosting the 25 projects summarized in **Listing of External Collaborations** (see page 163) representing 21 Universities, the Lawrence Livermore National Laboratory, the USDA Forest Service (Minnesota and Oregon), the US Environmental Protection Agency (EPA; Duluth, Minnesota) and the US DOE Joint Genome Institute. Over 100 persons are on our distribution listing for these funded projects and routinely participate in monthly teleconferences on SPRUCE science and project operational details. We continue to encourage collaborators to propose supplemental work in areas that are not fully represented by established working groups when they are complementary to ongoing work and do not compromise the decadal experimental plans.

2.2 Walker Branch (Task 2 – Completed)

Walker Branch Watershed is a forested watershed on the Oak Ridge Reservation. Previous studies in the watershed focused on understanding hydrological, biogeochemical, and ecological dynamics and responses to atmospheric deposition and climate variability. Work on the Walker Branch Watershed task was limited to finalizing datasets and publications from previous field studies. The long-term hydrology (precipitation, stream flow), stream chemistry, and climate datasets from Walker Branch Watershed were formatted to follow standard data archiving protocols, and more comprehensive data guides were completed from existing metadata and institutional knowledge. These updated datasets and data guides are now available on the ORNL TES SFA website and are accessible via the Walker Branch website (https://walkerbranch.ornl.gov). Four papers were completed that focused on in-stream biogeochemical dynamics (Griffiths and Tiegs 2016, Brooks *et al.* 2017, Hill and Griffiths 2017, Griffiths and Johnson 2018). Further, three papers synthesized C and N cycling in streams across the globe, including data from Walker Branch Watershed (Follstad Shah *et al.* 2017, Norman *et al.* 2017, Tank *et al.* 2018). Lastly, a deliverable focused on the development of a stream metabolism model has now shifted to focus on the completion of a manuscript on the long-term metabolism dataset.

2.3 Terrestrial impacts & feedbacks of climate variability, extreme events & disturbances (Task 6)

During the current SFA performance period (March 2015 to September 2018), the research supported by Task 6 has resulted in the publication of 42 peer-reviewed papers in journals with international circulation, two manuscripts under review, and two data sets with citable DOI's in addition to our AmeriFlux data product. Below we describe a few examples of research findings, focusing on those that have yet to be made publicly available.

2.3.1 Progress in MOFLUX site operations with strengthened belowground observations

The MOFLUX data acquisition system consists of EC/sun-induced chlorophyll fluorescence (SIF) instrumentation, meteorological and radiation sensors, vertical profiles of CO_2, H_2O, temperature and humidity, soil respiration systems, and vertical profiles of soil temperature and water content. The measurements are checked daily with an automated system. We also perform scheduled measurements of ecophysiological and biometric variables.

2.3.2 Progress in Task 6 Science

Technological and theoretical developments in SIF - SIF is a direct functional proxy for gross primary productivity (GPP) and highly sensitive to environmental changes. Major opportunities exist to advance terrestrial ecosystem science through integrated concurrent observations and theoretical understandings of dynamic ecosystem fluxes (e.g., energy, H_2O, CO_2) and SIF emission. We have focused on making simultaneous advances in measurement technology and theory needed for realizing these opportunities. On the technological front, a novel Fluorescence Automated Measurement Equipment (FAME) was developed for plug and play at EC sites, field-tested (Gu *et al.* 2018), and a US patent application has been filed by ORNL. The prototype was deployed at MOFLUX (Fig. 2.12) in September 2016 and operated continuously during the subsequent growing seasons. The FAME operating system and hardware configuration has also been optimized and new systems have been built to support other TES-SFA tasks.

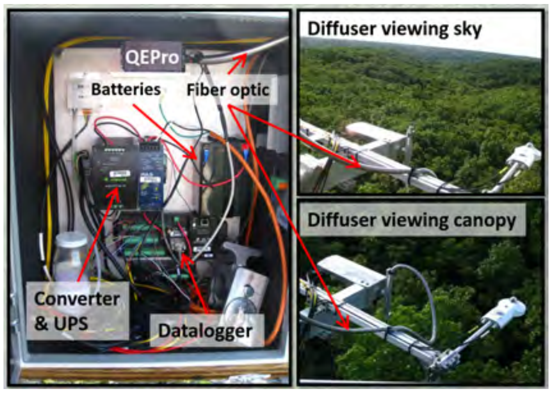


Fig. 2.12 Photographs of the prototype Fluorescence Automated Measurement Equipment (FAME) system deployed at MOFLUX. The left panel shows the interior of the thermostatically controlled enclosure that houses the spectrometer (QEPro) datalogger (CR1000), and power supplies. The right-most panels show the fiber optic to which a cosine diffuser (180° FOV) is affixed viewing the sky (upper) and canopy (lower). A smart motor is used to alternate the position of the diffuser. The net all wave radiometer (CNR4) is also visible at the right of both panels at right.

On the theoretical front, we have derived the fundamental equations governing SIF emission dynamics and the relationships between SIF and GPP for C3 and C4 photosynthesis (Gu *et al.* 2019). The fundamental equations reveal that SIF dynamics are driven by the absorbed light, but also affected by non-photochemical quenching (NPQ), fraction of open photosystem II (PSII) reaction centers (q_L), energy allocation, PSII resting state, canopy escape probability ε, etc. Although the dynamics are complex, canopy SIF observation greatly reduces the physical, physiological and biochemical complexity of estimating canopy photosynthesis and ecosystem stress because it integrates over this complexity. The SIF-GPP relationship is affected by q_L and ε for both C3 and C4 photosynthesis and also by stomatal and mesophyll resistances, chloroplastic CO_2 photocompensation point, dark respiration rate, and atmospheric CO_2 partial pressure, especially for C3 species. The theoretical advance brought about by our study will guide future SIF research and provide a new mechanistic modeling framework that complements the traditional dark reactions-centric biochemical model (Farquhar *et al.* 1980).

SIF observational studies - FAME data from MOFLUX showed that mean mid-day SIF increased rapidly during spring with a late-May to early-June peak, followed by a gradual decline through to the end of the growing season, and generally agreed with variations in plant water stress (Fig. 2.13). This seasonal pattern is broadly consistent with those of C and vegetation dynamics. A more in-depth probing of SIF dynamics at shorter timescales revealed consistent diurnal hysteresis in the light response and saturation of SIF at high incident PAR. There are several possible explanations for these observations that relate primarily to factors that decrease PAR absorption (e.g., diurnal leaf orientation changes and chloroplast repositioning) or alter energy partitioning in the light reactions of photosynthesis (i.e., upregulation of

NPQ). These key findings highlight the crucial need to better understand the factors controlling temporal SIF dynamics to unlock its full potential for monitoring ecosystem photosynthesis.

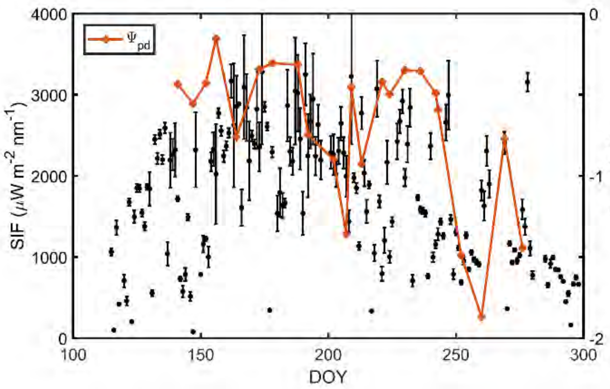


Fig. 2.13 Time series of mean mid-day SIF (left y-axis) and predawn leaf water potential (Ψ_{pd}, right y-axis) during the 2017 growing season. Error bars represent 1 standard error, for which the magnitude was largely dependent on the degree of variable cloudiness, which increases the noise in SIF retrievals.

<u>*Leaf-scale observational and modeling studies*</u> - Leaf-level pulsed amplitude modulation (PAM) fluorescence measurements revealed important temperature dependencies of the NPQ light response. Up regulation of NPQ at elevated temperatures and slow relaxation kinetics may partially explain the hysteresis in the canopy SIF light response. Diurnal cycles of leaf water potential (Ψ_L) differed among species, and in general displayed rapid changes in the morning with more muted variation during the afternoon. Afternoon SIF may be inhibited by the elevated water stress due to tree hydraulic limitations that persists from mid-day through the afternoon. Preliminary observations reveal diurnal patterns in leaf transmissivity (τ_L) with differences among species. In general, τ_L was lowest in early morning, increased through mid-day and declined later in the afternoon. These changes in optical properties could potentially be due to the repositioning of chloroplasts to decrease light absorption at high PAR, which has consequences for the supply of photons for driving the light reactions, and thus SIF emission. These comprehensive ecophysiological observations are crucial towards establishing a more thorough understanding of processes that drive variations in SIF, which is needed to support the development of appropriate models of SIF that are compatible with existing photosynthesis models.

A key factor in the uncertainty of the SIF-GPP relationship is that the dynamics of q_L and NPQ. q_L directly control linear electron transport from PSII to PSI and therefore the SIF-GPP relationships. NPQ competes with photochemical quenching for carbon dioxide (CO_2) reduction and indirectly affects the SIF-GPP relationships as well. For this reason, our modeling efforts have further focused on developing simple, yet mechanistically sound dynamic q_L and NPQ models to facilitate an improved understanding of SIF-GPP relationships. Modeling of q_L is still on-going while we have developed a dynamic NPQ model that accounts for the leaf irradiance history. The model simulates the induction and relaxation of NPQ on minute time scales. As a result, it is well suited for modeling NPQ and its effect on SIF-GPP relationships under fluctuating light conditions caused by rapidly developing and evolving cloud fields, which are a frequent phenomenon in nearly all vegetated climate zones. Initial tests show that the model accurately captures the transient processes of both light induction and dark relaxation of NPQ. The model has only four parameters and runs very efficiently, and thus has the potential to be implemented in large-scale models such as E3SM for simulating terrestrial SIF emission and photosynthesis.

<u>*Understanding drought impacts on ecosystem processes*</u> – We have probed the growing record of ecosystem flux, ecophysiological and biometric data sets to examine drought impacts on ecosystem functioning. This work has demonstrated links between simple metrics describing precipitation variability and both water stress and tree mortality at the species and ecosystem levels (Gu *et al.* 2015 and 2016a). We also found that the abiotic drought-stress likely triggered infection of fungal pathogens (*Biscogniauxia* spp.), which played a role in the mortality of white oak (*Quercus alba* L.) and black oak (*Q. velutina* Lam.) individuals (Wood *et al.* 2018). We also tested the Community Land Model (CLM) by asking the question: does the model behave like an ecosystem? (Gu *et al.* 2016b). Although CLM predicted seasonal and interannual variations in evapotranspiration reasonably well, its predictions of net C uptake were too small across the observed range of climate variability (i.e., climate sensitivity was underestimated) while carbon-water flux coupling was overestimated.

Photosynthetic and environmental controls of soil respiration - Using decade-long continuous measurements of soil respiration and eddy covariance records of net ecosystem CO_2 exchange at the MOFLUX site (Liu *et al.* 2019), we investigated the intrinsic linkage of photosynthesis and environmental factors with soil respiration (Fig. 2.14). Photosynthesis regulated soil respiration on diurnal scale with a time lag of 4 to 9 hours, with variations in this time lag affected by past trajectories of moisture and temperature. Photosynthesis exerted a more prolonged modulation on soil respiration during dry than wet seasons. Precipitation events affected the time lag between soil respiration and photosynthesis with a magnitude depending on the initial soil moisture level when precipitation started. Finally, we found that models of soil respiration were improved by incorporating photosynthesis as an input along with soil temperature and moisture. Our findings suggest that physiological and environmental processes jointly control soil respiration and are important for modeling soil respiration.

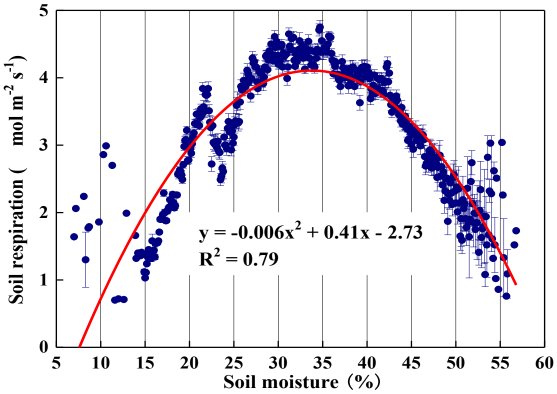


Fig. 2.14 Relationship between soil respiration and soil moisture.

Supporting collaborative research and data sharing - To support the AmeriFlux Management Project data standardization effort, we have reformatted all MOFLUX historical data since 2004 using the exact new AmeriFlux data format and variable naming conventions. We have made publicly available unique, important datasets collected by MOFLUX. For example, we have one of the best predawn leaf water potential datasets in the world (Fig. 2.15), available via the ORNL TES SFA data management effort (Pallardy *et al.* 2018). We have been continuously updating this dataset as new data are obtained. Additionally, we have been supporting the PhenoCam project of Prof. Andrew Richardson of Northern Arizona University. Also, two PhD students from Indiana University have visited the site to conduct field work, and collaborations will continue in the future with Dr. Kim Novick's (site PI of AmeriFlux Core Site US-MMS) research group. Dr. Lawren Sack at UCLA is planning to visit the site for field work during the growing season of 2019 to characterize organ-level plant hydraulic traits to complement ongoing ecosystem-level MOFLUX observations.

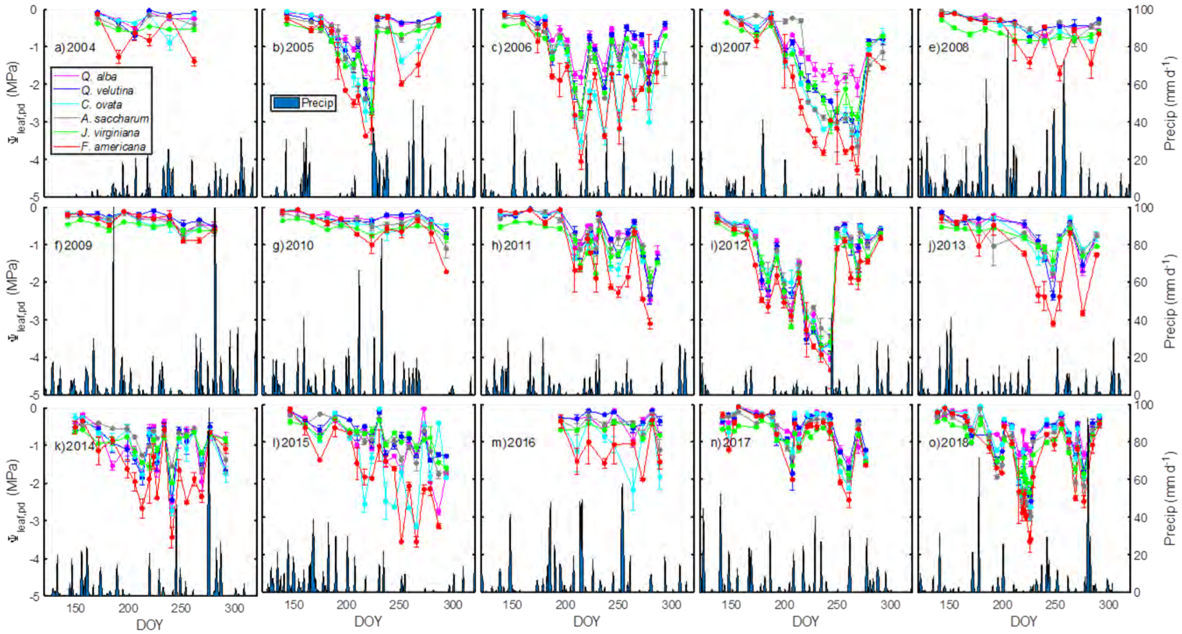


Fig. 2.15 Historical time series of predawn leaf water potential of six major species and precipitation at the MOFLUX site.

Outreach - Tours of the MOFLUX site were given to educate visitors about MOFLUX-specific, and wider ORNL TES-SFA research activities. Groups have included classes from the University of Missouri and Westminster College, the Missouri Chapter of the Nature Conservancy and the Missouri Chapter of the Society of American Foresters. MOFLUX personnel have also been invited to present MOFLUX-related science at a local high school and in classes at MU in the School of Natural Resources and the Division of Biological Sciences.

MODEL DEVELOPMENT AND EVALUATION*

2.4 Mechanistic Terrestrial Ecosystem Modeling (Task 3)

This task incorporates model development and MODEX activities at the point scales (Task 3.1), regional to global scales (Task 3.2), and at the level of mechanistic functional units (Task 3.3) to identify process contributions to the global climate C cycle forcing from terrestrial ecosystems. Development on the Multi-Assumption Architecture and Testbed (MAAT) has branched off to a new, higher-level subtask (task 3d; see below). Brief summaries of progress are presented along with tabular summaries of progress on proposed deliverables.

2.4.1 Task 3a – Improve ecosystem process models with site-level observations and experimental data

SPRUCE modeling – In April 2018, E3SM version 1 (including the land model ELM) was released to the public. ELMv1 contains developments initiated or co-funded by the ORNL TES SFA, including C and nutrient storage (Metcalfe *et al.* 2017) and phosphorus (P) cycling (Yang *et al.* 2017). We have created a SPRUCE-specific branch of ELMv1 (ELMv1-SPRUCE), which includes the representation of hummock-hollow microtopography and a *Sphagnum* plant functional type. This model has more realistic nutrient cycling but does not yet include the Microbe model developed by subcontractor Xiaofeng Xu of San Diego State University (Xu *et al.* 2014) and included in ELMv0-SPRUCE. We are currently resolving using the PFLOTRAN framework. We are continuing to maintain the previous version ELMv0-SPRUCE (formerly known as ALM-SPRUCE) for the purposes of predicting methane cycling and for comparison with v1. The *Sphagnum* photosynthesis submodel has been successfully implemented in both versions of the model and a publication is in preparation. This submodel predicts the reduction of moss

NPP with warming similar to what is currently being observed (Section 2.1.3). Following the high-profile publication by Richardson *et al.* (2018), we began to develop an improved phenology submodel for SPRUCE which we expect to be relevant for other ecosystems. Seasonal, species-specific phenology modeling has also been explored using pretreatment SPRUCE physiology data and was shown to have significant impacts on site level NPP (Section 2.4.3; Jensen *et al.* 2019). ELM-SPRUCE improvements, along with other wetland modeling tasks, are on the E3SM version 2 roadmap for integration in 2018 and 2019 with joint TES SFA and E3SM support. EcoPAD, an ecological forecasting framework for the SPRUCE site has been completed using the Terrestrial Ecosystem (TECO) model (University of Northern Arizona). EcoPAD has been demonstrated in three publications (Ma *et al.* 2017, Jiang *et al.* 2018a, Huang *et al.* 2017), and was successfully integrated with the SPRUCE Vista Data Vision software to provide continuously updated hind casts of selected variables (http://sprucedata.ornl.gov/). In January 2018, we contributed results from ELM-SPRUCE to workshops on hydrology and nutrient cycling, which helped to identify specific measurement and model shortcomings that are being addressed in this proposal. Several modeling groups have contributed to a SPRUCE model intercomparison project (SPRUCE-MIP), indicating a diversity of responses in pre-treatment C and methane fluxes. The MIP is currently being extended to cover treatment conditions.

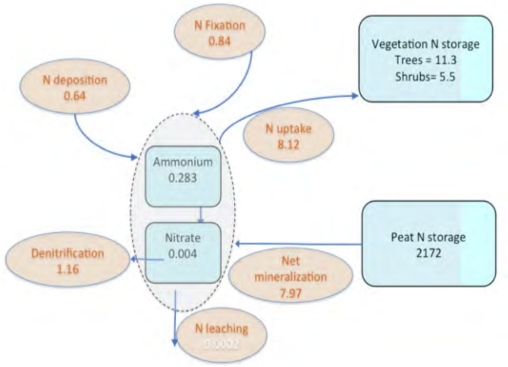


Fig. 2.16 Pre-treatment nitrogen budget as simulated by ELMv1-SPRUCE (yellow: fluxes in gN m^{-2} yr^{-1}; blue: pools in gN/m^{2}). At a nutrient cycling workshop held in January 2018, we compared the model and observed budgets and used this to prioritize model development tasks – e.g. the need for a better representation of organic N leaching, long-term peat accumulation, denitrification and N fixation.

Modeling at other sites - Beyond SPRUCE, we are also using the point version of ELM (version 1) at MOFLUX and additional AmeriFlux sites relevant for the TES SFA. We developed a site-level benchmarking package focused on model-data comparison with AmeriFlux data, which complements the ILAMB package and serve as a useful tool for SFA model development tasks. These model developments at SPRUCE improving 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 (UQ) 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 improves predictions of leaf area index (LAI) and carbon fluxes at the Missouri Flux eddy covariance site (Fig. 2.17).

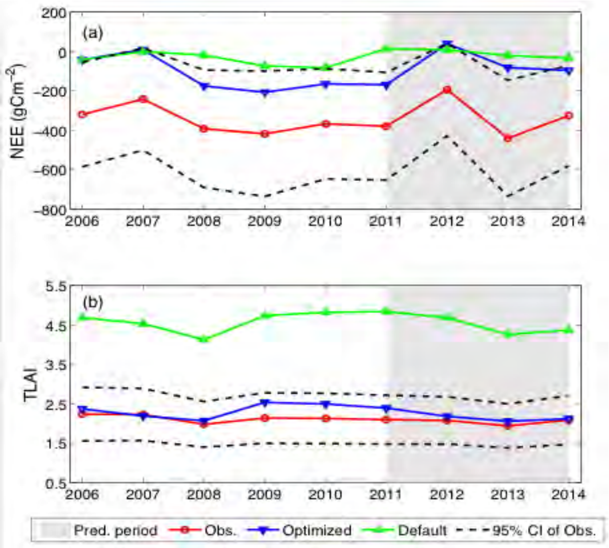


Fig. 2.17 3000 ELM simulations were performed, randomly varying 8 sensitive model parameters. These simulations were used to build a surrogate model of net ecosystem exchange (NEE) and leaf area index (TLAI) at the Missouri Ozark Flux site. This surrogate model was then calibrated using an efficient global optimization algorithm, and the optimized parameters were fed into ELM to perform new simulations. The optimized version of ELM performs much better than the default, especially for TLAI. For NEE, the interannual variability is represented better, although a significant bias remains. This is an indication that model structure (i.e., missing or incorrect process representation), rather than parametric uncertainty drives model error.

A novel tree stem-water model was also developed to capture the dynamics of stem-water storage and its contribution to daily transpiration. The module was incorporated into the Community Land Model, on which the ELM is based. The updated model was then used to test the sensitivity to stem-water content for an evergreen rainforest site in Amazonia, i.e., the BR-Sa3 eddy covariance site. With the inclusion of the stem-water storage, ELM produced greater dry-season latent heat flux that was closer to observations, facilitated by easier canopy access to stem-water, rather than solely dependent on soil water. Stored stem water of a single mature tree was estimated to contribute 20-80 kg/day of water to transpiration during the wet season and 90-110 kg/day during the dry season, thereby partially replacing soil water and maintaining plant transpiration during the dry season. Our study indicates that the inclusion of stem capacitance in ELM significantly improves model simulations of dry-season water and heat fluxes, in terms of both magnitude and timing, and a manuscript is in revision for *Agricultural and Forest Meteorology* (Yan *et al.* 2019).

2.4.2 Task 3b – Regional and Global Land Ecosystem Modeling

Contribution of environmental forcings to US runoff changes for the period 1950-2010 - We developed a detection and attribution (D&A) system for offline land model simulations and applied it to several use cases with ELM. Runoff in the United States is changing, and this study finds that the measured change is dependent on the geographic region and varies seasonally. Specifically, observed annual total runoff had an insignificant increasing trend in the US between 1950 and 2010, but this insignificance is due to regional heterogeneity with both significant and insignificant increases in the eastern, northern, and southern US, and a greater significant decrease in the western US. Trends for seasonal mean runoff also differ across regions. By region, the season with the largest observed trend is autumn for the east (positive), spring for the north (positive), winter for the south (positive), winter for the west (negative), and autumn for the US as a whole (positive). Based on the D&A analysis (Fig. 2.18) using gridded WaterWatch runoff observations along with semi-factorial land surface model simulations from the Multi-scale Synthesis and Terrestrial Model Intercomparison Project (MsTMIP), we find that while the roles of CO_2 concentration, N deposition, and land use and land cover appear inconsistent regionally and seasonally, the effect of climatic variations is detected for all regions and seasons, and the change in runoff can be attributed to climate change in summer and autumn in the south and in autumn in the west. We also find that the climate-only and historical transient simulations consistently underestimated the runoff trends, possibly due to precipitation bias in the MsTMIP driver or within the models themselves. This work was mainly supported by the TES SFA project and recently published in *Environmental Research Letters* (Forbes *et al.* 2018).

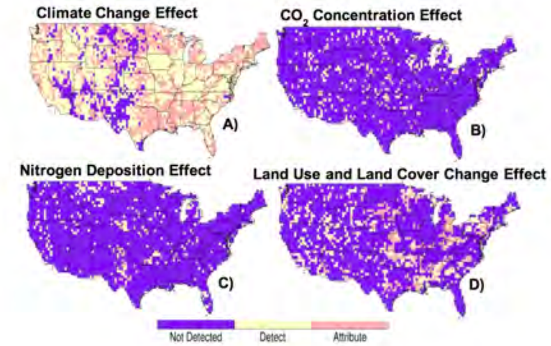


Fig. 2.18 Spatial patterns of D&A scaling factors. Not detected (purple) denotes a scaling factor whose corresponding 95% confidence interval was less than zero or included zero. If the 95% confidence interval was greater than zero but did not include one, the forcing was detected (yellow). A positive confidence interval was labeled as attributed (pink) if it included one.

Streamflow in the Columbia River Basin: Quantifying changes over the period 1951-2008 and determining the drivers of those changes – D&A analyses were performed using naturalized streamflow observations and routed land surface model runoff for 10 subbasins in the Columbia River Basin (CRB) during water years 1951–2008. The Energy Exascale Earth System Model (E3SM) and the Routing Application for Parallel computatIon of Discharge (RAPID) routing model were used to conduct semi-factorial simulations driven by multiple sets of bias-corrected forcing datasets. Four main potential drivers, including climate change (CLIM), CO_2 concentration (CO_2), N deposition (NDEP), and land use and land cover change (LULCC), were analyzed during the assessment (Fig. 2.19). All subbasins showed significant ($\alpha = 0.10$) declines in the observed amount of annual total streamflow, except for the Middle and Upper Snake and Upper Columbia Subbasins. These declines were led by significant decreases in June–October streamflow, which also directly led to significant decreases in peak and summer streamflow. Except for the Snake River Subbasins, LULCC had the same pattern of declines in monthly streamflow, but the period was shifted to May–September. NDEP also had significant trends in June–October; however, rather than decreases, the trends showed significant increases in streamflow.

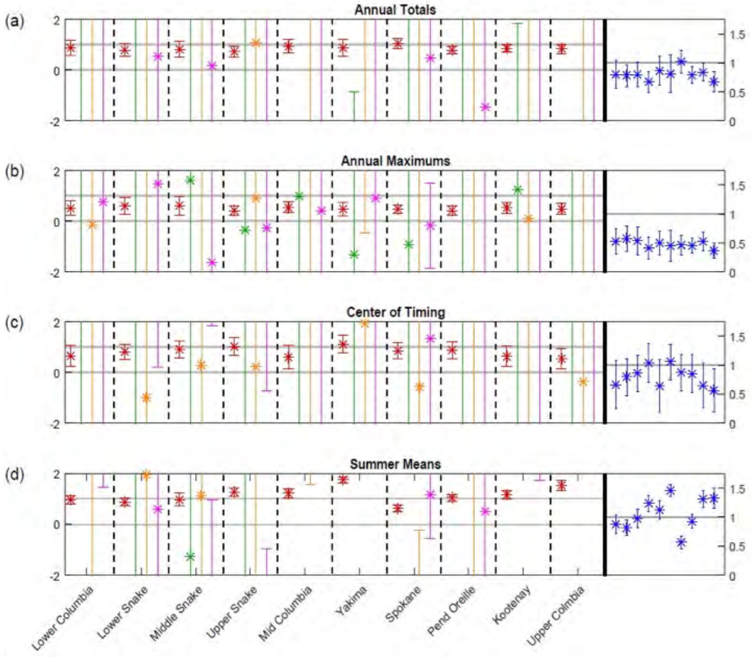


Fig. 2.19 Scaling Factor Estimates and Corresponding 95% Confidence Intervals for Annual Totals (a), Annual Maximums (b), Center of Timing (c), and Summer Means (d) using ALL and the Linear Combination of CLIM, CO_2, NDEP, and LULCC. Scaling factors for CLIM, CO_2, NDEP, and LULCC for each subbasin are shown on the left y-axis in red, green, orange, and magenta, respectively. Scaling factors for ALL (blue) are shown on the right y-axis in the same subbasin ordering. Light gray lines denote the values 0 and/or 1.

While there were significant trends in CO_2, NDEP, and LULCC, their signals of change were weak in comparison to the signal in CLIM and the natural internal variability found in streamflow. Overall, the detection and attribution analysis showed that the historical changes found in annual total, center of timing of, and summer mean streamflow could be attributed to changing climate and variability. This work was mainly supported by the TES SFA project and is under review at *Water Resources Research* (Forbes *et al.* 2018).

2.4.3 Task 3c - Functional Testing

Improving photosynthesis parameterization at SPRUCE – Observed pre-treatment interspecific seasonality in photosynthetic parameters ($V_{c,max25°C}$, $J_{max25°C}$ and $R_{d25°C}$) for *P. mariana*, *L. laricina* and the two dominant shrub species from the SPRUCE site were intoduced into ELM-SPRUCE to replace constant parameters (Jensen *et al.* 2019). Simulated NPP was enhanced using seasonal parameters. This pattern was particularly pronounced under simulations using the higher temperature and eCO_2 treatments of the SPRUCE experiment. These results show that the model's estimation of boreal ecosystem-level NPP could be significantly improved, especially in scenarios simulating future elevated temperatures and CO_2, by the inclusion of species-specific seasonal parameterization of key photosynthetic parameters.

Leaf-level functional units describing alternative formulations of leaf maintenance respiration ($R_{m,leaf}$) have been evaluated against pretreatment observations of dark respiration of *P. mariana*. Model formulations perform differentially when using their default parameterizations relevant to *P. mariana*, but these differences largely disappear when calibrated against observations using MCMC optimization. The default Q_{10} representation in ELM-SPRUCE performs as well or better than other more refined representations. The $R_{m,leaf}$ functional units are being evaluated against observations of foliar dark respiration from *P. mariana*, *L. laricina* and the two dominant shrubs collected from the SPRUCE treatment plots during the summer of 2017. Initial results for the Q_{10} formulation in *P. mariana* show no trends with warming or elevated [CO_2] in either the basal rate of respiration or the Q_{10} value. A manuscript is being prepared describing these results.

