# FY2021 PROGRESS REPORT OAK RIDGE NATIONAL LABORATORY'S TERRESTRIAL ECOSYSTEM SCIENCE — SCIENTIFIC FOCUS AREA

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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 subannual 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 Environments (SPRUCE) experiment that tests multiple levels of warming at ambient and elevated CO<sub>2</sub> 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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#### 1.0 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 Earth and Environmental Systems Sciences Division (EESSD) as outlined in the most recent Strategic Plan (US DOE 2018). The TES SFA addresses all five EESSD 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 and research results with the broader scientific communities.

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

The TES SFA is guided by the vision that sensitivities, uncertainties and recognized weaknesses of ESM predictions inform observations, laboratory and field experiments and the development of ecosystem process modeling. In turn, predictive understanding and findings from the field and laboratory and improved process modeling are incorporated, with the associated uncertainties, into ESMs as explicitly and expeditiously as possible. TES SFA research integrates laboratory and field experiments across a range of scales, observations from landscape greenhouse gas flux, field sites and remote sensing, and multiple process models. This integration is realized through the development and application of empirically-driven process model development, model-data fusion, model-data inter-comparison, model performance benchmarking, and uncertainty characterization and quantification. The integration occurs within the context of predictive Earth System modeling and within a framework of Earth system simulation using high-performance leadership-class computing.

TES SFA research is an iterative process (Fig. 1) translating mechanisms to ecosystem models with a quantitative understanding of model uncertainties. This process 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 predictions on decadal and century timescales. New measurements and experiments are employed to obtain new knowledge required to characterize, quantify, and reduce these uncertainties.

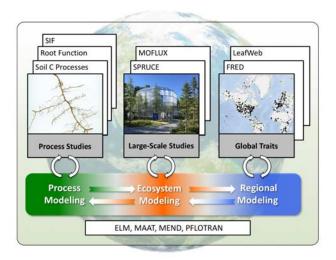


Fig. 1. Diagram of the TES SFA research philosophy and flow illustrating an iterative exchange between model projections, question or hypothesis development and the execution of observations and experiments to better understand impacts of multi-factor environmental changes on ecosystems.

Terrestrial ecosystem research requires the integration of biophysical, biochemical, physiological, and ecological process understanding. Terrestrial ecosystem models integrate these processes in a mathematically consistent, meta-hypothesis on the coupled operation of the C, hydrological, and energy cycles at hourly to multi-annual timescales and at ecosystem to landscape spatial scales. Terrestrial ecosystem models are built upon, validated by, and constrained by historical and contemporary observations and experiments. Nevertheless, the future 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 high-profile environmental change study, the Spruce and Peatland Responses Under Changing Environments experiment (SPRUCE), focuses on the combined response of multiple levels of warming at ambient or elevated CO<sub>2</sub> (eCO<sub>2</sub>) levels in a *Picea mariana–Sphagnum* peat bog in northern Minnesota. The experiment provides a platform for testing mechanisms that control vulnerability of organisms and ecosystem processes to important climate change variables which provide 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 (C) cycling, as well as long-term monitoring of landscape flux and sun-induced chlorophyll fluorescence (SIF) measurements at the Missouri flux (MOFLUX) site. TES SFA research on SPRUCE and MOFLUX covers a wide range of ecosystems in eastern North America from cool wet northern systems to warm and relatively dry systems on the forest-prairie transition in Missouri.

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, which focuses on the belowground ecosystem.

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 EESSD's 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.

# 2.0 SCIENCE QUESTIONS, GOALS AND MILESTONES

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 Section 4.

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

• <u>Long-term milestone</u>: Comprehensive predictive understanding of decadal peatland ecosystem responses to a range of technologically advanced warming and elevated [CO<sub>2</sub>] treatments in an ombrotrophic bog in northern Minnesota.

<u>Goal 2</u>: 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.

• <u>Long-term milestone</u>: 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.

<u>Goal 3</u>: 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.

• <u>Long-term milestone</u>: 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.

<u>Goal 4</u>: 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.

• <u>Long-term milestone</u>: Incorporate a flexible, comprehensive, and tested model of the belowground ecosystem into fully coupled ESMs.

<u>Goal 5</u>: 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.

• <u>Long-term milestone</u>: 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.

#### 3.0 TES SFA PROGRAM STRUCTURE AND PERSONNEL

Responsibility for the TES SFA resides within DOE's Climate and Environmental Sciences Directorate and is aligned with associated and related activities of the Climate Change Science Institute (CCSI) at ORNL. The organization chart for the TES SFA is presented in Fig. 2. The TES SFA includes a science and management organization to guide and direct research activities. The TES SFA Leadership Team, comprised of the individuals listed in Fig. 2, provides advice on the yearly SFA plans and budgets, monitors progress, adjusts project plans as appropriate, directs informatics development efforts, and resolves issues in a timely manner.

The TES SFA is supported by 24 dedicated ORNL scientific and technical staff including 5 current postdocs. Over 100 individuals from the USDA Forest Service, and various other collaborating universities and laboratories are participating in the SPRUCE and MOFLUX projects. 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 Coordinating Investigator and provides integrated leadership across tasks and coordinates financial management.
- Dr. Daniel M. Ricciuto is the Coordinating Investigator for terrestrial C-Cycle modeling activities.
- 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.

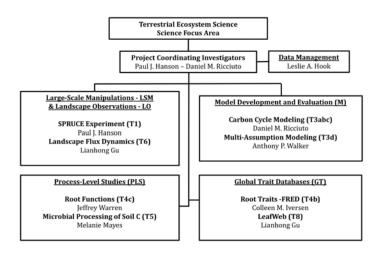


Fig. 2. Organizational chart for the TES SFA (2020 and 2021 status).

Individual Task lead responsibilities are as follows:

# Large Scale Manipulations (LSM) and Landscape Observations (LO) Task 1 – SPRUCE Personnel

<u>Experimental design, maintenance, and environmental documentation</u> – Paul Hanson leads operations of the SPRUCE infrastructure together with a team of ORNL structural and electrical engineers. Kyle Pearson (an ORNL employee located full-time in Minnesota) leads day-to-day onsite activities at the SPRUCE site with the help of a support technician (to be hired). Kyle is supported by Jeff Riggs (Lead Instrument Technician) to keep the treatments running and data streams flowing. Misha Krassovski, systems engineer, designed, implemented and now maintains the automated data acquisition systems.

<u>Plant growth, Net Primary Productivity (NPP) and phenology</u> – Paul Hanson is leading tree and shrub growth assessments with the participation of Jana Phillips. David Weston now leads the characterization of growth and community dynamics of the diverse *Sphagnum* communities. Dr. Richard Norby who retired in April 2020 has returned under subcontract to bridge this task while postdoctoral expertise is acquired. Belowground growth measurements are led by Colleen Iversen in collaboration with current postdoctoral staff, and with technical assistance from Joanne Childs and John Latimer. Vegetation phenology efforts are being led by Andrew Richardson (Northern Arizona University) with onsite manual observations collected by Kyle Pearson.

<u>Community composition</u> – Community compositional changes are being led by Brian Palik of the USFS with the participation of Rebecca Montgomery (Univ. of Minnesota). Chris Schadt leads efforts on microbial community changes and coordinates related efforts among the SPRUCE collaborators.

<u>Plant Physiology</u>—Plant physiological carbon and water relations and ecophysiological responses are led by Jeff Warren and current postdoctoral and technical staff. We are actively encouraging external participation in associated tasks: including collaborative research on gas exchange, carbohydrate dynamics, C partitioning, and woody and root respiration assessments.

<u>Biogeochemical cycling responses</u> – Work on hydrologic cycling and porewater biogeochemistry is led by Natalie Griffiths and Steve Sebestyen (USDA FS) with technical assistance from Keith Oleheiser. Colleen Iversen leads the subtask focused on plant nutrient availability in the shallow rhizosphere with technical assistance from Joanne Childs and John Latimer. C-Cycle observations focused on peat changes and C emissions are coordinated by Paul Hanson. Natalie Griffiths coordinates with Colleen Iversen, Randy Kolka (USFS), and external investigators on extensive decomposition studies. Verity Salmon coordinates compilation of peat, plant and porewater data for analysis of ecosystem-level N and P biogeochemical cycles.

<u>Modeling of terrestrial ecosystem responses to temperature and CO<sub>2</sub></u> – 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 is made up of the Response SFA research manager (Hanson), the local USFS contact (Kolka), the Technical Task leaders listed above, and an external SPRUCE advisory committee. The panel 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 6 – Lianhong Gu leads activities in the Coordinated Eco-physiology, Eddy covariance, and Sun-Induced chlorophyll Fluorescence Studies (CEESIFS) to advance integrative ecosystem science. Jeff Wood (University of Missouri) is subcontracted to operate the MOFLUX on-site activities. Other contributing staff include Colleen Iversen, Melanie Mayes, Anthony Walker, Jana Phillips and Joanne Childs.

#### **Model Development and Evaluation (M)**

Task 3abc – C-Cycle modeling activities are led by Daniel Ricciuto. Subtask contributions are made as follows: Wetlands [Xiaoying Shi, Xiaofeng Xu (San Diego State)], Allocation (Jiafu Mao, Dan Ricciuto), Photosynthesis (AnthonyWalker), rhizosphere (Xiaojuan Yang), ecological forecasting [Ricciuto, Yiqi Luo (NAU)], C flux reanalysis (Mao), wildfire analysis [Mingzhou Jin (UTK), Mao], global SIF analysis [Anping Chen (Colorado State University)], model reduction using representativeness (Kumar), and model intercomparisons (Ricciuto, Mao, Shi).

Task 3d – Multi-Assumption Systems Modeling task is being led by Anthony Walker to develop the Multi-Assumption Architecture Testbed (MAAT) for analyzing model process representations and to apply MAAT to specific TES-SFA science questions.

# **Process-Level Studies (PLS)**

**Task 4c** –Jeff Warren leads the initiative to experimentally link root function to specific root traits in collaboration with Colleen Iversen, post-docs and students.

**Task 5** – Melanie Mayes provides expertise in soil C cycling and Chris Schadt in microbial ecology to investigate microbial processes and develop the MEND model for soil C cycling.

#### **Global Trait Databases (GT)**

**Task 4b** – Colleen Iversen leads the root trait initiative including the development of a global root ecology database to inform the treatment of belowground processes in ecosystem models.

**Task 8** – Lianhong Gu supports and manages LeafWeb, a global database of biochemical, physiological and biophysical properties of leaves.

The TES SFA benefits from a SPRUCE advisory panel that is dedicated to providing guidance on the science and operation of our flagship experiment. In FY2021 the active membership of the SPRUCE Advisory Panel included: Molly Cavaleri (Michigan Technological University), Serita Frey (University of New Hampshire), Camilo Rey-Sanchez (University of California - Berkeley), Nigel Roulet (McGill University) and Daniel R. Engstrom (University of Minnesota, Emeritus).

# 4. PERFORMANCE MILESTONES AND METRICS

This section represents a summary of TES SFA activities accomplished since the review document dated June 2020. The material is organized by research theme and task with parenthetical identification of the goals addressed by each task. Task numbers are unchanged for reference across historical planning and review documents even though task titles may have been edited over time.

#### **Large-scale Manipulations and Landscape Observations**

Task 1: Spruce and Peatland Responses Under Changing Environments – SPRUCE (Goals 1,2,3,4,5)

Task 6: Coordinated Eco-physiology, Eddy covariance, and Sun-Induced chlorophyll Fluorescence Studies (CEESIFS) to advance integrative ecosystem science (Goal 1,2,3,4,5)

#### **Carbon-Cycle Focused work**

Task 3a: Improving process models with site-level observations and experimental data (Goals 1,2,3,4).

Task 3c: Functional Testing (Goals 1,2,3,4)

Task 3d: Multi-Assumption Systems Modeling (Goals 2,3,5)

#### **Process-Level Studies (PLS)**

Task 4c: Root function and modeling (Goals 2,3,4)

Task 5: Microbial processing of soil carbon (Goals 2,4)

# **Global Trait Databases (GT)**

Task 4b: Root traits characterization (Goals 2,3,4)

Task 8: LeafWeb data assimilation tool –New Task (Goal 3)

Following the description of progress for each TES SFA science task, a table of anticipated deliverables is provided with annotations regarding progress. Task-specific publications and completed manuscripts are listed by Task. Some citations may be repeated when multiple tasks contributed to the product. The number of new data sets established by each task are also noted with details presented in Appendix B.

#### 4AI. REVIEW OF SCIENTIFIC PROGRESS BY TASK

#### LARGE-SCALE MANIPULATIONS AND LANDSCAPE OBSERVATIONS

#### **Task 1: SPRUCE Infrastructure**

SPRUCE warming treatments ran full time throughout COVID-19 site-access limitations with limited interruptions other than those associated with scheduled maintenance. Warming treatments are maintained day and night throughout the year. The eCO<sub>2</sub> exposures are applied only during daytime hours during the active growing season (April through November). Table 1 shows the achieved whole-ecosystem warming treatments and eCO<sub>2</sub> treatments for the 2020 calendar year. Treatment data are archived in Hanson et al. (2016D).

Table T1.1. Mean annual air and soil temperatures and CO<sub>2</sub> concentrations by SPRUCE plot for 2020. Text in red correspond to elevated CO<sub>2</sub> treatments

Plot #s	Target Temperature Differential	Mean Air Temperature at +2 m	Mean Soil Temperature at -2 m	Ambient Daylight Mean Growing Season [CO <sub>2</sub> ]* at +2 m	Elevated Daylight Mean Growing Season [CO <sub>2</sub> ]** at +2 m
	(Delta °C)	(°C)	(°C)	ppm	ppm
Plots 7 & 21	Ambient	5.5, 5.2	5.5, 6.2	402	
Plots 6 & 19	+0	7.0,6.3	4.6 , 6.1	408	876
Plots 11 & 20	+2.25	9.1, 9.1	7.0 , 7.1	409	860
Plots 4 & 13	+4.5	11.5, 11.6	9.2, 9.3	408	877
Plots 8 & 16	+6.75	13.8 , 13.7	11.4 , 11.4	411	898
Plots 10 and 17	+9.0	15.9, 15.8	13.5 , 13.4	414	888

<sup>\*</sup>For the purpose of this enumeration the growing season runs from day of the year 92 through 295 to match the active season in the +9 °C treatment plots.