The leaf-level functional units of $R_{m,leaf}$ have been translated into options for representation of leaf maintenance respiration in ELM-SPRUCE. A suite of 10 alternative formulations (models) were encoded in an exploratory branch of ELM-SPRUCE. Stand-level C flux across pre-treatment years 2011-2015 was simulated. The various formulations made little difference in simulated $R_{m,leaf}$, canopy maintenance respiration ($R_{m,canopy}$), autotrophic respiration (R_a), NPP or net ecosystem production (NEP), largely because temperature was usually in the range over which the response functions are most similar and rarely exceeded 30°C. The impact of the alternative formulations of $R_{m,leaf}$ on model response to the SPRUCE experimental treatments was then simulated. In these simulations air temperature can exceed 35°C and differences in leaf-level temperature response became apparent in $R_{m,canopy}$, R_a, NPP and NEP. There was, however, a general narrowing of the differences when moving from the leaf to the stand. Effects of the different respiratory temperature-response formulations on 5-year mean annual NEP at +9.0°C ranged from -10 to 3%. With formulations representing acclimation, simulated net C loss was reduced by ~20% in some years. These results were presented at the 2018 American Geophysical Union (AGU) fall meeting and a manuscript is being prepared.

The functional testing framework is being used to evaluate the ELM decomposition submodel using long-term intersite decomposition experiment team (LIDET) data at 20 sites. The LIDET experiments are better suited to modeling as a functional unit, in which the environmental data is fed into the decomposition model directory, because performing the experiment in the full ELM introduces unrealistic nutrient and phenology feedbacks due to a misrepresentation of the scale of the experiment. Performing the LIDET experiment in the functional unit gives results that are more consistent with observed behavior (Fig. 2.20). A similar litter decomposition experiment is underway at SPRUCE, and we intend to use this framework to improve the decomposition model in peat environments.

In conjunction with the Optimization of Sensor networks for Climate Models (OSCM), we have extended a python-based functional testing framework to include the C cycle submodel of ELM (including phenology, growth, allocation and mortality). Using this simplified ELM (sELM), we can perform uncertainty quantification and model calibration much more efficiently. sELM is being used as a testbed for rapid model development of phenology and allocation algorithms, which can then be integrated and tested in the full ELM. We are also exploring machine learning and artificial intelligence (AI) approaches to build surrogate models of functional units, which may substantially improve model performance and allow scaling of ELM to pre-exascale architectures.

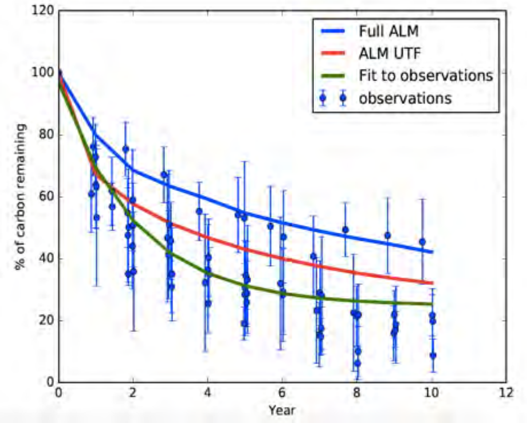


Fig. 2.20 Comparison of the functional testing and the full model approach to predicting loss of carbon in litter bags in the LIDET experiment. This figure summarizes the results for evergreen conifer forests over the 10-year period of the experiment. The unit test framework (UTF) outperforms the full version of the model because of unrealistic feedbacks described above.

2.4.4 Task 3d - Multi-Assumption Modeling – New Effort Started in FY2018

The goal of the Multi-Assumption Modeling task is to develop robust methods for formal and informal evaluation of model structural uncertainty, i.e. the uncertainty that arises in modeling a system when multiple competing hypotheses and assumptions exist to represent the mechanics of a process. To this goal, new software (the Multi-Assumption Architecture & Testbed, MAAT; Walker *et al.* 2018) and new mathematical methods (in collaboration with Ming Ye at Florida State University; Dai *et al.* 2017) have been developed, as well as using existing sensitivity analysis tools, such as Sobol methods for parameter sensitivity analysis (Saltelli *et al.* 2010). Given the potential and uniqueness in the approach, the “Formal Model Structural Uncertainty Analysis: Tools and Methods” sub-task of Task3a was elevated to the position of a task starting in FY18. Further goals of this task are to extract process understanding from observation and experiment data, to support model evaluation and new model development for improvements to ELM, contribute to ensemble modeling activities, and to promote robust modeling practice using multi-assumption methods. Model evaluation and development of leaf and canopy scale photosynthesis, has been supported by this task in the SPRUCE component of this SFA and NGEE-Tropics. MAAT allowed very flexible specification of alternative hypotheses in a model of *Sphagnum* photosynthesis, enabling the discovery of an interaction of *Sphagnum* photosynthesizing tissue area with the water table that described the main feature of seasonality *Sphagnum* in GPP (Walker *et al.* 2017).

In pursuit of promoting rigorous modeling practice, Anthony Walker convened a well-attended session on Multi-Hypothesis Modeling co-organized across hydrology and biogeoscience themes at the AGU Fall Meeting 2017. Dr. Walker was selected to give a plenary presentation on MAAT at the NACP and AmeriFlux PI Meeting in Washington DC, March 2017 and was invited to present MAAT to research groups at the University of Oxford and the University of Reading in the UK. For the NACP meeting, the presentation was competitively selected for the Emerging Technologies from the Local to Global Scale session alongside Berrien Moore’s presentation of NASA’s Geostationary Carbon Cycle Observatory (GeoCARB) mission. The promotion of these multi-assumption methods within the DOE and wider scientific communities has been successful in influencing the way models are framed (a number of talks at the 2018 AGU Fall Meeting) and developed (e.g. Plant Allocation and Reactive Transport Extensible Hypotheses [PARTEH] within the FATES model; https://github.com/NGEET/fates).

PROCESS-LEVEL STUDIES*

2.5 Partitioning in Trees and Soil (PiTS; Task 4a)

The $^{13}CO_2$ PiTS projects were very successful in bringing empiricists and modelers together to address poor representation of C flow in current terrestrial biosphere models. Three PiTS studies were completed prior to this triennial funding cycle, and final manuscripts and model exercises were completed in 2019. The studies manipulated (girdling or shading) and tracked ($\delta^{13}C$) C flow belowground, and two of the studies were used to assess the performance of C allocation modeling. The most exciting results indicate that much of the new C partitioned belowground was transported through fine roots to their associated mycorrhizal hyphae, where it was then rapidly respired in support of fungal growth and maintenance (Fig. 2.21). The rapid transfer of C from the plant to the fungi and subsequent release is a missing link in process-based Earth System models. Other results indicate that significant C (10-15% of foliar mass) is seasonally allocated to reproduction. But the model was not able to match the timing or rates of C flow to these different pools. The project suggests that additional MODEX efforts are needed to adequately incorporate both short-term and seasonal patterns of C allocation into the models. The project was not actively funded during this SFA cycle, but manuscripts and datasets continue to be produced from the effort (Mao *et al.* 2016b).

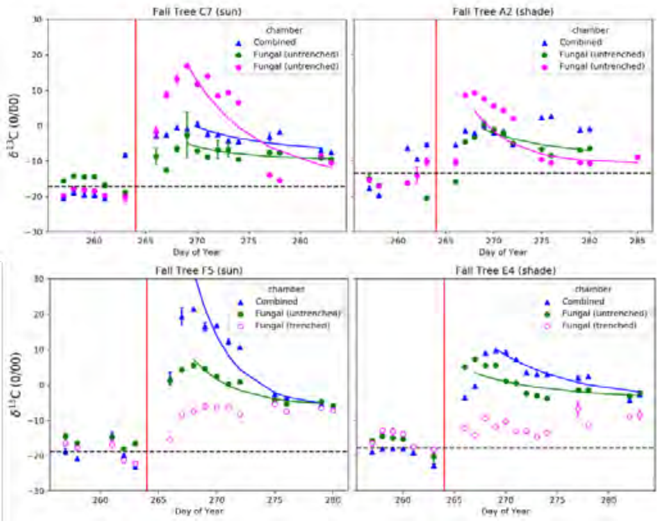


Fig. 2.21 Soil efflux of $^{13}CO_2$ following whole-tree labeling of shaded or full sun-exposed dogwood trees. Efflux is measured above soil collars that 1) contain bulk soil with roots and mycorrhizal hyphae (Combined) or 2) fungal hyphae only using a 61 µm root exclusion mesh that was connected to the surrounding soil (Fungal (untrenched)), or whose hyphal connections with the surrounding soil were severed (Fungal (trenched)).

2.6 Leveraging Root Functions to Inform Biosphere Models (Task 4c)

Based on our successful Tansley Review "Root structural and functional dynamics in terrestrial biosphere models" (Warren *et al.* 2015a) and leveraging the FRED database (Iversen *et al.* 2017), we developed a framework to improve fine-root functional representation in large-scale models through new data compilation and collection efforts, scaling and modeling. We are mechanistically assessing key root *functional* traits, including nutrient (see commentary by Walker 2018) and water uptake and linking these observations with a modeling environment that includes reactive transport (e.g., PFLOTRAN) and that may be linked to plant hydraulic traits (e.g., FATES, https://ngee-tropics.lbl.gov/news/1455-2/). Our initial focus has been to link root traits to their functional responses under drying conditions in context of water extraction rates (Dhiman *et al.* 2017) and respiration rates (Ficken & Warren 2019). We have also been focused on linking specific root ages, sizes and root order to actual root water uptake *in situ* by leveraging the neutron imaging facilities at ORNL.

We found that newer, younger roots have greater uptake capacity per unit surface area, but that total water uptake depended on the larger roots, with lower uptake rates (Fig. 2.22; Dhiman *et al.* 2017). Our results did not match Richard's equation model estimates based on root-free soil hydraulic properties, thus we initiated new work with an MS student from the University of Tennessee, Knoxville to comprehensively assess the impact of roots or mycorrhizal hyphae on soil water release curves, hydraulic conductivity and hydraulic redistribution, which should improve near surface soil hydraulic modeling.

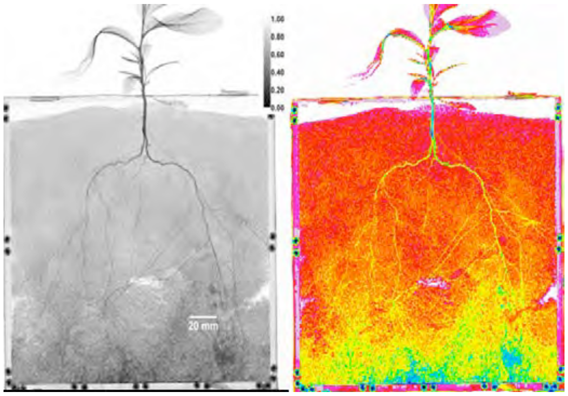


Fig. 2.22 Composite neutron images of 16 radiographs of an 11-week old poplar plant growing in sand, intensity indicates water content. Tracking water uptake through time, we quantified greater uptake rates for newer, younger roots.

2.7 Microbial Processing of Soil C (Task 5)

Soil microbes exert complex and nonlinear feedbacks on soil respiration and soil carbon storage, particularly in response to environmental changes in temperature and moisture. First-order models lack mechanisms to predict these complex responses, indicating the need for a new generation of microbial decomposition models. Here, we investigated the controls and effects of soil moisture on soil carbon stocks using the MOFLUX site, the 22-year Harvard Forest warming experiment, and heterotrophic respiration manipulations (trenching) in two forests in subtropical China. The role of microbial feedbacks was clear – drying conditions tended to increase soil carbon due to decreased microbial respiration and increased microbial dormancy, while prolonged warming increased the temperature sensitivity of microbial turnover and carbon use efficiency. Initial simulations with our Microbial ENzyme Decomposition (MEND) model using data from the subtropical forests indicate significant increases in soil carbon in response to projected decreases in soil moisture and increases in litterfall, while predicting minor changes in response to increasing soil temperature (Wang *et al.* 2019; Fig. 2.23). The implications are that the future trajectory of soil carbon storage could be more strongly affected by changes in soil moisture, than in soil temperature at these sites. MEND simulations at Harvard Forest indicate temperature increases in the manipulative field experiment reduce carbon use efficiency and increase turnover in both control and heated conditions, and the two decades of soil warming elevates the apparent temperature sensitivities of both parameters (Li *et al.* 2018b). We also compared the performance of MEND to other widely-used microbial models and found that the models exhibit divergent predictions to changes in drivers such as moisture, temperature, and clay content (Sulman *et al.* 2018). More importantly, existing field data were inadequate to determine the best model configuration. Consequently, our current efforts involve assembly of soil chamber respiration data from AmeriFlux sites worldwide to enable benchmarking and continued model improvements. A new set of incubation experiments investigating soil texture and moisture using loamy soils from MOFLUX, sandy soils from GA, and clayey soils from TX, shows that the soils have different moisture optima for highest CO_2 efflux. Results support earlier, long-term incubations involving paired forest and grassland soils from four locations that show site-specific parameters are essential for predicting lab incubation data (Kluber *et al.* 2017).

The E3SM Land Model (ELM, CLM-CN version) was used to simulate total soil respiration at MOFLUX using observations from 2005-2013. The default model parameters significantly underestimated soil water potential, annual soil respiration and gross primary production (GPP). Using a soil water retention model based on field measurements at MOFLUX, we improved the representation of GPP, but respiration was underestimated during peak growing seasons, and overestimated during drought and non-growing seasons (Liang *et al.* 2018). One potential reason may be lack of ELM representation of the seasonal cycle of microbial organisms and soil macroinvertebrates, which have high biomass and activity during peak growing seasons and tend to be dormant during non-growing seasons. However, the model showed good agreement with our new year-long measurements of heterotrophic respiration, so we are testing the sensitivity of soil C loss to moisture extremes and different recurrence intervals of droughts and wetting using the MOFLUX record. In ELM simulations, microbial respiration was more sensitive to drought than to wetting, and based on MEND, the decreased respiration and increased soil C was caused by large decreases in active microbial biomass, although decreasing substrate supply also plays a role.

Testing the MEND model at four field sites and in long-term incubations overall demonstrated the sensitivity of soil carbon stocks to critical feedbacks involving microbial biomass and physiology.

Finally, we led an interdisciplinary workshop sponsored by the Carbon Cycle Interagency Working Group to elucidate steps forward for microbial and soil C cycle models. As an outcome, we designed the "Millennial model" using 5 measurable soil C pools – particulate organic C, mineral-associated organic C, microbial biomass C, aggregate C, and low molecular weight C (Abramoff *et al.* 2017). Evaluating against the Century model, we found that the Millennial model predicts qualitatively similar changes in total SOC in response to single factor perturbations, but different responses to multiple factor perturbations. We attribute the differences to nonlinear microbial functions that result in complex feedbacks between drivers, respiration, and soil C. While progress has been made under this task, it is clear that additional efforts in benchmarking, multi-model evaluation, and model testing are needed to faithfully represent the complexities of how soil microbes affect soil C storage and respiration.

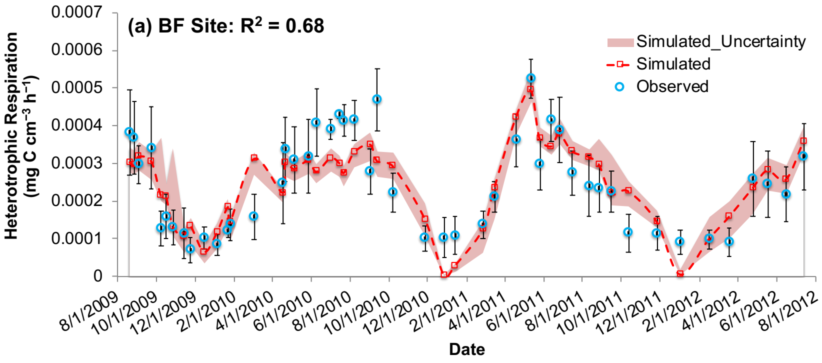


Fig. 2.23Comparison between observed and simulated heterotrophic respiration rate by the MEND model in an evergreen broadleaf forest. The vertical error bars are standard deviations for observations. The shaded band shows variability in simulations (95% confidence intervals) due to parameter uncertainty. Source: Wang *et al.* 2019.

GLOBAL TRAIT DATABASES*

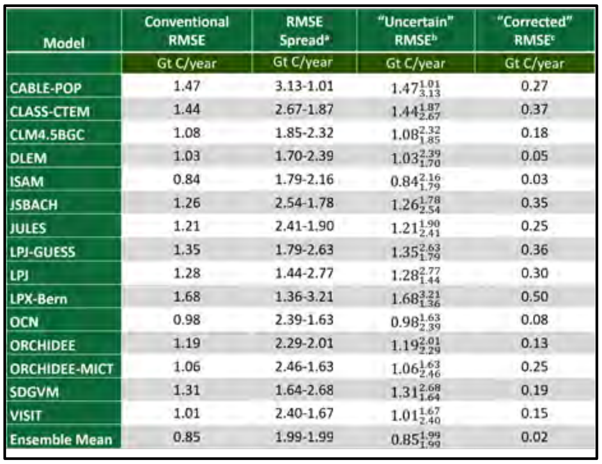
2.8 Fossil Emissions (Task 7 – Completed)

During FY2015-2016 Task 7 worked to: (1) maintain and improve a publicly-available database on carbon dioxide emissions from fossil fuel consumption, (2) confront the uncertainty in emissions estimates, and (3) utilize the carbon dioxide emissions database in terrestrial C budgets. Products include annual and monthly emissions data by country through 2014, which are available freely online (http://cdiac.ess-dive.lbl.gov/trends/emis/meth_reg.html), and significant strides in characterizing the uncertainty associated with carbon dioxide emissions from fossil fuel consumption (Andres *et al.* 2016; Ballentyne *et al.* 2015). Updated estimates of Chinese emissions were published in Nature (Liu *et al.* 2015). This task supported Robert Andres' prominent role in Global Carbon Project activities (LeQuéré *et al.* 2015) and in the Global Carbon Atlas (http://www.globalcarbonatlas.org). Andres also contributed to the Carbon Model Intercomparison Project (CMIP6) activities.

Beginning in FY2017, Task 7 was reformulated to focus on analysis and understanding of the implications of fossil-fuel emissions for terrestrial ecosystems and the terrestrial biosphere, moving away from estimates of fossil fuel emissions themselves. Given observations of the increase in atmospheric CO_2, estimates of anthropogenic CO_2 emissions and models of oceanic CO_2 uptake (LeQuéré *et al.* 2017), one can estimate net global CO_2 exchange between the atmosphere and terrestrial ecosystems as the residual of the balanced global C budget. Within the uncertainty in observations of atmospheric CO_2, anthropogenic emissions and oceanic uptake, this residual calculation is a sound estimate of the global behavior of terrestrial ecosystems over the past 60 years. This "residual land sink" is a benchmark against which the performance of global terrestrial biosphere models, including the land models of Earth System Models, should and has been evaluated (e.g., Huntzinger *et al.* 2017). However, the "within the uncertainty" above is an important caveat. Based on earlier work of Task 7, the uncertainty (2σ; 95% confidence interval) in fossil fuel emissions is 8.4% (Andres *et al.* 2014). Combined with uncertainty in other carbon budget components (LeQuéré *et al.* 2017), for example the 2σ uncertainty in land-use change emissions of 1.4 Pg C y-1, the 2σ uncertainty surrounding the global net terrestrial ecosystem CO_2

exchange is ±1.8 Pg C y-1. At the 2σ uncertainty bounds, terrestrial ecosystems may have been a cumulative sink as large as -237.15 Pg C (averaging 4.09 ± 0.15 Pg C y-1) or as small as 28.35 Pg C (averaging 0.49 ± 0.15 Pg C y-1).

We are preparing a manuscript examining how well global terrestrial biosphere models simulate the trend and interannual variability of the global-budget estimate of the terrestrial sink within the context of this uncertainty (e.g., which models fall outside the 2σ uncertainty and in what years. As part of this manuscript we are introducing a revised skill scores methodology which explicitly accounts for the uncertainty surrounding the global-budget estimate of the terrestrial sink (e.g., Table 2.1). In addition, if one adds land-use change emissions to the residual land-sink, one obtains a 60-year history of global Net Biosphere Production (NBP), the global extension of Net Biome Production (Chapin *et al.* 2006). We are preparing a manuscript which analyzes the time-series properties of this history.



Model	Conventional RMSE	RMSE Spread^{a}	"Uncertain" RMSE^{b}	"Corrected" RMSE^{c}
	Gt C/year	Gt C/year	Gt C/year	Gt C/year
CABLE-POP	1.47	3.13-1.01	$1.47^{1.01}_{3.13}$	0.27
CLASS-CTEM	1.44	2.67-1.87	$1.44^{1.87}_{2.67}$	0.37
CLM4.5BGC	1.08	1.85-2.32	$1.08^{2.32}_{1.85}$	0.18
DLEM	1.03	1.70-2.39	$1.03^{2.39}_{1.70}$	0.05
ISAM	0.84	1.79-2.16	$0.84^{2.16}_{1.79}$	0.03
JSBACH	1.26	2.54-1.78	$1.26^{1.78}_{2.54}$	0.35
JULES	1.21	2.41-1.90	$1.21^{1.90}_{2.41}$	0.25
LPJ-GUESS	1.35	1.79-2.63	$1.35^{2.63}_{1.79}$	0.36
LPJ	1.28	1.44-2.77	$1.28^{2.77}_{1.44}$	0.30
LPX-Bern	1.68	1.36-3.21	$1.68^{3.21}_{1.36}$	0.50
OCN	0.98	2.39-1.63	$0.98^{1.63}_{2.39}$	0.08
ORCHIDEE	1.19	2.29-2.01	$1.19^{2.01}_{2.29}$	0.13
ORCHIDEE-MICT	1.06	2.46-1.63	$1.06^{1.63}_{2.46}$	0.25
SDGVM	1.31	1.64-2.68	$1.31^{2.68}_{1.64}$	0.19
VISIT	1.01	2.40-1.67	$1.01^{1.67}_{2.40}$	0.15
Ensemble Mean	0.85	1.99-1.99	$0.85^{1.99}_{1.99}$	0.02

Table 2.1 Conventional model skill scores and skill scores modified to explicitly account for uncertainty in model benchmark. Model results from Le Quéré *et al.* (2017). a) Root Mean Square Error (RMSE) calculated on upper and lower uncertainty bounds. b) RMSE evaluated against the nominal value with superscript and subscript evaluated against the upper and lower 2σ uncertainty, respectively. c) Only values outside 2σ uncertainty are scored in the corrected RMSE.

2.9 Linking Root Traits to Function (Task 4b)

A fine-root ecology database (FRED) - Variation and tradeoffs within and among plant traits are increasingly being harnessed by empiricists and modelers to predict ecosystem processes in response to current and future environmental conditions. While fine roots play an important role in ecosystem processes, most fine-root traits are extremely underrepresented in global trait databases; e.g., <1% of data in the 'TRY' database describe fine-root functional traits.

To address the need for a centralized fine-root trait database that could be used to improve fine root representation in models, we compiled the Fine-Root Ecology Database (FRED) from published and unpublished data sources; data collection is ongoing and will continue for the foreseeable future. The first version of FRED (FRED 1.0) was released in 2017 via the website https://roots.ornl.gov (Iversen *et al.* 2016; 2017). FRED 1.0 contained ~50,000 species-specific trait observations from 1213 species, and ~20,000 trait observations collected from mixed plant communities, compiled from nearly 800 data sources. In total, these observations encompass more than 300 root traits. To facilitate empirical and modeling analyses, we also collected ancillary data related to vegetation, edaphic and environmental conditions; these encompassed ~ 270 additional data streams. FRED 1.0 was downloaded over 200 times, including 42 countries across six continents, but downloads were mainly focused in the United States, Europe, and China (http://roots.ornl.gov/overview).

To facilitate better quantification of relationships or tradeoffs between and among above- and belowground traits as suggested in a DOE-sponsored workshop (Koven *et al.* 2016; Kueppers *et al.* 2016), each version of the FRED database is being submitted to the TRY database under the 'public (open access)' data status. Recently, FRED was among the major contributions of trait data to TRY 4.0, adding about 250 new root traits and roughly doubling the number of root records compared a previous version.

FRED 2.0 was released in 2018 with 50% more root trait observations, particularly in the categories of root anatomy, architecture, chemistry, and morphology (Iversen *et al.* 2018, McCormack *et al.* 2018; Fig. 2.24). FRED 2.0 has more than 105,000 observations of more than 300 root traits, with data collected from more than 1200 data sources. Based on community input, we now report the numbers of root trait observations in FRED 2.0 associated with individual plant species (https://roots.ornl.gov/plant-species), and 2000 species names have now been harmonized to The Plant List. FRED 2.0 will be a part of the new TRY 5.0 upon its release in 2019.

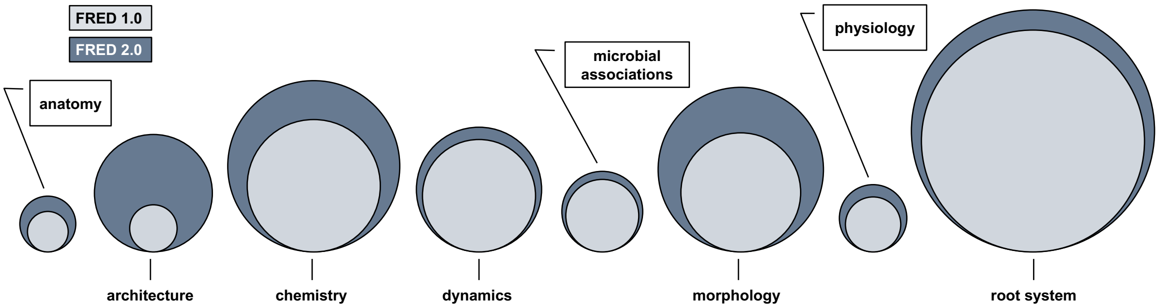


Fig. 2.24 Root trait observations included in FRED 2.0, grouped into broad trait categories according to McCormack *et al.* (2017); the area of each circle from FRED 1.0 and FRED 2.0 was scaled according to the observation numbers in each category. There was a 50% increase in root trait observations between FRED 1.0 and FRED 2.0, with the greatest increases in the categories of anatomy (88% increase), architecture (519%), chemistry (67%), and morphology (91%). More details on the observation numbers for other traits can be found at https://roots.ornl.gov/data-inventory.

FRED has provided the foundation for a number of national and international investigations, ranging from a better understanding of the diversity of root traits (McCormack *et al.* 2017), to understanding the drivers of global fine-root trait variation (Freschet *et al.* 2017), to a better understanding of the role of root traits in species successional patterns (Caplan *et al. in press*). Furthermore, FRED will be an integral part of an international root trait synthesis activity funded by the German Centre for Integrative Biodiversity Research (iDiv; https://www.idiv.de/sdiv/working_groups/wg_pool/sroot.html).

FRED is being used to inform the parameterization and conceptualization of fine-root traits in Version 1 of the E3SM land model, ELM. Our initial focus has been on: (1) fine-root turnover rates, which are a fixed parameter in ELM, (2) fine-root phenology, which in ELM is currently parameterized as a one-to-one relationship with leaf phenology, and (3) fine-root C/N ratios (currently equal to 42 for all plant functional types in ELM). Uncertainty analyses indicate that fine-root C/N ratio, allocation, and turnover are important controls over site-level GPP, while rooting depth distribution and phenology are less important (and the width of the peak in allocation phenology was more important than the timing).

2.10 Progress in LeafWeb and ESM support (Task 8)

LeafWeb (www.leafweb.org) is an automated online tool with primary objectives to (1) provide plant physiologists and photosynthesis researchers a reliable, convenient tool for analyzing leaf gas exchange and pulse amplitude modulated fluorescence measurements for key biochemical and physiological photosynthetic parameters, and (2) develop a global database of plant biochemical and physiological parameters needed for large-scale plant biological studies and cross-climate and cross-ecosystem modeling.

- The user interface was overhauled to meet the expectations of a modern web interface with simplified procedures for submitting data, retrieving and visualizing results of automatic data analysis. More importantly, the numerical analysis functionality is no longer tethered to a single machine. It currently resides on a cloud-based host but could easily be moved elsewhere. This change minimized interruption due to frequent computer software updates. As part of this change, LeafWeb migrated to www.leafweb.org. We have also upgraded the security settings of LeafWeb to meet the standard required by the US Department of Homeland Security.
- We implemented an algorithm to estimate C_4 photosynthesis model parameters, as per requests from LeafWeb users. The C_4 model implemented is the one commonly used in large-scale land surface models (e.g., the E3SM Land Model). Thus LeafWeb C_4 functionality will also be able to support C_4 photosynthesis modeling needs.

- We also implemented algorithms for analyzing A/Light, A/Temperature, or a combination of A/C_i/Light/Temperature curves. PAM data can also be included as part of the analysis to constrain the estimation of key photosynthetic parameters.
- On average, users from the US, South America, Europe and China submit about 2000 photosynthetic curves per year for LeafWeb analysis.

2.11 TES SFA Personnel Effort Not Defined in a Specific Task

TES SFA funding is also allocated to allow staff to take advantage of new scientific opportunities and to exercise their involvement in science development workshops, and to contribute to science responsibilities for both organized (Journal Editorships) and ad-hoc review processes (paper and proposal reviews), advising and mentoring students and post-doc, advising and limited participation on other DOE or university-led research projects, including contributions to non-SFA or funded manuscripts.

Several publications in our list of accomplishment come from affiliated work, and from past effort that has come to fruition with time (e.g., Asbjornsen *et al.* 2017; Eberhardt *et al.* 2015; Johnson *et al.* 2016; McDowell *et al.* 2016, 2018; Zhou *et al.* 2017ab).

3. RESEARCH PLANS FOR FY2019, FY2020 AND FY2021

This section describes our plans for research effort by TES SFA task during fiscal years 2019, 2020 and 2021. For ongoing tasks we assume a certain level background knowledge about the ongoing task and focus our discussion on active hypotheses to be tested or questions to be addressed. Further details of past effort can be found in cited articles or in past annual or triennial review reports (https://tes-sfa.ornl.gov/node/17). For new tasks or new approaches not covered in prior review documents (e.g., Task 3d and Task 6 methods) more discussion is allocated to describe our proposed effort.

LARGE-SCALE MANIPULATIONS AND LANDSCAPE OBSERVATIONS*

3.1 SPRUCE Future Plans and Deliverables (Task 1)

The motivation for SPRUCE (Hanson *et al.* 2017) was 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 (Section 2.1) provides a platform for testing mechanisms controlling vulnerability of organisms and ecosystems to important climate change variables. SPRUCE addresses key science questions for understudied high-C ecosystems essential for informing models of vegetation change under projected future climates:

1. Will belowground warming reverse 10,000 years of C accumulation in peatlands that store 1/3 of the Earth's terrestrial C?
    a. If the peatland turns into a C source, how much C release will occur?
    b. Will the released C be in the form of CO_2 or CH_4 with about 28 to 34 times the global warming potential of CO_2 at the end of this century (Myhre *et al.* 2013)?
2. 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?
3. Do critical air and soil temperature thresholds exist for ecosystem processes and organisms?
    a. What level of warming changes the annual C and water balance?
4. Will ecosystem function (e.g., hydrological and biogeochemical cycling) be compromised or enhanced by atmospheric and climatic change?

Recent review articles Crowther *et al.* (2016) and Gallego-Sala *et al.* (2018) continue to underscore the need for work on warming in high-latitude regions and peatlands to provide the quantitative information necessary to scale observations and experimental results within Earth System models.