In 2020, the unique isotopic signatures of air in the added  $CO_2$  treatments continued to be approximately -27 to -28  $\partial$  % for  $^{13}C$  and -540  $\Delta$  % for  $^{14}C$ . Through 5 full active seasons of eCO<sub>2</sub> exposures new tissue growth under eCO<sub>2</sub> has stabilizing at a new isotopic signatures commensurate with the experimental exposures to eCO<sub>2</sub> (Fig. T1.1). Tissue  $^{13}C$  and  $^{14}C$  signatures for *Sphagnum* and

<sup>\*\*</sup>Elevated CO<sub>2</sub> would approach 900 ppm in all plots if a specific active season definition were used for each warming treatment.

Maianthemum plants are different that for the taller plant species because they reincorporate respired forms of  $[CO_2]$  from the peat profile.

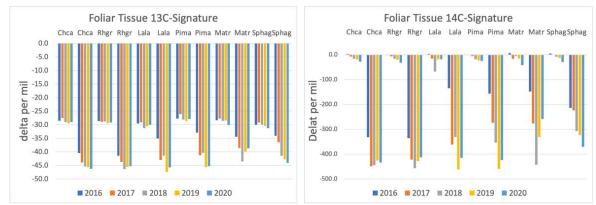


Fig. T1.1. Carbon isotope signatures for new above ground foliar tissue growth across plots and e $\rm CO_2$  treatments.

## Task 1: SPRUCE Response Data

Carbon Cycle Assessments for the S1 Bog —Our unprecedented, long-term, whole-ecosystem warming study has enabled an initial ecosystem-level analysis of ecosystem changes for the first three full years of whole-ecosystem warming. Warming caused variable responses for vegetation and consistent net losses of both CO<sub>2</sub> and CH<sub>4</sub> for a linear response of -31.3 gC m<sup>-2</sup> y<sup>-1</sup> °C<sup>-1</sup> (Hanson et al. 2020; Fig. T1.2). Carbon losses with warming of +2.25 to +9 °C were found to be 4.5 to 18 times faster than the historical rate of peatland C accumulation. Through 3-years of sustained active season exposure to eCO<sub>2</sub>, we have not yet observed a dominant and hypothesized increase in C uptake likely due to nutrient limitations.

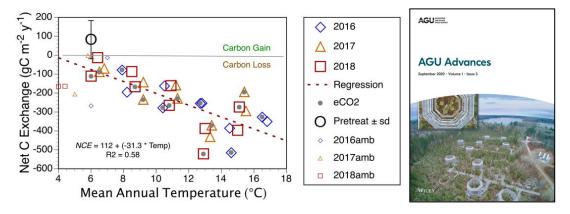


Fig. T1.2. Measured ecosystem net C exchange (NCE; g C m $^{-2}$  y $^{-1}$ ) for all treatment plots (+0, +2.25, +4.5, +6.75 and +9 °C treatments) plotted against the mean annual air temperature at +2 m for each plot in 2016, 2017 and 2018. NCE was calculated as the difference in measures of above- and belowground net primary production and C losses via heterotrophic CO<sub>2</sub> efflux, net CH<sub>4</sub> efflux, and combined total organic C and dissolved inorganic C efflux. Treatment plots receiving elevated atmospheric CO<sub>2</sub> exposures (eCO<sub>2</sub>) are indicated by a solid grey circle within the plot symbol. Also shown is the NCE for pretreatment conditions in 2014-2015 [open circle  $\pm$  SD from Griffiths et al., (2017) modified based on new estimates of heterotrophic contributions]. Non-enclosed ambient plot data for 2016, 2017, and 2018 are shown as small open symbols, and are provided for reader reference.

Because COVID-19 protocols kept us from routine access to the SPRUCE site in 2020 we do not have independent evaluations of the NCE for each treatment plots for 2020.

<u>Sphagnum production and Community Response</u> – Norby et al. (2019) documented the rapid loss of the <u>Sphagnum</u> community from the <u>SPRUCE</u> treatment plots through a significant linear effect of

minimum water table elevation on *Sphagnum* NPP. This work continues in 2020 and 2021 with the addition of a shading study established to determine the extent to which light limitations might be driving the loss of *Sphagnum* spp. from the peatland vegetation community.

<u>Understanding Sphagnum benefits to warming through microbiome interactions</u> – Our previous research showed that SPRUCE warming manipulations alter the <u>Sphagnum</u> – associated microbiome and influences maximal rates of N<sub>2</sub>-fixation (Carrell et al. 2019). This is important as N<sub>2</sub>-fixing microbial associates are critical for <u>Sphagnum</u> production and competitive success, along with the provision of N inputs to the ecosystem. Due to COVID related restrictions on travel to the SPRUCE site, we decided to focus on laboratory experiments examining the environmental conditions and metabolic basis for <u>Sphagnum</u> symbiosis with its main microbial associate – cyanobacteria. Ecological research has shown that peatland N<sub>2</sub> fixation activity is stimulated by the addition of pH raising bicarbonate, whereas <u>Sphagnum</u> growth remained unaffected, suggesting that <u>Sphagnum</u> – cyanobacteria symbiosis is decoupled at high pH.

To test the hypothesis that variable pH conditions influence Sphagnum-Nostoc symbiosis, we grew Sphagnum angustifolium collected from SPRUCE and Nostoc at pH 3.5, 5.5, and 8.5. Symbiosis outcome was evaluated by comparing the growth of Sphagnum in direct contact with Nostoc (designated Nostoc/Sphagnum symbiosis), relative to individual growth in isolation and the sum of individual growth (designated Nostoc+Sphagnum). There was a clear benefit to symbiosis in the low pH (3.5) environment: when the species were grown together under these conditions, the change in weight was greater than the sum of individual growth (Fig. T1.3; W = 35; one-tailed, FDR adjusted p = 0.00866). However, the growth benefit was not clearly observed at pH of 5.5 or 8.5. When evaluated alone, Sphagnum growth was higher at pH 5.5 (32.1 mg  $\pm$  26.2) than at 3.5 (13.8 mg  $\pm$  14.0) or 8.5 (24.2 mg  $\pm$  15.4). In contrast to the host plant, Nostoc grown alone grew more as pH increased: growth was 21-fold higher at pH 8.5 (29.8 mg  $\pm$  39.4) than at pH 3.5 (1.38  $\pm$  9.17). Thus, the symbiosis is only mutualistic at low pH.

These observations demonstrate that changing environmental conditions can drastically influence species interactions, including the *Sphagnum – nostoc* symbiosis. By leveraging EMSL and JGI resources through a FICUS award, we are currently exploring the consequences of warming and metabolic exchange for this critical plant – microbe symbiosis.

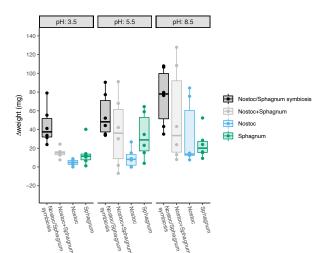


Fig. T1.3: Sphagnum and Nostoc growth analysis across variable pH conditions. At pH 3.5, growth was highest when both organisms were grown together. Growth of Sphagnum grown individually or with Nostoc across a pH gradient were determined by change in wet weight (mg) of organisms grown in BG11 (n=6). Samples labeled with "symbiosis" represent the two organisms grown together, and Nostoc+Sphagnum shows the sum of individual growth of each organism alone.

<u>Aboveground vegetation production</u> – A paper on shrub-layer production growth through the first 4 seasons of manipulations has been published (McPartland et al. 2020) showing mixed responses, with some species showing increases with warming (*Rhododendron*, an ericaceous shrub) and others showing dramatic losses (*Maianthemum*, a forb). Yet unpublished tree growth data show initial negative responses for *Picea* (black spruce) that have dissipated with time and developing positive responses for *Larix* (*larch*); changes are hypothesized to be driven by nutrient availability increases under warming (see below).

<u>Belowground Dynamics</u> - The dynamics and distribution of fine roots in ecosystems underlain by organic soils are some of the least understood processes in belowground ecology. Building on our work to understand fine roots in an ombrotrophic bog prior to initiation of climate change treatments (Iversen *et al.*, 2018, *Plant & Soil*), we leveraged on-going data collection (e.g., from manual and automated minirhizotrons, root ingrowth cores, and ion-exchange resins; data citations: Childs *et al.* 2019, 2020; Iversen *et al.* 2017a, b, 2021; Malhotra *et al.* 2020) to ask two main questions:

1. How does warming affect root and fungal growth, and how are belowground dynamics related to edaphic and environmental conditions?

We have shown previously that the root length of ubiquitous ericaceous shrubs is increased by as much as 130% per degree of warming at SPRUCE (Malhotra *et al.* 2020, *PNAS*). Building on this observed belowground response, we have focused on the distribution and dynamics of fine roots and their associated mycorrhizal fungi in response to warming. Using novel, high-resolution minirhizotrons, we found that not only has warming increased the abundance of ericaceous shrub roots in shallow peat, it has increased the abundance of ectomycorrhizal fungal rhizomorphs, especially in deep peat, and extended the belowground active season by 62 days. In turn, tree roots and associated ectomycorrhizas and fungal hyphae were more abundant in the cooler enclosures (Fig. T1.4). Taken together, changes in the dynamics and distribution of roots and hyphae in response to warming may reduce peat C accumulation (Defrenne *et al.*, 2021, *PPP*). Along with this publication, post-doctoral researcher Dr. Defrenne led the development of an interactive website that allows scientists and the public to peer belowground in the SPRUCE experimental enclosures (https://colleeniversen.ornl.gov/inside-the-spruce-bog).

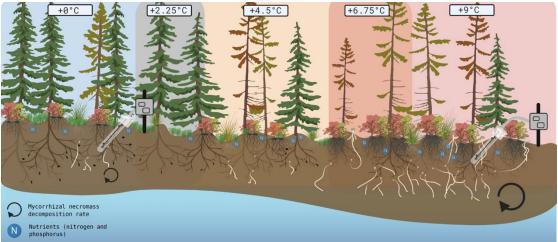


Fig. T1.4. Defrenne *et al.* (2021) focused on two automated, high-resolution minirhizotron tubes installed at the coldest and warmest ends of the experimental temperature gradient, respectively. The dark-green coniferous trees represent black spruce (*Picea mariana*) and the light-green and brown trees represent larch (*Larix laricina*). The small bushes represent ericaceous shrubs, the light-green plants represent *Sphagnum* mosses, and the light-green herbs represent graminoid species. The black root tips represent *Cenoccoccum geophilum* ectomycorrhizas that mostly associate with spruce while the light-colored root tips represent rhizomorph-forming ectomycorrhizas that mostly associate with larch. Created with BioRender.com

2. Does warming increase plant-available nutrients over time and throughout the peat profile?

Using ion-exchange resins deployed across peat depths and microtopographic positions (Iversen *et al.* in preparation; data citation: Iversen *et al.*, 2017), we found that: (1) warming increased resin-available NH<sub>4</sub>-N and PO<sub>4</sub>-P, but the magnitude of the response increased over time and varied across the highly heterogeneous bog surface and with peat depth (Fig. T1.5). These dynamics were generally unaffected by elevated  $[CO_2]$  or the relatively minor changes in water table depth with warming. (2) Relative increases

in resin-available NH<sub>4</sub>-N and PO<sub>4</sub>-P with warming were similar, though resin-available NP ratios increased with peat depth. Resin-available nutrient dynamics were only loosely correlated with inorganic and organic porewater nutrients, likely representing different processes. Furthermore, we observed complex interactions with the declining nutrient requirements of ubiquitous non-vascular *Sphagnum* mosses in response to warming. Predictions of peatland nutrient availability under climate change scenarios must account for microtopography, peat depth, and the interplay between vegetation nutrient acquisition and microbial activity.

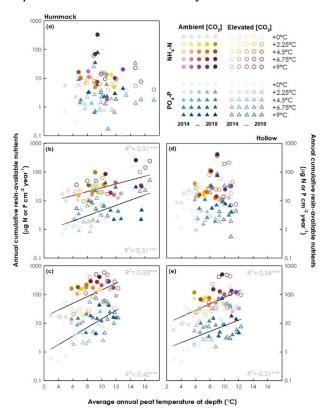


Fig. T1.5 Annual, cumulative NH<sub>4</sub>-N or PO<sub>4</sub>-P adsorbed to ion-exchange resins regressed against annual average peat temperature at a depth closest to the depth of resin incubation at multiple peat depths in hummock and hollow microtopography along a gradient of whole-ecosystem warming and warming combined with elevated [CO2]. Each data point is one enclosure, in years 2014 to 2018. Closed symbols are warming only, while open symbols are the same warming gradient repeated at elevated [CO<sub>2</sub>]. More intense colors correspond with more recent years. Letter insets correspond to depth of resin incubation (a, b, and c are 10, 30, and 60-cm depths in hummocks and d and e are 10 and 30-cm depths in hollows, respectively). Asterisks indicate level of significance corresponding to linear regression, where  $R^2$  is the adjusted  $R^2$ of NH<sub>4</sub>-N regression (upper right of each panel) or PO<sub>4</sub>-P regression (lower right of each panel); note the log-scale of the y-axis.