The SPRUCE experiment described in Hanson *et al.* (2017) is focused on WEW treatments that were initiated August 2015 and have operated to date. These treatments will continue 24 hours a day throughout 2019, 2020 and 2021 under this proposal, and eCO_2 treatments will be operated during daytime hours throughout the active growing season (typically May through October). Performance data are available in Hanson *et al.* (2016D) in Appendix F.

Before the initiation of warming treatments, we hypothesized that warming would increase CO_2, CH_4 and DOC losses from the bog ecosystem proportionate to temperature increases unless they became limited by drying in the warmest treatment plots. Processes to be enhanced by warming included aerobic decomposition, methanogenesis, and priming of such activities due to eCO_2 enhanced delivery of C substrates to the belowground system. Water evaporation from bog surfaces and *Sphagnum*, and transpiration use by rooted plants were also expected. Initial hypotheses related to vegetation growth were varied. We projected that *Sphagnum* would do poorly with warming as has been observed (Section 2.1.3), but we expected that rooted plant species would benefit at lower levels of warming from the availability of nutrients released from the decomposition of older peat. We also anticipated that eCO_2 treatments would enhance root growth. As described in Section 2.1, some of these hypotheses have been supported while others have not. Nevertheless, given that we are early in the operation of the SPRUCE study (only 3 of a planned 10-year operation) we propose to sustain measurement efforts and support for external collaborators in the next 3-year cycle while adding effort in a few new areas described below.

Vegetation Phenology (Richardson, Hanson) – Manual phenology observations (Heiderman *et al.* 2018D; 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 over the next three years to evaluate any long-term changes in response.

Shrub-layer NPP and Tree Growth (Hanson) – Destructive assessments of shrub-layer live stocks and annual production (Hanson *et al.* 2018Da) will continue in August 2019 and 2021, but we will skip the destructive assessment in 2020 to save the experimental footprint while nondestructive evaluation of community plots (R. Montgomery, University of Minnesota) continues annually. 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 annual terrestrial laser scanning in May and August for canopy height and volume changes under contract with Nancy Glenn's group at Boise State University.

Sphagnum Moss and Related Processes (Weston, Norby) – *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. Recent results show that *Sphagnum* productivity at the SPRUCE site declines with increasing temperature, and there is some initial evidence that eCO_2 may also reduce productivity (Norby *et al.* 2019). However, the specific mechanisms driving this consequential observation are unknown, likely a combination of temperature, water, light and nutrients. Prior results show that warming treatments have reduced the water table depth and water availability, increased mineralization and thus nutrient availably, and boosted the growth and leaf area of shrubs (McPartland *et al.* 2019). We will use experimentation and modeling to explicitly test 1) how warming influences *Sphagnum* physiology, fitness and CO_2 exchange, 2) the susceptibility of warming exposed moss to secondary stressors from extreme weather events (drought) and species interactions (e.g., shading by shrubs, hyaline microbiome and associated N-fixing bacteria), and 3) the impact of warming on tissue metabolic composition (including nutrients, non-structural carbohydrates (NSC) and phenolics) and implications for decomposition across *Sphagnum* species. In addition, ongoing annual *Sphagnum* production and community cover measurements will be expanded to include periodic in situ non-destructive seasonal production estimates that better link growth to phenology and environmental conditions. Results will be used to add detailed parametrization to our *Sphagnum* net ecosystem exchange model (NEEs, Walker et al. 2017) for continued improvement. We will strive for continuous data – model integration and ask how warming influences our ability to predict NEE across environmental conditions.

To address these tasks, we will expand our field observations of the *Sphagnum* community net ecosystems exchange (NEE_S) measures with clear-top LiCOR 8100s to include a mixture of permanent and movable units to ensure observations are made in all SPRUCE enclosures. Each 8100 unit will be equipped with cameras to assess seasonal phenology (e.g., sporophyte production), growth estimates, and degree of desiccation (based on color shift from green to lighter-green/white). *Sphagnum* will be sampled seasonally for detailed gas exchange and chemistry (chlorophyll, amino acids, NSCs). Additional field and controlled laboratory manipulations will be used to identify mechanisms of *Sphagnum* decline under warming and warming-induced shifts in the degree of dehydration between precipitation events. *Sphagnum* will be propagated in growth chambers at ORNL under three different growth temperature regimes based on actual prior SPRUCE temperature patterns (0, +4.5, +9 °C). Two different watering regimes will be used: (1) maintaining field capacity or (2) based on actual prior SPRUCE precipitation records that allow for significant water stress. Net carbon uptake, camera-based and destructive assessment of degree of desiccation, gravimetric water content, gas exchange and chemistry will be assessed prior to, during and after drought stress to assess degree of resilience. Results will be used to confirm and scale ongoing NEE responses measured at SPRUCE under similar warming and precipitation regimes, and to refine our *Sphagnum* model. As time permits, and to further assess the mechanisms underlaying observed SPRUCE *Sphagnum* responses, we will consider additional laboratory and field manipulations of secondary responses to treatments, including shading, increased nutrient availably, or potential CO_2-induced changes in the pH of hyaline cells.

Preliminary data suggest that *Sphagnum* exposed to SPRUCE warming conditions have variable tissue C:N and P – (Norby, *in review*). We hypothesize that *Sphagnum* species and genotypes will decompose differently based on their metabolic profiles and that the decomposition response for a single species of genotype will vary across warming treatments. For example, measurements within SPRUCE suggested that N mineralization rates are increasing with warming, and therefore *Sphagnum* with higher N content, which will be reflected in the metabolic profile, might more easily decompose then the same *Sphagnum* genotype grown at a lower temperature with less nutrient availability. To test this hypothesis within and across *Sphagnum* species, we will leverage our collaborations with DOE JGI and EMSL who are providing metabolic profiles and DNA sequencing for two *Sphagnum* populations (DOE JGI Community Science Program 504399; and FICUS 504306). Using these resources, we will select three species: *S. fuscum, S. magellanicum, and S. fallax,* and 12 individual genotypes from an *S. fallax* pedigree (6 low, 6 high decomposers) for a litter decomposition experiment. *Sphagnum* will be collected and deployed in litterbags within each enclosure (15 bags x 10 enclosures x 3 replicates x 2 retrieval dates) and will be retrieved after 1 year to measure mass loss during the early phase of decomposition. Results from this unique approach will allow us to link genes to metabolite profiles, and metabolite profiles to decomposition rates, thereby providing a mechanistic understanding of warming by decomposition interactions.

Woody Plant Physiology (Warren) – Woody vegetation plays a dominant role in interannual net carbon exchange between the expansive boreal forest and the atmosphere, and the structure and composition of the forest has strong controls on surface energy balance. Thus any change in vigor, or shift in dominance between plant functional types (e.g., evergreen *Picea* vs deciduous *Larix*, or trees vs shrubs) will have significant effects on ecosystem function. Our key objectives are to mechanistically quantify the underlying species-specific physiological or morphological changes that may induce shifts in competitive ability and relative species composition. The SPRUCE plant physiology task continues to focus on both carbon physiology and plant water relations in response to WEW and eCO_2. Key planned tasks include 1) quantifying and assessing thermal acclimation of photosynthesis and foliar respiration, 2) quantifying and scaling plant water use, 3) quantifying vulnerability thresholds in hydraulic conductivity and assessing hydraulic acclimation, 4) assessing morphological and anatomical plasticity and 5) assessing plant stress, damage and mortality.

Photosynthetic and respiratory thermal acclimation enables plants to adjust to warming temperatures by shifting their photosynthetic thermal optimum and increasing net photosynthesis at higher temperatures (Way and Yamori 2014). Yet, different species or plant functional types vary in their thermal plasticity (Dusenge *et al.* 2018), indicating the need to quantify species-specific acclimation to better parameterize models (Smith and Dukes 2013), especially for the northern latitudes (Rogers *et al.* 2017). At SPRUCE, two years after initiating the warming treatments and one year after CO_2 additions, we collected more than 1000 photosynthesis-CO_2 temperature response (A-Ci) and foliar dark respiration temperature response curves to assess thermal acclimation to temperature and $CO_{2,}$ and to compare with pretreatment measurements (Jensen *et al.* 2015, 2019). Data are currently being analyzed and will be developed into an initial response manuscript. Based on the results, in this SFA we propose to revisit foliar thermal acclimation in 2020, after 5 years of treatments. This will allow us to examine short term foliar acclimation and longer-term whole plant acclimation to treatments (e.g., including hydrological, anatomical and biochemical changes related to shifts in resource availability such as water and nutrients). We are working closely with the ELM-SPRUCE modeling team to leverage results for model improvement.

Based on measurements of water table depth, soil moisture and sap flow there is greater annual evapotranspiration in the warmer plots, partially due to a longer active season (Richardson *et al.* 2018). The *Picea* trees are maintaining the same daily maximum sap flow as temperature increases, but the *Larix* trees are increasing sap flow, leading to significant water potential stress. We plan to expand sap flow measurements and continue to monitor water potentials to maximize our future ability to track and measure these critical responses. We will also contribute scaled data for the plot-level hydrology budget project, which is led across groups and will inform focused hydrological parameterization and bounding of ELM-SPRUCE. In FY19-FY20, we are also planning to initiate plant hydraulics measurements for the four main woody species. This will build on pretreatment pressure-volume and hydraulic vulnerability curves of the trees that indicates root and foliar hydraulic limitations in *Picea*, and hydraulic vulnerabilities in *Larix*. This work will assess if the SPRUCE treatments have changed functionality of xylem conductivity, vulnerability to embolism, capacitance or the turgor loss point. In addition, we are assessing how the SPRUCE treatments have changed the anatomy of xylem, including annual growth, cell wall thickness, cell diameters, mean hydraulic diameter and theoretical hydraulic conductivity.

We also expect the SPRUCE treatments to change plant biochemistry and morphological traits, including nonstructural carbohydrates, pigments, nutrients, sapwood to leaf area index, foliar size, foliar display, leaf mass per area. As part of the intensive A-Ci curve campaigns, material will be retained to assess the species-specific plasticity in these traits. In addition, we will continue to collaborate with the LIDAR task, to assess how shrub and tree structure is affected by treatments, and to tease apart potential species-specific competitive advantages under the SPRUCE treatments.

Based on our prior and ongoing observations, some trees in the warmest plots are currently displaying damage, including top dieback, branch tip damage and whole tree mortality, that may or may not be related to prior spring freeze damage (Richardson *et al.* 2018). In addition, the shrubs have shown significant winter desiccation/freeze damage due to a reduction in the insulating snow layer with warming, yet still achieve greater NDVI than cooler plots (McPartland *et al.* 2019). While both *Rhododendron* and *Chamaedaphne* are semi-evergreen shrubs that carry leaves overwinter, *Rhododendron* maintains greater leaf function in the second year (and subjectively has greater density in the warmer plots, TBD). Consequently, ELM-SPRUCE simulated net primary productivity is enhanced for *Rhododendron* when it is treated as an evergreen shrub but reduced for *Chamaedaphne* when treated as a deciduous shrub (Jensen *et al.* 2019), indicating a need to further assess differences between these species and the appropriate PFT parameters for use in the model. As such, we are focused on assessing the trade-offs between growth, foliar stress and hydraulic safety by assessing gas exchange, fluorescence, water use efficiency, non-structural carbohydrates, water potential, pigments, sap flow and foliar greenness. Together, these data will be able to attribute reduced fitness or competitive abilities to specific trait response to environmental conditions, which can be used to interrogate results in ELM-SPRUCE, and refine both mechanistic representation of key processes and their parameterization.

Belowground Processes at SPRUCE (Iversen) – The dynamics and distribution of fine roots in ecosystems underlain by organic soils are some of the least understood processes in belowground ecology (Reader and Stewart 1972, cf. Murphy & Moore 2010, Iversen *et al.* 2015, Iversen *et al.* 2018). Building on our work to understand fine roots in an ombrotrophic bog prior to initiation of climate change treatments (Iversen *et al.* 2018), we will leverage on-going data collection (e.g., from manual and automated minirhizotrons, root ingrowth cores, and ion-exchange resins) to ask two main questions: (1) How does warming affect the phenology of root and fungal growth, and how is belowground phenology related to aboveground phenology, as well as edaphic and environmental conditions? (2) How does warming affect the distribution of fine roots throughout the peat profile, and their relationship with soil nutrient and water availability?

Root and fungal phenology – We will use images collected since 2014 using manual minirhizotrons to investigate the timing of root production of ericaceous shrub and tree roots throughout the growing season, and whether these dynamics match a lengthening of the growing season observed aboveground in response to warming (Richardson *et al.* 2018). Further, we 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. Preliminary investigation, based on the ability to obtain minirhizotron images from warmed plots earlier in the spring and later into the fall (and sometimes year-round) indicates that the growing season is also longer belowground. Furthermore, preliminary ^{13}C data from root ingrowth cores in plots receiving elevated [CO$_2$] indicates that fine roots in warmed plots may be incorporating new C into their tissues more quickly (Malhotra *et al. in preparation*), and we will continue to follow these responses to quantify the turnover of root C.

Fine roots are assisted in nutrient and water acquisition by their fungal partners. We will use novel, prototype automated minirhizotrons to investigate the interactions among fine roots and their mycorrhizal partners, and whether these interactions differ among species that associate with ericoid (ericaceous shrubs) compared with ectomycorrhizal (*P. mariana* and *L. laricina*) fungi.

The distribution of fine roots throughout the soil profile – We have hypothesized that an observed drawdown of the water table level with warming will result in deeper rooting distributions in the bog, and we are continuing to track this response in the root ingrowth cores and manual minirhizotron images (Fig.

3.1ac). In addition, minirhizotron images are providing a novel glimpse at how the surrounding rhizosphere changes with peat depth. For example, we are able to observe whether each image is saturated (i.e., whether it is above- or below the water table level), something that we hypothesized would be possible at the onset of the project (Iversen *et al.* 2012); a preliminary comparison of these data with plot wells indicates that minirhizotron images may provide finer spatial-scale resolution of the effects of warming on the water table level (Fig. 3.1b). 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 bubble formation, and the gasses therein, in collaboration with other project partners.

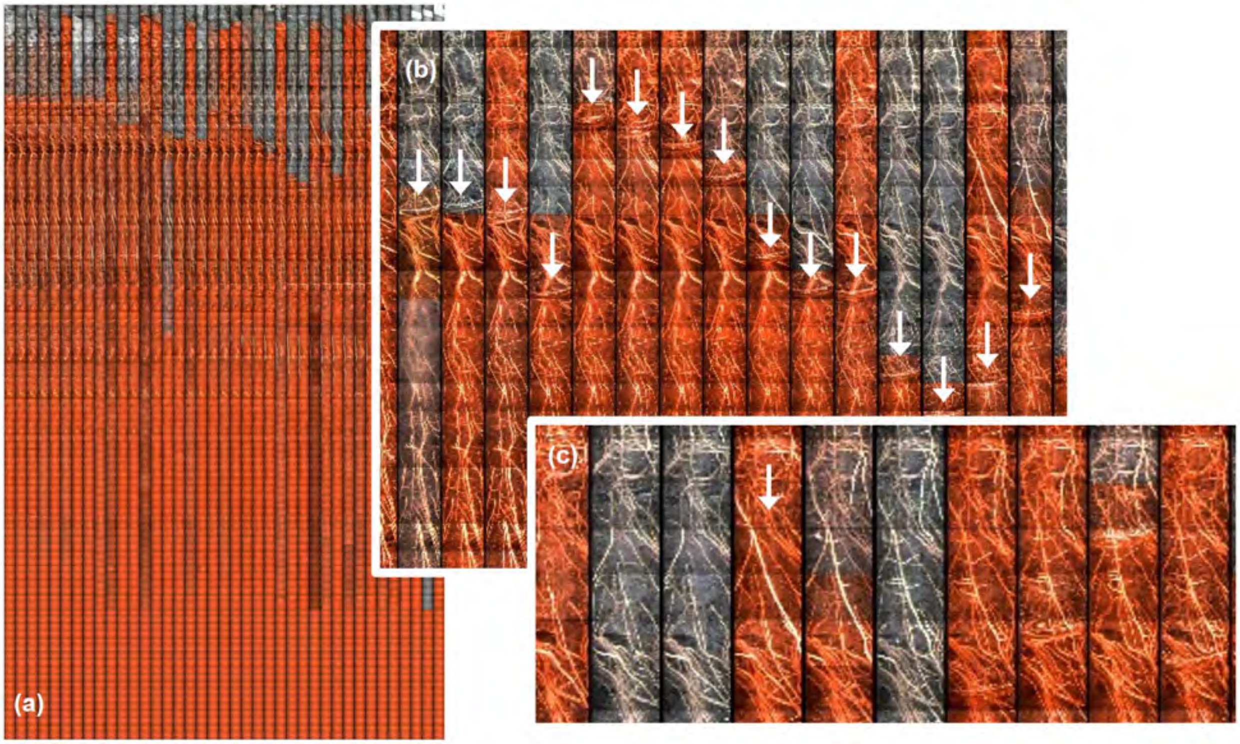


Fig. 3.1 Compiled minirhizotron images from one minirhizotron installed in a hummock in a SPRUCE enclosure with no warming, but with elevated [CO_2]. (a) All ~weekly imaging sessions from 2017, where each column is one imaging date with a stack of ~80 images from 0 cm depth (surface) to ~95 cm depth (deepest depth; there are no roots). (b) Image subset from mid-May through early September to show that the water table level (white arrows) is visible in the minirhizotron images, and changes from week to week (the largest change is ~ 7 cm between June 7 and June 15; there were two large precipitation events that week). (c) Image subset to indicate the birth and growth of a fine root (beginning at white arrow on August 25), including the production of lateral roots over a period of 2 weeks. The color changes in the images are adjustments of the camera lighting to ambient lighting as the camera moves further into the minirhizotron tube.

<u>Nutrient Cycling and Plant-available Nutrients (Iversen et al.)</u> – As a result of the last triennial review and with the endorsement of the SPRUCE experiment advisory panel, the SPRUCE group hosted workshops on the water and nutrient cycles for N and P in January 2018. Those workshop results are leading to summary manuscripts and have pushed the group to add new measurement objectives on nutrient turnover.

We will continue to quantify the availability of soil N and P for plant uptake using arrays of ion-exchange resins installed across hummock-hollow microtopography and throughout the peat profile. Preliminary evidence indicates that warming is increasing plant-available N and P, but we hypothesize that the N and P cycles will respond to warming at different rates, and that this will be reflected in vascular and non-vascular plant tissue in a species-specific manner, depending on the nutrient limiting growth of that particular species. While ion-exchange resins provide the best non-destructive way to monitor the effects on warming and elevated [CO_2] on plant-available nutrients in a long-term experiment, these data are necessarily qualitative (i.e., nutrient adsorbed per surface area of the resin), which can inform patterns of nutrient cycling in terrestrial biosphere models but do not serve as a quantitative model evaluation. On the advice of our science advisory board and project modelers, in summer 2018 we began to quantify net N mineralization (i.e., net N available for plant uptake per gram of dry peat) in surface peat across the SPRUCE enclosures. We are simultaneously quantifying other edaphic factors, including moisture and pH, and these data will be used to inform our understanding of plant-available N and its responses to warming and elevated [CO_2], and also serve as a data stream for model evaluation and quantitative assessments of the nitrogen budget in each enclosure.

<u>*Microbial Community Activity and Change (Schadt)*</u> – Currently our efforts are focused on understanding the response of these communities over time using metagenomics-based approaches. Analyses of datasets from 2015 and 2016 are nearing completion, and DNA samples from the 2017 and 2018 growing seasons are in queue for sequencing. Our recent studies have shown that a large proportion of the microbial community can be binned into distinct genome types (MAGs) that vary in abundance with depth peat layer depths (Fig. 3.2). Collectively, these genomes represent >70% of all microbial DNA sequences recovered from intermediate and deep peat communities. We expect that analyses of genome-resolved communities will enable an improved assessment of treatment effects and can serve as reference sequences for other efforts investigating SPRUCE peatland microbiology. These approaches show much greater resolution than prior 16S rRNA-based methods used for assessment, as well as greater ability to infer important changes in microbial functions that are directly linked to each identified MAG. Similar methods have recently proved valuable in Arctic peatland and permafrost systems (McCalley *et al.* 2014; Woodcroft *et al.* 2018). These data again are showing striking patterns with depth and diverse communities where we have been able to identify 336 unique microbial genomes (Fig. 3.2). While 2015-2016 samples indicate little treatment effect on microbial abundances, the recent observations of increased CH_4 flux, increased resin-available nutrients and changes in plant productivity suggest that the 2017-18 WEW microbial samples could show direct treatment effects, particularly in the upper peat profile. Future efforts will leverage these microbial community data to track changes in MAG abundance with treatments and also in collaboration with other SPRUCE site investigators conducting rRNA gene-based assessments (Kostka) and detailed biochemical analyses (Wilson/Chanton) in order to model microbial physiological responses *in situ*.

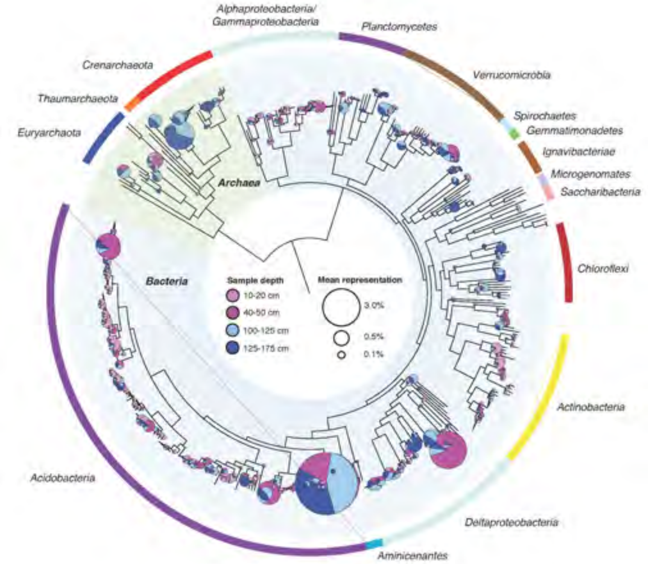


Fig. 3.2 Phylogenic relatedness, taxonomic affiliations, and abundances of recovered SPRUCE peatland metagenome-assembled genomes (MAGs). Phylogenetic tree constructed using RAxML on an alignment of 11 ribosomal protein sequences and visualized with the Interactive Tree of Life (iTOL) software. Each branch on the tree represents a non-redundant MAG. The size of each pie chart is proportional to the mean abundance of each MAG across 45 SPRUCE metagenomes samples collected in 2016 (see key). Pie chart colors represent mean distribution of each MAG at each of the four sampling depths.

Going forward we will employ multiple approaches to track the responses of these MAGs to change over time and treatments through: 1) Metagenomic sequencing of peat samples collected in 2018 and annually going forward, 2) QPCR-based analyses designed to specifically track the most abundant MAGs at finer seasonal scales using the analyses of DNA derived from porewater samples and 3) RNA-based analysis that will allow us to track the activity of the MAGs rather than just relative abundance. Metagenomic analysis will be carried out in collaboration with the DOE-Joint Genome Institute and their Community Sequencing (CSP) and Biological and Environmental Research Support Science (BERSS) Programs. Based on our prior results we plan to sample 4 depths in each plot multiplexed at 3 samples per lane of Illumina 2x250bp sequencing. Trimmed metagenomic sequence reads will be recruited to MAG assemblies in order to track abundance of each MAG over space and time within the SPRUCE experiment. QPCR analysis will target both at functional gene markers for important processes (e.g., *mcrA* for methogens and *pmoA* for methanotrophs) as well as phylogenetic markers for prominent MAGs. Porewater-based sampling will be used to allow greater temporal and spatial resolution than is possible with peat metagenomics due on the sampling frequency of peat. We expect that increasing the temporal resolution of our analyses will allow us to link microbiome responses to other response variables from the SPRUCE treatments such as water table depth and plant derived available carbon and nutrients. Finally, in addition to the DNA-based metagenomic approaches we have been successfully employing, we will work to develop RNA-based approaches that can be used to match the activity of the microorganisms. At a minimum we will track activity using the QPCR based approaches described above on RNA samples, however we are hopeful that by both scaling up our extractions and as recent sequencing technology improvements that have reduced required RNA requirements for meta-transcriptome sequencing to 10s of ng rather than 100s, we will be able to carry out metatranscriptomic analysis in parallel with the peat metagenome analyses.

Net C Exchange and Isotopic Tracer Work (Hanson, Griffiths, McFarlane et al.) – We will continue community level point-in-time assessments of daytime net ecosystem exchange of CO_2 and darkened plot values for ecosystem respiration (Hanson *et al.* 2016) at approximately monthly intervals during the active season in all years. We will conduct limited reevaluation of vegetated vs. non-vegetated plots for and assessment of heterotrophic contributions to flux. Community measurements of CH_4 flux will be obtained with all measurements. In 2020, we will fund Karis McFarlane, at Lawrence Livermore National Laboratory to measure the ^{13}C and ^{14}C composition of CO_2 and CH_4 emitted from the bog in 2020 and will be contrasted with her team's observations from 2014, 2015, and 2016 when SPRUCE manipulation treatments were being initiated (Guilderson *et al.*, in prep). These earlier results showed respired CO_2 and CH_4 was dominated by relatively young carbon sources (< 15 years old) and unresponsive to deep peat heating (Fig. 3.3). As was done previously, surface emitted gases will be collected from the large collars and end-members for the isotopic values of respired CO_2 and CH_4 determined using a Keeling plot approach for CO_2 (Phillips *et al.* 2015) and isotopic mixing models (e.g., McCallister and del Giorgio 2012) to correct for background atmospheric CH_4. These data will address whether several years of WEW treatments have increased the release of older peat-derived carbon to the atmosphere as CO_2 or CH_4 and provide insight into the mechanisms behind warming and elevated CO_2 treatment effects on carbon gas fluxes.

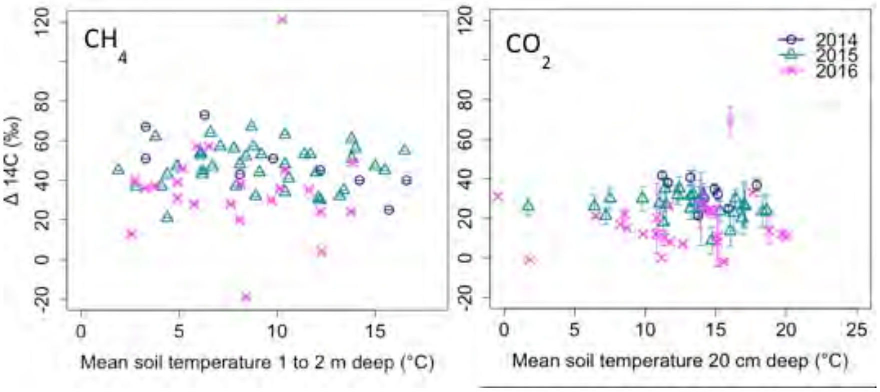


Fig. 3.3 No significant effect of temperature or deep-peat or early warming treatments were observed for ^{14}C of emitted CH_4 or CO_2 during 2014-2016 growing seasons.

Plot-scale assessments of C gain and loss will be reevaluated in 2020 through the combination of NPP data (from *Sphagnum*, shrub-layer and tree growth measures) with the measured flux of CO_2 and CH_4 gases and basin TOC losses (Griffiths *et al.* 2017) We will focus on the cumulative response data through 4-years of manipulation (2016 through 2019) using a regression of the plot results under control and warming treatments with and without eCO_2 treatments. Overall results will be contrasted with direct observations of bog elevation change (Cahoon *et al.* 2002, Hanson *et al.* 2018D) which have been trending downwards since the initiation of warming treatments.

Organic Matter Decomposition (Griffiths, Kolka, Iversen et al.) – While we have observed little effect of warming and eCO_2 on organic-matter breakdown during the initial phases of decomposition, we hypothesize that as decomposition progresses, we may begin to see responses to warming across all litter types. In the next three years, we will continue the long-term organic-matter decomposition measurements, which will include continuing to retrieve and process litterbags that are currently in the enclosures. Additionally, for selected harvests we will subsample litter for amplicon based assessment of microbial communities (bacteria/archaea 16S rRNA genes + fungal ITS rRNA genes) to understand how these may differ by substrate and warming treatment and interact with decomposition rates. The final litterbag retrieval for the mixed species decomposition experiment will occur in 2019 (end of a 4-year-long experiment). Litterbags from the single species decomposition experiment will be retrieved in 2020 (year 5), with the final set of litterbags scheduled to be retrieved in 2025 (year 10). The first set of peat decomposition ladders will be retrieved from the enclosures after 3 years (2020), and future retrievals are planned for 6 and 9 years. Lastly, we plan to continue our biannual measurement of cotton strip decomposition as the cotton strips, which are 95% cellulose, have provided evidence that labile C decomposition is responsive to warming treatments. After the next 3 years of cotton strip decomposition data are collected, we will explore the drivers (e.g., temperature, precipitation) of interannual variation in labile C decomposition.

We also propose a new experiment comparing the decomposition of litter from plants grown in the warmer (+9 °C), ambient and eCO_2 enclosures to litter from plants grown in the cooler (+0 °C), ambient and eCO_2 enclosures. We hypothesize that litter from the ambient CO_2, +9 °C enclosure will decompose faster than litter from the eCO_2, +9 °C enclosure because eCO_2 is expected to increase the C:N ratio of litter. Further, we hypothesize that litter from the +9 °C enclosures will decompose faster than litter from the +0 °C enclosures, if greater N mineralization with warming increased the N content of vegetation. If we determine that (1) there are chemical differences in litter from these 4 enclosures, and (2) enough litter (from *Picea*, *Larix*, or *Rhododendron*) can be collected from these 4 enclosures without affecting the carbon and nutrient balance of the system, then we will carry out an experiment comparing the decomposition of litter collected from these 4 enclosures over a 4-year period. The experiment will take place outside of the enclosures to minimize the effect of environmental factors and focus on the effect of litter quality on decomposition rate.

Post-Treatment Evaluation of Peat Characteristics (Hanson, Iversen, Phillips) – Changing peatland elevations, increasing isotopic signatures of litterfall, and enhanced losses of CO_2 and CH_4 with warming (Section 2.1) suggest that resampling of peatland C, elements, ash and bulk density should be done in 2020 or 2021. Preliminary characterization as described in Tfaily *et al.* (2014) and Iversen *et al.* (2014D) will be repeated when isotopic signatures of input C stabilize (Fig. F1 in Appendix F). 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*).

Hydrology and Water Chemistry (Griffiths, Sebestyen) – The responses of outflow volume and chemistry and porewater chemistry have not been consistent over the first three years of WEW and eCO_2. For instance, TOC concentrations have increased to a larger degree in the warm plots in 2018 compared to the previous two years. Therefore, to capture the longer-term responses of water chemistry and hydrology to warming and eCO_2, we will continue the bimonthly sampling from the piezometers and the weekly sampling from the outflow system for water chemistry analyses. We will also continue the high-frequency measurements of lateral outflow (i.e., stream flow) from each enclosure. These data will be used to better understand the water chemistry and hydrology responses to WEW and eCO_2. The data will also be used in the estimation of ecosystem-scale C flux responses and to better understand responses of plant-available nutrients to warming and eCO_2. The lateral outflow and TOC flux results will also be used to parameterize the ELM-SPRUCE model. Lastly, as part of the hydrology task, we plan to develop and test methods to better quantify the inputs and dynamics of snow (spatial variation within an enclosure, inputs via drift between the enclosure wall and the corral) and throughfall (volume and chemistry) under the shrub layer.

Modeling SPRUCE Response Mechanisms – Individual SPRUCE measurement tasks provide process-based quantitative regression algorithms for potential use within the higher order modeling activities described under Task 3a. The goal of process modeling 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.

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, site access and participation in annual peat coring efforts. A key part of this effort is the support for annual/periodic sampling of the peat column in an organized manner to sustain the experimental plots for continued observations.

Table 3.1 outlines the major SPRUCE activities anticipated for the next 3-year funding cycle.

Table 3.1 – Future deliverables for SPRUCE

Date	Deliverable	Status
FY2019 Deliverables		
Dec 2018	Manuscript on 3-year *Sphagnum* production and community change - Norby	Submitted
December 2018	Publish manuscript on pretreatment gas exchange: "Simulated projections of boreal forest peatland ecosystem productivity are sensitive to observed seasonality in leaf physiology." Jensen *et al.*	Completed
March 2019	Publish manuscript of initial tree response to whole-ecosystem warming (Dusenge *et al.*2018)	Completed
March 2019	Publish manuscript of initial shrub responses to whole-ecosystem warming and eCO2 (Ward *et al.*)	Underway
March 2019	Publish manuscript of pretreatment and initial woody plant water responses to whole-ecosystem warming and CO2 (Warren *et al.*)	Underway
June 2019	Complete analysis of initial respiratory and photosynthetic acclimation to temperature based on 1000 A-Ci curves collected in 2017	Underway
September 2019	Manuscript on 3-Year tree growth and associated TLS Data – Graham/Hanson	Planned
September 2019	Manuscript on multi-year plant-available nutrient response to warming (Iversen *et al.*)	Underway
September 2019	Complete draft manuscript on the responses of lateral outflow and TOC concentration and fluxes to the first 3 years of warming (Griffiths *et al.*)	Planned
September 2019	Complete plant hydraulics measurements on the four main species	Planned
All Year	Sustain continuous SPRUCE treatments and automated data collection efforts	Underway
FY 2020 Deliverables		
December 2019	Publish manuscript on initial woody plant acclimation to whole-ecosystem warming and eCO_2	Planned
December 2019	Manuscript on 3-Year shrub community growth – Collaborators/Hanson	Planned
January 2020	Publish manuscript on initial responses of woody plant morphology	Planned
August 2020	Complete 2nd field campaign to collect A-Ci curves to test respiratory and photosynthetic acclimation to temperature	Planned
September 2020	Manuscript on root-fungal interactions with warming and drying	Planned
September 2020	Manuscript on plot-scale C-Budget changes from warming and eCO2	Planned
All Year	Sustain continuous SPRUCE treatments and automated data collection efforts	Planned
FY 2021 Deliverables		
November 2020	Complete field collection of litterbags from the 3 main decomposition experiments (t=4 y mixed species bags, t=5 y single species bags, t=3 y peat bags)	Planned
January 2021	Complete morphological and biochemical assessments of ACi curve samples	Planned

September 2021	Publish manuscript on tree and shrub physiological damage based on NSC, fluorescence, d^{13}C, greenness	Planned
March 2021	Complete draft manuscript on the effects of *Sphagnum* on litter decomposition (Griffiths *et al.*)	Planned
September 2021	Manuscript on root phenological responses to warming	Planned
September 2021	Complete manuscript on ^{13}C and ^{14}C of surface emissions of CO_2 and CH_4	McFarlane *et al.* Planned
All Year	Sustain continuous SPRUCE treatments and automated data collection efforts	Planned

3.2 Coordinated Ecophysiology, Eddy Covariance, Sun-Induced Chlorophyll Fluorescence Studies to Advance Integrative Ecosystem Science (Task 6)

Task 6 has its roots in the Missouri Ozark AmeriFlux (MOFLUX) project. Over the years (2004 – 2018), this Task has evolved from an original focus on eddy covariance to a concerted effort of observation and modeling that bridges the scales and approaches of ORNL TES SFA activities across contrasting ecosystem types. The progress made so far has advanced several research fronts in ecosystem science from fundamental theories and applications of eddy covariance (e.g., Gu *et al.* 2005, 2012, & 2013) to key ecosystem processes (e.g., Gu *et al.* 2007, 2008, 2015, Wood *et al.* 2018, Wood *et al.* 2019) to state-of-the-art ecosystem models (e.g., Sun *et al.* 2014, Gu *et al.* 2016b). Task 6 must now evolve again. For FY 2019, 2020 and 2021, Task 6 will conduct Coordinated Ecophysiology, Eddy Covariance, and Sun-Induced chlorophyll Fluorescence Studies (CEECSIFS) to advance integrative ecosystem science.

CEECSIFS is driven by the exciting advances we have made during the last research cycle (2015-2018, see Section 2.3) in new technologies for integrated sun-induced chlorophyll fluorescence (SIF) and eddy covariance (EC) observations (Gu *et al.* 2018) and in modeling photosynthesis from the side of light reactions enabled by SIF measurements (Gu *et al.* 2019). The light reactions approach complements the traditional, dark reactions-centric biochemical model (Farquhar *et al.* 1980) and represents a potential paradigm shift in predictive photosynthesis research with implications on carbon and water cycle modeling. CEECSIFS intends to bring this potential paradigm shift into reality.

Following the tradition of past renewals, CEECSIFS will also continue research topics that leverage the strategic location of MOFLUX within the geographically and ecologically distinct prairie-forest biome/precipitation transition in the central United States where there is no other AmeriFlux, National Ecological Observatory Network (NEON) or Long Term Ecological Research Network (LTER) presence. These topics include the effects of drought, climate variability and extreme events on ecosystem fluxes and tree growth/mortality, the coupling between above- and below-ground processes, and the testing, evaluation and improvement of integrated ecosystem models. These research topics require uninterrupted long-term datasets and their continuation will enable AmeriFlux's representation of the US Midwest.

Under CEECSIFS, Task 6 will continue to be an integral part of the overall scientific mission of ORNL TES SFA and serve as a bridge between observational science (manipulative experiments and fundamental process studies) and modeling tasks. This will be achieved via concerted efforts of integrated SIF and EC observations between SPRUCE and MOFLUX and via continuing collaboration with TES SFA modeling activities in Task 3. By conducting research in two contrasting ecosystem types (upland deciduous forest vs spruce bog) and by integrating observation and modeling across scales, CEECSIFS will ensure that any theoretical and methodological advances will be tested rigorously for generality and will be relevant to large scale modeling efforts of importance to other DOE BER programs (e.g., the Energy Exascale Earth System Model).

Accordingly, the following subtasks are planned for FY 2019, 2020, and 2021:

Task 6a - Fundamental studies of photosynthesis from the side of light reactions
Task 6b -Building a solid foundation for ground-based SIF research
Task 6c - Interdisciplinary measurements and process understanding at the MOFLUX site
Task 6d - Integrated shrub-level SIF/EC measurements at the SPRUCE site

3.2.1. Fundamental studies of photosynthesis from the side of light reactions (Task 6a)

For the last several decades, predictive studies of photosynthesis have primarily focused on the side of dark reactions, led by the widely-used biochemical model of photosynthesis (FyCB; Farquhar *et al.* 1980; extended by Sharkey *et al.* 1985). In the FvCB model, the dark reactions (the Calvin cycle) are mechanistically represented to determine, with a high degree of process fidelity, the activity of Rubisco, regeneration of the substrate of Rubisco (RuBP), triose phosphate utilization (TPU), and their control on the rate of carboxylation. In contrast, the light reactions are only represented by a single empirical function that calculates the potential, rather than actual, electron transport rate. The potential electron transport rate is only the actual rate if carboxylation is limited by RuBP regeneration. In our recent efforts to develop a theoretical framework to guide SIF research, we have successfully derived the mechanistic equations for modeling photosynthesis from the side of light reactions, using first principles (Gu *et al.* 2019). For the C_3 photosynthetic pathway, these equations express the gross primary production (GPP) as:

$$GPP = \frac{C_c-\Gamma^*}{4C_c+8\Gamma^*}\frac{q_L\Phi_{PSIImax}}{(1+NPQ)(1-\Phi_{PSIImax})+q_L\Phi_{PSIImax}}\beta\alpha_{grn}PAR. \quad (1)$$

$$SIF = \frac{1-\Phi_{PSIImax}}{(1+k_{DF})[(1+NPQ)(1-\Phi_{PSIImax})+q_L\Phi_{PSIImax}]}\varepsilon\beta\alpha_{grn}PAR. \quad (2)$$

$$GPP = \frac{C_c-\Gamma^*}{4C_c+8\Gamma^*}q_L\frac{\Phi_{PSIImax}(1+k_{DF})}{(1-\Phi_{PSIImax})\varepsilon}SIF. \quad (3)$$

Here, C_c is the chloroplastic CO_2 partial pressure; Γ^* is the chloroplastic CO_2 photocompensation point; q_L is the fraction of open photosystem II (PSII) reaction centers; $\Phi_{PSIImax}$ is the maximum photochemical quantum yield of PSII of a fully dark-adapted leaf; NPQ is the nonphotochemical quenching (NPQ) parameter; β is the absorbed photon energy allocated to PSII; α_{grn} is the absorptance of photosynthetically active radiation (PAR); k_{DF} is the ratio of the rate constant of constitutive thermal dissipation to fluorescence; ε is the escape probability of SIF photons. Key inputs to Eqn 1 - 3 (q_L, NPQ, and $\Phi_{PSIImax}$) can be obtained from the Pulse Amplitude Modulated (PAM) fluorometry (Baker *et al.* 2008).

Eqn 1 and 2 mechanistically describe the light responses of GPP and SIF, respectively, while Eqn 3 mechanistically relates SIF to GPP. If valid, these equations could have far-reaching implications for photosynthesis and SIF research and carbon cycle modeling across different disciplines. *The goal of Task 6a is to verify the validity of these theoretical equations, explore their potentials and identify priorities for their broad applications in modeling photosynthesis and SIF by collecting and analyzing coordinated SIF, EC and PAM fluorimetry data sets.*

The benefit of using SIF as an input for modeling photosynthesis from the side of light reactions is a reduction in the number of dynamic inputs (Eqn 3 vs. Eqn 1). The elimination of NPQ from Eqn 3 is particularly important because NPQ consists of multiple components that respond to changing environmental conditions at multiple scales and is thus very difficult to predict (Zaks *et al.* 2012). Eqn 3 is also mathematically simpler and requires fewer parameters than the FvCB model. It is possible that Eqn 1 - 3 could complement the FvCB model for future photosynthesis research.

Eqn 1 and 3 use C_c as an input. The corresponding equations that use atmospheric CO_2 partial pressure C_a, as an input are derived in Gu *et al.* (2019). A crucial knowledge gap that must be addressed to apply Eqn 1 - 3 for modeling GPP and SIF is how the inputs vary with environmental conditions and across the depth of the canopy. Among the inputs, k_{DF} is determined by the physical properties of chlorophyll molecules and is believed to be a scaling constant (~19, Gu *et al.* 2019). $\Phi_{PSIImax}$ has been found to be highly conserved across species under unstressed conditions (~ 0.83) although it can decrease as a result of photoinhibition (Papageorgiou & Govindjee 2004). All other inputs are variables and respond to variations in environmental conditions. We will conduct coupled PAM fluorometry and gas exchange measurements at the MOFLUX site using a hydraulic boom lift during each growing season. The PAM fluorometry measurements will be used to determine q_L, NPQ, and $\Phi_{PSIImax}$ while gas exchange measurements will be used to verify the validity of Eqn. 1. Unfortunately, Eqn 2 and 3 cannot be directly verified at the leaf level because current PAM fluorometry outputs fluorescence in relative units, not absolute energy units. As a first-order check for the validity of Eqn 2 and 3, we will assume the canopy is a big leaf and apply Eqn 2 and 3 directly to the canopy level. α_{grn} at the canopy scale will be determined by line quantum sensors that have been already installed at the top and bottom of the canopy at the

MOFLUX site. ε will be estimated from canopy reflectance using the approach of Yang and van der Tol (2018). We will convert the wavelength-specific SIF measured by FAME (see Task 6b) to broadband SIF (Yang *et al.* 2017). The predicted broadband SIF with Eqn 2 will be compared with the converted broadband SIF. With these efforts, Task 6a will be able to answer the following questions:

- How do q_L and NPQ vary with canopy depth and environmental conditions, particularly heat and drought stress? And can they be predicted?
- Does SIF predicted with Eqn 2 agree with SIF measured with FAME?
- Does Eqn 1 predict leaf gas exchange measurements?
- Do big-leaf GPP estimates from Eqn 1 and 3 agree with each other, and with GPP inferred from EC measurements using mechanistically-based partitioning methods (see Task 6c)?

The work planned for Task 6a will pave the way for implementing the light reactions-based photosynthesis modeling in a multi-layer model in the future.

3.2.2 Building a solid foundation for ground-based SIF research (Task 6b)

While the importance of SIF for studying photosynthesis in natural environments has been well-recognized (Gu *et al.* 2019), SIF research is still in its infancy. Measuring SIF remains a challenging task and requires an extraordinary attention to technical details (Gu *et al.* 2018). Multiple SIF measurement systems have been developed independently using different design philosophies and approaches (e.g., Yang *et al.* 2018, Grossmann *et al.* 2018, Gu *et al.* 2018), which is advantageous for the community given the nascent state of SIF measurement science. However, for SIF research to move forward, the community needs to develop design criteria to optimize SIF instrumentation and a standard protocol to guide ground-based SIF measurements, retrieval and data quality control. As DOE-supported AmeriFlux investigators, we developed FAME specifically for integrated SIF/EC measurements (Gu *et al.* 2018). We are committed to building a solid foundation for ground-based SIF research and working with the community to advance SIF measurement techniques. *Task 6b will improve SIF instrumentation and retrieval methods and refine SIF measurement protocols and data quality control criteria.*

We will target two aspects of the design and operation of FAME to improve its robustness and ease of use in the field at EC flux sites: 1) streamlining the procedure for absolute irradiance calibration and 2) improving the control of spectrometer body temperature. Absolute irradiance calibration ensures SIF data comparability over time and across sites. Currently, two people are needed to safely complete the calibration procedure at the top of a flux tower—one operating and monitoring the status of FAME using a computer interfaced with the datalogger, the other physically placing the lamp on the fore-optics. We will implement a system that allows the tower operator to easily control FAME sampling using physical switches in an external control box, with LED indicators providing information on the sampling mode and system readiness. This will make calibrations easier for a single tower operator to perform.

The absolute temperature and thermal stability of a spectrometer critically affects the quality of obtained spectral data. Currently FAME uses a thermoelectric cooler (TEC) with a unipolar temperature controller to control the ambient temperature of the spectrometer to be not above 25 ^{o}C. This allows the internal spectrometer TEC to maintain the temperature of the detector at -10 ^{o}C to minimize thermal noise. However, with this approach it is possible for the spectrometer body, and thus the optical bench temperature to drift when ambient temperatures drop below 25 ^{o}C because the current FAME system has no heating capability. Drifting optical bench temperatures can affect the spectral stability of the detector. We will experiment with two approaches to more stringently controlling the body temperature of the spectrometer at 25 ^{o}C. The first approach is to replace the unipolar temperature controller with a bipolar temperature controller. The second approach is to apply the two-stage temperature stabilization scheme of Grossmann *et al.* (2018). In this scheme, the first stage uses a TEC to cool the air inside the enclosure to 18 ^{o}C. In the second stage, a polyimide film insulated flexible heater is used to heat the spectrometer to 25 ^{o}C. We will select an approach that provides adequate temperature stability for the optical bench of the spectrometer with minimal operational cost or maintenance burden and with maximal flexibility for applications in tropical to arctic ecosystems.

In addition to a high-performance measurement system, robust retrieval methods are also needed to obtain high-quality SIF data. Currently, all SIF retrieval methods (Meroni et al 2009, Guanther *et al.* 2012) use ordinary optimization procedures to infer SIF from measured incoming and outgoing irradiance samples. These methods assume that only outgoing irradiance samples contain measurement errors while incoming irradiance samples are error-free. This assumption is strictly invalid because both incoming and outgoing irradiance samples are measured with the same spectrometer and therefore potentially the same type of error. We will implement orthogonal optimization methods to replace ordinary optimization methods for SIF retrievals.

Another issue with current retrieval methods is that they all assume incoming (E_I) and outgoing (E_O) irradiance samples are perfectly matched in time. Unfortunately, this assumption is also not true because E_I and E_O are measured by the same spectrometer sequentially with different integration times. Between sampling E_I and E_O, sky conditions may have changed, leading to mismatched E_I and E_O and errors in retrieved SIF. We have found that the spectral shape of the incoming solar irradiance is rather stable even when absolute intensities vary significantly (unpublished data). We will exploit this finding to recast the retrieval algorithm based on normalized incoming solar irradiance (i.e., spectral shape). We will test and compare the spectral shape-based orthogonal retrieval methods with conventional methods using simulated incoming and outgoing irradiance measurements.

With these research efforts, Task 6b will be able to deliver

- An improved design of FAME
- A reliable SIF retrieval solution for cloudy conditions

We will document our SIF operational experiences and communicate our findings to other SIF investigators, through direct contacts, papers, and conference presentations, in a timely matter to benefit the SIF research community worldwide.

3.2.3 Interdisciplinary measurements and process understanding at the MOFLUX site - Task 6c

MOFLUX is an adjunct core site in the AmeriFlux network and has been playing a key role in AmeriFlux and FLUXNET network syntheses because of its strategic location within the geographically and ecologically distinct prairie-forest ecotone / precipitation transition in the central United States. It is also one of the very few flux sites in the world that is now instrumented with fully integrated EC-SIF measurements. Thus, it is essential for MOFLUX to sustain its contribution to AmeriFlux and FLUXNET. MOFLUX will continue long-term measurements of meteorology, EC and soil fluxes, ecophysiology, and biometry to support AmeriFlux and FLUXNET missions. Regular predawn leaf water potential and tree mortality monitoring will also remain so that we can build up the valuable datasets that are among the best in the world. These datasets are key for understanding and predicting potential shifts in species composition in the prairie-forest ecotone in response to climate change.

We initiated continuous measurements of SIF and canopy absorption of PAR in the last funding cycle. Exploratory measurements of q_L, NPQ, $\Phi_{PSIImax}$, and diurnal leaf water potentials and transmittance to PAR were also made to support the interpretation of the dynamics of SIF observed at the canopy scale. The leaf transmittance measurements were made to test the hypothesis that chloroplasts can reposition themselves in response to diurnal variations in incident PAR to either enhance or reduce light absorption. It has been suggested that chloroplasts line up just below the cell surface to maximize interception in low light, and retreat to the cell walls to reduce light absorption and minimize photodamage in high light (Kasahara *et al.* 2002). If so, chloroplast repositioning should affect α_{grn} and therefore SIF (see Eqn 2). Our preliminary measurements of leaf transmittance of PAR appeared to support this hypothesis. But more measurements are needed to ensure the observed pattern is a common phenomenon. Measurements of SIF and canopy absorbed PAR have now become an integral part of MOFLUX long-term continuous data streams and will continue in FY2019, 2020 and 2021. q_L, NPQ, $\Phi_{PSIImax}$, and leaf transmittance in PAR will also be measured regularly in time and across the depth of the canopy to support Task 6a.

Synthesis under Task 6c will focus on addressing a recalcitrant challenge in the EC community—the partitioning of net ecosystem CO_2 exchange (NEE) into GPP and ecosystem respiration (Wohlfart and Gu 2015). We will develop novel partitioning approaches based on our theoretical advances in modeling light reactions of photosynthesis. Eqn 1 and 3, transformed with ambient CO_2 partial pressure as an input (Gu *et al.* 2019), will be used to quantify GPP in an inversion framework. We will use joint measurements of NEE frm EC and soil respiration from automated soil CO_2 efflux chambers (Li-Cor 8100A) deployed at the MOFLUX site. The joint use of NEE and soil respiration measurements will potentially allow us to infer above-ground respiration as part of the partitioning effort. Additionally, we will apply traditional methods of empirical light/temperature response functions to partition NEE (Gu *et al.* 2002, Reichstein *et al.* 2005). The GPP estimates from different partitioning methods will be compared with each other and also with the GPP values predicted with the forward models in Task 6a.

The combined activities of Task 6a and 6c will yield multiple independent GPP estimates, which will be objectively evaluated with the goal of developing a mechanistically sound partitioning approach. While this plurality is a major step forward towards the eventual goal of reliable GPP estimation at large scales, it also begs the question: how do we know which GPP estimate to trust if these independent methods don't agree with each other? Unfortunately, this question cannot be answered unequivocally because the truth is an unknown and largely immeasurable. However, the robustness of different GPP estimates can be assessed by investigating the dynamic behaviors of GPP estimates, their responses to environmental variations (PAR, temperature, vapor pressure deficit, etc.) and relationships with other ecosystem functional variables such as evapotranspiration and soil respiration. As part of Task 6c research, we will develop a set of objective criteria for evaluating the robustness of GPP estimates.

Key questions to be answered in Task 6c include:

- Can SIF be used to partition NEE into GPP and ecosystem respiration?
- Can the mechanistic light response function (i.e., Eqn 1) be used to partition NEE into GPP and ecosystem respiration?
- What are the objective criteria for evaluating the robustness of GPP estimates obtained with different methods?

We expect a successful execution of Task 6c will have an immediate impact on how flux data can be analyzed for developing deeper understanding of key ecosystem processes.

3.2.4 Integrated shrub-level SIF/EC measurements at the SPRUCE site (Task 6d)

For Task 6d, measurements and analyses of integrated shrub-level SIF/EC will be conducted at the SPRUCE site during FY 2019, 2020, and 2021. The objectives are to support the SPRUCE modeling efforts to scale up findings from manipulative experiments of temperature and CO_2 treatments and to understand biotic and abiotic controls of CO_2, CH_4 water vapor and sensible heat fluxes in bogs. Integrated SIF/EC measurements can be potentially used to infer GPP of shrubs and *Sphagnum* species at the SPRUCE site, using approaches developed in Task 6a and 6c.

An EC-only system has been operational in Plot #2 (an open control plot) since 2015. An integrated SIF/EC system was tested in Plot #17 (an enclosed plot) for two days in September 2018. Because of the short duration of the test, we did not find conclusive evidence to either reject or support the applicability of EC technique in an enclosed environment with forced turbulence. However, the test did show that SIF can be measured at the shrub level inside a SPRUCE enclosure. We will continue the within-enclosure integrated SIF/EC test in FY 2019. We will examine the diurnal cycles of observed EC fluxes of CO_2, CH_4 and water vapor and SIF and compare the obtained fluxes with those from automated chambers and large-dome manual chambers that have been in use by other SPRUCE investigators. We will determine whether the EC fluxes show reasonable diurnal cycles and good agreement with measurements simultaneously made with other techniques. If we are convinced that the EC technique can work in an enclosed environment with forced turbulence, we will regularly rotate the integrated SIF/EC system among different treatment plots. If it turns out the EC technique cannot be reliably employed in enclosed plots, we will permanently install the integrated SIF/EC system at a location close to the end of Transect #4 to measure shrub-level EC fluxes and SIF. Electrical service will need to be extended to Transect #4. This shrub-level integrated SIF/EC system can complement the potential above-canopy integrated SIF/EC observation in the future.

Task 6d intend to answer the following questions:

- Can the EC technique be applied in an enclosed environment with artificial turbulence?
- Can SIF be used to estimate GPP in a bog?
- What processes control fluxes of CO_2, water and methane at daily, weekly, monthly time scales for the S1 Bog peatland?

Table 3.2– Task 6 Deliverables

Date	Deliverable	Status
May 2019	Submit 2018 MOFLUX data to AmeriFlux	Annual delivery
Summer 2019	PAM fluorometry and leaf gas exchange measurements at MOFLUX	Planned
Summer 2019	Test of the integrated SIF/EC system in SPRUCE enclosures	Planned
Dec. 2019	Manuscript on SIF retrieval methods	Planned
April 2020	Complete spectroradiometer body temperature control design and test	Planned
May 2020	Submit 2019 MOFLUX data to AmeriFlux	Annual delivery
Sept 2020	Report on EC applicability in SPRUCE enclosures	Planned
Dec 2020	Manuscript on within-canopy variations of PAM parameters	Planned
April 2021	Complete the development and test of LED/resistor circuit and software for streamlining the FAME absolute irradiance calibration	Planned
May 2021	Submit 2020 MOFLUX data to AmeriFlux	Annual delivery
Sept 2021	Manuscript on NEE partitioning based on SIF	Planned
Oct 2021	Manuscript on the dynamics of CO_2, SIF, CH_4, water vapor and sensible heat at the SPRUCE site	Planned

MODEL DEVELOPMENT AND EVALUATION*

3.3 Mechanistic Terrestrial Ecosystem Modeling Future Plans (Task 3abc)

This proposed task integrates data from SPRUCE, MOFLUX, and other DOE-funded flagship experiments, observation networks, and related activities into models to identify and reduce terrestrial process and parameter uncertainties in the global Earth system. The Energy Exascale Earth System Model (E3SM) and its land model component (ELM) provide consistent frameworks to integrate process knowledge, field experiments and observations to improve predictive understanding of the Earth system. Task 3ab involves the algorithmic development of specific process-based submodels within ELM targeted to improve predictions understanding in key aspects of wetland, boreal and temperate deciduous forest systems. This subtask involves both site-scale and regional modeling, and combines previous Tasks 3a and 3b. The complexity and computational expense of ELM require novel methods for model prediction, evaluation and diagnostics to understand key uncertainties. Task 3c therefore expands on the previous emphasis on model functional units by developing a comprehensive ELM testbed for ecological forecasting and uncertainty quantification assisted by machine learning. This new testbed will use artificial intelligence (AI) and surrogate modeling to aid in model design, validation and uncertainty quantification. New Task 3d (detailed below) will develop a comprehensive framework for quantifying model structural uncertainty, the Multi-Assumption Architecture & Testbed (MAAT). Modeling activities for Tasks 3abc over the next 3-year cycle will address the following key science questions, with model improvements taking place in task 3ab and model evaluation and uncertainty quantification in task 3c:

1. Will the refinement of phenology algorithms, inclusion of seasonality in photosynthetic and respiratory parameters, and representation of sun-induced chlorophyll fluorescence in ELM help to improve model predictions compared to observations at SPRUCE and MOFLUX?
2. Will an improved representation of root phenology and function in ELM, informed by trait measurements and combined with improvements in microbial modeling (task 5), result in stand-scale model predictions of CO_2, CH_4, nutrient and energy fluxes that are consistent with observations?

3. To what extent does accurately predicting the response of *Sphagnum* to warming at SPRUCE require integration of physiology and flux measurements, improved representation of site hydrology, and inclusion of competition with other plant functional types for above and belowground resources?
4. How important is fire disturbance in predictions of decadal-scale regional responses to climate change in peatland and boreal ecosystems?

3.3.1 Improve ELM submodel process representation (Task 3ab)

Site-level observations have been used to test and improve ELM, including at SPRUCE (Shi *et al.* 2015, Griffiths *et al.* 2017), MOFLUX (Gu *et al.* 2016, Lu *et al.* 2017, Liang *et al.* 2019) and a broader distribution of FLUXNET sites (Ricciuto *et al.* 2018). Regional datasets have been used to improve ELM and understand the contributions of various drivers (Forbes *et al.* 2018, Forbes *et al.* 2019, Mao *et al.* 2015) In the future, this project will develop parts of ELM associated with specific submodels (Fig 3.4) focused on SPRUCE and MOFLUX, but using additional datasets to make these developments regionally relevant when possible. For SPRUCE simulations, we will utilize ELM-SPRUCE (formerly CLM-SPRUCE; Shi *et al.* 2015) designed to capture the SPRUCE bog microtopography and specific plant types. Gridded simulations covering temperate and boreal regions will be performed and evaluated using ILAMB (Collier *et al.* 2018) and other benchmarking software. Model improvements made in these tasks will be integrated into a branch of the publicly available E3SM repository (https://github.com/E3SM-Project/E3SM). We will coordinate SFA development activities with the NGEE and E3SM ecosystem projects, and project staff also involved in the E3SM project (Ricciuto, Shi, Yang) will merge code developments into E3SM versions 3 and 4 for testing in the coupled Earth system.

We have identified several specific areas (detailed below) to pursue model development that will help to improve model predictions of carbon dioxide, energy and methane fluxes at SPRUCE, MOFLUX, and more broadly at a regional scale. Carbon fluxes at SPRUCE are especially sensitive to leaf respiration parameters at SPRUCE and across a wide range of ecosystems (Griffiths *et al.* 2017, Ricciuto *et al.* 2018). Using observed pre-treatment interspecific seasonality in $V_{\mathrm{cmax},25^\circ}$, $J_{\mathrm{max},25}$ and $\mathrm{R}_{\mathrm{d},25}$ for black spruce in ELM-SPRUCE has had significant effects on modeled carbon fluxes when compared to the default version (Jensen *et al.* 2019). Thus, we will improve model representations of canopy photosynthesis and leaf respiration, informed by leaf-to-canopy scale measurements. The response of phenology to experimental treatment at SPRUCE has been shown to be significant (Richardson *et al.* 2018), while model representations are still lacking (Richardson *et al.* 2012). If the high levels of warming associated with SPRUCE become reality in future climates, wildfires in boreal zones will likely increase.

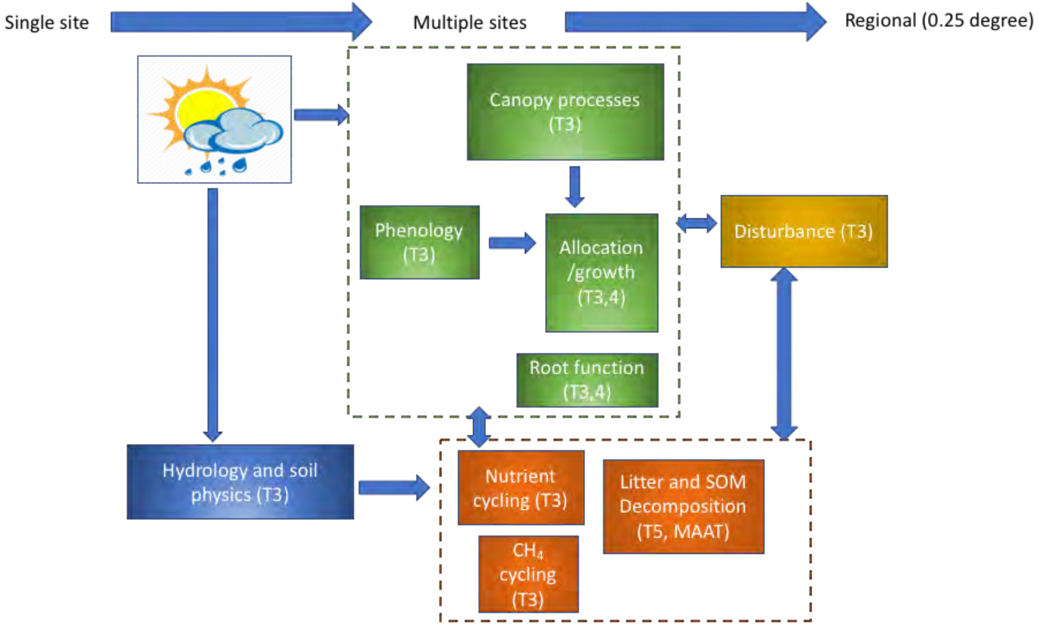


Fig. 3.4 Major process submodels in ELM (colored boxes) and flow of information among these submodels (arrows). Areas in the green box represent plant processes, while areas in the brown boxes represent belowground biogeochemical processes. A task or subtask is devoted to model process improvements in each of these submodels. We will also develop machine learning-based surrogate models for each of these submodels (Task 3c), allowing efficient model testing and calibration while accounting for feedbacks within ELM. MAAT (Task 3d) will be used to conduct a deep dive into model structural uncertainty for SOM decomposition, root function, and *Sphagnum* photosynthesis.