<u>Woody Plant Physiology</u> – The primary focus of FY2020/2021 was on processing lab samples, analyzing automated data streams, synthesizing multiple datasets and publications. We continued our focus on linking the visible presence of foliar or branch tip damage on the woody species in the warmest plots to existing physiology data, including for individual trees (e.g., water potential, sap flow, carbohydrates, nutrients). Using the past four years of plant water stress we see divergent hydraulic strategies between the two tree species, as spruce exhibited a more conservative response to warming through reduced stomatal aperture and reduced water stress, while larch maintained open stomata which led to greater water stress – a strategy that favors C uptake, but at greater hydraulic risk (Dusenge et al. 2021, Warren et al. 2021). Based on continued and planned laboratory and field hydraulic disfunction and vulnerability measurements we have several new papers developing that build from these initial papers to link physiological and detailed hydraulic mechanisms to foliar and branch physiological stress.

We also used microscopy techniques to analyze wood anatomy samples and image processing was employed to extract xylem area, ring width, lumen area and density – characteristics linked to hydraulic function. This work demonstrated that the eCO<sub>2</sub>, in combination with the warming treatment significantly increased xylem wood production in branches (Fig. T1.6), which can facilitate greater water movement though the stem. This treatment response is a dramatic acclimation for both species that could enable them to overcome the severe heat/water stress imposed by the temperature treatments.

We are finalizing analysis and manuscript development of the 2017 extreme physiology gas exchange campaign that measured photosynthetic capacity and thermal acclimation (e.g., optimal temperature of photosynthesis (A), carboxylation capacity ( $V_{cmax}$ ), maximum rate of electron transport ( $J_{max}$ ), and dark

respiration). Thermal acclimation was correlated with changes in the T<sub>opt</sub> of for both tree species (Fig. T1.7), and for *Chamaedaphne* in August, but no change in T<sub>opt</sub> was exhibited by *Rhododendron*. Surprisingly, there was little acclimation of tree foliar respiration to whole ecosystem warming (although respiration was correlated to maximum carboxylation capacity of Rubisco), and we are pushing through a MODEX effort on understanding this response and its implications for net carbon balance under warming. There was some evidence for acclimation to eCO<sub>2</sub> by down-regulating photosynthetic capacity in *Picea* and *Rhododendron*, but not for the other species. If acclimation to eCO<sub>2</sub> is not accounted for, the current models will over-predict gross primary production (GPP). If acclimation to elevated temperatures is not accounted for, the current models will underpredict GPP. As such, the physiology team continues to work directly with the modeling team to ensure results are correctly informing and helping to refine the model structure.

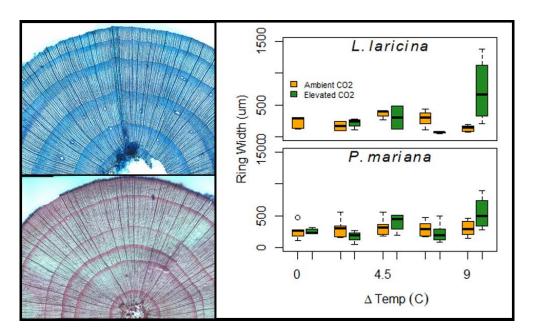


Fig. T1.6. Stained sections of branch xylem for spruce (top) and larch (bottom) with annual growth rings clearly visible; the outer most ring is 2019 and second ring is the 2018 ring. The images depict the 2018 growth rings response across treatments, illustrating greater widths for  $eCO_2 + 9$  branches.

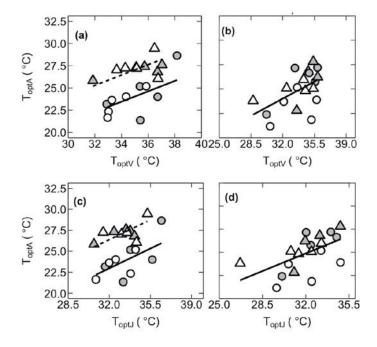


Fig. T1.7. Shifts in thermal optimum of net photosynthesis was driven by warming-induced shifts in thermal optima of maximum carboxylation capacity of Rubisco ( $V_{cmax}$  -  $T_{optV}$ ) and maximum rate of electron transport ( $J_{max}$  -  $T_{optJ}$ ) for both larch (left) and spruce (right).

We also completed a manuscript describing how drought during budbreak in spruce can impact branch development and foliar display (Jensen et al. 2021). Since evergreen species retain active leaves for multiple years, spring drought impacts on plant vigor could be carried forward into subsequent years. Additionally, we processed 4 years of sap flow data. From these data we extracted sap flow initiation and cessation dates for each tree across the treatments and found that the growing season defined by active sap flow was extended by 41 days for *P. mariana* and by 34 days for *L. laricina* in the +9 plots compared to controls. We were able to access the site briefly to sample material from the four woody species to maintain our analyses of annual summer and winter non-structural carbohydrate (NSC) dynamics. We also were able to collect foliar material from trees that we are specifically tracking due to visible physiological stress and damage to analyze for NSC and complete nutrient workup. Five years of NSC samples collected by the physiology team are currently being organized and processed - data will support three different manuscripts, one focused on shrub herbivory (esp., *Chamaedaphne*) in the warmer plots, one on physiological stress in targeted trees, and one on interannual and seasonal NSC dynamics over time.

<u>Outflow and Porewater Chemistry</u> – Data collection on the water chemistry task was somewhat affected by COVID-19. Due to site access constraints, the task focused on collecting weekly samples from the outflow systems as these data are critical for whole-system elemental flux/budget calculations. Porewater sampling was thus put on hold at the start of the 2020 field season. Porewater sampling began in July 2020 (sampling typically begins in February/March of each year).

Solute concentrations in outflow continued to respond to warming. Higher total organic C (TOC; Fig. T1.8A) concentrations in outflow were observed in warmer enclosures, and TOC concentrations were positively related to annual peat soil temperature (Fig. T1.8B) and negatively related to water table height (Fig. T1.8C; lower water tables corresponded to higher TOC concentrations). In contrast, responses of total N (TN) and total P (TP) concentrations to warming were variable, and only TN concentrations were negatively correlated with water table height. Total nutrient and TOC concentrations were most responsive to warming in near surface porewaters; minimal changes were observed below 1 m depth. The same drivers of TOC concentration in outflow (peat temperature, water level) were found to drive annual patterns in TOC concentrations in near surface porewater. However, at deeper depths, water level was no longer a driver of variation in TOC concentrations, as expected. A manuscript describing outflow and porewater chemistry responses is being drafted.

Keith Oleheiser, who has primarily supported the SPRUCE water chemistry task for multiple years in a subcontracting position, was hired by ORNL in 2021 as a technician. Keith will continue his role in providing support to the SPRUCE water chemistry task and SPRUCE decomposition tasks, as well as providing support to other SPRUCE field and operations tasks as needed.

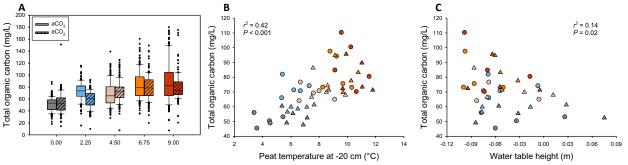


Fig. T1.8. (A) Box plots of total organic carbon (TOC) concentrations in lateral outflow (i.e., stream flow) from SPRUCE enclosures and responses to warming over five years (2016-2020). (B) Relationships between annual mean TOC concentrations and (B) annual mean peat temperature at 20 cm depth and (C) annual mean water table height.

<u>Decomposition</u> – The five-year retrieval of litterbags planned for fall 2020 was put on hold due to COVID-19. Instead, litterbags will be retrieved after 6 years of incubation in fall 2021, with one final (10-

year) retrieval date planned in 2025. Biannual cotton strip retrieval occurred in 2020 and these data continue to reveal strong effects of warming on labile C decomposition (cotton strips are 95% cellulose), with greater decomposition rate of cotton in warmer enclosures throughout the peat profile.

A five-year-long decomposition study that took place outside of the enclosures and that examined the effect of intrinsic (litter quality) versus extrinsic (soil moisture, temperature, porewater chemistry) drivers on moss decomposition was completed and submitted to Oikos (Shelley et al. in revision). A key finding was that litter chemistry was the main driver of the early phases of decomposition, and environmental drivers became more important in the later phases. These findings suggest that warming effects (an extrinsic driver) may become more apparent as the SPRUCE decomposition measurements continue. More generally, because most litter decomposition studies in peatlands are generally of short duration (< 3 y), these results suggest that longer-term studies are needed to better understand the multiple controls on litter decay in peatlands.

N and P Nutrient Cycling – Field observations were used to construct comprehensive nitrogen (N) and phosphorus (P) budgets for the S1 Bog prior to the implementation of SPRUCE treatments (Salmon et al, accepted). Pools and fluxes of these co-limiting nutrients were also compared to output from ELM-SPRUCE. Results showed that N accumulated in the bog ecosystem at  $0.2 \pm 0.1$  g N m<sup>-2</sup> y<sup>-1</sup>, similar to annual N fixation rates within the *Sphagnum* moss layer. Annual P inputs were generally balanced by losses from the bog ecosystem. Plant functional types (PFTs) varied in their degrees of N versus P limitation, allocation across tissues, and internal recycling of N and P. The model ELM-SPRUCE captured N pools and fluxes across PFTs accurately, but representation of P cycling could be improved. Establishing a benchmark for N and P cycling at this site as well as within the ELM-SPRUCE model represents a crucial step toward predicting the C storage capacity of peatland ecosystems in the  $21^{st}$  century.

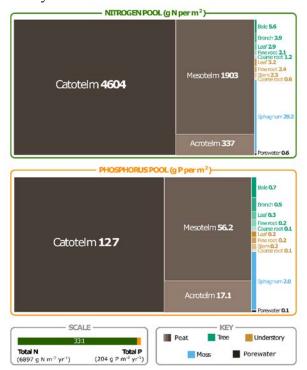


Fig. T1.9. N and P pools across biotic and abiotic components of the S1 Bog ecosystem. Area of the boxes for each N and P pool reflect pool sizes. Note the different scales used to depict storage of these two nutrients: the total ecosystem N pool is 33x larger than the ecosystem P pool.

<u>Microbial Community Responses</u> – Initial studies of the responses to in situ experimental warming of the SPRUCE chambers indicated that the peat microbial communities and decomposition rates were resistant to elevated temperatures in the first years of experimental warming (Wilson et al., 2016). While metagenomic analyses of samples from 2015 and 2016 showed a strong depth stratification of microbial community profiles there was little evidence of changes in the structure or abundance of microbial communities with the treatment regimes at SPRUCE. This past year a more in-depth analysis using

combined evidence from metagenomics, proteomics and metabalomic analysis has shown that while abundance profiles have not changed there has been a distinct shift in the microbial activities and substrate preferences toward methanogenic microbial activity and metabolisms that is shifting deeper within the peat profile, with both temperature and  $CO_2$  treatments (Fig. T1.10 – Wilson et al. 2021).

These are likely resulting greater prevalence of CH<sub>4</sub> vs CO<sub>2</sub> fluxes at the site observed in recent years (Wilson et al 2021). This past year in collaboration with the Joint Genome Institute we have also completed metagenomic sequencing for an additional 48 samples from 2018 that have resulted in approximately 32Gbp of additional sequence data (compared to approx. 15 Gbp obtained from 2016 samples). Analyses of these samples is ongoing, however given the large vegetation and other biogeochemical changes that have been noted, combined with additional resolution in the dataset, the analyses will reveal further changes along these lines even deep within the profile.

Concurrently with the above metagenomic work, we have been conducting a series of manipulative experiments to understand important microbial processes at play in peatland biogeochemical processes. A series of incubation studies has shown that in addition to methanogenesis via the more well-known acetoclastic and hydrogentrophic pathways, a more specialized form of methylotrophic methanogensis involving the utilization of methylated aromatic compounds (MACs) is also present within the S1 bog system. Community analysis of these data is being completed but shows very high spatial variability across plots and depths. New studies of microbial contributions to peat and litter decomposition were also begun this year. Peat "decomposition ladder" samples to provide depth resolved understanding of surface decomposition patterns (in collaboration with R. Kolka and N. Griffiths). Samples were harvested after two years of in-situ incubations in the chambers in late fall of 2020 and amplicon based analyses of microbial community profiles associated with each depth are ongoing.

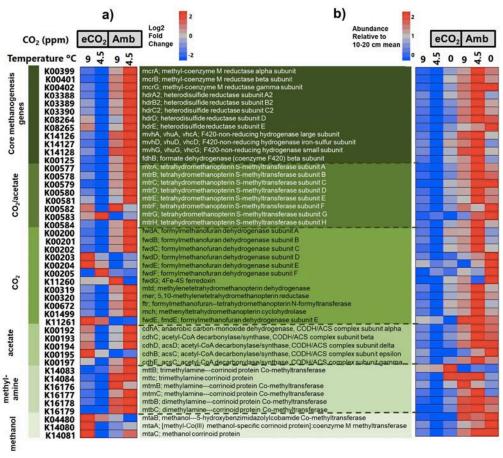


Fig. T1.10. Shifts in microbial catabolic pathways in response to experimental warming. Panel (a) contains a heatmap presenting the relative abundances of enzymes associated with the methanogenic (or potentially reverse methanogenic) pathways from the short-read data from the 45 cm depth. The values for each gene

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were normalized by the log2 fold change relative to the control (0C) for each of eCO2 and ambient CO2 (Amb) treatments. Panel (b) provides the same data normalized relative to the mean relative abundance of all soil short-reads (by rows). In both panels, genes are grouped according to pathway and KO numbers are given to the left of each row, while the identifications from KEGG are given in the middle. "Core methanogenesis genes" are genes used by all methanogens regardless of pathway. The other categories encompass genes unique to the pathway indicated (e.g. acetoclasty or methylotrophy etc).

<u>SPRUCE field activities and COVID-19</u> – Site access restrictions imposed on SPRUCE researchers in 2020 limited field activities by ORNL and cooperators stationed away from the SPRUCE research site in northern Minnesota. Full-time and onsite ORNL and contractor staff and key USDA Forest Service personnel were able to sustain SPRUCE warming and eCO<sub>2</sub> treatments throughout 2020. All automated data streams were uninterrupted by COVID-19 and the task based measurements executed by on site staff were also collected on schedule. As mentioned above, 5-year sampling of the peat profile was executed as scheduled, but the automated and monthly CO2 and CH4 flux data sets dependent on remote ORNL staff were not collected in 2020.