Developing a predictive understanding of boreal responses to climate change necessarily must include disturbance, especially wildfire in a modeling context. Peatlands contain large amounts of carbon and may be especially vulnerable (Turetsky *et al.* 2015). Another important model development need is to improve the representation of nitrogen and phosphorus cycling. Understanding nutrient cycling at SPRUCE was identified as a key priority at a recent workshop in January 2018. Peatland hydrology plays a critical role in the stability of peatland carbon changes and regional water dynamics (Lafleur *et al.* 2003, Kettridge *et al.* 2013, Mezbahuddin *et al.* 2016). Accurate modeling of relevant peatland hydrological processes thus has broad implications for improved simulations of surface budgets of energy, water and carbon, especially for the boreal region.

Along with model developments in Tasks 4, 5 and 6 these model improvements will be integrated together in the ELM framework (Fig 3.4) with functional unit and surrogate representations for each submodel (Task 3c). Site simulations will be conducted at SPRUCE, MOFLUX, and selected similar FLUXNET sites (e.g. Mer Bleue, Lost Creek, Morgan Monroe State Forest). Pan-boreal simulations will be conducted at 0.25 x 0.25-degree resolution using the improved model, and assessed using remote sensing (e.g., Landsat surface reflectance data, NASA's MODIS fire product MCD64A1). To investigate the sensitivity of major land-atmosphere exchange variables to the model changes, we will perform multiple factorial offline simulations (Mao *et al.* 2013 and 2015). We will vary combinations of land use change, atmospheric CO_2, nitrogen deposition, and aerosol deposition to separate the individual effects of selected natural and anthropogenic drivers on fluxes and stocks of interest.

Canopy Processes – We will develop a species-specific formulation that accounts for observed seasonal variation of key photosynthetic parameters based on the phenological state or leaf age and calibrate it using leaf-level observations. 10 alternative leaf respiration formulations (e.g. Heskel *et al.* 2016) have been coded in ELM and have been shown to affect net carbon fluxes at SPRUCE under the warming scenarios. We will continue to evaluate these formulations and quantify the related uncertainties at SPRUCE, MOFLUX, and over North America. We will also incorporate a leaf-level sun-induced chlorophyll Fluorescence (SIF) module (developed in Task 6 along with Thum *et al.* 2017, van der Tol *et al.* 2009 and 2014) into the canopy component of ELM, and lead the new model evaluation and calibration using site measurements of SIF and gross primary production (e.g., those from the SPRUCE and MOFLUX), and from the latest satellite products (e.g., those from the GOSAT, GOME-2, OCO-2, and OCO-3). This work will be coordinated with Task 6 and the E3SM next generation development (NGD) projects.

Phenology - We will first comprehensively assess state-of-the-art phenology models using the SPRUCE observations (Richardson *et al.* 2018) for three dominant boreal vegetation types: *Picea* trees, *Larix* trees, and mixed shrub, and from them select the best candidate submodels for further investigation. For the spring onset process, we will examine four widely used models: alternating (Murray *et al.* 1989), parallel (Landsberg 1974), sequential (Kramer 1994), and unified (Chuine 2000), evaulating each for their performance in terms of trends and interannual variability. For the autumn offset modeling, we will intercompare two models that assume leaf senescence is regulated by temperature and daylength (Jolly *et al.* 2005, Delpierre *et al.* 2009). For each vegetation type, the best candidate models will be selected based on Akaike information criterion (AIC) and residual sum of squared errors between model results and phenology observations (e.g., budburst date from field observation and PhenoCam derived phenology indicator during the period 2015-2018). We will incorporate the selected phenology models into ELM.

Disturbance – The current ELM fire model has a relatively detailed representation in the impacts of socioeconomic factors on fire events (Li *et al.* 2018a and 2018b). However, its characterization of fire process, estimation of fire burned area, and calculation of fire feedbacks still requires improvement, especially over peatlands and boreal areas. Instead of using relative humidity and soil wetness, we will derive the fuel combustion probability by utilizing fire potential indices (e.g., the Nesterov Index, McArthur Forest Fire Danger Index, Canadian Fire Weather Index, and Keetch-Byram Drought Index). We will update the cloud-to-ground lightning index, which is used to measure the ignition events based on total flashes, from the latitude-only dependence to both latitude and altitude dependence (Bourscheidt *et al.* 2009). For the constraint of anthropogenic ignition potential, we will replace the present monotonic decreasing function of human density using the historical human-caused fire counts (Thonicke *et al.* 2010). We will link the wind-spread rates to the terrain slope and adjust the simulated burned areas (Van Wagner and Pickett 1985). We will then use the simulated carbon density, burned area, and the burned depth to estimate the fire-induced carbon emissions in both the above- and below-ground biomass (Yang *et al.* 2014). We will replace the fixed ELM fire duration (set as 1 day) using the fire distinguishing probability or fire duration probability (Venevsky *et al.* 2002). We will also consider possible power grid effects and add impacts from barriers such as rivers and roads to better model the fire driving factor and spread extent especially for the high-resolution regional simulations.

Nutrient Cycling and Root Function – Specific model development includes implementation of nutrient acquisition schemes and associated carbon cost into ELM. Through collaborations with Josh Fisher (Jet Propulsion Laboratory), we expect to incorporate the Fixation and Uptake of Nitrogen (FUN) model into ELM in 2019. With the FUN structure in the model, we will introduce different nutrient acquisition schemes (both N and P), synthesize data to better constrain these schemes, and investigate how the introduction of different nutrient acquisition schemes and associated carbon cost affects terrestrial carbon cycle feedbacks. We have identified several areas of N and P cycling in ELM that need to be improved, including N fixation, nitrification and denitrification, phosphatase activity and organic N and P leaching. N fixation is a key input of N to peatland ecosystems. Measurements from SPRUCE and other studies show that N fixation in peatland can be comparable to the highest rate of N fixation in a global synthesis (Cleveland *et al.* 1999). Field observations also suggest that P availability is also a key factor in controlling N fixation, in addition to N availability (Toberman *et al.* 2015). We propose to develop a new N fixation scheme that reflects the effect of N and P availability on fixation by utilizing the N fixation measurements at SPRUCE and other field sites. We propose to improve the representation of leaching in ELM v1 -SPRUCE, mainly by including organic N and P leaching. Measurements from SPRUCE show high phosphatase activity indicating potential P limitation for plants/microbes. The different trends in the vertical profile of C:N and C:P ratios also suggest that microbes/plants utilize N and P differently through phosphatase activity, preferential uptake of N vs. P through mycorrhizae, etc. We propose to improve model representation of phosphatase activity in the peat profile by working with various streams of measurements.

Root turnover is poorly constrained in current ELM – a fixed parameter assuming the same as leaf turnover rate. We will link root turnover with root traits such as specific root length and root chemistry, and environmental factors such as soil moisture, temperature, and nitrogen (N) and phosphorus (P) availability. We propose to: (1) investigate the emerging pattern of root phenology at ecosystem scale from field observations, (2) redefine root phenology (e.g., decouple from leaf phenology) in ELM based on observations, and (3) evaluate impacts of new root phenology scheme on plant nutrient acquisition and ecosystem carbon dynamics. We will investigate how the introduction of two functional root pools affect model-simulated ecosystem responses to changes in CO_2, warming and drought. We will utilize the FRED database to parameterize and constrain the new fine root model. Specifically we propose to; (1) link water/nutrient uptake kinetics to refined root functional classes (absorptive vs. transport fine roots) based on root traits such as specific root length, C:N ratio, C:P ratio, and mycorrhizal association; (2) leverage the effort on enabling FUN in ELM to incorporate C cost associated with nutrient uptake; and (3) include how mycorrhizal fungi (implicitly as part of the suite of fine-root traits) affect nutrient uptake, particularly for immobile nutrients like phosphorus.

Methane – A microbial functional group-based methane module was developed to predict methane production and consumption from laboratory incubation experiments in conjunction with the NGEE Arctic project (Xu *et al.* 2015). In collaboration with Xiaofeng Xu (SDSU), further improvement is underway in terms of detailed biogeochemical processes along the soil column. New data-model integration efforts will include primarily model improvement on carbon isotopic methane, model parameterization, testing at additional sites, model sensitivity analysis, and model synthesis.

Biogeochemical observations from Scott Bridgham at Oregon State University, Adrien Finzi from Boston University, Paul Hanson and Natalie A. Griffiths at ORNL, and Jeff Chanton at Florida State University will be used for model evaluation and parameterization at SPRUCE. We propose 3 overall efforts. The first effort will integrate the CH_4 module into the PFLOTRAN reactive transport model, which has an ELM interface that was developed as part of the NGEE Arctic project. This will be done in conjunction with efforts in task 5 to improve the soil organic matter decomposition model. Next, we will incorporate isotopic C (^{14}C) into the CH_4 module within the ELM-SPRUCE model to develop the ability to trace C flow. A new pool will be separated from all existing soil C and microbial C pools; this ^{14}C pool will be linked with existing isotopic capability for decomposition cascade. Finally, we will validate and apply the improved ELM-SPRUCE model in simulating C flow within soil profile under elevated CO_2 and atmospheric warming treatments. Through the mechanistic model simulations, we will further explore the impacts of elevated atmospheric CO_2 and warming on belowground biogeochemistry and further the surface CH_4 flux in the S1 Bog. We will pay particular attention to the C source for surface CH_4 flux; the different age of C along soil profile and acetoclastic and hydrogenotrophic methanogenesis will be quantified for their contributions to the observed surface CH_4 flux.

Peatland Hydrology - For ELM, the soil water potential is simply calculated from volumetric water content based on the Clapp & Hornberger model (Clapp and Hornberger 1978), and was demonstrated to not capture well the soil water retention curve (Liang *et al.* 2018). Moreover, ELM was shown to significantly underestimate the total evapotranspiration at the SPRUCE S2 bog (Shi *et al.* 2015), which is likely induced by the weak representation of the impacts of soil water stress on the stomatal conductance Verhoef and Egea (2014). To improve the simulated responses of peatland hydrology to future climates, we will first implement the Modified Campbell Model (MCM) (Dimitrov *et al.*, 2010; Mezbahuddin *et al.*, 2015) to estimate the peat moisture retention. We will then investigate how soil water stress affects plant transpiration using new detailed SPRUCE observations and characterize such relationships using a more appropriate approach. For example, to calculate the water stress factor using the water potential as the independent variable combining with the reliable soil hydraulic parameters and chemical signaling which ensure feedbacks between the entire soil-root-xylem-leaf system (Verhoef and Egea 2014). In addition, we will continue to improve the lateral transport between the hummocks and hollows to better predict the soil water table depth. Since the moss layer buffers the exchanges of land-atmosphere water fluxes at the soil surface (Turetsky *et al.* 2012, Wu *et al.* 2016), it would be realistic to treat moss species as the top soil layer in land surface model. Based on the generic moss modeling applied in the ELM_SPRUCE (related paper is under preparation, Shi *et al.* 2019), we also propose to parameterize the moss layer as the first soil layer in the ELM_SPRUCE and to calibrate the new schemes using the SPRUCE measurements. Furthermore, we will improve the representation of moss *Sphagnum* photosynthesis in the ELM_SPRUCE based on the approach reported by Walker *et al.* (2017). We will finally investigate to what extent those new schemes together affect the total peatland water, energy, carbon and nutrient dynamics, and how the peatland hydrology responds to warming and elevated CO_2 concentration scenarios.

Table 3.3 – Future Task 3ab Deliverables

Date	Deliverable	Status
2019	Complete integration of FUN into ELM Complete integration of methane module into ELM-PFLOTRAN Integrate mechanistic formulation for seasonal photosynthetic variation Complete manuscript on structural uncertainty in leaf respiration T-response Complete manuscript on methane cycling using ELMv0-SPRUCE	Planned
2020	Complete new phenology submodel Complete improved fire submodel Complete Improved nutrient cycling submodel (organic leaching, improved N fixation) Complete manuscript on model evaluation with improved nutrient cycling	Planned
2021	Regional benchmarking of ELM including all new improvements Complete ELM forcing factor simulations and publish results Publish results of improved ELM-SPRUCE model	Planned

	Integration of new model features into E3SM code base	

3.3.2 Machine learning assisted UQ and ecological forecasting in ELM (Task 3c)

Evaluation, calibration and uncertainty quantification of ELM are challenging because of model complexity, strong nonlinearity, and significant computational requirements (Lu *et al.* 2018). In the previous phase of this task, we developed a model functional testing platform, which allows for the testing of specific submodels using existing ELM output without having to rerun the full ELM (Wang *et al.* 2015). This platform has allowed new insights about the behavior of these submodels, but it has not led to increased simulation efficiency due to large memory and communication requirements. Surrogate models, especially those based on artificial intelligence (AI) technologies, have the potential to greatly increase the efficiency of ELM and submodel evaluation (Lu *et al.* 2019). Here we propose an AI-based surrogate modeling framework dynamic testing, uncertainty quantification (UQ) and development platform for ecosystem functions represented as functional units within ELM. Surrogate model units can be run alone, or as part of ELM. These AI surrogates will allow rapid UQ for ELM as a whole, or may assist model development by connecting process based code with surrogates of the other ELM submodels to understand the implications of new functions in the full ELM.

This flexible testing platform may take as inputs either ESM-generated drivers or measurable external forcings at experimental sites and will generate spatial-temporal driving data for specific ecosystem functions. This will dramatically reduce the data dependency in generating standalone functional units describing specific processes for further ecosystem experimental design, testing of new algorithms, UQ or module-based integration. Model development may be done within functional units, allowing for more efficient coding, simulation and evaluation. These standalone units, if sampled sufficiently over the possible space of parameters and drivers, can also be substituted by AI-based surrogate models trained on the behavior of the functional units across the sample space. Spatially resolved AI-based surrogate models demonstrate improved accuracy over traditional surrogate approaches with 1% of the required computation (Lu *et al.* 2019). Model parameter calibration (e.g. Lu *et al.* 2018) and sensitivity analysis (e.g. Griffiths *et al.* 2017) will be performed using these surrogate models. Model development focused on a specific submodel (e.g. canopy photosynthesis) can use the surrogate representations of other expensive submodels (Fig. 3.5), allowing the model developer to understand the feedbacks within the full land model in the context of uncertainty while retaining the ability for rapid evaluation. The surrogate representations will necessarily have some loss of fidelity, but we expect to minimize this loss through improved neural-net (NN) training capabilities on HPC and new algorithms. In addition, we will exploit multifidelity techniques such as multi-level Monte Carlo (Giles *et al.* 2015) to perform uncertainty propagation while considering multiple model structures. We will perform simulations at single gridcell, multiple gridcells, and gridded regions. Single gridcell simulations (e.g. at SPRUCE or MOFLUX) provide a simple testbed for experimental sites with extensive data.

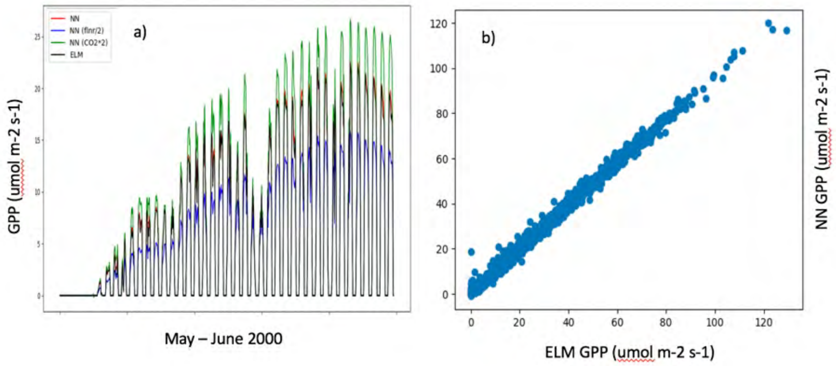


Fig. 3.5 (a) Performance of a GPP neural network (NN)-based surrogate model (red) compared to the ELM output over a two-month period at the US-UMB flux site. The NN is trained using 50,000 hourly outputs from a global simulation over a large range of atmospheric drivers and parametric variations (e.g. specific leaf area and leaf C:N ratio), and has high accuracy (R^2= 0.99, see (b)). The NN is significantly faster than the

ELM module and can be used to explore parameter and driver uncertainty, for example halving the fraction of leaf N in RuBisCO (blue), or doubling CO_2 concentration (green) (see (a)).

We will then use these approaches to develop an ecological forecasting system for ELM to predict ecosystem behavior over synoptic to interannual timescales. EcoPAD, developed by collaborator Yiqi Luo (Northern Arizona University (NAU)), successfully demonstrated near real-time data assimilation and forecasting at SPRUCE using the TECO model (Jiang *et al.* 2018a Ma *et al.* 2017). Computational expense requires the integration of the above surrogate modeling methods to enable this capability for ELM-SPRUCE. Forecasting is fully automated, runs on a regular basis and placed on a web server (https://sprucedata.ornl.gov). We will also track model skill over time, quantifying improvements from model process development and parameterization. This forecasting system will reveal key process uncertainties and inform measurement campaigns by assessing the importance of specific observations at specific times. As part of an upcoming workshop sponsored by NAU, we will integrate additional models into the EcoPAD system to enable a new type of model intercomparison at SPRUCE that includes data assimilation. For ELM, this approach will then be extended to MOFLUX, and enabled for regional simulations using gridded observations and regional surrogate models.

Table 3.4 – Future Task 3c Deliverables

Date	Deliverable	Status
2019	Integrate ELM into EcoPAD (without assimilation) and display output on website Develop GPP, hydrology, phenology and decomposition functional units/surrogates	Planned
2020	Develop root function, nutrient cycling, disturbance functional units/surrogates Integrate SIF module into ELM and the canopy functional unit Enable data assimilation capability with ELM-EcoPAD Integrate 4 additional models into EcoPAD for SPRUCE intercomparison	Planned
2021	Complete high-resolution and regional simulations Publish multi-model SPRUCE intercomparison	Planned

3.3.3 Multi-Assumption Modeling (Task 3d)

The idea central to this new task is that ecosystem models are systems of inter-connected mechanistic hypotheses and assumptions that represent ecosystem processes. Viewing models in this way connects them directly with the language of experiments and observations, and recognizes that multiple hypotheses or assumptions for many of the processes represented in a model is the norm (Walker *et al.* 2018). Few methods and tools exist to rigorously evaluate the epistemic uncertainty (Beven, 2016) that arises due to uncertainty in how a system works, i.e. when multiple competing hypotheses and assumptions exist to represent cause and effect in ecosystem processes.

With this motivation, new software (the Multi-Assumption Architecture & Testbed, MAAT; Walker *et al.* 2018) and new mathematical methods (collaboration with Ming Ye at Florida State University; Dai *et al.* 2017) were developed during the previous phase of the TES-SFA. MAAT is a novel software framework designed specifically for formal and informal evaluation of alternative model process representations. MAAT, open-source (https://github.com/walkeranthonyp/MAAT) and written in R, is flexible object-oriented software comprising a domain-agnostic model-ensemble builder that can automatically manipulate modularized code to efficiently generate multiple models that vary in process representation (sometimes referred to as multi-physics), parameter values, and boundary conditions (Fig. 3.6). MAAT allows full global process-representation and parameter uncertainty analysis (Walker *et al.* 2018), allowing the quantitative evaluation of mechanistic hypotheses in a systems context and the influence on model output of each of the processes of a given system. Current MAAT multi-assumption models are a fully developed leaf photosynthesis model and in-development canopy photosynthesis and canopy structure models.

Goals of the Multi-Assumption Systems Modeling Task are to facilitate robust, quantitative process understanding, model evaluation, and new model development in the context of multiple process assumptions across the TES-SFA, for DOE BER terrestrial ecosystem modeling efforts in ELM and FATES, and in the wider scientific community, by:

1) representing current SFA and DOE supported models in the open-source MAAT multi-assumption code base that includes new and commonly used hypotheses and assumptions;
2) evaluating alternative hypotheses against observed and experiment data in a systems framework with full quantitative accounting of the uncertainty, e.g. biophysical drivers of *Sphagnum* photosynthesis (Walker *et al.* 2017);
3) developing robust methods to evaluate model structural uncertainty and to leverage DOE supported leadership computing facilities (LCFs).

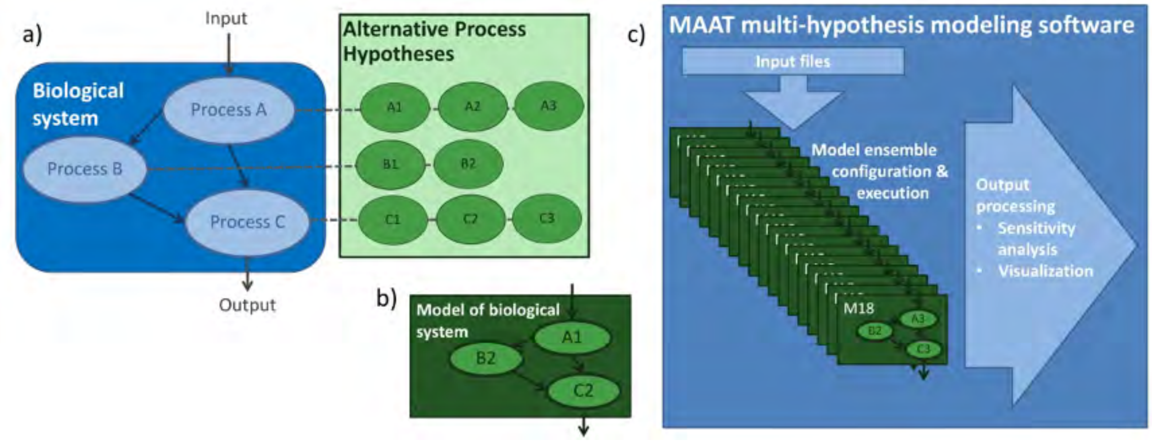


Fig. 3.6. Multi-assumption systems modeling in MAAT. a) Schematic of an arbitrary real-world system comprised of three processes, each with multiple alternative mechanistic hypotheses: three for process A, two for process B, and three for process C. b) A modeler is faced with the choice of which hypothesis to use for each process in their model: a conventional model uses only a single hypothesis for each process, while in this trivial example a total of 18 possible system models exist. c) MAAT allows a modeler to use all available hypotheses by generating an ensemble of all 18 possible system models in a single execution.

It is widely recognized, though often overlooked, that the addition of processes to a model can increase epistemic uncertainty and can have unintended consequences (Medlyn *et al.* 2015). Nevertheless, the incorporation of nutrients, roots, and microbes in ESMs is an active area of research. DOE recognize the assessment of epistemic uncertainty in plant-microbe models as a high priority. The DOE Virtual Ecosystems Workshop Report (U.S. DOE, 2015) identified a “virtual plant-soil model” as one of three key research opportunities and the DOE Data-Model Needs for Below-ground Ecology Workshop Report (U.S. DOE, 2014) specified the need to “Develop functional testing platforms for assessing belowground processes in models”. However, to-date, a software capability that can properly evaluate and quantify epistemic uncertainty in plant and microbe models is not available. For the FY2019-2021 phase of the TES-SFA the Multi-Assumption Modeling Task plans to build on existing ties with SFA tasks and to develop new ties to SFA tasks (Tasks 4 and 5), using MAAT to evaluate epistemic uncertainty in plant and microbial models.

Continuing to support scientific questions in the SPRUCE *Sphagnum* task, we plan a formal model evaluation and parameter estimation for *Sphagnum* photosynthesis and respiration based on 8100 net carbon flux data. Walker *et al.* (2017) identified a strong water table control on *Sphagnum* photosynthesis seasonality when the water table is close to the *Sphagnum* surface. Alternative models describing this interaction will be tested, with full parameter estimation and formal model evaluation using information criteria (e.g. AIC), to inform ELM-SPRUCE development (Shi *et al.* 2015). It is also planned to investigate the links between *Sphagnum* photosynthesis and respiration, including the partitioning of autotrophic and heterotrophic respiration.

To support Task 5 it is planned to draw together microbe enabled soil decomposition models into multi-assumption soil decomposition model. This will facilitate rapid model development and evaluation. We intend to develop the multi-assumption soil decomposition model in MAAT with the Microbial

Enzyme Decomposition (MEND) model (Wang *et al.* 2013). First order kinetics models of decomposition such as CENTURY (popular in many ESMs) and the sequential decomposition cascade (the default in ELM v1) will also be incorporated. Building on Sulman *et al.* (2018), it is planned to analyze soil decomposition models at the process level to identify key uncertain processes.

A high-priority in the DOE community and the ecosystem modeling community is the development of functional roots in models (e.g. U.S. DOE, 2014; Warren *et al.* 2015; see Task 4bc). A multi-assumption model of root function and nutrient acquisition will be developed in MAAT. Development will start by building on recently developed nutrient acquisition modules of ecosystem models and incorporating more detailed mechanistic models, such as the model that accounts for alternative nutrient transport pathways and mechanistic uptake functions (Mcmurtrie and Nasholm, 2018). Nutrient uptake hypotheses will include hypotheses of competition with microbes for nutrients, such as microbial priority, relative demand (Oleson *et al.* 2010), and the trait-based Equilibrium Chemistry Approximation (Tang, 2015). An exploration of the key processes causing uncertainty in root nutrient acquisition is planned. MAAT conceptualizations of fine roots will draw on the root trait data available in the Fine-Root Ecology Database (Iversen et al. 2017; Task 4b) as well as root observations being made in Task 4c and at SPRUCE and MOFLUX.

To expand the capabilities of MAAT it is planned to develop Markov-chain Monte Carlo parameter estimation algorithms and programming with big data in R (pbdR) methods to run on ORNL LCF computers. The advanced DREAM MCMC algorithm (Vrugt *et al.* 2009) will be coded within MAAT to allow for rapid and robust parameter estimation. Monte Carlo ensembles required for many of the analysis algorithms in MAAT can be computationally costly and require High Performance Computers (HPC). MAAT currently operates on HPCs using packages from the R base package which use forking for parallelization. Forking requires shared memory and thus can only be run over a single compute-node, and not across nodes. To fully exploit ORNL's HPC resource, we will develop cross-node parallel processing functionality by incorporating ORNL's "pbdr" suite of R packages (Ostrouchov *et al.* 2012).

Table 3.5 – Task 3d Deliverables

Date	Deliverable	Status
April 2019	State-of-the-art MCMC routines enabled in MAAT	Code
Oct 2019	Parameter estimation and hypothesis testing in SPRUCE *Sphagnum* photosynthesis and respiration data 2014-2018	Publication
April 2020	pbdr enabled MAAT to run on OLCF	Code
April 2020	Multi-assumption soil decomposition model	Code
Sept 2020	Multi-assumption root nutrient acquisition model	Code
April 2021	Structural and parametric uncertainty quantification of soil decomposition models	Publication
Sept 2021	Structural and parametric uncertainty quantification of root nutrient acquisition and nutrient competition models	Publication

PROCESS-LEVEL STUDIES*

Sections 3.4 and 3.5 describe TES SFA process-level studies designed to emphasize quantification and conceptualization of plant and ecosystem characteristics that are inadequately captured by terrestrial biosphere models. Our goals are to provide data and an improved theoretical basis for the inclusion and use of these processes within terrestrial biosphere models. This research is targeted and designed to be conducted, evaluated, and incorporated into models and the funding recycled to other pressing questions or areas of uncertainty.

3.4 Root Function (Task 4c)

The root function task was designed to quantify mechanistic root responses to environmental conditions, with particular focus on linking root function to root traits and providing data that could be useful to model root function in land surface models. Our key objective is to assess the root-soil rhizosphere interface and the flow and control of C, nutrient and water exchanges across the rhizosphere to provide new insights of root function. Planned tasks include: (1) assessing how root and mycorrhizal hyphae impact soil hydraulic properties, (2) linking root water uptake to traits using advanced imaging techniques, (3) assessing root and hyphal respiration rates in response to stress, and (4) along with the Root Traits task (Section 3.6), leverage new data into a modeling framework.

Over the course of the prior SFA, our efforts have leveraged neutron imaging to explore root water uptake dynamics and linkage to specific root traits, such as diameter, age or order (Warren *et al.* 2013, Decarlo *et al.* 2019). Our most recent manuscript modeled water uptake based on measured changes in soil water content, but the model failed to recreate the actual soil water dynamics, revealing the impact of significant root modification of soil hydraulic properties (Dhiman *et al.* 2018). Other recent studies acknowledge the potential importance of the impacts of roots (Helliwell *et al.* 2017) or *mycorrhizal hyphae* (Querejeta 2017) on soil properties, which is directly linked to model estimates of soil water availability. As such, we propose to investigate how roots and their associated *mycorrhizal hyphae* shift soil hydraulic properties; measurements will be made on soil columns that are root free, contain plant roots and/or contain fungal *hyphae*. Data should help refine reactive transport modeling in the uppermost, root-dense soil layers and lead to improvements in PFLOTRAN, ELM or FATES model soil parameters.

Dynamics of the soil-root interface in the rhizosphere is another emerging research topic where the display of roots (traits) is directly linked to root functions such as nutrient or water uptake. The rhizosphere acts as the mediator between roots and bulk soil, which is important for both carbon and nutrient cycling. Recent research indicates that root turnover and exudate release into the rhizosphere, along with soil microbial populations can enhance the wettability of the soil, making it more hydrophilic, or alternately more hydrophobic, such that the near root hydration can be greater than or less than the bulk soils (Carminati *et al.* 2010, Ahmed *et al.* 2016, DeCarlo *et al.* 2019). Root hydraulic redistribution and release into the rhizosphere can also affect upper soil water dynamics, and potentially impact nutrient availability (Newmann and Cardon 2012). Thus, the rhizosphere is critical and dynamic interface that controls and mediates the exchange of water, nutrient and carbon between the plant and the soil. Yet the sub-mm thick rhizosheath surrounding fine roots in the soil is particularly delicate, requiring advances in measurement techniques. As such, we propose to leverage ORNL capabilities in x-ray and neutron imaging/scattering techniques to assess rhizosphere characteristics and dynamics *in situ*. Novel understanding could provide the relevant architecture to assess mechanistic root function, and link to root traits that can be used to scale modeled function to the landscape level (McCormack *et al.* 2015, Warren *et al.* 2015).

One of the key root functional traits assessed during our earlier work on the carbon partitioning PiTS project, was the high respiration rate of *mycorrhizal* fungi. In fact, root-exclusion soil containing *hyphae*, and bulk soil containing roots and *hyphae* had a similar magnitude of soil surface efflux of new C based on ^{13}C tracking. Thus, a large part of the carbon allocated belowground was transferred to root-associated *mycorrhizal hyphae* where it was rapidly respired. This is a key part of the carbon cycle that is strongly linked to resource uptake and can be differentially impacted by stressors such as drought (Ficken & Warren 2019). Carbon partitioning in ELM is still rudimentary, and based on fixed proportions, indicating a need to further assess the C allocated belowground, and its fate. Here, we plan to leverage ongoing and planned work within our group focused on root versus microbial respiration dynamics, and how changing environmental conditions can impact both belowground allocation, and rapid release through respiration. There is synergy in this task with work at MOFLUX and the National Institute of Standards and Technology (NIST), and extensive laboratory measurements are planned for roots from the SPRUCE site. Specifically, root systems will be sampled initially from outside the SPRUCE plots, then respiration-temperature response curves generated (from 5 - 65 °C) that will be used to parameterize root response to temperature in ELM-SPRUCE modeling. To test for respiratory acclimation to treatments, there is the potential for limited, destructive small-scale root system harvesting and measurements from shrubs and trees within the SPRUCE treatment plots. We will also consider additional root and fungal respiratory work linked to detailed root trait analysis planned for diverse species at the Morton Arboretum in concert with the Root Traits task (Task 4b) As such, we will develop and deploy *in situ* root and soil hyphal separation collars for surface CO_2 efflux measurement by Morton Arboretum staff. Data will be linked to detailed root and leaf phenology, growth allocation and environmental conditions to examine species-specific and fungal-symbiont specific responses to internal and external forcing.

Table 3.6 – Task 4c Root Function Deliverables

Date	Deliverable	Status
FY2019 Deliverables		
December 2018	Publish manuscript on root respiratory response to drought: "Sensitivity and recovery of soil respiration to extreme drought in AM and ECM mesocosms." (Ficken & Warren 2019)	Completed
August 2019	Develop and demonstrate successful root respiration temperature response curve techniques	Planned
September 2019	Complete initial assessment of root and hyphal impacts on soil hydraulic properties	Underway
September 2019	Publish new manuscript on root rhizosphere water dynamics based on neutron imaging	Underway
FY 2020 Deliverables		
January 2020	Develop and build *in situ* root and soil hyphal respiration separation chambers	Planned
	Install respiration separation chambers in key projects, TBD	Planned
June 2020	Publish manuscript on root and hyphal impacts on soil hydraulic properties	Planned
FY 2021 Deliverables		
September 2021	Publish dataset and manuscript on root respiration in response to whole-ecosystem warming at SPRUCE	Planned

3.5 Microbial Processing of Soil C (Task 5)

Organic matter decomposition in nearly all ESMs, including the ELM, relies on linear, first-order decomposition rates based on empirical data and modified by edaphic factors like clay content. ESMs produced a six-fold difference in predicted soil organic matter (SOM) stocks in CMIP5 (Todd-Brown *et al.* 2013). From a global-change perspective, first-order models cannot mathematically account for the impacts of changes in inputs that are observed due to elevated CO_2 and nitrogen fertilization on SOM decomposition, or priming of SOM, because increased organic inputs will simply result in increased SOM stocks (Cotrufo *et al.* 2013, Todd-Brown *et al.* 2014, Wang *et al.* 2014, Li *et al.* 2014, Wieder *et al.* 2015, van Groenigen *et al.* 2015, Shi *et al.* 2018). Environmental changes such as increasing temperature can alter microbial biomass and decomposition rates through physiological acclimation or shifts in community composition, with variable and interacting effects on SOM stocks (Haruruk *et al.* 2015, Liang *et al.* 2018). New results from the SPRUCE site are showing the potential for changes in microbial community and function with warming. First-order models cannot represent the complexity of microbial community responses or changes in inputs, and therefore have difficulties predicting conditions in response to climate and environmental changes (Abramoff *et al.* 2017).

It is for these reasons that a new generation of nonlinear models with explicit microbial pools has arisen. Decay rates in nonlinear microbial models depend on both the SOC substrate and the catalyst, e.g., enzymes and/or microbial biomass (Wang *et al.* 2013, Wieder *et al.* 2015). Our recent efforts have focused on: (1) explicitly modeling microbial decomposition at the field scale (Wang *et al.* 2019), (2) incorporating moisture sensitivity into our Microbial Enzyme Decomposition (MEND) model (Liang *et al.* 2018, Wang *et al.* 2019), and (3) determining the sensitivity of microbial parameters to warming (Li *et al.* 2018). We have also discovered that the suite of microbial models currently in use has highly divergent responses to changes in inputs and increases in temperature (Sulman *et al.* 2018), indicating that the proper configuration of microbial models is far from settled. Lack of appropriate benchmarking data is also a well-known problem (Luo *et al.* 2015) that further inhibits our ability to determine the most appropriate microbial model structure (Sulman *et al.* 2018).

The following hypotheses will be tested in this task: (1) decreasing soil moisture will alter microbial biomass and activity, resulting in decreases in CO_2 fluxes and increases in SOM stocks; and (2) increases in temperature will result in changes to microbial physiology that also influence SOM stocks and CO_2 fluxes, but the effect of various feedbacks must be considered to understand the direction and magnitude of the changes. We propose to use the long-term and manipulative data from the two flagship TES field sites (i.e., MOFLUX and SPRUCE) to determine the role of microbial respiration in soil carbon cycling, and in particular to understand the sensitivity to changes in soil moisture, increased temperature, and increased atmospheric CO_2 concentrations. We will focus on the MEND model which includes explicit microbes and enzymes, and the "Carbon, Organisms, Rhizosphere and Protection in the Soil Environment" (CORPSE) model (Sulman *et al.* 2017), which is capable of considering the priming response of soil microbes to mycorrhizal exudation, a common response to elevated CO_2. We will work closely with the new Task 3d (Multi-Assumption Architecture & Testbed (MAAT) modeling) which is testing how different configurations of these models and others represent microbial and root respiration. We will perform companion lab-scale experiments designed to isolate the roles of soil moisture, temperature, and soil texture on carbon decomposition. Comparison of the models with lab and field data will provide a basis for defining the configuration of a microbial module in the ELM-PFLOTRAN framework which is being developed at ORNL under the NGEE Arctic project. Coupling the microbial module with PFLOTRAN and ELM will enable consideration of a number of processes necessary to resolve our hypotheses, e.g., plant functional type that controls organic matter inputs, as well as vertically-resolved carbon cycling and soil hydrology.

Role of Drought and Soil Moisture – Results of application of ELM to the MOFLUX site show that the model overestimated GPP and dramatically overestimated soil respiration during the drought of 2012 (Fig. 3.7). The model also tends to overestimate soil respiration outside of peak growing season, and to underestimate soil respiration during peak season (Fig. 3.8), despite solid improvements in accurately accounting for the soil water potential (Liang *et al.* 2018). This may be related to lack of consideration of seasonal microbial and root dynamics in ELM but could also be related to the lack of dynamic root and leaf carbon allocation (Song *et al.* 2013, El Masri *et al.* 2013). Also, recent work suggests that photosynthesis influences soil respiration through the supply of exudates to the subsurface, resulting in a predictable daily lag time for peak respiration (Liu *et al. in review*) which is not considered in ELM.

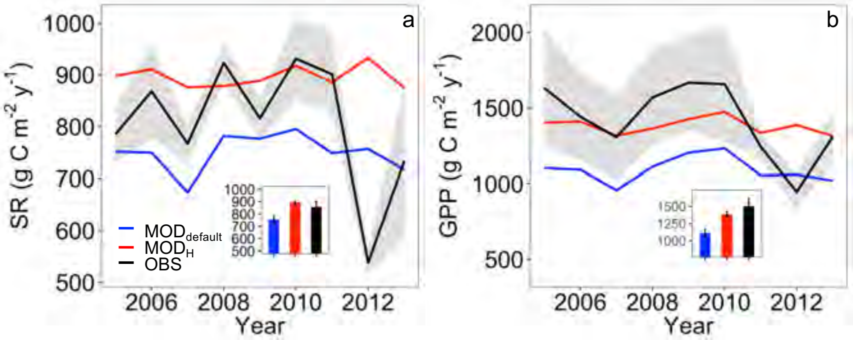


Fig. 3.7 Annual soil respiration (SR) and gross primary production (GPP). Blue and red lines are model outputs before (MOD$_{default}$) and after (MOD$_H$) soil water potential improvement, respectively. Black lines and grey area are the observed (OBS) mean and 1 sigma (i.e., standard deviation) range, which were calculated from eight field replications for SR, and from three different net ecosystem exchange partitioning methods for GPP. The inserted bar plots are mean annual average ± 1 sigma across 2005-2011. From Liang *et al.* (2018).

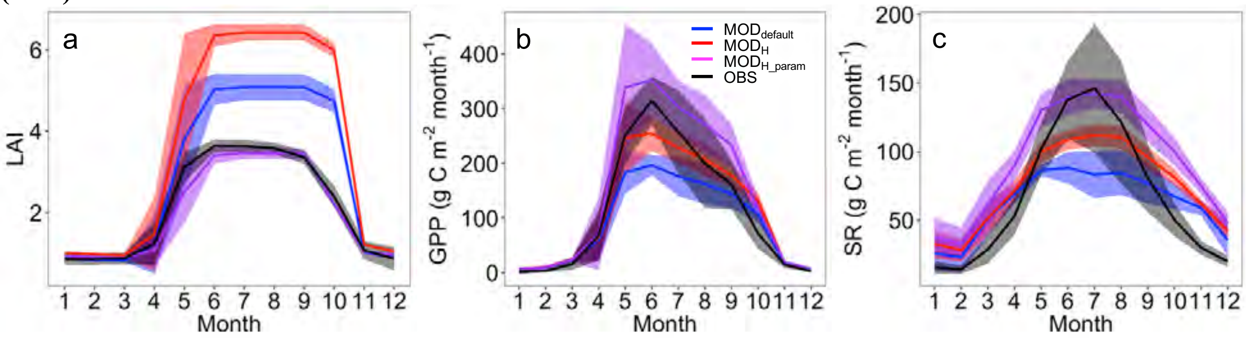


Fig. 3.8 The annual mean cycles of leaf area index (LAI), gross primary production (GPP) and soil respiration (SR). OBS: observation; MOD$_{default}$: model output before soil water potential improvement; MOD$_H$: model output after soil water potential improvement by the Hanson model; MOD$_{H\_param}$: model

output after soil water potential improvement by the Hanson model and parameter adjustments. From Liang *et al.* (2018).

While better consideration of soil moisture has improved predictions of soil respiration and GPP for the MOFLUX site (Fig. 3.7), more work is needed. To that end, in FY19 we are performing a set of incubation experiments on three soils with dramatically different textures (sandy, loamy, clayey), and determining CO_2 fluxes as a function of 5 different moisture contents ranging from air-dried to fully saturated. Initial results show that sandy and loamy soils show peak respiration at intermediate moisture conditions, whereas clay soils show peak respiration under saturated conditions. In addition, we have planned a drought-rewetting incubation experiment with the MOFLUX soils. When completed, we will use the data to continue to improve the sensitivity of moisture to soil texture in ELM. We will attempt to unify the moisture functions for soil carbon dynamics in soils with different textures, and provide moisture scalars for the carbon cycling processes in mechanistic models, such as ELM and MEND. We are working to improve ELM's drought sensitivity, also using MOFLUX's long-term data to construct projections of different drought frequencies and intensities. Initial results with the MEND model, which includes only belowground processes, are showing much greater model sensitivity to drought versus wetting, where soil CO_2 emissions are reduced as a function of intensified soil moisture extremes, which is a consequence of increased matric stress on microbial C assimilation and increased osmotic stress-induced dormancy status of the microbial community, which are considered explicitly in MEND. However, the concomitant changes to vegetative inputs are just now being included by performing the same simulations in ELM; these are expected to modify the strong responses seen by the belowground-only model MEND. Since February 2017, the MOFLUX site has four of its total 16 soil flux chambers where heterotrophic respiration has been isolated through trenching. Companion samples on root biomass and length, root and soil respiration, soil microbial biomass carbon and nitrogen, and other soil characteristics have been collected quarterly and are undergoing analyses currently. Initial tests with ELM show good agreement between observed and modeled data in 2017, but we expect different performance in the relatively strong dry season in 2018. This set of observations, coupled with the long-term measurements at MOFLUX, will enable a better understanding of how moisture affects both root and microbial respiration, which we will use to improve ELM and MEND beyond results shown in Figs. 3.7 and 3.8. If the problem is related to microbial respiration, coupling ELM with MEND will result in better fidelity against the data, and will clearly point to the need to include an explicit microbial function in ELM.

Building and Testing a Coupled Microbial-ELM Model at MOFLUX – While Task 3a is focused on porting the methane microbe model into ELM, we recognize that ELM still lacks basic representation of aerobic microbial decomposition of soil organic matter. Thus, beginning in FY20, we will use the long-term data stream from the MOFLUX site, as well as our site-level measurements since 2017, to enable the development and testing of a vertically-resolved microbial model in ELM. Again, close collaboration with Task 3d will facilitate the choice of model configuration, while keeping in mind the lessons learned in an informal microbial model intercomparison described above (Sulman *et al.* 2018), as well as consideration of belowground processes not yet represented in microbial models (Abramoff *et al.* 2017). Task 3d will be used to help focus on appropriate structures for the microbial model, by comparing MEND, CORPSE, and other concepts. The coupled PFLOTRAN-ELM framework developed at ORNL under the NGEE-Arctic project will be used to incorporate the new model configuration into an offline version of ELM. Additional data on root growth and function at MOFLUX, in addition to the measurements taken since 2016 described above, are also available through the mini-rhizotrons currently installed at the site. Additional lab-scale incubation experiments will likely be needed to test specific aspects of the model, and the specifics of those experiments will emerge from the model testing. Finally, we will also incorporate the concept of lag-times of photosynthate supply to the belowground microbe-root communities (Liu *et al.* in review), which may result in improved diurnal fidelity of the model to the site data. It will be particularly interesting to see how drought conditions affect this process, particularly in light of our MEND model results that suggest decreased CO_2 fluxes and increased soil carbon storage under drought (Wang *et al.* 2019). This task is expected to yield a functional microbial model that has been tested at the MOFLUX site, and that is sufficiently sensitive to important constraints on vegetation and microbial productivity, such as soil moisture, drought, seasonality, and diurnal variations in respiration.

The Coupled Microbial-ELM Model at AmeriFlux Sites and at SPRUCE – In the third year of this project, we will begin to test the coupled Microbial-ELM model at SPRUCE. We will use the voluminous SPRUCE data to develop predictive capabilities for physiological acclimation and the priming effect in the model, while recognizing that specific laboratory incubation experiments may be needed to identify site-specific microbial model parameters such as carbon use efficiency. We will also begin to reconcile our efforts with those of Xiaofeng Xu at SDSU and his ELM-Microbe model that is focused on methane cycling (Task 3a). The ultimate outcome (which will extend into the next SFA cycle) will be a fully functional model that is capable of representing both CO_2 and CH_4 fluxes from the SPRUCE site, while considering essential microbial acclimation processes that occur with warming (e.g., Li *et al.* 2018) as well as changes in exudation and photosynthesis that occur with elevated CO_2 (Sulman *et al.* 2017). Fully considering these effects on soil respiration is needed in order to predict future climate that will be dominated by these kinds of conditions. This work will result in the incorporation and testing of a functional microbial model in ELM, through the ELM-PFLOTRAN framework. Finally, this set of coupled models and experiments will answer basic questions about microbial community responses to warming and labile carbon supply that underpin the community-wide desire to include microbes in ESMs.

Table 3.7 – Task 5 – Soil C Deliverables

Date	Deliverable	Status
2019	Accounting for the sensitivity of soil CO_2 emissions to soil moisture and texture	Underway
2020	Development and initial offline testing of microbial model coupled to ELM at MOFLUX	Planned
2021	A plan for applying microbial model coupled to ELM at SPRUCE	Planned

GLOBAL TRAIT DATABASES*

3.6 Root Traits (Task 4b)

FRED has been and will continue to be a freely-available resource for the broader community of root and rhizosphere ecologists and terrestrial biosphere modelers (McCormack *et al.* 2018). We propose to continue to use existing data to better understand the variation in root traits within and among species and across the globe, to harvest data from completed studies not yet in FRED (e.g., data from agricultural systems), and to make new measurements that improve the data available to inform our understanding of belowground processes and below- and aboveground linkages.

Using FRED 2.0 to Answer Important Questions In Belowground Ecology – We are using FRED 2.0 to test for the existence of a root economics spectrum (e.g., Weemstra *et al.* 2016); preliminary analysis indicates that fine-root trait variation does not mirror patterns observed aboveground. We hypothesize that this is due to the difference in structure and functional variety of fine roots compared with leaves, and also because of the close association between roots and mycorrhizal fungi. We will use the empirical root trait relationships derived using FRED 2.0 to parameterize a heuristic model that includes the traits and functional contributions of mycorrhizal fungi for a more holistic view of belowground resource acquisition strategies.

Furthermore, we propose to conduct a global assessment of the variation in root traits by implementing a hierarchical Bayesian model (e.g., Ogle *et al.* 2014) 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. With this statistical framework, we will quantify intra- versus inter- specific trait variation, trait covariation, and trait trade-offs related to a suite of limiting ecosystem processes. Results from this analysis will also guide the design of plant functional types in terrestrial biosphere models that better consider the covariation in belowground plant traits (i.e., Root Functional Types).

While FRED represents the largest compilation of root-trait data in the world, analyses of these data must consider whether FRED is representative of biomes and plant species across the world, and if not, where future data collection efforts should be concentrated (e.g. Metcalfe *et al.* 2018). We will use representativeness analysis (e.g., Hargrove and Hoffman, 2004, Hoffman *et al.* 2013) using base layers related to vegetation type, soil characteristics, climatic conditions, and topography to ask which areas of the world are most similar in their fine-root traits, where this changes depending on the trait of interest, and where data are lacking that would allow us to develop a more comprehensive understanding of root trait variation across the world.

We will continue to be involved in international collaborations, including the sROOT working group (https://www.idiv.de/sdiv/working_groups/wg_pool/sroot.html) within the German Centre for Integrative Biodiversity Research (iDiv). Furthermore, FRED 2.4 has been integrated into TRY 5.0, to be released in early 2019, and we will continue to interface with the TRY data team to facilitate below- and aboveground linkages. We are also developing a collaboration with the International Soil Carbon Network to develop linkages between fine-root trait data and soil carbon data (Malhotra *et al.* 2018).

Improving the Next Generation of the FRED Database – Data collection is ongoing and will continue for the foreseeable future, with the release of version 3.0 of FRED expected in early 2020. For the release of FRED 3.0, we will draw upon the data management capabilities within ORNL's Environmental Sciences Division to convert the FRED database, which is currently stored as a flat file (.csv format), to a database with a flexible online interface for data access and which can seamlessly integrate with the TRY database. This will allow users to interact more precisely with FRED, and to download the subset of root traits or ancillary data from specific species or geographic regions that inform their scientific questions.

Making New Measurements to Inform Our Understanding of FRED Observations – The data in FRED are necessarily a mixed compilation of root traits and ancillary data from a subset of plant species, quantified using a variety of methodologies. These important, but somewhat disconnected, pieces of a very large puzzle need to be placed into a solid framework to advance our global understanding of belowground processes. We propose to further develop this framework by making a series of interconnected below- and aboveground measurements on the same plants, using the same methodology, and in the same ecosystem. We will select a phylogenetically and ecologically diverse suite of tree species from mature forestry plots at Morton Arboretum, Chicago (in collaboration with M.L. McCormack) to determine how belowground strategies for resource acquisition differ across ecologically important and model-relevant plant groups. We will quantify commonly-measured root traits and critical but less frequently measured processes that link root traits with their function, including root phenology and lifespan, associations with mycorrhizal fungal partners, and belowground plant responses to environmental variation. We will make explicit linkages among below- and aboveground traits and edaphic and environmental conditions through monitoring of leaf traits and phenology, stem growth and phenology, temporal patterns of soil moisture and temperature, and external factors including light availability, temperature, and precipitation. These new observations will serve as a solid framework for linking below- and aboveground data within and among species to more effectively use the diversity of traits in FRED and other developed resources (e.g. TRY) to understand above- and belowground linkages across the globe.

Table 3.8 Task 4b - Root Trait Deliverables

Date	Deliverable	Status
2019	Manuscript on belowground resource acquisition strategies	Underway
2020	Manuscript on hierarchical Bayesian model of root-trait variation in FRED 2.0	Planned
2021	FRED 3.0 available to community as a relational database	Planned

3.7 LeafWeb (Task 8)

For FY 2019, 2020, and 2021, LeafWeb (www.leafweb.org) will continue to apply the principle of SErvices in Exchange for Data Sharing (SEEDS) to support ORNL TES SFA missions. So far, Leafweb has been primarily focused on analyzing and gathering leaf gas exchange measurements from global researchers. Given the exciting new developments in SIF research and modeling photosynthesis from the side of light reactions, it is clear that this focus is now too narrow. Currently, Leafweb users are able to include only the photochemical quantum yield of photosystem II measured with Pulse Amplitude Modulated (PAM) fluorometry as a column in the gas exchange data files they submit to LeafWeb for analyses. However, many different variables are measured with PAM fluorometry and these variables are all crucial for studying the dynamics of SIF and its relationship with GPP (e.g., NPQ, q_L, $\Phi_{PSIImax}$, see Task 6a). Also, users may measure leaf gas exchange and PAM fluorometry separately. For example, they may use a monitoring PAM to measure fluorescence parameters. In this case, no gas exchange measurements would be made simultaneously and the current version of Leafweb would not be able to accept these separately measured PAM data.

We will redesign Leafweb so that it can accept the submission of leaf gas exchange and PAM fluorometry data for analyses either simultaneously or separately. Users will be able to submit all PAM parameters. To attract users to submit comprehensive PAM fluorometry datasets, we will explore novel ways to conduct online analyses and graphic displays for these datasets. For example, we will implement a model fitting for light responses of q_L and NPQ (Serôdio and Lavaud, 2011). Users will be able to extract characteristic response constants from the fitting and compare them across species and habitats. These constants can be used to study species adaptation to environments and stress. Meanwhile the PAM data gathered can be used to better understand and parameterize Eqn 1- 3 in Task 6a for modeling photosynthesis from the side of light reactions.

Additionally, we will add data search capabilities to LeafWeb to provide quick access to specific input and result sets matching given query parameters. We will also improve guidance for users to submit input files in the correct format. We have found that most issues encountered by LeafWeb are due to incorrect formatting of input data. More clear guidance on input data format will reduce the occurrence of these issues and improve users' LeafWeb use experience.

Table 3.9 – Task 8 LeafWeb Deliverables

Date	Deliverable	Status
Aug 2019	Clear data formatting guidance provided in the LeafWeb site	Planned
Dec 2019	Completion of software for PAM data analysis	Planned
May 2020	LeafWeb ready to accept full PAM fluorometry data	Planned
Dec 2020	Completion of data search capabilities	Planned
July 2021	Completion of graphic display capabilities for PAM data	Planned
Oct 2021	Manuscript synthesizing the dynamics of NPQ and q_L for modeling photosynthesis	Planned

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4. MANAGEMENT AND TEAM INTEGRATION

4.1 Organizational Structure and Key Personnel

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

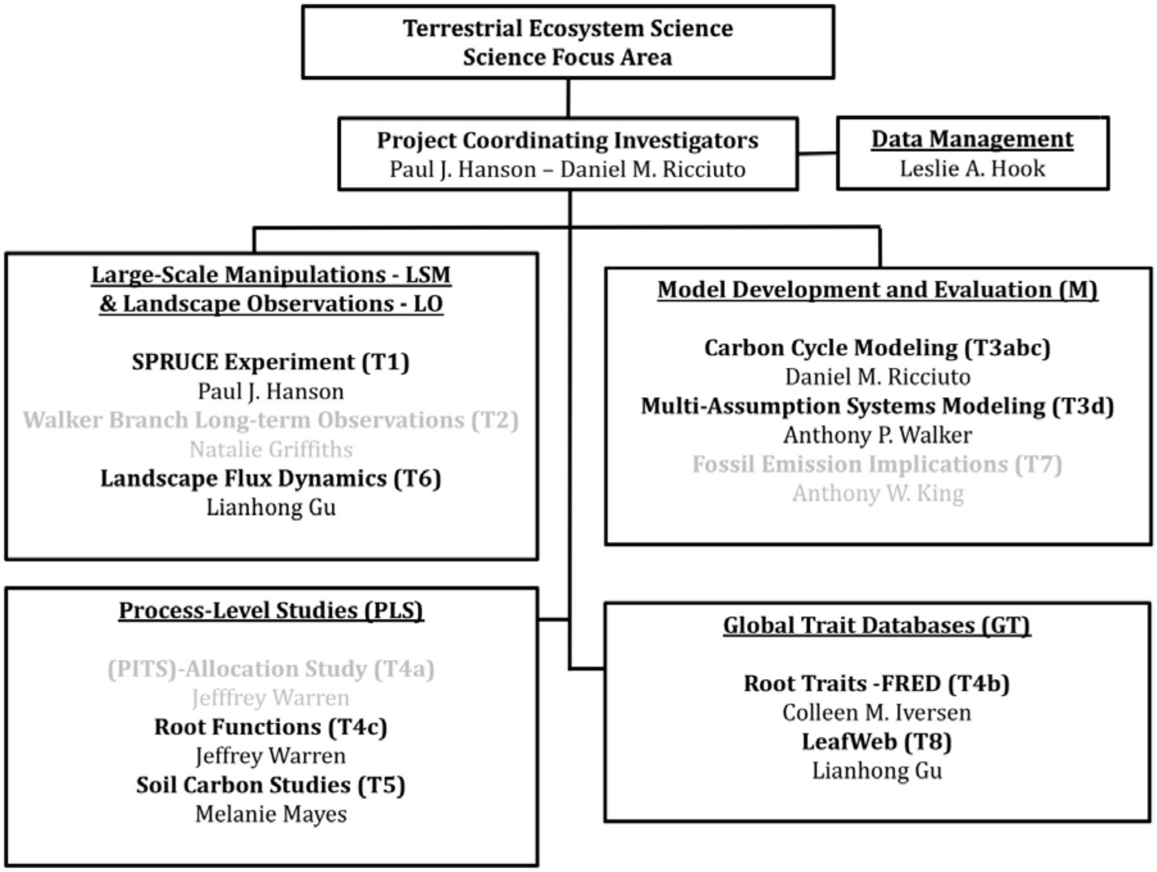

Fig. 4.1 – Organizational chart for the TES SFA effective October 2018.

Dr. Paul J. Hanson is the Principal Investigator (PI) for the TES SFA, and Dr. Daniel M. Ricciuto is the PI for the C-Cycle modeling tasks which are integrated across the TES SFA. Task Leads described in Fig. 4.1 and Section 6 are given independent science and financial responsibility to achieve the goals of their respective tasks. Responsibility for the TES SFA resides within the Energy and Environmental Sciences Directorate and is aligned with associated and related activities of the Climate Change Science Institute (CCSI).

4.2 Project Planning and Execution

Periodic (typically monthly) teleconferences are held between the TES SFA Coordinators and DOE BER. Technical Coordinators and Task Leads meet at least monthly with their respective teams and staff to evaluate program integration and to ensure that research tasks are progressing and are being performed appropriately.

Budget planning for the TES SFA is a cooperative activity between the PIs and Task Leads and ORNL accounting staff. When annual funds are received they are distributed among the TES SFA Task leads and SPRUCE Sub-Task Leads according to the funding schedule laid out in Table B3. Task Leads are expected to manage their funds throughout the fiscal year without exceeding planned funding levels. If task or subtask overages do occur near the end of the fiscal year the PI (Dr. Hanson) will seek to cover such cost over runs from limited carry-over funding from the prior fiscal year. If such funds are insufficient the PI may consult with Task Leads having excess funds to balance the overall TES SFA budget.

4.3 Collaborative Research Activities

A variety of collaborations, both within the TES SFA and externally, are being fostered to provide necessary expertise or effort in areas critical to the completion of research tasks (see page 163). 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 PLAN

Understanding fundamental responses of ecosystem biogeochemical cycles to climatic and atmospheric change is the aim of the Terrestrial Ecosystem Science Scientific Focus Area (TES SFA). The data generation tasks include large ecosystem manipulations, C-Cycle observations, database compilation, and fundamental process studies integrated and iterated with modeling activities.

- The centerpiece is the SPRUCE experiment, a large-scale experimental manipulation testing multiple levels of warming at ambient and eCO_2 on the C feedbacks from a *Picea*-*Sphagnum* ecosystem. SPRUCE has implemented a highly instrumented experimental platform for the long-term observation of the mechanisms controlling the vulnerability of organisms, ecosystems, and ecosystem functions to increases in temperature and exposure to eCO_2 treatments within the northern peatland high-C ecosystem.
- Other TES SFA efforts aim to improve mechanistic representation of processes within terrestrial biosphere models by furthering our understanding of fundamental ecosystem functions, and their response to environmental change. These tasks include smaller-scale, process-level manipulations to quantify root trait and function research, and mechanistic studies of soil C-cycling. The TES SFA supports the long-term monitoring of landscape flux measurements at the Missouri flux (MOFLUX) site and complementary measurements to better interpret responses.

All data collected at the SPRUCE facility, 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 are submitted to the respective SPRUCE or TES SFA data archive in a timely manner such that data will be available for use by project scientists and collaborators and, following publication, the public, through the SPRUCE (https://mnspruce.ornl.gov) and TES SFA (https://tes-sfa.ornl.gov) websites.

TES SFA data management plans and policies align with the Office of Science's digital data management policies. A more detailed DMP is provided in Appendix D.

Collaboration across BER Projects- TES SFA participants (Paul Hanson and Daniel Ricciuto are serving as members of the U.S. Department of Energy's (DOE) Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS–DIVE) Archive Partnership Board (APB). In this capacity the TES SFA stays current with community expectations for data and model archiving.

DOI Registration - The TES SFA now registers DOIs for all data products using the OSTI (DOE Office of Scientific and Technical Information) E-Link System. SPRUCE products as 10.25581/spruce.0XX/zzzzzz and TES SFA products as 10.25581/ornlsfa.0XX/zzzzzz. Comprehensive metadata can be entered that will facilitate the eventual transfer of metadata, documentation, and data to the DOE's Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) archive.

Gigabit Internet Connection at SPRUCE field site - This new fiber optic connection facilitates better access to data logger controls, soil flux chamber instruments, real-time PhenoCam images, the eddy covariance (EC) flux system, and a mobile integrated EC/SIF (solar-induced chlorophyll fluorescence) system. The fiber optic connection replaces a slower satellite link for the 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.