# **SPRUCE Deliverable Progress**

The SPRUCE project is now in its 5<sup>th</sup> full year of operation with science measurement and modeling tasks representing the dominant effort. The COVID-19 pandemic will have some impacts on the field work that can be accomplished in 2020. The following deliverables cover SPRUCE activities for FY2019 and FY2020.

Task 1 – SPRUCE Deliverable Status FY2020 through FY2021

Date	Deliverable	Status
2020 All Year	Sustain continuous SPRUCE treatments and automated data collection efforts	Completed
September 2019	Manuscript on multi-year plant-available nutrient response to warming	Iversen et al. – final draft with co-authors
May 2020	Submission of SPRUCE manuscript describing initial morphological and xylem anatomical responses to treatments.	Postponed for further data collection
August 2020	Complete 2 <sup>nd</sup> 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	Completed Defrenne et al. 2021
September 2020	Manuscript on plot-scale C-Budget changes from warming and eCO <sup>2</sup>	Completed
2021 All Year	Sustain continuous SPRUCE treatments and automated data collection efforts	On Schedule
March 2021	Publish manuscript on drought impacts on spring branch development	Complete
March 2021	Publish manuscript on initial sap flow and water relations	Complete
April 2021	Publish manuscript on initial gas exchange and acclimation	Complete
August 2021	Complete summer remote sensing / woody physiology campaigns	Planned
August 2021	Publish manuscript on woody plant water stress and hydraulic failure	Underway
September 2021	Complete summer shrub sampling for foliar chemistry linked to herbivory	Planned
September 2021	Publish manuscript on initial sap flow timing and seasonal dynamics	Underway
September 2021	Manuscript on root phenological responses to warming	Planned
October 2021	Publish manuscript on warming induced physiological stress	Underway
October 2021	Publish manuscript on photosynthetic acclimation to SPRUCE treatments	Planned
December 2021	Publish manuscript on 5 years of non-structural carbohydrate dynamics	Planned

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- Shelley, S.J., D.J. Brice, C.M. Iversen CM, Kolka RK, Sebestyen SD, Griffiths NA (2021) Deciphering the shifting role of intrinsic and extrinsic drivers on moss decomposition in peatlands over a 5-year period. *Oikos* (in revision).
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peatland CH<sub>4</sub> emission under warming and eCO<sub>2</sub>elevated CO<sub>2</sub>: A modeling study. *Global Change Biology* (in review).

Yuan F, Wang Y, Ricciuto DM, Shi X, Yuan F, Hanson PJ, Thornton PE, Xu X (2020) An Integrative Model for Soil Biogeochemistry and Methane Processes: II. Warming and Elevated CO<sub>2</sub> Effects on Peatland CH4 Emission. *Journal of Geophysical Research - Biogeosciences* (accepted).

#### Task 1 Data Sets

Fourteen new Task 1 data sets have been prepared and posted (Childs et al. 2020D; Dusenge et al. 2020D; Hanson et al. 2021D; Iversen et al. 2021D; McPartland et al. 2019D; Norby et al. 2020D; Phillips et al. 2021D; Schädel et al. 2020Da and 2020Db; Sebestyen et al. 2020D and 2021D; Shelley et al. 2021D; Warren et al. 2021D; Wilson et al. 2021D all in Appendix B).

# Task 6: Coordinated Eco-physiology, Eddy covariance, and Sun-Induced chlorophyll Fluorescence Studies (CEESIFS) to advance integrative ecosystem science (formerly MOFLUX)

<u>MOFLUX site updates</u> – Effective Jan 1, 2021, the site Co-PI of MOFLUX, Dr. Jeff Wood was converted to a tenure-track position at the University of Missouri (MU). He continues to serve as MOFLUX co-PI with reduced time commitment to the project. A technician hired to assist Wood's effort on the project reported to work on June 1, 2021.

As part of the University of Missouri Agricultural Experiment Station's "virtual field day" events in 2020, we produced a number of educational/outreach videos about MOFLUX activities. These were officially released with the Baskett Wildlife Research and Education Center's virtual field day (<a href="https://baskett.missouri.edu/field-day/">https://baskett.missouri.edu/field-day/</a>). Our undergraduate summer student even wrote and recorded original music for the <a href="https://baskett.missouri.edu/field-day/">MOFLUX video</a>.

<u>MOFLUX field activities and Covid-19</u> – Out of an abundance of caution, and uncertainty at the start of the 2020 growing season, we scaled-MOFLUX field activities. This entailed maintaining automated data streams, and continuing the collection of our standard ecophysiological and biometric data sets. We had initially been planning to do more leaf-level work including gas exchange/chlorophyll fluorescence and water potential measurements and these activities were put on hold for 2020 due to the need of more than two people working together at the site. We will resume these activities during the 2021 growing season.

<u>CEESIFS science updates</u>—We continue to leverage the unique combination of observations and modeling to understand processes including photosynthesis, and ecosystem responses to drought. Specific avenues of inquiry include (i) fundamental photosynthesis modeling, (ii) coupling of photosynthesis with soil respiration (and its components), and (iii) ecosystem-scale hydraulics and water relations. MOFLUX Co-PI Wood contributed to an AmeriFlux network-level analysis of flux footprint representativeness analysis.

<u>Photosynthesis modeling</u> – Plants balance the light and C reactions of photosynthesis to ensure the normal functioning of photosynthetic apparatus and long-term species survival. Convergence is expected on prediction of photosynthesis from either the light or C reactions. Historically, C reactions have been the focus of mechanistic modeling, which does not provide a systems framework needed by emerging research frontiers that must deal with the whole photosynthetic machinery. We developed a closed biophysical (photophysical) representation of the light reactions for lake and puddle photosynthetic unit connectivity to model photosynthesis, fluorescence, and the balance between the light and C reactions. Closure was achieved by modeling photochemical and non-photochemical electron transport regulations (PNPETR). The light reaction equations, derived from the law of conservation of energy in photosystems, are coupled with the PNPETR model to resolve all dynamic light reaction variables plus CO2 assimilation rate. This photophysical model of photosynthesis accurately predicts fluorometry and gas exchange

measurements of multiple crop and tree species across broad environmental conditions (Fig. Task 6.1). We found that the lake and puddle formulations perform equally well. Model inference from measurements show that species share essentially identical photochemical quenching responses to intercellular CO2 concentration but differ in non-photochemical quenching responses, suggesting regulated heat dissipation is key to understanding species difference in photosynthetic efficiency. Our new model has broad applications. It establishes the light-reaction mechanism for photosynthetic remote sensing via sun-induced chlorophyll fluorescence, provides insights for crop engineering, and complements C reaction models to form a comprehensive framework for systems modeling of photosynthetic responses to climate change. A manuscript on the photophysical model of photosynthesis is now under preparation.

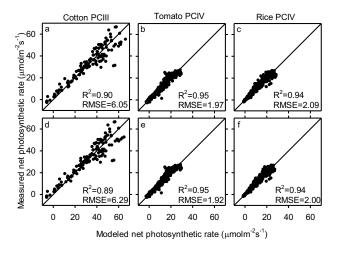


Fig. T6.1. Comparison of measured and modeled Anet with either the lake (first row) or puddle (second row) model formulation of the light reaction equations and the modeled NPQE, qL and qP. Predictor combination III (PCIII, PAR + temperature + CO2 + O2) was used for cotton (left column). PCIV (PAR + CO2 + O2) was used for tomato (middle column) and rice (right column)

With our completion of the photophysical model development (above), we have turned our attention to the photochemistry of photosynthesis. The goal of this new modeling effort is to establish the missing mechanistic link between the photophysics (above) and the biochemistry of the C reactions (represented by the FvCB model). To achieve this goal, we use two levels of complexity in representing the states and redox reactions of complexes and electron carriers along the electron transport chain from photosystem II (PSII) to Cytochrome b6f complex (Cyt). Since we are only interested in steady state, we assume that the downstream transport from Cyt to plastocyanin (PC) to PSI to the eventual electron acceptors in the C reactions is in balance with the upstream transport. Further, we assume that any feedbacks from the downstream to the upstream transport act via the dynamics of Cyt redox state. We challenge the validity of these representations and assumptions with joint leaf fluorometry and gas exchange measurements made on C3 and C4 species under a wide range of climate and environmental conditions, including CO2 and light responses at multiple O<sub>2</sub> and temperature levels. The species used cover crops, deciduous and evergreen trees, grasses, and lianas.

The first representation (denoted as DA, Fig. Task 6.2) defines the states of PSII based on whether the electron donor (D) and acceptor (A) are reduced or oxidized. The second, more complex representation (denoted as Q<sub>A</sub>Q<sub>B</sub>, Fig. Task 6.3) groups PSII based on the redox conditions of the tightly bound plastoquinone (Q<sub>A</sub>) and the loosely bound plastoquinone (Q<sub>B</sub>). Both the DA and Q<sub>A</sub>Q<sub>B</sub> representations consider not only regular open / closed (i.e., reversible) reaction centers but also the irreversible reaction centers which include the inhibited PSII under stress, QB-nonreducing PSII, and cushion PSII. Cushion PSII is introduced here because electron transport through PSII occurs in an uneven relay race fashion. At the start of the relay, the electron donor can only acquire the energy of one photon and donates one electron at a time. Also, Q<sub>A</sub> can only transfer one electron at a time. Down the chain, however, Q<sub>B</sub> has to acquire two electrons before picking up two protons from the stroma and joining the free plastoquinone (PQ) and plastoquinol (PQH2) pool. This unevenness means that the acceptors of some PSII reaction centers must have already been in a reduced state to provide cushion before any electron transport downstream is possible. Both the DA and Q<sub>A</sub>Q<sub>B</sub> representations model the electron transport chain down to the oxidation of the reduced and protonated plastoquinone by Cyt. These two representations permit us

to gauge the level of complexity needed to collapse the regulatory mechanisms of electron transport into an informative model. We expect to complete this new model development by the end of FY2022.

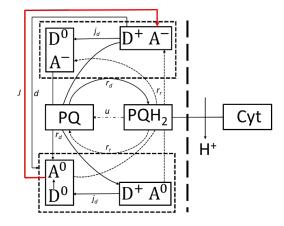


Fig. T6.2. The DA model representation of photosynthetic linear electron transport. Lower case letters denote rate constants of redox reactions while J denotes energy-requiring transfer of electron from donor to acceptor.

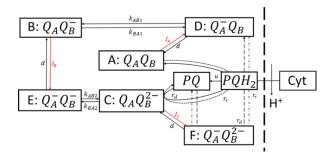


Fig T6.3. The  $Q_AQ_B$  model representation of photosynthetic linear electron transport. Lower case letters denote rate constants of redox reactions while  $J_A$ ,  $J_B$ , and  $J_C$  denote energy-requiring transfer of electron from donor to acceptor.

<u>Coupling of photosynthesis with soil respiration</u> – In collaboration with Dr. Melanie Mayes (ONRL, TES-SFA Task 5 Lead), we have been measuring soil respiration on trenched and untrenched plots to enable the partitioning of soil respiration into its heterotrophic and autotrophic components. A manuscript focusing on the coupling of photosynthesis to soil respiration and its components is in preparation (for *Agricultural and Forest Meteorology*). We found that the relative importance of heterotrophic (autotrophic) respiration increases (decreases) as ecosystem drought stress intensifies (Fig. T6. 4). We developed a three-way CO<sub>2</sub> flux-partitioning algorithm that separates net ecosystem exchange into aboveground plant respiration, below-ground root and soil respiration, and gross primary production. We found that on annual time scale, belowground soil respiration dominates over aboveground plant respiration in total ecosystem respiration, but the relative contributions of different sources vary seasonally. A new manuscript is in review in *Agricultural and Forest Meteorology*.

Ecosystem-scale hydraulics and water relations: – We have conducted novel ecosystem scale analyses by combining eddy covariance observations with leaf water potential measurements. One manuscript has been completed on the dynamics of ecosystem hydraulic conductance ( $K_{eco}$ ). We submitted the manuscript to Nature Communications and are presently appealing the 1<sup>st</sup> decision. In another manuscript (in preparation for Global Change Biology), we leveraged observations during the major 2012 drought to conduct an ecosystem scale "pressure-volume" analysis to derive the ecosystem scale wilting point,  $\Psi_{EWP}$  (Fig. Task 6.5). The  $\Psi_{EWP}$  is an integrated ecosystem property that defines the point at which vegetation is no longer able to readily extract soil water and leaves are at or near their turgor loss point.

<u>Collaborative research activities</u> – Over the last year, several collaborative research activities, leveraged on the ongoing ecosystem monitoring at MOFLUX, were initiated. As part of an initiative by Dr. Anthony Walker of ORNL, we have installed 16 automated band dendrometers (4 species, each with 4 bands) at MOFLUX. They installed dendrometers on the same species at Walker Branch in TN. A

collaborator at Morton Arboretum, Dr. Luke McCormick, has also banded the same species. This multisite collaboration will help to enable improved understanding of growth dynamics for species growing in different climates and on different soils.

Dr. Sean Zeiger, at Lincoln University, an Historically Black College and University (HBCU) in Jefferson City MO, installed 5 sub-canopy weather stations at the end of the MOFLUX vegetation plot transects. He is interested in microclimate variability, particularly with respect to soil moisture variations and rainfall interception by the canopy. In the future, Dr. Zeiger is also interested in quantifying runoff in ephemeral streams around the MOFLUX tower.

Dr. Christian Frankenberg of CalTech sent two GPS units to deploy at MOFLUX, one on the tower and the other in the sub-canopy space. The canopy water content and vegetation optical depth can be retrieved based on the attenuation of the GPS signal. This will enhance our ability to study forest drought responses, as well as understanding canopy SIF dynamics.

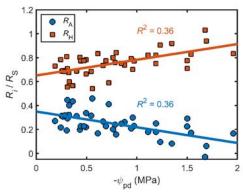


Fig. T6.4. Intensifying ecosystem drought stress as represented by the community predawn leaf water potential  $(\psi_{\rm pd})$  increases and decreases the relative contribution of heterotrophic  $(R_{\rm H})$  and autotrophic  $(R_{\rm A})$  respiration to total soil respiration  $(R_{\rm S})$ , respectively.

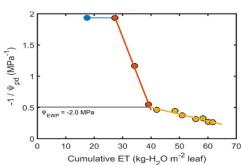


Fig. T6.5. Ecosystem "pressure-volume" analysis in reciprocal  $\Psi_{pd}$  – cumulative ET space. The ecosystem wilting point ( $\Psi_{EWP}$ ) corresponds to the change point in the slope during the strong decline in the  $-1/\Psi_{pd}$  vs. cumulative ET plot.

Task 6. Deliverable status FY2020 Through FY2022

Date	Deliverable	Status
Sept 2020	Report on EC/SIF applicability in SPRUCE enclosures	The system moved to non-enclosed Plot 2 due to interference with existing measurements in the enclosed plot
December 2020	Manuscript on within-canopy variations of PAM parameters	Measurements not conducted due to covid-19
April 2021	Complete the development and test of LED/resistor circuit and software for streamlining the FAME absolute irradiance calibration	Complete
May 2021	Submit 2020 MOFLUX data to AmeriFlux	Complete
Oct 2021	Submit a manuscript on photophysical modeling of photosynthesis	Planned
Dec 2021	Submit a manuscript on photochemical modeling of photosynthesis	Planned
May 2022	Submit 2021 MOFLUX data to AmeriFlux	Planned

- Task 6 Publications/Manuscripts
- Chang CY, Zhou R, Kira O, Marri S, Skovira J, Gu L, Sun Y (2020) An Unmanned Aerial System (UAS) for concurrent measurements of solar-induced chlorophyll fluorescence and hyperspectral reflectance toward improving crop monitoring. *Agricultural and Forest Meteorology* 294. <a href="https://doi.org/10.1016/j.agrformet.2020.108145">https://doi.org/10.1016/j.agrformet.2020.108145</a>
- Chen A, Mao J, Ricciuto D, Xiao J, Frankenberg C, Li X, Thornton PE, Gu L, Knapp AK (2021) Moisture availability mediates the relationship between terrestrial gross primary production and solar-induced fluorescence: Insights from global scale variations. Global change biology 27: 1144-1156.
- Chu H, ... Wood JD and 68 other authors (2021) Footprint representativeness of eddy covariance flux measurements across AmeriFlux sites. *Agricultural and Forest Meteorology* 301–302:108350, <a href="https://doi.org/10.1016/j.agrformet.2021.108350">https://doi.org/10.1016/j.agrformet.2021.108350</a>.
- Denham SO, Oishi AO, Miniat CF, Wood JD, Yi K, Benson MC, Novick KA (2021) Eastern US deciduous tree species respond dissimilarly to declining soil moisture but similarly to rising evaporative demand. *Tree Physiology* 41:944-959, <a href="https://doi.org/10.1093/treephys/tpaa153">https://doi.org/10.1093/treephys/tpaa153</a>.
- Griffis TJ, Roman DT, Wood JD, Deventer MJ, Fachin L, Rengifo J, Castillo DD; Lilleskov E, Kolka R, Chimner RA, del Aguilla J, Wayson C, Hergoualc'h K, Baker JM, Cadillo-Qurroz H, Ricciuto DM (2020) Hydrometeorological sensitivities of net ecosystem carbon dioxide and methane exchange of an Amazonian palm swamp peatland. *Agricultural and Forest Meteorology* 295:108167, doi: <a href="https://doi.org/10.1016/j.agrformet.2020.108167">https://doi.org/10.1016/j.agrformet.2020.108167</a>.
- He L, Wood JD, Sun Y, Magney T, Dutta D, Köhler P, Zhang Y, Yin Y, Frankenberg C (2020) Tracking seasonal and interannual variability in photosynthetic downregulation in response to water stress at a temperate deciduous forest, *Journal of Geophysical Research: Biogeosciences* 125:e2018JG005002. doi: <a href="https://doi.org/10.1029/2018JG005002">https://doi.org/10.1029/2018JG005002</a>.
- Hu C, Griffis TJ, Baker JM, Wood JD, Millet DB, Yu Z, Lee X (2020) Modeling the sources and transport processes during extreme ammonia episodes in the U.S. Corn Belt, *Journal of Geophysical Research: Atmospheres* 125:e2019JD031207, doi: 10.1029/2019JD031207.
- Hu C, Griffis TJ, Frie A, Baker JM, Wood JD, Millet DB, Yu Z, Yu X, Czarnetzki AC (2021) A multiyear constraint on ammonia emissions and deposition within the U.S. Corn Belt. *Geophysical Research Letters* 48, e2020GL090865, <a href="https://doi.org/10.1029/2020GL090865">https://doi.org/10.1029/2020GL090865</a>.
- Kira O, Chang C Y-Y, Gu L, Wen J, Hong Z, Sun Y (2021) Partitioning net ecosystem exchange (NEE) of CO2 using solar-induced chlorophyll fluorescence (SIF). *Geophysical Research Letters* 48, e2020GL091247.
- LeRiche EL, VanderZaag AC, Wood JD, Wagner-Riddle C, Dunfield K, McCabe J, Gordon R (2020) Does overwintering change the inoculum effect on methane emissions from stored liquid manure? *Journal of Environmental Quality* 49:247–255, doi: <a href="https://doi.org/10.1002/jeq2.20003">https://doi.org/10.1002/jeq2.20003</a>.
- Meng L, Zhou Y, Gu L, Richardson AD, Peñuelas J, Fu Y, Wang Y, Asrar GR, De Boeck HJ, Mao J, Zhang Y, Wang Z (2021) Photoperiod decelerates the advance of spring phenology of six deciduous tree species under climate warming. *Global Change Biology* (in press). https://doi.org/10.1111/gcb.15575
- Yu X, Millet DB, Wells KC, Griffis TJ, Chen X, Baker JM, Conley SA, Smith ML, Ghvakharia A, Kort EA, Plant G, Wood JD (2020) Top-down constraints on methane point source emissions from animal agriculture and waste based on new airborne measurements in the US Upper Midwest, *Journal of Geophysical Research: Biogeosciences* 125:e2019JG005429, doi: https://doi.org/10.1029/2019JG005429.
- Wang Y, Zhang H, Ciais P, Groll D, Huang Y, Wood JD, Ollinger S, Tang X, Prescher A-K (2021) Microbial activity and root carbon inputs are more important than soil carbon diffusion in simulating soil carbon profiles. *Journal of Geophysical Research: Biogeosciences* 126:e2020JG006205. <a href="https://doi.org/10.1029/2020JG006205">https://doi.org/10.1029/2020JG006205</a>.

#### CARBON-CYCLE FOCUSED WORK

# Task 3abc: Mechanistic Carbon Cycle modeling

This task incorporates model development and MODEX activities at the point scales (Task 3a), regional to global scales (Task 3b), and at the level of mechanistic functional units (Task 3c) to identify process contributions to the global climate C cycle forcing from terrestrial ecosystems. Brief summaries of progress are presented along with tabular summaries of progress on proposed deliverables.

<u>ELM-SPRUCE CH4 modeling</u> – A series of two papers reporting the CH4 module of the ELM-SPRUCE model has been accepted; these papers introduce the incorporation of the microbial-functional group-based CH4 module into the ELM-SPRUCE model and its application to the warming and eCO2 impacts on CH4 processes at the S1 bog (Ricciuto et al 2021; Yuan et al., 2021). The model reproduced the observed vertical distributions of dissolved organic C and acetate concentrations. The seasonality of acetoclastic and hydrogenotrophic methanogenesis – two key processes for CH4 production – and CH4 concentration along the soil profile were accurately simulated. Meanwhile, the model estimated that plant-mediated transport, diffusion, and ebullition contributed to approximately 23.5%, 15.0%, and 61.5% of CH4 transport, respectively. The model application to the S1 bog examined the mechanistic processes of how warming and eCO2 affect methanogenesis and methanotrophs along soil profile. We found that warming and eCO2 stimulate peatland CH4 emissions through different mechanisms. The stimulating impact of warming is primarily through the stimulation of microbial processes. The stimulating impact of eCO2 is primarily through enhanced substrate availability by increased photosynthesis.

The isotopic component of the CH<sub>4</sub> module has been successfully developed (Fig. T3.1). The pools and fluxes of <sup>13</sup>C and <sup>14</sup>C are added to all C pools and processes associated with CH<sub>4</sub> processes in the ELM-SPRUCE; for example, the dissolved organic C has additional pools of <sup>13</sup>C and <sup>14</sup>C (in current simulations <sup>14</sup>C is kept off). On the SPRUCE all hands meeting in May 2021, the preliminary results of the isotopic CH<sup>4</sup> module have been presented; further improvement and testing are ongoing. A manuscript will be developed to publish this effort in the second half of the 2021.

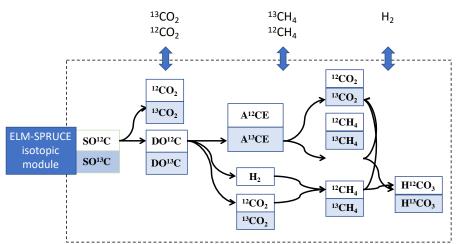


Fig. T3.1. A diagram showing isotopic processes and pools component of the ELM-SPRUCE methane module (ACE: acetic acid; SOC: soil organic C; DOC: dissolved organic C; <sup>14</sup>C is not shown but is kept in the code)

<u>ELM-SPRUCE soil and vegetation modeling</u> — With the comprehensive measurements at SPRUCE, we are able to evaluate model performance at the process level. It was found that ELMv1-SPRUCE simulated net C exchange (NCE) responses to warming is consistent with field observations under ambient CO<sub>2</sub> conditions. However, ELM-SPRUCE fails to capture the observed general lack of response to eCO<sub>2</sub> concentrations (Hanson et al., 2020). A more detailed analyses of model results suggest that model simulated eCO<sub>2</sub> responses is mostly in the non-structural C (NSC) pool. Ward et al. (2019) showed

that NSC in two shrub species increased significantly under eCO<sub>2</sub> condition. Preliminary data for spruce and larch also show significant increase of NSC under eCO<sub>2</sub> (J. Peters, unpublished data). A more detailed evaluation of NSC responses between model and observations is underway. We also compared simulated ANPP responses to warming with field observations for each PFT at SPRUCE site. It was found that although ELM-SPRUCE simulated shrub NPP compares well with observations at lower temperature treatment, ELM-SPRUCE fails to capture the observed increasing productivity with warming. Malhotra et al. (2019) suggested the increased productivity of shrub is mainly due to the significant increase of find root length, which allows plants to have greater access of soil nutrients. Since ELM-SPRUCE does not explicitly represent root traits such as specific root length and the linkage between root traits and nutrient uptake, we designed two simulations to test if the increased shrub productivity is due to greater access to nutrients for plants: (1) the default shallow root (2) the deeper fine root to allow plants to have greater access to nutrients. Simulations results show that with deeper fine roots, shrub productivity is greatly increased, consistent with observations. This suggests that it is critical to improve the representation of fine root traits and nutrient uptake in ELM-SPRUCE.

Sphagnum mosses modeling – We developed a Sphagnum moss PFT and associated processes within the ELM-SPRUCE model and used the updated model to examine the ecosystem response to warming and eCO<sub>2</sub> at a temperate bog ecosystem. The new model can capture the seasonal dynamics of moss Sphagnum GPP and predict reasonable annual values for Sphagnum NPP. The model predicts that different PFTs responded differently to warming levels under both ambient and eCO<sub>2</sub> concentration conditions. The NPP of two dominant tree PFTs showed contrasting responses to warming scenarios (increasing with warming for Larix but decreasing for black spruce), while shrub NPP had similar warming response to Larix. Hummock and hollow Sphagnum showed opposite warming responses: hollow Sphagnum shows generally higher growth with warming, but the hummock Sphagnum demonstrates more variability and strong dependence with water table height. The ELM-SPRUCE predictions further suggest that the effects of CO<sub>2</sub> fertilization can change the direction of the warming response for the bog peatland ecosystem (Shi et al., 2021).

<u>Canopy Processes</u> – Effective use of solar-induced chlorophyll fluorescence (SIF) to estimate and monitor gross primary production (GPP) in terrestrial ecosystems requires a comprehensive understanding and quantification of the relationship between SIF and GPP. We derived the GPP/SIF ratio from multiple data sources as a diagnostic metric to explore its global-scale patterns of spatial variation and potential climatic dependence. We found that the growing season GPP/SIF ratio varied substantially across global land surfaces, with the highest ratios consistently found in boreal regions; spatial variation in GPP/SIF was strongly modulated by climate variables; and the most striking pattern was a consistent decrease in GPP/SIF from cold-and-wet climates to hot-and-dry climates. Furthermore, we show that GPP/SIF can be empirically modeled from climate variables using a machine learning (random forest) framework, which can improve the modeling of ecosystem production and quantify its uncertainty in global terrestrial biosphere models. Relevant work is detailed by Chen et al. (2020) and is highlighted in a Commentary by Jeong and Park (2020).