5.1 Data Products:

SPRUCE has archived and shared with the public 44 data products along with 18 products for the ongoing TES SFA tasks (Appendix B). There are currently 8 products, available to the project only, that are awaiting publication of paper and a few others in a development queue at any one time. The products include regularly updated time-series of SPRUCE environmental data, peat analyses, modelling archives, 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, V2), and characterization of SPRUCE plots (e.g., elevation). In the next funding cycle the TES SFA will do the following:

Implement Data Sharing and Archiving System - A new set of data management resources to support project-level data sharing, search, and archiving will be implemented for SPRUCE and TES-SFA. This system will leverage existing DOE BER investments in data management technology from NGEE Arctic and the ORNL Critical Interfaces SFA to provide enhanced data management support to the project by adopting standards-based, open-source approaches to ensure efficiency across DOE BER projects and interoperability with OSTI for generation of DOIs. The improved "Data Sharing and Archiving System" will include an Online Metadata Editor for metadata input and data upload; Data DOI Application for reserving and registering DOIs; Data Search and Access including DOI Landing Pages; and Data Product Management capability for data upload, storage, processing, access control, etc.

Initiate Transfer of Selected Data Products to DOE ESS-DIVE Archive- Data management staff will work with ESS-DIVE archive staff to develop and implement a workflow for transfer of selected SPRUCE data products to the ESS-DIVE Archive. Data and documentation will be reviewed and updated as needed. Product metadata will be reviewed and updated as needed to meet archive requirements and to ensure efficacious data search and discovery. It will be determined if OSTI DOI transfers are needed. We will evaluate the transfer process and release of SPRUCE products to the public through the Archive's search capabilities. If needed, metadata will be enhanced to maximize data discovery and access.

5.2 SPRUCE and TES SFA Websites Upgrades

The SPRUCE and TES SFA Websites will be upgraded to the latest version of Drupal (content management system) while transferring the websites to the ORNL Web Services organization for all future DRUPAL maintenance, security updates, and upgrade services. Website content will still be managed by TES SFA Staff.

6. PERSONNEL

ORNL is uniquely positioned to deliver the science required to support the vision of the TES SFA. The original team (established in 2009) has undergone several staff changes but has been supplemented by developing staff in both the modeling and experimental areas and by acquisition of key technical support 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. We have brought together exceptional multidisciplinary expertise and are retaining and building staff flexibility to support new research priorities as they are identified.

- Dr. Paul J. Hanson is the TES SFA Coordinating Investigator. He provides integrated leadership across tasks, and coordinates financial management. Dr. Hanson has 33 years of experience as a plant physiologist and environmental ecologist. He operated and managed the long-term (14-year) Throughfall Displacement Experiment on the Oak Ridge Reservation, and coordinated the multi-lab Enriched Background Isotope Study. He currently manages a 29-member Ecosystem Science Group within the Environmental Sciences Division at ORNL, is a Subject Editor for *Global Change Biology*, and is coordinating investigator for the SPRUCE study.
- Dr. Daniel M. Ricciuto is the coordinating investigator for terrestrial C-cycle modeling. Dr. Ricciuto is a staff scientist in the Terrestrial Systems Modeling Group in the Climate Change Science Institute (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. Leslie A. Hook serves as the Data Management Coordinator. He brings expertise and technical skills for data policy, management, and archive planning and implementation. Working with web site developers, he has developed and maintained task-specific web sites with project information, resources, and public data access.

Individual Task leads take responsibility for their respective continuing or future initiatives as follows (person-specific annual effort is summarized in Table 5.1).

Task 1

Experimental Design, Maintenance and Environmental Documentation – Paul Hanson leads the development of the SPRUCE experimental infrastructure together with a team of ORNL structural and electrical engineers. W. Robert Nettles (an ORNL employee located full-time in Minnesota) leads the day-to-day onsite activities at the SPRUCE site. He is supported by Jeff Riggs (Lead Instrument Technician) to keep the treatments running and data streams flowing. Misha Krassovski, system engineer, designed and implemented automated data acquisition system for SPRUCE.

Plant Growth Phenology and NPP – Paul Hanson, Colleen Iversen, Richard Norby and postdoctoral research staff are splitting efforts in this area. Paul Hanson is leading tree and shrub growth and vegetation phenology with the participation of W. Robert Nettles and Jana Phillips. Richard Norby leads characterization of growth and community dynamics of the diverse *Sphagnum* communities occupying the bog surface beneath the higher plants. Richard Norby will be transitioning to part-time status in 2019 and withdrawing from active participation in this SFA, but he will maintain an advisory role to ensure a smooth transition on tasks he formerly led. Belowground measurements are led by Colleen Iversen, with technical assistance from Joanne Childs and Deanne Brice. Camille Defrenne has agreed to join the TES SFA as a post-doc beginning in May 2019. She will be based at ORNL (supervised by Colleen Iversen) but will travel to the SPRUCE experimental site as needed. Her main focus will be to link fine-root traits with ecosystem processes at SPRUCE.

Community Composition – Community compositional changes are being led by Brian Palik of the USDA Forest Service (USFS). Chris Schadt at ORNL leads efforts on microbial community changes, and coordinates related efforts among the SPRUCE collaborators.

Plant Physiology – Characterization of pre- and post- treatment plant physiological responses are led by Jeff Warren, past and planned postdoctoral staff, and unfunded University collaborators, particularly Danielle Way of the University of Western Ontario. 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.

Biogeochemical Cycling Responses – Work on hydrologic cycling is led by Steve Sebestyen (USFS) and Natalie Griffiths (ORNL). Colleen Iversen leads the subtask focused on plant nutrient availability in the shallow rhizosphere, with technical support from Deanne Brice and Joanne Childs. C-cycle observations focused on peat changes and C emissions are coordinated by Paul Hanson, with technical support from Jana Phillips and Deanne Brice. Natalie Griffiths and Randy Kolka (USFS) are leading efforts on measuring related decomposition processes.

Modeling of Terrestrial Ecosystem Responses to Temperature and CO_2 –Daniel Ricciuto coordinates efforts to utilize and incorporate experimental results into improved modeling frameworks for understanding the peatland C-cycle and its feedbacks to climate together with Xiaoying Shi, and Jiafu Mao.

A coordinating panel consisting of the Response SFA research manager (Hanson), the local USFS contact (Kolka), the Technical Task leaders listed above, and members from the scientific community make up the experimental advisory panel. This group serves as the decision-making body for major operational considerations and the decision making body for vetting requests for new research initiatives to be conducted within the experimental system.

Task 3abc – Terrestrial ecosystem modeling activities are led by Daniel Ricciuto. Subtask contributions are made as follows: Canopy Processes (A. King, D. Ricciuto, Jiafu Mao), Phenology and disturbance (Jiafu Mao), Nutrient cycling and root function (X. Yang), Methane Modeling (X. Xu), peatland hydrology (X. Shi), surrogate model development using machine learning (D. Lu, D. Ricciuto), ecological forecasting (D. Ricciuto, Y. Luo)

Task 3d – Anthony Walker and postdoc.

Task 4b – Colleen Iversen leads this task developing a path forward for improving the representation of fine roots in models by developing a global root ecology database (FRED) and improving model structure to better reflect empirical knowledge.

Task 4c – Jeff Warren leads this task to experimentally link root function to specific root traits in collaboration with Colleen Iversen and Luke McCormack (Morton Arboretum), and modelers Dan Ricciuto, Dan Lu and Anthony Walker who are considering ways to apply root function to models.

Task 5 – Melanie Mayes provides expertise in soil C cycling, postdoc Junyi Liang in process modeling, and Chris Schadt in microbial ecology, in order to develop improved process understanding to model soil C cycling. Tennessee State University faculty Jianwei Li and University of Tennessee faculty Sindhu Jagadamma provide key modeling and experimental support, respectively. Microbial model testing initially began with incubation experiments and has now evolved into field site testing at MOFLUX, the Harvard forest warming experiment, and two sites in subtropical China.

Task 6 – Lianhong Gu leads activities in measuring and analyzing landscape fluxes of trace gases, water vapor, energy, and SIF. Jeffrey D. Wood (University of Missouri) leads onsite activities in Missouri for the Task. Other contributing staff include Melanie Mayes, Colleen Iversen, Anthony Walker, and Joanne Childs.

Task 8 – Drs. Lianhong Gu, Anthony Walker and Dali Wang support LeafWeb.

Table 5.1 – FY2019 annual person hours by TES SFA Task (160 hours = 1 person month). Hours for some persons change in FY2020 and FY2021.

Personnel Contributing to Tasks	Task 1*	Task 3abc	Task 3d	Task 4b	Task 4c	Task 5	Task 6	Task 8
Scientific Staff								
Griffiths N	900							
Gu L	700						640	160
Hanson P	1600							
Hook L	500							
Iversen C	700			400				
King A		640						
Lu D		180						
Mao J		880						
Mayes M						480		
Norby R	320							
Ricciuto D		600						
Schadt C	320					80		
Shi X		640						
Walker A			730					
Wang D		480						
Warren J	960				360			
Weston D	400							
Yang X		720						
USFS In Kind – Science**	880							
Postdoctoral Staff								
SPRUCE PDs 1,2,3	6552							
MAAT PD			1872					
Soil C PD						1872		
Root Trait PD				1872				
Root Function PD					936			
Technical and Support staff								
Brice D (ORNL)	1500							
Childs J (ORNL)	1500							
Krassovski (ORNL)	900							
Nettles WR (ORNL-MN)	1872							
Phillips (ORNL)	1020				500			
Riggs (ORNL-Inst.)	900							
Wood (Univ. of Missouri)							1872	
USFS In-Kind Technical*	1320							
Estimated Annual Person Hours By Task	22,844	4140	2602	2272	1796	2432	2512	160

*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.

Recent Personnel Actions – Richard J. Norby is transferring to part-time status in the next funding cycle and Gangsheng Wang has left ORNL in FY2018. Past postdoctoral researchers Avni Malhotra and Eric Ward have also moved on to new positions. New postdoctoral researchers are being hired to replace staff that have moved on.

Succession Planning – We use various methods to prepare for and 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. We are currently leveraging some of those internal funds for a new entry or mid-level staff hire to complement current staff. The recruitment process is focused on ecosystem ecology to find a colleague that fits in best with our program; key interests include belowground ecology, physiology, remote sensing and modeling.

Within the TES SFA, task accomplishments and budget management are executed at an overarching level by the Coordinating Investigators with feedback from all Task leads. However, individual 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.

7. 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 infrastructures, including a new field support building (Building 1521), greenhouses, the Joint Institute for Biological Sciences, and renovations in support of molecular ecology. Funding is often allocated annually based on need and general utility to the acquisition of multi-user instrumentation that will benefit multiple users and projects. For example: ORNL acquired a Columbus Instruments Micro-Oxymax Respirometer for lab-scale incubations, and it is capable of detecting CO_2, CH_4, H_2S, H_2, and O_2.

The TES SFA is supported by world-class capabilities at ORNL. The National Leadership Computing Facility provides an open, unclassified resource that we will use to enable breakthrough discoveries 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 (ARM Archive) and the NASA Distributed Active Archive Center for Biogeochemical Dynamics (NASA-DAAC) provide additional expertise in the area of data management. ORNL is also home to the High Flux Isotope Reactor and the Spallation Neutron Source, which we is or can be used to understand physical, chemical, and biological complexity in plant and soil processes.

Other facilities to be used include the Lawrence Livermore National Laboratory – Center for Accelerator Mass Spectrometry (LLNL-CAMS) provides large volume, high precision ^{14}C measurements for ecosystem tracer studies. Pacific Northwest National Laboratory's Environmental Molecular Science Laboratory combines advanced instrumentation such as high-throughput mass spectrometry, advanced microscopy instruments, and NMR instruments with high performance computing.

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Listing of External Collaborations

TES SFA FUNDED EXTERNAL COLLABORATION

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.

Task 1: SPRUCE – 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 assessments 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 (John Latimer), on-site hydrology and porewater biogeochemistry sampling and analysis (Keith Oleheiser), support for on-site operations (Kyle Pearson), and occasional summer student support.

Task 3: Terrestrial Ecosystem and Carbon Cycle Modeling – 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 (Northern Arizona University) for software development and development of data assimilation techniques at the SPRUCE and MOFLUX sites for ecological forecasting. We will establish an unfunded collaboration with Joshua Fisher (JPL) to incorporate new methods for modeling nitrogen cycling into CLM.

Task 6: – MOFLUX – We will contract with Dr. Jeffrey D. Wood at the University of Missouri for full-time management and support of the operation of the MOFLUX tower. Dr. Wood will also manage and execute a variety of science objectives as outline in the description of Task 6 in Section 3.2.

Task 8: LeafWeb – A programmer will be contracted to maintain the web presence of LeafWeb.

INVESTIGATOR-INITIATED SPRUCE COLLABORATIONS (TASK 1)

The following research proposals were developed by the listed investigators and institutions to take advantage of the TES SFA investments in the SPRUCE experiment. 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. **The response of soil carbon storage and microbially mediated carbon turnover to simulated climatic disturbance in a northern peatland forest: revisiting the concept of soil organic matter recalcitrance**. Principal Investigators: Joel E. Kostka, Georgia Institute of Technology & Jeff Chanton, Florida State University (2012-2013)
2. **Understanding the mechanisms underlying heterotrophic CO_2 and CH_4 fluxes in a peatland with deep soil warming and atmospheric CO_2 enrichment**. Principal Investigators: Scott D. Bridgham, University of Oregon & Jason Keller, Chapman University (2013 to present, with renewal pending)
3. **Mercury and sulfur dynamics in the spruce experiment.** Principal Investigators: Brandy Toner and Ed Nater, University of Minnesota & Randy Kolka and Steve Sebestyen, USDA Forest Service MN (2103 to present)
4. **Improving models to predict phenological responses to global change**. Principal Investigator: Andrew D. Richardson, Harvard University (2013 to present)
5. **Lichen community responses to warming.** Principal Investigators: Bruce McCune, Oregon State University, Sarah Jovan, USDA Forest Service OR (2013 to present)
6. **Fungal, bacterial, and archaeal communities mediating C cycling and trace gas flux in peatland ecosystems subject to climate change**. Principal Investigator: Erik Lilleskov, Michigan Technological University with Joint Genome Institute Support (2013 to present)
7. **Toward a predictive understanding of the response of belowground microbial carbon turnover to climate change drivers in a boreal peatland**. Principal Investigators: Joel E. Kostka Georgia

Institute of Technology & Jeffrey P. Chanton, William T. Cooper Florida State University (2014 to present)

8. **Can microbial ecology inform ecosystem level c-n cycling response to climate change?** Principal Investigators: Kirsten Hofmockel, Iowa State University & Erik Hobbie, University of New Hampshire (2014 to present)
9. **Peatland Mercury Cycling in a Changing Climate: A Large-Scale Field Manipulation Study.** Carl Mitchell, University of Toronto - Scarborough (2014-present)
10. **Effects of experimental warming & elevated CO_2 on trace gas emissions from a northern Minnesota black spruce peatland: measurement and modeling**. Principal Investigator: Adrian Finzi, Boston University (2014-present)
11. **Functioning of wetlands as a source of atmospheric methane: a multi-scale and multi-disciplinary approach**. Principal Investigator: Karis McFarlane and Xavier Mayali, Mike Singleton, Ate Visser, Jennifer Pett-Ridge, Brad Esser, Tom Guilderson Lawrence Livermore National Laboratory (2014-present)
12. **Using microbial enzyme decomposition models to study the effects of peat warming and/or CO_2 enrichment on peatland decomposition**. Principal Investigator: Brian H. Hill and Colleen M. Elonen, Terri M. Jicha, Mary F. Moffett US Environmental Protection Agency (2014-present)
13. **The role of the *Sphagnum* microbiome in carbon and nutrient cycling in peatlands - JGI's Community Science Program**. Joel E. Kostka and Gen Glass Georgia Institute of Technology, David Weston Oak Ridge National Laboratory, Erik Lilleskov USDA Forest Service – Houghton, MI, Jon Shaw Duke University, and Susannah Tringe at the Joint Genome Institute (2015-present)
14. **Soil fauna biodiversity sampling at SPRUCE**. Zoë Lindo University of Western Ontario. (starting in 2015)
15. **Monitoring warming and elevated CO_2 induced changes in photosynthetic efficiency via canopy spectral reflectance.** Michael J. Falkowski University of Minnesota, Evan Kane Michigan Technological University, Brian Benscoter Florida Atlantic University, & Randy Kolka US Forest Service (starting in 2015?)
16. **Wood decomposition rates and functional types in a shifting climate.** Jonathan Schilling & Jason Oliver, University of Minnesota, & Randy Kolka US Forest Service.
17. **Microbial growth and carbon and nutrient use partitioning under peatland warming and elevated CO2.** Jessica Gutknecht, University of Minnesota
18. **Modeling porewater stable carbon isotopes of CH_4 and CO_2 to estimate in-situ microbial rates.** Rebecca Neumann, University of Washington
19. **SPRUCE Plot-scale LIDAR**, Nancy F. Glenn, Lucas Spaete, Jake Graham Boise State University
20. **Linking experiments with models.** Principal Investigator: Yiqi Luo, University of Oklahoma.
21. **Quantification of aqueous Fe(II)/Fe(III) fluxes from SPRUCE treatment plots.** Principal investigator: Steven Hall, Iowa State University
22. **Mechanistic modeling of methane cycle at SPRUCE.** Principal investigator: Xiaofeng Xu, San Diego State University
23. **Mast seeding patterns in response to climate change**. Principal Investigator: Jalene M. LaMontagne, DePaul University, (2017-present).
24. **Deep C: Deep soil carbon cycling in a warming world – the molecular marker perspective.** Principal Investigators: Michael W.I. Schmidt and Guido L.B. Wiesenberg, University of Zurich (2017-2020).
25. **Measuring the surface-atmosphere exchange budgets of CO_2 and CH_4 from peatlands using micro-meteorological flux measurements.** Principal Investigator: M. Julian Deventer, University of Minnesota. (2017-present).
26. **Improving models to predict phenological responses to global change.** Principal Investigator: Andrew D. Richardson, Northern Arizona University (2018-continuing).
27. **Nitrogen fixation and its coupling to methane dynamics in the peat moss (*Sphagnum*) phytobiome of northern peatlands.** Principal Investigator: Joel Kostka, Georgia Institute of Technology (2018-present)

APPENDIX A: TES SFA Publications

Published, accepted and in press articles completed since the last triennial review (i.e., March 2015 through September 2018). We have published 166 papers which equals 55 publications per year, or on average 5.2 Publications FTE^{-1} where an FTE is a full-time equivalent research professional.

32 Participants since March 2015 included in the count of FTEs: Andres, Iversen, Griffiths, Gu, Guha, Hanson, Hook, Johnston, King, Kluber, Krassovski, Liang, Liu, Lu, Malhotra, Mao, Mayes, Norby, Painter, Ricciuto, Schadt, Shi, Yang, Walker, Wang D, Wang G, Ward, Warren, Weston, Wood, Wullschleger, and Xu.

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7. Chen M, Griffis TJ, Baker JM, Wood JD, Meyers T, Suyker A (2018a) Simulating the long-term carbon budget across agricultural sites using CLM4-Crop, *Agricultural and Forest Meteorology* 256-257:315-333, doi: 10.1016/j.agrformet.2018.03.012.
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10. Dai H, Ye M, Walker AP, Chen X (2017) A new process sensitivity index to identify important system processes under process model and parametric uncertainty. *Water Resources. Research* 53:2577-3522, doi:10.1002/2016WR019715.
11. Dhiman I, Bilheux HZ, DeCarlo KF, Painter SL, Santodonato LJ, Warren JM (2018) Quantifying root water extraction after drought recovery using sub-mm in situ empirical data. *Plant and Soil* 424:73-89; doi: 10.1007/s11104-017-3408-5.

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APPENDIX B: TES SFA Data Sets and Software

ORNL TES-SFA Data Policy: Archiving, Sharing, and Fair-Use

The open sharing of ORNL TES-SFA data, modeling products, and documentation among researchers, the broader scientific community, and the public is critical to advancing the mission of DOE's Program of Terrestrial Ecosystem Science. The policy is applicable to all TES-SFA participants including ORNL, cooperating independent researchers, and to the users of data products. Data collected by TES-SFA researchers, results of analyses and syntheses of information, and model algorithms and codes will be quality assured, documented, and archived and will be made available to the public. Archived data products are freely available to the public. Users should acknowledge the contribution of the data provider with the citation (with DOI) as provided in the documentation and acknowledge the U.S. DOE Program for Terrestrial Ecosystem Science.

TES-SFA data policies are consistent with the most recent DOE policies for "Public Access to the Results of DOE-Funded Scientific Research"

https://mnspruce.ornl.gov/sites/default/files/DOE_Public_Access%20Plan_FINAL.pdf

and the "Statement on Digital Data Management"

http://science.energy.gov/funding-opportunities/digital-data-management/

A complete copy of our data policy may be found at:

http://tes-sfa.ornl.gov/sites/default/files/TES_SFA_Data_Policy_20130510_Ver_1_approved.pdf

TES SFA Software:

1. The Multi-Assumption Architecture and Testbed (MAAT v1.0) is now open source, available at https://github.com/walkeranthonyp/MAAT.

SPRUCE Public Data Sets:

1. 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, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/SPRUCE.016
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3. Griffiths NA, Hook LA, Hanson PJ (2016D) **SPRUCE S1 Bog and SPRUCE Experiment Location Survey Results, (2015)** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/spruce.015
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9. Hanson PJ (2015D) **SPRUCE S1-Bog and SPRUCE Experiment Aerial Photographs.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/spruce.012
10. Hanson PJ, Brice D, Garten CT, Hook LA, Phillips J, Todd DE (2012D) **SPRUCE S1-Bog Vegetation Allometric and Biomass Data: 2010-2011**. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/spruce.004.
11. Hanson PJ, Phillips JR, Riggs JS, Nettles WR, Todd DE (2014D) **SPRUCE Large-Collar in Situ CO_2 and CH_4 Flux Data for the SPRUCE Experimental Plots**. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/spruce.006.
12. Hanson PJ, Riggs JS, Dorrance C, Nettles WR, Hook LA (2015D) **SPRUCE Environmental Monitoring Data: 2010-2014.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. doi: http://dx.doi.org/10.3334/CDIAC/spruce.001. (Includes recent additions of annual data files.)
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14. Hanson PJ, Riggs JS, Nettles WR, Krassovski MB, Hook LA (2015D) **SPRUCE Deep Peat Heating (DPH) Environmental Data, February 2014 through July 2105.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/spruce.013
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39. Walker AP, Carter KR, Hanson PJ, Nettles WR, Philips JR, Sebestyen SD, Weston DJ (2017D) **SPRUCE S1 Bog *Sphagnum* CO_2 Flux Measurements and Partitioning into Re and GPP**. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/spruce.039
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41. Wilson RM, Tfaily MM, Keller JK, Bridgham SD, Zalman CM, Hanson PJ, Pfeifer-Meister L, Chanton JP, and Kostka JE (2017D) **SPRUCE Geochemical Changes in Porewater from Northern Peatlands at Multiple Depths in Field Samples and over Time in Peat Incubations**. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/spruce.042
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43. Zalman CA, Meade N, Chanton J, Kostka JE, Bridgham SD, Keller JK (2017D) **SPRUCE Methylotrophic Methanogenesis in Sphagnum-dominated Peatland Soils - CH_4 and CO_2 Production in Laboratory Incubations.** Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.25581/spruce.047/1413216

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SPRUCE Project-only Access Data Sets (to be made public following article publications):

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47. Hanson PJ, Phillips JR, Brice DJ, Hook LA (2018Da) **SPRUCE Shrub-Layer Growth Assessments in S1-Bog Plots and SPRUCE Experimental Plots beginning in 2010**. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.25581/spruce.052/1433837
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49. Hanson, PJ, Phillips JR, Riggs JS, Nettles WR (2017D) **SPRUCE Large-Collar in Situ CO_2 and CH_4 Flux Data for the SPRUCE Experimental Plots: Whole-Ecosystem-Warming**. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/spruce.034
50. Hanson PJ, Phillips JR, Wullschleger SD, Nettles WR, Warren JM, Ward EJ (2018Dc) **SPRUCE Tree Growth Assessments of Picea and Larix in S1-Bog Plots and SPRUCE Experimental Plots beginning in 2011**. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.25581/spruce.051/1433836
51. 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, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.25581/spruce.054/1444106
52. McPartland MY, Kane ES, Falkowski MJ, Kolka R, Turetsky MR, Palik B, Montgomery RA (2019D) **SPRUCE: LAI Data from SPRUCE Experimental Plots, 2017-2018.** Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.25581/spruce.058/1491566

Other TES SFA Public Data Sets and Tools:

1. Griffiths NA, Tiegs SD (2016D) **Walker Branch Watershed: Temperature Response of Organic-Matter Decomposition in a Headwater Stream.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/ornlsfa.003
2. Griffiths NA, Johnson LT (2018D) **Walker Branch Watershed: Effect of Dual Nitrogen and Phosphorus Additions on Nutrient Uptake and Saturation Kinetics**, 2011-2012. Carbon Dioxide

Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.25581/ornlsfa.015/1484490

3. Iversen CM, McCormack ML, Powell AS, Blackwood CB, Freschet GT, Kattge J, Roumet C, Stover DB, Soudzilovskaia NA, Valverde-Barrantes OJ, van Bodegom PM, Violle C (2017D) Viewpoints: A global Fine-Root Ecology Database to address belowground challenges in plant ecology. *New Phytologist* 215: 15-26. https://doi.org/10.1111/nph.14486
4. Iversen CM, Powell AS, McCormack ML, Blackwood CB, Freschet GT, Kattge J, Roumet C, Stover DB, Soudzilovskaia NA, Valverde-Barrantes OJ, van Bodegom PM, Violle C (2016D) **Fine-Root Ecology Database (FRED): A Global Collection of Root Trait Data with Coincident Site, Vegetation, Edaphic, and Climatic Data, Version 1.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. Access on-line at: http://dx.doi.org/10.3334/CDIAC/ornlsfa.005.
5. Iversen CM, Powell AS, McCormack ML, Blackwood CB, Freschet GT, Kattge J, Roumet C, Stover DB, Soudzilovskaia NA, Valverde-Barrantes OJ, van Bodegom PM, Violle C (2018D) **Fine-Root Ecology Database (*FRED*): A Global Collection of Root Trait Data with Coincident Site, Vegetation, Edaphic, and Climatic Data, Version 2.** Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. Access on-line at: https://doi.org/10.25581/ornlsfa.012/1417481
6. Jagadamma S, Mayes MA, Steinweg JM, Wang G, Post WM (2014D) **Organic Carbon Sorption and Decomposition in Selected Global Soils.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/ornlsfa.002
7. Kluber LA, Phillips JR, Wang G, Schadt CW, Mayes MA (2017D) **Soil Respiration and Microbial Biomass from Soil Incubations with ^{13}C Labeled Additions.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. http://dx.doi.org/10.3334/CDIAC/ornlsfa.010
8. **LeafWeb.** LeafWeb is a TES SFA-funded web-based tool for the automated numerical analyses of leaf gas exchange measurements. LeafWeb is a Service-in-Exchange-for-Data-Sharing (SEEDS) Project. With the approval of the user, the data LeafWeb receives are preserved and added to a global database of biochemical, physiological, and biophysical properties of single leaves to support studies of plant functions and terrestrial carbon cycle modeling. Access LeafWeb at http://leafweb.ornl.gov/.
9. **Missouri Ozark Flux (MOFLUX) Measurement Data.** TES SFA-funded site characterization and flux measurement data, starting in 2004 and continuing, are archived by the AmeriFlux Program. Data and can be accessed at http://ameriflux.ornl.gov/fullsiteinfo.php?sid=64.
10. Mulholland PJ, Griffiths NA (2016D) **Walker Branch Watershed: Hourly, Daily, and Annual Precipitation**. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/ornlsfa.006
11. Mulholland PJ, Griffiths NA (2016D) **Walker Branch Watershed: 15-minute and Daily Stream Discharge and Annual Runoff**. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/ornlsfa.007
12. Mulholland PJ, Griffiths NA (2016D) **Walker Branch Watershed: Daily Climate and Soil Temperature Data**. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/ornlsfa.008
13. Mulholland PJ, Griffiths NA (2016D) **Walker Branch Watershed: Weekly Stream Water Chemistry**. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/ornlsfa.009

14. Pallardy, SG, Gu, L, Wood, JD, Hosman, KP, Sun, Y, Hook, L. (2017D) **Predawn Leaf Water Potential of Oak-Hickory Forest at Missouri Ozark (MOFLUX) Site: 2004-2017**. United States: N. p., 2018. http://dx.doi.org/10.3334/CDIAC/ornlsfa.004
15. Shi X, Wang D (2014D) **GSOD Based Daily Global Mean Surface Temperature and Mean Sea Level Air Pressure** (1982-2011)", doi: 10.15149/1130373.
16. **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.
17. **Walker Branch Watershed Long-Term Data Archive.** Repository for TES SFA-funded data collections of long-term hydrology, stream ecology, chemistry, and biogeochemistry measurements and research. Data can be accessed at http://walkerbranch.ornl.gov/.
18. Warren JM, Iversen CM, Garten Jr CT, Norby RJ, Childs J, Brice D, Evans RM, Gu L, Thornton P, Weston DJ (2013D) PiTS-1: **Carbon Partitioning in Loblolly Pine after ^{13}C Labeling and Shade Treatments**. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/ornlsfa.001.

TES SFA Data Sets in the NASA Oak Ridge National Laboratory Distributed Active Archive Center (ORNL DAAC):

1. Barr AG, Ricciuto DM, Schaefer K, Richardson A, Agarwal D, Thornton PE, Davis K, Jackson B, Cook RB, Hollinger DY, van Ingen C, Amiro B, Andrews A, Arain MA, Baldocchi D, Black TA, Bolstad P, Curtis P, Desai A, Dragoni D, Flanagan L, Gu L, Katul G, Law BE, Lafleur P, Margolis H, Matamala R, Meyers T, McCaughey H, Monson R, Munger JW, Oechel W, Oren R, Roulet N, Torn M, Verma S (2013) **NACP Site: Tower Meteorology, Flux Observations with Uncertainty, and Ancillary Data.** Data set. Available on-line [http://daac.ornl.gov] from Oak Ridge National Laboratory Distributed Active Archive Center, Oak Ridge, Tennessee, USA http://dx.doi.org/10.3334/ORNLDAAC/1178.
2. Huntzinger DN, Schwalm CR, Wei Y, Cook RB, Michalak AM, Schaefer K, Jacobson AR, Arain MA, Ciais P, Fisher JB, Hayes DJ, Huang M, Huang S, Ito A, Jain AK, Lei H, Lu C, Maignan F, Mao J, Parazoo N, Peng C, Peng S, Poulter B, Ricciuto DM, Tian H, Shi X, Wang W, Zeng N, Zhao F, Zhu Q, Yang J, Tao B (2016) **NACP MsTMIP: Global 0.5-deg Terrestrial Biosphere Model Outputs (version 1) in Standard Format.** ORNL DAAC, Oak Ridge, Tennessee, USA, https://doi.org/10.3334/ORNLDAAC/1225.
3. Ricciuto DM, Schaefer K, Thornton PE, Davis K, Cook RB, Liu S, Anderson R, Arain MA, Baker I, Chen JM, Dietze M, Grant R, Izaurralde C, Jain AK, King AW, Kucharik C, Liu S, Lokupitiya E, Luo Y, Peng C, Poulter B, Price D, Riley W, Sahoo A, Tian H, Tonitto C, Verbeeck H (2013) **NACP Site: Terrestrial Biosphere Model and Aggregated Flux Data in Standard Format.** Data set. Available on-line [http://daac.ornl.gov] from Oak Ridge National Laboratory Distributed Active Archive Center, Oak Ridge, Tennessee, USA. http://dx.doi.org/10.3334/ORNLDAAC/1183.
4. Ricciuto DM, Schaefer K, Thornton PE, Cook RB, Anderson R, Arain MA, Baker I, Chen JM, Dietze M, Grant R, Izaurralde C, Jain AK, King AW, Kucharik C, Liu S, Lokupitiya E, Luo Y, Peng C, Poulter B, Price D, Riley W, Sahoo A, Tian H, Tonitto C, Verbeeck H (2013) **NACP Site: Terrestrial Biosphere Model Output Data in Original Format.** Data set. Available on-line [http://daac.ornl.gov] from Oak Ridge National Laboratory Distributed Active Archive Center, Oak Ridge, Tennessee, USA. http://dx.doi.org/10.3334/ORNLDAAC/1192.
5. Wei Y, Hayes DJ, Thornton MM, Post WM, Cook RB, Thornton PE, Jacobson A, Huntzinger DN, West TO, Heath LS, McConkey B, Stinson G, Kurz W, de Jong B, Baker I, Chen J, Chevallier F, Hoffman F, Jain A, Lokupitiya R, McGuire DA, Michalak A, Moisen GG, Neilson RP, Peylin P,

Potter C, Poulter B, Price D, Randerson J, Rodenbeck C, Tian H, Tomelleri E, van der Werf G, Viovy N, Xiao J, Zeng N, Zhao M (2013) **NACP Regional: National Greenhouse Gas Inventories and Aggregated Gridded Model Data.** Data set. Available on-line [http://daac.ornl.gov] from Oak Ridge National Laboratory Distributed Active Archive Center, Oak Ridge, Tennessee, USA http://dx.doi.org/10.3334/ORNLDAAC/1179.