<u>Phenology</u> – We introduced new seasonal-deciduous phenology schemes into version 1.0 of ELM and evaluated their performance against the SPRUCE PhenoCam observations from 2015 to 2018 (Meng et al., 2021). We found that phenology simulated by the revised ELM (i.e., earlier spring onsets and stronger warming responses of spring onsets and autumn senescence) was closer to observations than simulations from the original algorithms for both the deciduous conifer and mixed shrub layers (Fig. T3.2). Moreover, the revised ELM generally produced higher C and water fluxes during the growing season and stronger flux responses to warming than the default ELM. A parameter sensitivity analysis further indicated the significant contribution of phenology parameters to uncertainty in key C and water cycle variables, underscoring the importance of precise phenology parameterization. This phenological modeling effort demonstrates the potential to enhance the E3SM representation of land-climate interactions at broader spatiotemporal scales, especially under anticipated eCO<sub>2</sub> and warming conditions.

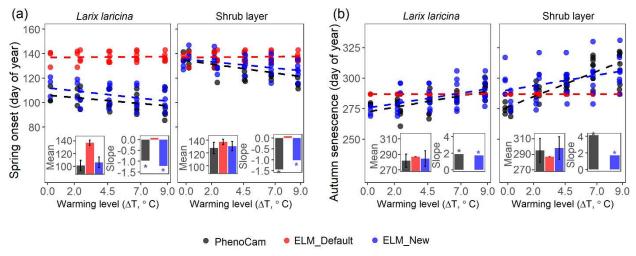


Fig. T3.2. Observed and simulated responses of spring onset (a) and autumn senescence (b) to warming at SPRUCE. Linear regression lines are shown as dashed lines. The mean phenology across all warming and  $CO_2$  levels and slopes of phenology against warming levels are shown in the subfigures. The error bars in the subfigures represent the standard deviations of phenology across all warming levels. Significance P < 0.1 from two-tailed Student's t test. Spring onset was during 2016 to 2018, and autumn senescence was during 2015 to 2018.

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

<u>Uncertainty quantification and functional units</u> – We are developing machine learning workflows to enable uncertainty quantification at SPRUCE, MOFlux, and other observation sites of interest. A new method has been developed for model-independent data assimilation (MIDA; Huang et al., 2021). The Offline Land Model Testbed (OLMT; <a href="https://github.com/dmricciuto/OLMT">https://github.com/dmricciuto/OLMT</a>) has been updated to include automated parameter sensitivity analysis and model calibration techniques. It is currently being applied at SPRUCE to visualize model uncertainty. We are also developing an AI-enabled ELM diagnostic and validation framework that will speed-up the ELM function validation at different spatial-temporal scales. This leverages work being done in the E3SM next generation development (NGD), taking advantage of GPU architectures that we will use to increase the efficiency of MODEX at regional to global scales.

Task 3abc Deliverable status FY2020 and FY2021

Date	Deliverable	Status
2020	Complete new phenology submodel	Completed (Meng et al., accepted)
	Complete improved fire submodel	Underway (Tang et al., accepted)
	Complete manuscript on model evaluation with	Completed (Salmon et al., accepted)
	improved nutrient cycling	
	Develop root function, nutrient cycling, disturbance	Underway
	functional units/surrogates	•

	Integrate SIF module into ELM and the canopy	Partially completed (Chen et al., 2020;
	functional unit	Chen et al., accepted)
	Enable data assimilation capability with ELM-EcoPAD	Completed (Huang et al., in review)
	Integrate 4 additional models into EcoPAD for SPRUCE	Underway
	intercomparison	
2021	Regional benchmarking of ELM including new	Complete
	improvements	
	Complete ELM forcing factor simulations and publish	Underway
	results	
	Publish results of improved ELM-SPRUCE model	Complete (Shi et al., 2021; Meng et al,
		accepted)
	Integration of new model features into E3SM code base	Underway
	Complete high-resolution and regional simulations	Underway
	Publish multi-model SPRUCE intercomparison	Underway

#### Task 3abc Publications

- Chen A, Mao J, Ricciuto D, Lu D, Knapp AK (2021) Season changes in GPP/SIF ratio and their climatic determinants across the Northern hemisphere. *Global Change Biology* (accepted).
- Chen A, Mao J, Ricciuto D, Xiao J, Frankenberg C, Li X, Gu L, Knapp A (2020) Moisture availability mediates the relationship between terrestrial gross primary production and solar-induced fluorescence: Insights from global scale variations. *Global Change Biology* https://doi.org/10.1111/gcb.15373.
- Huang X, Lu D, Ricciuto DM, Hanson PJ, Richardson AD, Lu X, Weng E, Nie S, Jiang L, Hou E, Steinmacher IF, Luo Y (2021) A Model-Independent Data Assimilation (MIDA) module and its applications in ecology, *Geosci. Model Dev. Discuss.* [in press], https://doi.org/10.5194/gmd-2021-33 (in review)
- Meng L, Mao J, Ricciuto D, Shi X, Richardson A, Hanson P, Warren J, Zhou Y, Li X, Zhang L, Schädel C (2021) Evaluation and modification of ELM seasonal deciduous phenology against observations in a Southern boreal peatland forest. *Agricultural and Forest Meteorology (accepted)*
- Ricciuto D, Xu X, Shi XY, Wang Y, Song X, Schadt C, Griffiths N, Mao JF, Warren JM, Thornton PE, Chanton J, Keller JK, Bridgham S, Gutknecht J, Sebestyen S, Finzi AC, Kolka R, Hanson PJ (2021). An integrative model for soil biogeochemistry and methane processes: I. Model structure and sensitivity analysis. *Journal of Geophysical Research Biogeosciences* (accepted).
- Shi X, Ricciuto DM, Thornton PE, Xu X, Yuan F, Norby RJ, Walker AP, Warren J, Mao J, Hanson PJ, Meng L, Weston D, Griffiths NA (2021) Extending a land-surface model with Sphagnum moss to simulate responses of a northern temperate bog to whole ecosystem warming and elevated CO<sub>2</sub>, *Biogeosciences* 18:467–486, https://doi.org/10.5194/bg-18-467-2021
- Tang R, Mao J, Jin M, Chen A, Yu Y, Shi X, Zhang Y, Hoffman F, Xu M, Wang Y (2021) Interannual variability and climatic sensitivity of global wildfire activity. *Advances in Climate Change Research* (accepted).
- Yuan F, Wang Y, Ricciuto DM, Shi X, Yuan F, Hanson PJ, Bridgham S, Keller JK, Thornton PE, Xu X (2021) An Integrative Model for Soil Biogeochemistry and Methane Processes: II. Warming and elevated CO<sub>2</sub> Impacts on Peatland CH<sub>4</sub> Emission. *Journal of Geophysical Research-Biogeosciences* (accepted).

# Task 3d: Multi-Assumption Systems Modeling

Ecosystem models are composed of inter-connected quantitative hypotheses and assumptions intended to represent the mechanics of an ecosystem's component processes. Viewing models in this way connects them directly to the language of experiments and observations and recognizes that multiple hypotheses or assumptions is the norm for many of the processes represented in a model (Walker *et al.* 2018). However, few methods and tools exist to rigorously incorporate and evaluate these multiple competing and quantitative hypotheses. With this motivation, new open-source 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 specifically for formal and informal evaluation of alternative model process representations. In this Phase, Task 3d is primarily focussed around understanding how alternative process hypotheses lead to variability in below-ground processes.

FY21 has seen good progress within Task 3d. The manuscript titled "Multi-hypothesis analysis of Farquhar and Collatz photosynthesis models reveals unexpected influence of empirical assumptions" has been published in Global Change Biology (Walker et. al., 2021). Science results were described in the previous report and in a BER Highlight.

Matt Craig's (post-doc on Task 3d) paper titled "Biological mechanisms may contribute to soil C saturation patterns" has recently been published in Global Change Biology (Craig et al., 2021). This paper uses the first generation of the multi-assumption soil C (C) model in MAAT, as well as a new data synthesis, to investigate the mechanisms underlying soil C saturation (i.e. the limits to soil C storage as organic inputs increase). Whereas models typically represent an assumption that this phenomenon is driven by soil texture, we show that soil C saturation could also be driven by constraints on soil microbes. To do this, we compiled data from field and laboratory experiments and found evidence of microbial population limits as organic inputs increase. Then, we simulated these limits in a soil C model and found that apparent saturation could occur even without assuming an innate upper limit. The results imply that more realistic representations of microbes in soil C models could help us predict how soils will respond to environmental change and could help us manage soils to store more C.

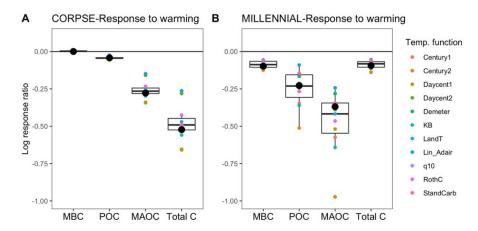


Fig. T3.3 Simulated response of soil carbon (C) pools (microbial [MBC], particulate [POC], mineral-associated [MAOC], and total C) to 10 years of warming for two contemporary soil C models (CORPSE and MILLENNIAL) using 12 different temperature response functions. The function typically employed in each model (Arrhenius in CORPSE and modified Daycent2 in MILLENNIAL) is shown in black.

We continue development of the multi-assumption soil C model in MAAT. Modern soil C models are numerous, represent different hypotheses about the dominant processes governing soil C dynamics, and increasingly employ more complicated representations of microbial and mineral interactions. Thus, there has been an explosion of potential soil C model configurations leading to highly divergent model predictions about soil C responses to global change. Systematic evaluation of this process-level uncertainty is critical to guide future empirical studies and model development. Thus, our goals are to 1) develop a generalizable model structure that can assimilate state-of-the-art soil decomposition models and 2) use this tool to probe the sources of inter-model uncertainty. In addition to our progress on generalizing soil C models reported in Craig et al. (2021), we have incorporated four modern soil C models into MAAT: MEND (Wang et al., 2013), MIMICS (Wieder et al., 2014), MILLENIAL (Abramoff et al., 2018), and CORPSE (Sulman et al., 2014). We are using MAAT to explore the extent to which specific process representations lead to variable predictions among these models. As one example, we find that the choice of a temperature response function leads different soil C trajectories in a model warming experiment, but the sensitivity of specific pools varies among models (Fig. T3.3). We plan to submit a manuscript on this project within the next year.

Task 3d Deliverable status FY2020 and FY2021

Date	FY20 Deliverables	Status
December 2021	2. Parameter estimation and hypothesis testing in SPRUCE Sphagnum	On hold, seeking
(revised last	photosynthesis and respiration data 2014-2018	candidate
annual report)		
April 2020	3. pbdr enabled MAAT to run on OLCF	50 % complete
April 2020	4. Multi-assumption soil decomposition model	70 % complete
April 2021	6. Structural and parametric uncertainty quantification of soil decomposition model	Complete (Craig
		et al 2021)
September 2021	5. Multi-assumption root resource acquisition model	In Progress
Sept 2021	7. Structural and parametric uncertainty quantification of root nutrient acquisition	In Progress
	and nutrient competition models	

# **FY20 Papers and Datasets**

- Craig ME, Mayes MA, Sulman BN, Walker AP (2021) Biological mechanisms may contribute to soil carbon saturation patterns. *Global Change Biology* 27:2633–2644. https://doi.org/10.1111/gcb.15584
- Craig ME, Walker AP (2021) Biological mechanisms may contribute to soil carbon saturation patterns: Modeling archive. Oak Ridge, TN: Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy. https://doi.org/10.25581/ornlsfa.022/1768048
- Friedlingstein P, O'Sullivan M, Jones MW, Andrew RM, Hauck J, Olsen A, Peters GP, Peters W, Pongratz J, Sitch S, Le Quéré C, Canadell JG, Ciais P, Jackson RB, Alin S, Aragão LEOC, Arneth A, Arora V, Bates NR, ... Zaehle S (2020). Global Carbon Budget (2020) *Earth System Science Data* 12:3269–3340. https://doi.org/10.5194/essd-12-3269-2020
- Jung M, Schwalm C, Migliavacca M, Walther S, Camps-Valls G, Koirala S, Anthoni P, Besnard S, Bodesheim P, Carvalhais N, Chevallier F, Gans F, Goll DS, Haverd V, Köhler P, Ichii K, Jain AK, Liu J, LombardozziD, ... Reichstein M (2020) Scaling carbon fluxes from eddy covariance sites to globe: Synthesis and evaluation of the FLUXCOM approach. *Biogeosciences* 17:1343–1365. https://doi.org/10.5194/bg-17-1343-2020
- Keller AB, Brzostek ER, Craig ME, Fisher JB, Phillips RP (2021) Root-derived inputs are major contributors to soil carbon in temperate forests, but vary by mycorrhizal type. *Ecology Letters* 24:626–635. https://doi.org/10.1111/ele.13651
- Mushinski RM, Payne ZC, Raff JD, Craig ME, Pusede SE, Rusch DB, White JR, Phillips RP (2021) Nitrogen cycling microbiomes are structured by plant mycorrhizal associations with consequences for nitrogen oxide fluxes in forests. *Global Change Biology* 27:1068–1082. https://doi.org/10.1111/gcb.15439
- Walker AP, Johnson AL, Rogers A, Anderson J, Bridges RA, Fisher RA, Lu D, Ricciuto DM, Serbin SP, Ye M (2021) Multi-hypothesis comparison of Farquhar and Collatz photosynthesis models reveals the unexpected influence of empirical assumptions at leaf and global scales. *Global Change Biology* 27:804–822. https://doi.org/10.1111/gcb.15366

### PROCESS-LEVEL STUDIES (PLS)

# Task 4c: Linking Root Traits to Function

The root function task was developed to improve understanding of root function and implications for modeling. We continue to leverage the unique capabilities of the neutron imaging facilities at ORNL for assessment of root traits, function and interactions with soil microbes and soil physicochemical attributes. Our prior work quantified these dynamics, including root-specific water uptake linked to traits, such as diameter or order (Dhiman et al., 2019). Subsequent modeling of these data revealed that roots and mycorrhizae may affect soil hydraulic properties, which have a direct impact on ELM and other process-based modeling efforts. We are finalizing analysis of subsequent laboratory and neutron-imaging based confirmation of the modeling results, and a manuscript is in preparation for submission later this year. Other neutron imaging work has led to development of new software for automated root and soil water analysis, and its application revealed rhizosphere development is linked to root size across species. Two manuscripts developed from that work by a student that has since moved on were postponed - PI Warren and neutron scattering scientists are developing a plan for reanalysis, revision and resubmission of those papers (DeCarlo et al. 2021a, b). Data are directly applicable to models that assess mechanistic soil to root hydraulics, such as ELM-FATES.

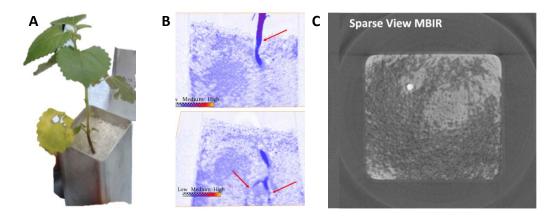


Fig. 4c.1. (A) Fatoua villosa (mulberry weed) plant in sample chamber; (B) axial slices from fast neutron computed tomography (NCT) showing stem/root system in situ (arrows); (C) NCT radial slice reconstructed based on machine learning algorithms showing belowground stem (white dot).

Our neutron imaging of belowground systems continues to develop (Fig. 4c.1). A techniques paper on the use of the HFIR CG1D beamline, including application to a plant-soil system was developed and a video production of the technique is pending filming (Bilheux et al. 2021). We have also been focused on developing faster neutron computed tomography (NCT) acquisition times to improve measurement of soil and root water dynamics in 3D (Venkatakrishnan et al, 2021) and new beamtime was awarded this FY for further experimentation and development of the necessary machine learning techniques. We remain engaged in the broader development of neutron imaging techniques with a focus on plant and soil water, nutrient, and C dynamics. A complementary study of bioenergy wood pyrolysis using multimodal NCT and X-ray CT sequentially was successful (Ossler et al. 2021) and similar multimodal techniques can be applied to belowground systems. We have also participated in new future beamline proposals for the Spallation Neutron Source (SNS) that leverage more advanced techniques, such as neutron interferometry and Bragg edge imaging, and which could enable unprecedented insight in soil, rhizosphere and root function in situ. In addition, we are drafting a comprehensive review article on neutron imaging in the Geosciences (with a focus on soil and root dynamics) for submission to Annual Reviews.

We continue to focus on assessing linkages between root traits, mycorrhizae and root respiratory (Rs) response to environmental dynamics in order to improve autotrophic vs heterotrophic Rs modeling. In collaboration with the Root Traits Task, and to provide additional physiology data to FRED, we have established a relationship with The Morton Arboretum to assess root, hyphal and soil respiration

dynamics for tree species with divergent root traits. As such, we constructed 108 root/fungal exclusion collars that are currently being installed in different monoculture stands at Morton. Collars will be periodically measured for respiration rates and linked to above/below ground traits and environmental conditions to provide novel root functional data for models that increasingly consider root function. This effort has synergy with MAAT, MOFLUX and NIST research efforts.

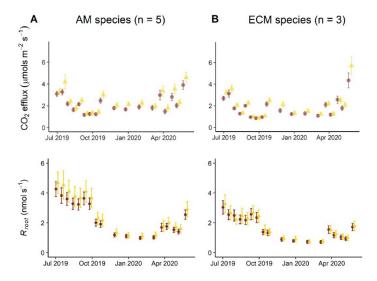


Fig. 4c.2. (A) Soil CO<sub>2</sub> efflux rates for arbuscular mycorrhizal species (Liriodendron tulipifera, Liquidambar styraciflua, Cercis canadensis, Acer rubrum, and Nyssa sylvatica) and (B) ectomycorrhizal (Pinus taeda, Fagus grandifolia, and Oxydendrum arboretum); and rates of fine root system respiration (Rroot) indicating greater rates for arbuscular mycorrhizal species. Dark symbols are treated with fungicide/bactericide and have lower root respiration rates.

Analysis and manuscript preparation was completed for an *in-situ* root respiration project facilitated by a DOE Office of Science Graduate Student Research (SCGSR) Program fellowship. This study focused on assessing root traits and their linkages to seasonal respiration *in situ* using a novel measurement system that assessed a single 3<sup>rd</sup> or 4<sup>th</sup> order root system while attached to mature temperate tree species. In that study, rates of root system CO<sub>2</sub> efflux ranged between 10 and 90 µmols m<sup>-2</sup> sec<sup>-1</sup>, with ectomycorrhizal species having slightly greater rates than arbuscular mycorrhizal species. (Fig. 4c.2; Hogan et al. under review).

Task 4c. Deliverable status FY2020 and FY2021.

Date	Deliverable	Status
January 2020	Revise and resubmit (2) manuscripts on root rhizosphere water dynamics based on neutron imaging	Postponed
October 2020	Building root/hyphal separation chambers and shipment to Morton Arboretum	Completed
April 2021	Publish new manuscripts on neutron imaging techniques and analysis	Completed
May 2021	Publish manuscript on above/belowground physiological acclimation to warming in <i>Populus trichocarpa</i>	Under review
July 2021	Use neutron beamtime to further develop analysis techniques for assessing root function <i>in situ</i> using fast neutron imaging	Underway
August 2021	Develop and test measurement techniques of root respiration of woody root systems at SPRUCE (outside plots)	Planned
December 2021	Develop comprehensive review article on neutron imaging in the Geosciences (including root, rhizosphere and soil dynamics)	Underway
December 2021	Publication on root and mycorrhizal impacts on soil hydraulic properties	Underway

Task 4c New Publications and Manuscripts

Bilheux HZ, Cekanova M, Warren JM, Meagher MJ, Ross R, Bilheux JC, Venkatakrishnan S, Lin JYY, Zhang Y, Pearson MR, Stringfellow E (2021) Neutron radiography and computed tomography of biological systems. *Journal of Visualized Experiments* https://doi.org/10.3791/61688

- DeCarlo KF, Caylor K, Bilheux H, Warren JM (2020a) Integrating fine root morphology and soil distance mapping to characterize the plant-soil interface. *Plant and Soil* (in revision).
- DeCarlo KF, Bilheux JC, Bilheux H, Caylor K, Warren JM (2020b) RootProcessing: An open-source python package for root/soil analysis at the neutron imaging beamline at ORNL. *Plant and Soil* (in revision).
- Hogan JA, Baraloto C, Ficken C, Clark MD, Weston D, Warren JM (2020) The physiological acclimation and growth response of *Populus trichocarpa* to warming. *Physiologia Plantarum (in press)*
- Hogan JA, Labbé JL, Carrell AA, Franklin J, Hoyt KP, Valverde-Barrantes OJ, Baraloto C, Warren JM (2021) Functional variability in specific root respiration translates to differences in belowground CO<sub>2</sub> efflux in a temperate deciduous forest. *Geoderma* (under review)
- Ossler F, Finney CEA, Warren JM, Bilheux JC, Zhang Y, Mills RA, Santodonato LJ, Bilheux HZ (2021) Dynamics of hydrogen loss and structural changes in pyrolyzing biomass utilizing neutron imaging. *Carbon* 176:511-529. <a href="https://doi.org/10.1016/j.carbon.2020.11.060">https://doi.org/10.1016/j.carbon.2020.11.060</a>
- Venkatakrishnan S, Ziabari A, Hinkle J, Needham AW, Warren JM, Bilheux HZ (2021) Convolutional neural network based non-iterative reconstruction for accelerating neutron tomography. *Machine Learning Science and Technology* 2(025031):1-18 <a href="https://doi.org/10.1088/2632-2153/abde8e">https://doi.org/10.1088/2632-2153/abde8e</a>

#### Task 5: Microbial Processing of Soil C

Experimental and modelling studies continued to focus on the key role of microbial activity in influencing CO<sub>2</sub> emissions and soil C cycling and particularly to understand the role of soil moisture which has been neglected in the literature in comparison to temperature.

In association with the MOFLUX Task 6, we continued soil core sampling and site monitoring of the four soil chambers that were trenched to isolate heterotrophic respiration (ongoing since 2017). We are working to understand connections between below-ground microbial respiration and canopy photosynthesis at MOFLUX using novel combination of trenching experiments and sun-induced chlorophyll fluorescence measurements (Wood et al. under preparation). Following our recent work with the ELM model at MOFLUX (Liang et al. 2019), the Microbial Enzyme Decomposition model (MEND) was parameterized with 11 years of observations to predict long-term (100 year) soil organic C (SOC) dynamics under five extreme moisture scenarios with different frequencies and severities (Liang et al. accepted pending minor revisions). Results showed that the changes in active microbial biomass C and the corresponding turnover rates of SOC pools were more sensitive to extreme soil drying than soil wetting, due to decreases in active microbial biomass, dissolved organic C substrate, and extracellular enzyme concentrations associated with the extreme dryness simulations, which were not able to be compensated by increases under wetting conditions. As a result, the decomposition of SOC and CO<sub>2</sub> emissions were reduced.

Recently published lab and field experiments performed by Dr. Shikha Singh support these predictions. Dr. Singh defended her PhD at the University of Tennessee in December 2020, and she was supported by Task 5 throughout her dissertation work. As mentioned last year, a moisture manipulation experiment – drought, rainfed, and irrigated – in a soybean field in western Tennessee showed decreases in CO<sub>2</sub> emissions, microbial biomass, enzyme activity under the imposed drought compared to rainfed and irrigated conditions (Singh et al., 2021a). Then, a set of lab experiments involving 3 different soil textures (sandy soils, loamy soils from MOFLUX, and clayey soils) were conducted over a range of soil moistures and over steady-state and transient conditions. The steady state moisture manipulation experiment showed different moisture optima for highest microbial respiration for different textured soils. Extractable organic C was greatest under dry conditions, and C degrading enzyme activity was lowest, indicating lower microbial activities for all soil textures (Singh et al., 2021b). The transient incubation experiment sought to understand mechanisms fueling rapid decomposition following the wetting of dry soils ("Birch effect"), by comparing the different textured soils that were air-dried and at water holding capacity, under both steady-state and transient conditions. We found higher cumulative SOC loss under transient moisture state compared to steady state, and that different mechanisms contributed to the Birch

effect in different textured soils (Fig. T5.1). In sandy soil, metabolite accumulation and changes in bacterial community structure were the most important Birch effect drivers; while in loamy and clayey soils, metabolite accumulation and release of aggregate protected C were more important (manuscript under preparation). Therefore, the response of microbial respiration to changing soil moisture will strongly depend on the sensitivity to textural differences.

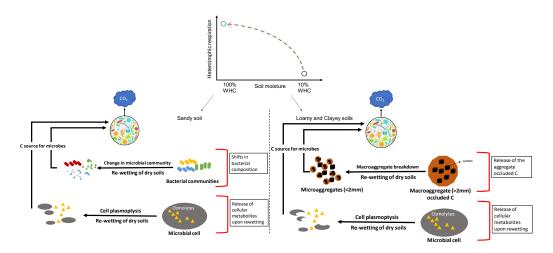


Fig. T5.1. Conceptual model of microbial responses to transient changes in soil moisture, as a function of soil texture. Source (Singh 2020).

Dr. Siyang Jian defended his PhD at Tennessee State University (note, TSU is an Historically Black College) in July of 2020, and he was also supported by Task 5 throughout his dissertation work. His paper, explained in last year's report, about how MEND microbial parameter values are affected by the length of the incubations from which they were generated, was published in *Nature Communications* (Jian et al. 2020). The paper compares model predictions with a meta-analysis of field-scale warming experiments and suggests that parameters from short-term incubations are most applicable to predicting changes in SOC stocks associated with short-term warming experiments; and parameters from long-term incubations are most applicable to predicting changes in SOC stocks associated with long-term warming experiments. The implications are that both incubations and field-scale warming experiments conducted over short-time frames will tend to predict large losses of SOC stocks that are not sustained when experiments are allowed to continue over longer time frames. Microbial community acclimation and the resultant changes in fitted microbial parameters with time is the most likely cause. Dr. Jian is preparing an additional paper exploring the extent to which model microbial parameters from incubation experiments can be generalized across multiple sites. Initial results suggest that model microbial parameters are highly site-specific.

Finally, in a modeling collaboration with Task 3 (Multi-Assumption Architecture and Testing), we found that apparent saturation of SOC can occur as a result of limitations in microbial biomass (Craig et al. 2021). The model simulations look very similar to the widely recognized phenomena of mineral saturation, and the results therefore suggest that multiple factors can give the appearance of a saturation effect in SOC cycling models.

<u>COVID-19 Delays</u> – The microbial biomass sampling at SPRUCE was delayed from 2020 to 2021 due to travel restrictions associated with Covid-19.

<u>Future Plans</u> - We are developing a whole-ecosystem modeling strategy for the MOFLUX and SPRUCE sites using ELM, PFLOTRAN, and MEND. We are planning to do seasonal sampling of microbial biomass at SPRUCE to complement and enhance existing site data. We will offer samples to the microbiology task in SPRUCE, Georgia Technological University, and

the University of Minnesota in the hopes of comparing multiple types of microbial characterizations in the samples. We will continue seasonal sampling at MOFLUX.