6. Wei Y, Liu S, Huntzinger D, Michalak AM, Viovy N, Post WM, Schwalm C, Schaefer K, Jacobson AR, Lu C, Tian H, Ricciuto DM, Cook RB, Mao J, Shi X (2014) **NACP MsTMIP: Global and North American Driver Data for Multi-Model Intercomparison.** Data set. Available on-line [http://daac.ornl.gov] from Oak Ridge National Laboratory Distributed Active Archive Center, Oak Ridge, Tennessee, USA. http://dx.doi.org/10.3334/ORNLDAAC/1220.
7. Yang X, Post WM, Thornton PE, Jain A (2014) **Global Gridded Soil Phosphorus Distribution Maps at 0.5-degree Resolution.** Data set. Available on-line [http://daac.ornl.gov] from Oak Ridge National Laboratory Distributed Active Archive Center, Oak Ridge, Tennessee, USA. http://dx.doi.org/10.3334/ORNLDAAC/1223.
8. Yang X, Post WM, Thornton PE, Jain A (2014) **A Global Database of Soil Phosphorus Compiled from Studies Using Hedley Fractionation.** Data set. Available on-line [http://daac.ornl.gov] from Oak Ridge National Laboratory Distributed Active Archive Center, Oak Ridge, Tennessee, USA. http://dx.doi.org/10.3334/ORNLDAAC/1230.

TES SFA Task 7 Data Sets:

1. Andres RJ, Boden TA, Marland G (2013) **Annual Fossil-Fuel CO_2 Emissions: Mass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1751-2010**. ORNL/CDIAC, electronic database. doi 10.3334/CDIAC/ffe.ndp058.2013.
2. Andres RJ, Boden TA, Marland G (2013) **Monthly Fossil-Fuel CO_2 Emissions: Mass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1950-2010**. ORNL/CDIAC, electronic database. doi 10.3334/CDIAC/ffe.MonthlyMass.2013.
3. Andres RJ, Boden TA, Marland G (2013) **Annual Fossil-Fuel CO_2 Emissions: Isomass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1751-2010**. ORNL/CDIAC, electronic database. doi 10.3334/CDIAC/ffe.AnnualIsomass.2013.
4. Andres RJ, Boden TA, Marland G (2013) **Monthly Fossil-Fuel CO_2 Emissions: Isomass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1950-2010**. ORNL/CDIAC, electronic database. doi 10.3334/CDIAC/ffe.MonthlyIsomass.2013.
5. Andres RJ, Boden TA, Marland G (2013) **Annual Fossil-Fuel CO_2 Emissions: Global Stable Carbon Isotopic Signature, 1751-2010**. ORNL/CDIAC, electronic database. doi 10.3334/CDIAC/ffe.db1013.2013.
6. Boden TA, Marland G, Andres RJ (2013) **Global, Regional, and National Fossil-Fuel CO_2 Emissions.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. doi 10.3334/CDIAC/00001_V2013.
7. Andres RJ, Boden TA, Marland G (2013) **Annual Fossil-Fuel CO_2 Emissions: Mass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1751-2009.** ORNL/CDIAC, electronic database. doi 10.3334/CDIAC/ffe.ndp058.2012.
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9. Andres RJ, Boden TA, Marland G (2013) **Annual Fossil-Fuel CO_2 Emissions: Isomass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1751-2009.** ORNL/CDIAC, electronic database. doi 10.3334/CDIAC/ffe.AnnualIsomass.2012.
10. Andres RJ, Boden TA, Marland G (2013) **Monthly Fossil-Fuel CO_2 Emissions: Isomass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1950-2009.** ORNL/CDIAC, electronic database. doi 10.3334/CDIAC/ffe.MonthlyIsomass.2012.

11. Andres RJ, Boden TA, Marland G (2013) **Annual Fossil-Fuel CO_2 Emissions: Global Stable Carbon Isotopic Signature, 1751-2009.** ORNL/CDIAC, electronic database. doi: 10.3334/CDIAC/ffe.db1013.2012.
12. Andres RJ, Boden TA (2016) **Annual Fossil-Fuel CO_2 Emissions: Uncertainty of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1751-2013**. ORNL/CDIAC, electronic database. doi: 10.3334/CDIAC/ffe.AnnualUncertainty.2016.
13. Andres RJ, Boden TA (2016) **Monthly Fossil-Fuel CO_2 Emissions: Uncertainty of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1751-2013.** ORNL/CDIAC, electronic database. doi: 10.3334/CDIAC/ffe.MonthlyUncertainty.2016.
14. Andres RJ, Boden TA, Marland G (2016) **Annual Fossil-Fuel CO_2 Emissions: Mass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1751-2013**. ORNL/CDIAC, electronic database. doi:10.3334/CDIAC/ffe.ndp058.2016.
15. Andres RJ, Boden TA, Marland G (2016) **Monthly Fossil-Fuel CO_2 Emissions: Mass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1950-2013.** ORNL/CDIAC, electronic database. doi:10.3334/CDIAC/ffe.MonthlyMass.2016.
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17. Andres RJ, Boden TA, Marland G (2016) **Monthly Fossil-Fuel CO_2 Emissions: Isomass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1950-2013**. ORNL/CDIAC, electronic database. doi:10.3334/CDIAC/ffe.MonthlyIsomass.2016.
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20. Andres RJ, Boden TA, Marland G (2015) **Monthly Fossil-Fuel CO_2 Emissions: Mass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1950-2011**. ORNL/CDIAC, electronic database. doi:10.3334/CDIAC/ffe.MonthlyMass.2015.
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22. Andres RJ, Boden TA, Marland G (2015) **Monthly Fossil-Fuel CO_2 Emissions: Isomass of Emissions Gridded by One Degree Latitude by One Degree Longitude, 1950-2011**. ORNL/CDIAC, electronic database. doi:10.3334/CDIAC/ffe.MonthlyIsomass.2015.
23. Andres RJ, Boden TA, Marland G (2015) **Annual Fossil-Fuel CO_2 Emissions: Global Stable Carbon Isotopic Signature, 1751-2011.** ORNL/CDIAC, electronic database. doi:10.3334/CDIAC/ffe.db1013.2015.
24. Boden TA, Andres RJ, Marland G (2012) **Global, Regional, and National Fossil-Fuel CO_2 Emissions: 1751-2009.** ORNL/CDIAC, electronic database. doi 10.3334/CDIAC/00001_V2012.
25. Boden TA, Andres RJ, Marland G (2015) **Global, Regional, and National Fossil-Fuel CO_2 Emissions: 1751-2011.** ORNL/CDIAC, electronic database. doi:10.3334/CDIAC/00001_V2015.
26. Boden TA, Andres RJ, Marland G (2016) **Global, Regional, and National Fossil-Fuel CO_2 Emissions: 1751-2013. ORNL/CDIAC, electronic database.** doi:10.3334/CDIAC/00001 V2016.
27. Global Carbon Project (2013) **Global Carbon Atlas**. http://www.globalcarbonatlas.org.
28. Global Carbon Project (2015) **Global Carbon Atlas.** http://www.globalcarbonatlas.org.
29. Maksyutov S, Takagi H, Belikov DA, Saeki T, Zhuravlev R, Ganshin A, Lukyanov A, Yoshida Y, Oshchepkov S, Bril A, Saito M, Oda T, Valsala VK, Saito R, Andres RJ, Conway T, Tans P, Yokota T (2012) **Estimation of regional surface CO_2 fluxes with GOSAT observations using two inverse modeling approaches.** Proc. SPIE 8529, Remote Sensing and Modeling of the Atmosphere, Oceans, and Interactions IV, 85290G. doi:10.1117/12.979664.

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APPENDIX C: Progress-to-Date Deliverables Tables

These tables not the status of past proposed deliverables. They are derived from the 2015 proposal and any updates by Task noted in subsequent annual reports for FY2016, FY2017 and FY2018 (add URL for reports).

Table C.1 – Deliverables for SPRUCE Task 1

Date	Deliverable	Status
Remaining FY2015 Deliverables		
March 2015	Submission of manuscript describing vertical pore water profiles in the S1 Bog.	Completed –Griffiths and Sebestyen 2016
March 2015	Submission of baseline SPRUCE water relations manuscripts	Expanded to include initial responses - in progress for 2019 (Warren *et al.*)
June 2015	Full deployment of remaining SPRUCE sensors in all treatment plots	Completed
Sep 2015	Manuscript on peat age and historical C accumulation from ^{14}C data.	Complete – McFarlane *et al.* 2018
Sep 2015	Initial whole-ecosystem response measurements for all tasks	Completed
Sep 2015	Submit High-profile paper(s) describing results from deep peat heating	Completed – Wilson *et al.* 2016
Sep 2015	A manuscript on a 2-year preliminary investigation of fine-root dynamics in the S1 Bog is currently being prepared	Completed – Iversen *et al.* 2018
FY 2016 Deliverables		
Oct 2015	Recruit strong plant physiologist / ecophysiologist post docs	Complete x2
Jan 2016	Whole-Ecosystem Warming Technique Paper	Completed – Hanson *et al.* 2017
Jan 2016	Manuscript detailing spatial variation in porewater profiles in S1	Completed –Griffiths and Sebestyen 2016
Oct 2016	Full season of task measurements under whole-ecosystem warming	Completed
Oct 2016	Manuscript on root-fungal interactions using AMR technology	Incomplete pending image analysis
FY 2017 Deliverables		
January 2017	Draft manuscript comparing porewater chemistry across peatlands (S1 Bog, S2-Bog, Bog Lake Fen).	Paper in progress for 2019
Aug 2017	Submission of baseline SPRUCE water relations manuscript. Submit sap flow and water potential data to TES SFA data archive.	Paper in progress for 2019
Oct 2017	Full season of task measurements under whole-ecosystem warming	Completed
Sept 2017	Submission of baseline SPRUCE carbon physiology MODEX manuscript for all major woody species. Submit A-Ci and A-Q data to TES SFA data archive.	Completed – Jensen *et al.* 2018, Jensen et al (in press)
Sept 2017	Submission of SPRUCE manuscript describing initial response of photosynthesis and respiration of *Picea mariana* and *Larix laricina* under whole-ecosystem warming and elevated [CO_2], and TES SFA data archive.	Paper in progress for 2019 - Dusenge *et al.*
Dec 2017	Manuscript on initial rhizosphere responses to warming and elevated [CO_2]	Incomplete pending image analysis
FY2018 Deliverables		
Oct 2017	Submission of SPRUCE manuscript describing initial response of photosynthesis and respiration of *Chamaedaphne calyculata* and *Rhododendron groenlandicum* under whole-ecosystem warming and elevated [CO_2], and TES SFA data archive.	Paper in progress for 2019 (Ward *et al.*)

Summer 2018	Complete draft manuscript on the moss decomposition study.	Litterbag retrieval in 2019 Manuscript in 2019
Jan 2018	Based on prior results, plan physiological campaigns for 2018	Completed
Oct 2018	Full season of task measurements under whole-ecosystem warming	Completed

Table C.2 – Walker Branch Task 2 Deliverables.

Date	Deliverable	Status
Summer 2015	Submit paper on uncertainty in nutrient uptake kinetics.	Completed – Brooks *et al.* 2017
Fall 2015	Draft paper on dual N and P uptake in streams.	Completed – Griffiths and Johnson 2018
Fall 2016	Complete development of stream metabolism model and analyze various climate change scenarios.	Shifted to paper summarizing long-term metabolism dataset. Paper in progress for 2018.
Fall 2017	Manuscript on effects of climate change on stream C cycling.	Shifted to paper summarizing long-term metabolism dataset. Paper in progress for 2018.

Table C.3 – Task 3a Deliverables

Date	Deliverable	Status
2016	Document CLM_SPRUCE with improved microbial model and simulations from multi-model SPRUCE ensemble; Prototype ecological forecasting system at SPRUCE	Ma et al. 2017
2017	Completion of CLM_SPRUCE model with improved *Sphagnum* and photosynthesis, evaluated with initial treatment data; Complete 3D PFLOTRAN simulations for supersites	Completed – Walker *et al.* 2017
2018	- Document ecological forecasting system - Deliver model to E3SM	Complete In progress

Table C.4 – Task 3b Deliverables

Date	Deliverable	Status
2016	Collection and compilation of the SIF, NDVI, ET, biomass, SR and river flow data; the online and offline D&A methodology testing and development	Planned
2017	The CLM-SIF module validation; experimental design and ensemble model simulations; D&A study of the NDVI and river flow	Planned
2018	Finish the global optimization framework, and produce the global GPP time series; D&A study of the global GPP	Planned

Table C.5 – Task 3c Deliverables

Date	Deliverable	Status
FY2016	Functional testing for "root" modules and integration with UQ methods	Planned
FY2017	Functional testing for ecosystem dynamics and hydrological components and module structure UQ development	Planned
FY2018	Regional CLM functional testing and multiscale UQ with observational datasets	Underway

Table C.6 – Task 4a PiTS Future Deliverables

Date	Deliverable	Status
Oct 2016	Finish existing PiTS data and model analysis and finalize publications and archived datasets	In progress for 2019 (Warren *et al.*)
Oct 2016	Levering PiTS results, assess if additional partitioning-specific MODEX activities should be established	Underway (Walker, Iversen, Warren)
Future	Initiate PiTS Phase II activities, as warranted	Underway (Walker, Iversen, Warren)

Table C.7 – Task 4b Root Trait Deliverables

Date	Deliverable	Status
Jan 2016	Fine-root ecology database (FRED) – Accessible to the broader community of root and rhizosphere ecologists and modelers through TES SFA and TRY.	**Complete**
Sep 2016	Synthesize and highlight global patterns and trends in root traits, and root trait variation within and among model-defined plant functional types.	Planned
April 2017	Break-out session hosted at annual DOE PI meeting to continue engagement of broader community and leverage above- and belowground trait linkages and data collected in other DOE-funded efforts (SPRUCE, NGEEs, PiTS, FACE, AmeriFlux)	Planned
Sep 2017	Sensitivity analyses linking PFT root parameterizations with ecosystem function using FRED and CRM.	Planned
Sep 2018	New model structure that includes an additional fine-root pool. Fine roots will be divided into absorptive and transport fine roots, and trait-function relationships will be overlaid on new pools using synergy of Tasks 4b and 4c. A new round of sensitivity analyses using FRED and CRM will be conducted based on new model structure.	Planned

Table C.8 – Task 4c Root Function Deliverables

Date	Deliverable	Status
Dec 2015	Leverage existing data sets (e.g., FACE water content, water use, root distribution) and apply root uptake models for uncertainty and sensitivity analyses	Deferred to Root Traits task, new MAAT task, (Ricciuto *et al.* in prep)
March 2016	Based on data/modeling results, define scale of interest/scope of task	Completed
July 2016	Recruit strong root physiology/hydraulics post doc	Funds redirected to modeling (Painter, King) and new MS student
Oct 2016	Begin directed laboratory and field-based experiments to quantify water and nutrient uptake kinetics by root functional classes in response to environmental conditions as justified by model uncertainty and sensitivity analyses	Completed, with focus narrowed to water uptake rates linked to root traits, drought
Oct 2017	Begin deployment of Rhizosphere Ecology Laboratory for integrative assessment of belowground dynamics	Based on Funding
Oct 2018	Manuscript publication of water and nutrient uptake kinetics by root functional classes	Dhiman *et al.* 2017, DeCarlo *et al.* in prep

Table C.9 – Task 5 Soil Carbon Deliverables

Date	Deliverable	Status
05/17	Complete temperate grassland v forest, short-term, long-term isotope study	Completed; Kluber *et al.* 2017D
03/17	Incorporate soil moisture effects and test against MOFLUX field scale experimental data in ELM and MEND model	Completed; Liang *et al.* GMD manuscript
12/17	Model temperate grassland v forest short-term, long-term isotope study using MEND	Ongoing
5/18	Complete lab-scale moisture – texture sensitivity experiments	Ongoing
9/18	Incorporate flexible C:N ratio into MEND	Completed
new	Modeling soil carbon loss in response to intensified soil moisture extremes using MEND and ELM	Ongoing

Table C.10 – Task 6 MOFLUX *et al.* Deliverables

Date	Deliverable	Status
Mar 2016	Submit 2015 MOFLUX data to AmeriFlux	**Completed**
Jun-Jul 2016	Install new instruments for expanded process work.	**Completed**

Summer 2016	Measure vadose Zone Soil Water, Shallow Groundwater Flow	Scaled back due to the leave of Univ Missouri PI. Shallow groundwater flow not measured.
March 2017	Submit 2016 MOFLUX data to AmeriFlux	Completed
Summer 2017	Quantify relationship between SIF- and EC-based GPP estimates at two contrast ecosystems	Completed
Summer 2017	Datasets for 2017 solar eclipse study (added task)	High-frequency turbulence flux data collected from more than 20 AmeriFlux sites
Dec 2017	Report on species-specific relationships between root morphometrics and nutrient content	Incomplete; pending image analyses
Dec 2017	Development of new SIF instrumentation (added task)	Completed, patent filed
Dec 2017	Development of SIF instrumentation control software (added task)	Completed, copyright filed
March 2018	Submit 2017 MOFLUX data to AmeriFlux	**Completed**
2018	Funding-dependent installation of EC instrument systems at the S1 Bog	ongoing
Summer 2018	Report on the potential EC application in large open-top enclosures	On-going
Sep 2018	Report on spatial heterogeneity of soil moisture, root growth and soil efflux	Manuscript in review
Oct 2018	Effects of 2017 solar eclipse on terrestrial ecosystem fluxes (added task)	One manuscript submitted
Oct 2018	Description of a novel SIF instrumentation (added task)	Manuscript in press

Table C.11 – Future Task 7 Deliverables

Date	Deliverable	Status
FY 2016-18	Create monthly emission inventories at the scale of states and months at a global scale	Completed 2016
FY 2016-18	Create annual and monthly distributions of emissions	Completed 2016
FY 2016	Explore and publish uncertainty estimates associated with annual emissions	Andres et al. 2016
FY 2016-18	Create closer fossil fuel-terrestrial biosphere ties	King et al. in progress

Table C.12 – Task 8 LeafWeb Deliverables

Date	Deliverable	Status
FY 2016	Parallelize LeafWeb background processing algorithms so that multiple users can be served and multiple datasets can be analyzed simultaneously	Completed
FY 2016	Transfer the LeafWeb system from CDK to ORNL’s supercomputing clusters	Completed
FY 2017	Enable joint A/Ci, A/light and leaf fluorescence analyses	Completed
FY 2017	Enable analyses for C4 species	Completed
FY 2018	Redesign the LeafWeb user interface to accommodate the added functionalities	Completed

APPENDIX D: 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 Program of Terrestrial Ecosystem Science. Active data sharing facilitates delivery of SFA products to our stakeholders.

Data Types and Sources

The SPRUCE experiment is the key component of the SFA. SPRUCE has implemented an experimental platform for the long-term observation of the mechanisms controlling the vulnerability of organisms, ecosystems, and ecosystem functions to increases in temperature and exposure to eCO_2 treatments within the northern peatland high-carbon ecosystem. Data acquisition and real time display of SPRUCE experimental plot monitoring data are fully implemented. More than 1,100 sensors are deployed across 16 instrumented plots. Data types include: the automated environmental data collected by in situ sensors; manual and automated measurements of responses of vegetation communities, species, and individual plants -- both above and belowground; characterization of the physical and chemical properties of soil/peat; characterization of experimental plot hydrology, water quality and carbon constituents; innovative characterization of the microbial community, and measurements of soil gas fluxes. Also included are model development products – input drivers, codes, and outputs.

Ongoing TES SFA tasks generate a diverse collection of data products including: the long-term monitoring of landscape flux measurements at the Missouri flux (MOFLUX) site and supporting site environmental and vegetation community data; the extensive literature compilation of plant root traits and corresponding environmental data (i.e., FRED, V2); and mechanistic studies and modeling of soil C-cycles (i.e., MEND).

Content and Format

The TES SFA 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. The TES-SFA registers DOIs for all data products using the OSTI (Office of Scientific and Technical Information) E-Link System. Comprehensive metadata can be entered that will facilitate the transfer of metadata, documentation, and data to the DOE's Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) archive.

The TES SFA is implementing a new set of data management resources to support project-level data sharing, search, and archiving for SPRUCE and TES-SFA tasks. The new tools leverage existing DOE investments in data management and expertise from across ORNL DOE BER projects to provide enhanced data management support. The ORNL Online Metadata Editor (OME) is a Web-based tool that allows users to create and maintain robust metadata stored as eXtensible Markup Language (XML) files, the preferred metadata output format, with output that conforms to and satisfies widely-adopted metadata standards – specifically Federal Geospatial Data Committee (FGDC) and ISO11915 metadata standards. The OME captures information about the investigators specific task, parameters, time periods, quality assurance, and locations associated with the data. Users may upload data products plus additional documentation using the OME. The preferred non-proprietary file format for pubic 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.

Sharing and Preservation

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 in a timely manner such that data will be available for use by project scientists and collaborators and, following publication, the public, thru the SPRUCE (https://mnspruce.ornl.gov) and TES SFA (https://tes-sfa.ornl.gov) websites.

Code Sharing

Public release of SPRUCE-specific E3SM code will be 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 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. For reproducibility, publications using model output will include information about the specific release or development branch 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.

Timeline

The diverse set measurements vary greatly in their temporal measurement frequency, ranging from, for example, 30-minute averages of 1-minute 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 (VDV); 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, etc., 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:

Level 1 Quality 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.

Level 2 Quality **i**ndicates 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 as a result 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, etc. These products should be submitted to the archive for long-term storage but will not be shared.

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 that are displayed in charts, figures, images, etc. In addition, the underlying digital research data used to generate the displayed data will be made as accessible as possible.** In this context, research data is defined as the data required to validate the published results and modeling codes, inputs, and output for reproducibility of results. The research data products, as accessible through the TES SFA data archive, should be cited in the publication with a registered DOI.

Data Fair Use Policy:

The data provided for public access are freely available and were furnished by the SPRUCE Team at ORNL, the U.S. Forest Service, and cooperating independent researchers who encourage their use. Users of these data products and project information should do the following:

- 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.
- 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, (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: SPRUCE Experiment, ORNL, ORNL TES SFA, U.S. DOE Office of Science, Marcell Experimental Forest, Northern Research Station, U.S. 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 Archive

At the conclusion of the SPRUCE and TES-SFA projects, or per an agreed upon schedule, research data will be provided to DOE's Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE). ESS-DIVE will archive and publicly share digital research data obtained from observational, experimental, and modeling research that is funded by the DOE's Office of Science under its Terrestrial Ecosystem Science (TES) programs within the Environmental Systems Science (ESS) activity.

The ORNL TES SFA agrees to the ESS-DIVE data contributor license and specifies that research data may be served to the public with Creative Commons Attribution 4.0 data usage rights. Metadata will always be available under Creative Commons Public Domain data usage rights. 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.

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. Stored data are protected from loss due to system failures or inadvertent deletion by routine and tested backup protocols.

Rationale

The open sharing of all data and results from TES SFA research and modeling tasks among researchers, the broader scientific community, and the public is critical to advancing the mission of DOE's Program of Terrestrial Ecosystem Science. Active data sharing facilitates delivery of SFA products to our stakeholders. TES SFA researchers continue to develop and deploy the data systems, repositories, tools, and integration capabilities needed for the collection, QA, 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 U.S. 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.*

APPENDIX E: AmeriFlux Letter of Support

BERKELEY LAB Lawrence Berkeley National Laboratory

EARTH & ENVIRONMENTAL SCIENCES

Dr. Margaret S. Torn
Senior Scientist and Senior Program Advisor
Climate & Ecosystem Sciences Division, Berkeley Lab
Adjunct Professor, ERG, UC Berkeley
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January 31, 2019

Lianhong Gu
Environmental Sciences Division and Climate Change Science Institute
Oak Ridge National Laboratory
Oak Ridge, TN 37381

Dear Dr. Gu,

I am writing to express the value of continued operation of the Missouri Ozark AmeriFlux (MOFLUX) site from the perspective of the AmeriFlux Management Project (AMP), which I lead.

The MOFLUX site plays a valuable role in the AmeriFlux Network in three ways. First, MOFLUX is currently the only site in the Network that is located in the prairie-forest transition. This is an important geographic and ecological biome/climate transition in North America, and MOFLUX occupies the western edge of the deciduous forests, providing one boundary for the flux-tower climate gradient that is capped in the north by the Wisconsin and Michigan sites. Second, we are glad to have MOFLUX be part of the long-term, high quality core sites, because of its location and the rich, well-curated data that the site and PI produce. We consider MOFLUX an independently funded (i.e., not AMP-funded) core site because they make comprehensive observations and upload their data promptly to the publically available archive. One measure of MOFLUX data quality is the fact that the site has been included in nearly all AmeriFlux synthesis studies that include forests. Finally, one of the big pushes we are making in AmeriFlux for the next few years is to get more sites to study belowground processes. The other is to promote the use of emerging techniques to quantify gross primary production. The MOFLUX program to link belowground processes to canopy functions, and to use solar-induced fluorescence to partition GPP/respiration have been at the vanguard of these efforts.

These are the key reasons why I see MOFLUX as a valuable site in the network. I look forward to continuing to work with you and hearing about MOFLUX progress in the future.

Sincerely yours,

Margaret Torn

Margaret Torn
Lead, AmeriFlux Management Project

Lawrence Berkeley National Laboratory

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APPENDIX F: SPRUCE Treatment Performance Data

Table F1 shows the achieved whole-ecosystem warming treatments and eCO_2 treatments for 2016, 2017 and the 2018 calendar years. Treatment data are archived in the Hanson *et al.* (2016D) data set.

Table F1. Mean annual air and soil temperatures and CO_2 concentrations by SPRUCE plots and all years of whole-ecosystem warming and the percent of time that temperature (half-hour 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.

Plot #s	**Target Temperature Differential**	**Mean Annual Air Temperature at +2 m and [% of Days within 0.5°C of target differential for half hour data]**	**Mean Annual Soil Temperature at -2 m and [% of Days within 0.5°C of target differential for half hour 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	(Δ°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, 401	-----
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], 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]

*Growing seasons were DOY 168 to 321 for 2016; DOY 98 to 312 for 2017; and DOY 93 to 309 for 2018. Daylight hours were 0800 through 1800.

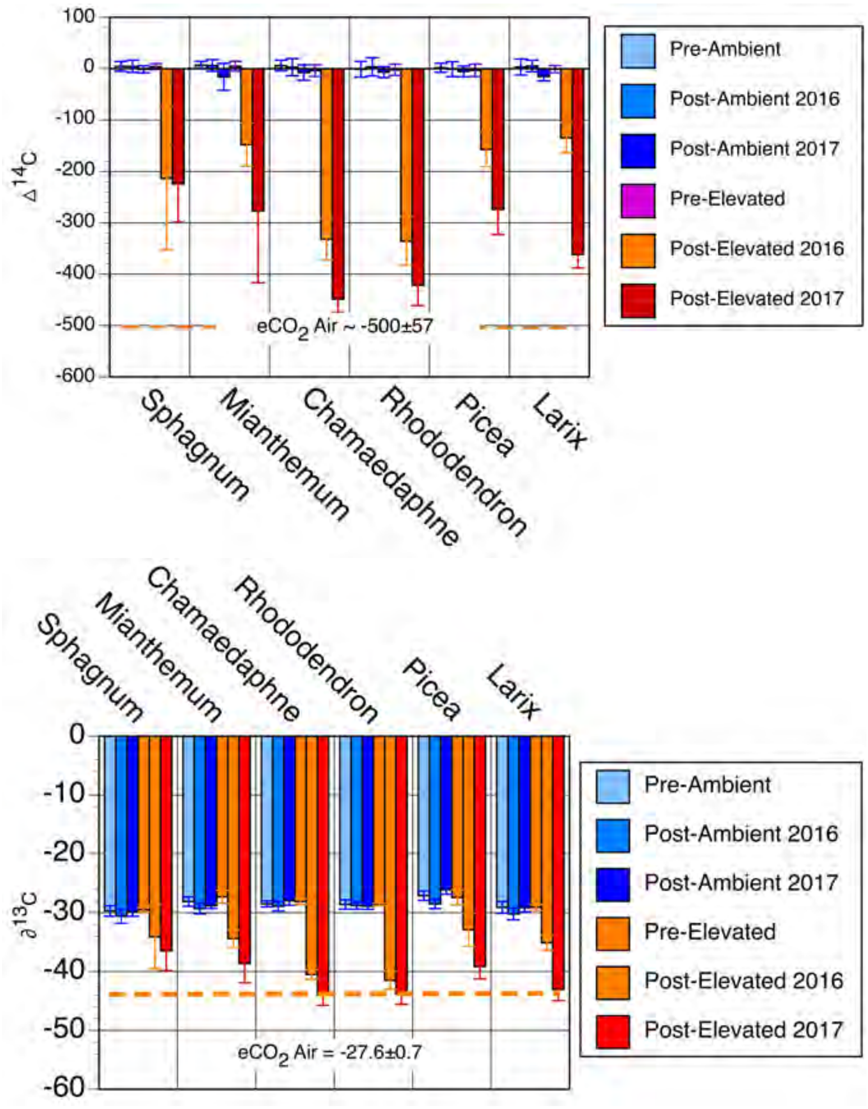

Fig. F1. Isotopic signatures for ^{14}C (upper) and ^{13}C (lower) new aboveground foliar tissue growth across plots and eCO_2 treatments.