Task 5. Deliverable Status FY2020 and FY2021

Date	Deliverable	Status
2020	Accounting for the sensitivity of soil CO <sub>2</sub> emissions to soil moisture and texture	Completed
2021	Development and initial offline testing of microbial model coupled to ELM at MOFLUX	Planned

# Task 5 Publications/Manuscripts/Datasets

- Craig ME, Mayes MA, Sulman BN, Walker AP (2021) Biological mechanisms may contribute to soil carbon saturation patterns. *Global Change Biology* 27:2633-2644, https://doi.org/10.1111/gcb.15584
- Jian S, Li J, Wang G, Kluber LA, Schadt CW, Liang J, Mayes MA (2020) Multi-year incubation experiments boost confidence in model projections of long-term soil carbon dynamics. *Nature Communications* 11:5864, doi:10.1038/s41467-020-19428-y.
- Liang J, Wang G, Singh S, Jagadamma S, Gu L, Schadt CW, Wood JD, Hanson PJ, Mayes MA (2020) Intensified soil moisture extremes decrease soil organic carbon decomposition: a mechanistic modeling analysis. *Journal of Geophysical Research Biogeosciences* (accepted pending minor revisions).
- Rewcastle KE, Moore JAM, Henning JA, Mayes MA, Patterson CM, Wang G, Metcalfe DB, Classen AT (2020) Investigating drivers of microbial activity and respiration in a forested bog. *Pedosphere* 30:1351145, doi:10.1016/S1002-0160(19)60841-6.
- Singh S, Mayes MA, Shekoofa A, Kivlin S, Bansal S, Jagadamma S (2021) Soil organic carbon cycling in response to simulated soil moisture variation under field conditions. *Scientific Reports* 11:10841 https://doi.org/10.1038/s41598-021-90359-4.
- Singh S, Jagadamma S, Liang J, Kivlin S, Wood J, Wang G, Schadt CW, DuPont J, Gowda P, Mayes MA (2021) Differential organic carbon mineralization responses to soil moisture in three different soil orders under mixed forested system. *Frontiers in Environmental Science* Article 682450 (in press).

#### Task 5 Dissertations

- Jian, Siyang (2020) Evaluation And Improvement of the Microbial Enzyme Decomposition (MEND) Model Against Multiple Incubation Experiments. PhD dissertation, Department of Agricultural and Environmental Sciences and Department of Biological Sciences, Tennessee State University, Nashville, TN.
- Singh, Shikha (2021) *Soil Moisture Sensitivity to Microbial Processing of Soil Organic Carbon*. PhD dissertation, Department of Biosystems Engineering and Soil Science, University of Tennessee, Knoxville, TN.

# GLOBAL TRAIT DATABASES (GT)

# Task 4b: Leveraging root traits to inform terrestrial biosphere models

<u>The Fine-Root Ecology Database</u> – 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. Over the past year, we have: (1) used existing data to better understand the variation in root traits within and among species and across the globe, (2) released the third version of FRED (FRED 3.0) as a searchable database, (3) continued facilitate data harvest from underrepresented ecosystems, and (4) continued to make new measurements that improve the data available to inform our understanding of belowground processes and below- and aboveground linkages.

<u>Using FRED 2.0 to answer important questions in belowground ecology</u> – Dr. Yao Liu, an ORNL post-doc co-advised by Drs. Anthony Walker and Colleen Iversen, accepted a position as a senior lecturer

at Northumbria University in the UK in September 2020, and continues to complete a manuscript on a hierarchical Bayesian assessment of the variation in root traits in FRED in relation to environmental conditions, phylogeny, and mycorrhizal symbiosis (Liu et al., *in preparation*). Furthermore, a number of groups have also used FRED as a resource to answer their own scientific questions (<a href="https://roots.ornl.gov/publications">https://roots.ornl.gov/publications</a>).

The FRED team has continued to be involved in international collaborations (<a href="https://roots.ornl.gov/synthesis-activities">https://roots.ornl.gov/synthesis-activities</a>). For example, the sROOT working group within the German Centre for Integrative Biodiversity Research (iDiv) from 2018 to 2020 leveraged FRED 2.0 to develop a 'Ready to Use' database that is a species-specific subset of FRED and TRY (Guerrero-Ramirez et al. 2021, Global Ecology and Biogeography, data citation: Guerrero-Ramirez et al. 2021), resulting a series of papers focused on the global variation in fine-root traits within the multidimensional Root Economics Space (Bergmann et al. 2020, Science Advances) and along environmental gradients (Laughlin et al. 2021, Nature Ecology & Evolution), and within and among above- and belowground plant traits (Weigelt, Mommer et al. 2021, New Phytologist Tansley Review, in press).

FRED 3.0 is now available as a searchable database! — We released the third version of the Fine-Root Ecology Database (FRED 3.0) in March 2021 (data citation: Iversen et al. 2021). We worked with web developers within ORNL's Information Technology Services Division over multiple years to encode the observations in FRED into database form (Microsoft Azure), and to develop a user interface (programmed using Vue.js for the user interface and Node.js for the data interface) that allows users to filter the observations in FRED according to their scientific needs. The user interface is accessed via <a href="https://roots.ornl.gov/public-release">https://roots.ornl.gov/public-release</a>. FRED 3.0 has more than 150,000 observations of more than 330 root traits, with data collected from more than 1400 data sources. FRED is focused on fine roots (roots traditionally defined as less than 2 mm in diameter) but accepts data collected from roots of all sizes.

We highlighted FRED 3.0 as a community resource for belowground ecologists and modelers alike (Fig. T4b.1) in an editorial that accompanies a Virtual Special Issue in *New Phytologist*, where we compiled more than 40 recent papers on the topic 'Filling gaps in our understanding of belowground plant traits across the world' (Iversen and McCormack, *New Phytologist*, *in press* to be released in July 2021).

Root traits from the tundra and the tropics are still underrepresented in FRED – The root trait framework developed by the FRED team has also been leveraged to develop a 'Root Traits Handbook' and companion paper advocating for increased quantification of functional root traits (Freschet et al. 2021a, New Phytologist, early view; Freschet et al. 2021b, New Phytologist, in press). FRED is also providing the foundation for new, biome-specific working groups related to the Arctic (the 'Arctic Underground', PIs Hewitt and Mack) and the tropics ('Tropical Forest Root Traits', PI Cusack).

<u>Making new measurements to inform our understanding of FRED observations</u> – The data in FRED are necessarily a mixture of root traits and ancillary data, quantified using a variety of methodologies. These observations need to be placed into a comprehensive framework that will allow us to more effectively use the diversity of traits in FRED to understand above- and belowground linkages across the globe. To advance this framework, we are making new observations across a phylogenetically and ecologically diverse suite of tree species from mature forestry plots at The Morton Arboretum, Lisle, IL (in collaboration with M.L. McCormack; see data portal here: <a href="http://mrootlab.info/">http://mrootlab.info/</a>). A new ORNL postdoc, Dr. Bin Wang, co-advised by Drs. Dan Ricciuto and Colleen Iversen, will use data from FRED to improve the representation of fine-root conceptualization and function in ELM, informed by linkages among root, leaf, and wood phenology as measured across plant functional types at Morton Arboretum.

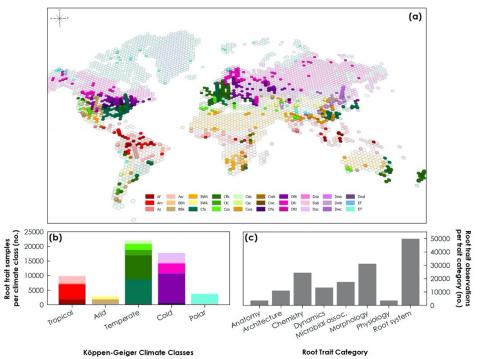


Fig. 4b.1. FRED 3.0 observations are distributed unevenly across the globe (map from Iversen & McCormack 2021, New Phytologist, in press). For the purposes of this map, land cover within a Köppen-Geiger climate classification zone (Kottek et al., 2006, 10.1127/0941-2948/2006/0130) was aggregated into hex bins that are extruded in three-dimensional space based on the number of root trait samples collected in each bin. Map courtesy of Chris DeRolph. (b) The number of root trait samples collected from each Köppen-Geiger climate subclass (e.g., Kottek et al., 2006), summed within each climate class. (c) The distribution of observations in FRED 3.0 across broad categories of root traits; for more information about the trait categories, see <a href="https://roots.ornl.gov/data-inventory">https://roots.ornl.gov/data-inventory</a>.

Task 4b. Deliverable status FY2020 and FY2021

Date	Deliverable	Status
2020	Manuscript on heleviores and resource acquisition strategies	Completed
2020	Manuscript on belowground resource acquisition strategies	(McCormack et al., 2019)
2020	Manuscript on hierarchical Bayesian model of root-trait	Underway
2020	variation in FRED 2.0	(Liu et al., in final prep)
	FRED 3.0 available to community as a relational database	Completed
2020		https://roots.ornl.gov/public-release
2020		(Iversen & McCormack 2021,
		New Phytologist, in press)
2021	Manuscript leveraging FRED 3.0 and Morton observations	·
	to inform representation of root pools and dynamics in	Planned
	ELM	

#### Task 4b Publications/Manuscripts

Bergmann J, Weigelt A, van der Plas F, Laughlin DC, Kuyper TW, Guerrero-Ramirez N, Valverde-Barrantes OJ, Bruelheide H, Freschet GT, Iversen CM, Kattge J, McCormack ML, Meier IC, Rillig MC, Roumet C, Semchenko M, Sweeney CJ, van Ruijven J, York LM, Mommer L. 2020. The fungal collaboration gradient dominates the root economics space in plants. *Science Advances* 6:eaba3756.

Freschet GT, Roumet C, Comas LH, Weemstra M, Bengough AG, Rewald B, Bardgett RD, De Deyn GB, Johnson D, Klimešová J, Lukac M, McCormack ML, Meier IC, Pagès L, Poorter H, Prieto I, Wurzburger N, Zadworny M, Bagniewska-Zadworna A, Blancaflor EB, Brunner I, Gessler A, Hobbie SE, Iversen CM, Mommer L, Picon-Cochard C, Postma JA, Rose L, Ryser P, Scherer-Lorenzen M, Soudzilovskaia NA, Sun T, Valverde-Barrantes OJ, Weigelt A, York LM, Stokes A. 2021a. Root

traits as drivers of plant and ecosystem functioning: current understanding, pitfalls and future research needs. *New Phytologist* (in press), https://doi.org/10.1111/nph.17072.

Freschet, GT, Pagès L, Iversen CM, Comas LH, Rewald B, Roumet C, Klimešová J, Zadworny M, Poorter H, Postma JA, Adams TS, Bagniewska-Zadworna A, Blancaflor EB, Brunner I, Cornelissen JHC, Garnier E, Gessler A, Hobbie SE, Lambers H, Meier IC, Mommer L, Picon-Cochard C, Rose L, Ryser P, Scherer-Lorenzen M, Soudzilovskaia NA, Stokes A, Sun T, Valverde-Barrantes OJ, Weemstra M, Weigelt A, Wurzburger N, York LM, Batterman SA, Bengough AG, Gomes de Moraes M, Janeček Š, Salmon V, Tharayil N, McCormack ML. 2021b. A starting guide to root ecology: strengthening ecological concepts and standardizing root classification, sampling, processing and trait measurements. *New Phytologist* (in press).

Guerrero-Ramirez N, Mommer L, Freschet GT, Iversen CM, McCormack ML, Kattge J, Poorter H, van der Plas F, Bergmann J, Kuyper TW, York LM, Bruehlheide H, Laughlin DC, Meier IC, Roumet C, Semchenko M, Sweeney CJ, van Ruijven J, Valverde-Barrantes OJ, Aubin I, Catford JA, Manning P, Martin A, Milla R, Minden V, Pausas JG, Smith SW, Soudzilovskaia NA, Ammer C, Butterfield B, Craine JM, Cornelissen JHC, de Vries F, Hickler T, Isaac ME, Kramer K, König C, Lamb E, Medlyn B, Onipchenko VG, Read Q, Reich PB, Rillig MC, Sack L, Shipley B, Tedersoo L, Valladares F, van Bodegom P, Weigelt P, Wright J, Weigelt A. 2021. Global Root Traits (GRooT) Database. *Global Ecology and Biogeography* 30:25-37.

Iversen CM, McCormack ML. 2021. Filling gaps in our understanding of belowground plant traits across the world: A Virtual Special Issue. *New Phytologist* (in press)

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Weigelt A, Mommer L, Andraczek K, Iversen CM, Bergmann J, Bruelheide H, Freschet GT, Guerrero-Ramírez NR, Kattge J, Kuyper TW, Laughlin DC, Meier IC, van der Plas F, Poorter H, Fan Y, Roumet C, van Ruijven J, Sabatini FM, Semchenko M, Sweeney CJ, Valverde-Barrantes OJ, York LM, McCormack ML. 2021. An integrated framework of plant form and function: The belowground perspective. New Phytologist (in press)

#### Task 8: LeafWeb

Website development – Leafweb support libraries have been updated to better serve users. These changes are mostly not noticeable from an end-user perspective, but over 30 support libraries have been updated with bug and security fixes, including Umbraco 7.15.3, Hangfire 1.7.7, Bootstrap 3.4.1 to 4.3.1, and Entity Framework to 6.3. The Bootstrap upgrade in particular made Leafweb usable on mobile devices. We have added data search capabilities to Leafweb. The search interface is now available on the Search and Manage Queue pages. Over 100 uploaded data samples with errors were analyzed to find common formatting issues for users. A document was added to explain how to avoid these errors. These analyses also led to developing additional coding strategies that are more tolerant to non-lethal formatting errors (i.e., errors that do not affect Leafweb parameter optimization outputs). User accounts have been created for users who use Leafweb frequently so that they can manage the data they submitted. A batch download function has been added to allow fast and easy download of Leafweb inputs and outputs. Finally, all Leafweb pages have been adjusted to better accommodate mobile devices, as well as remain fully functional for the desktop.

The update of Leafweb is still ongoing. Leafweb will be updated and tested with the latest support modules. This includes over 40 updates on the Website portion and over 20 on the background processing program Piscal server. During the last phase of development, an advanced search was added to Leafweb providing capabilities to quickly access specific data sets matching given query parameters. This will now

be extended to retrieving individual Leafweb output results instead of the entire archive. A new result page will be offered to display individual Leafweb input file results - instead of the entire inputs currently displayed. This will show fields such as Latitude, Longitude, CO2S, PARi, Tleaf, and PhPS2 directly in the search results.

Since adding the ability to register users during the last development, the number of bots attempting to access Leafweb has greatly increased. CAPTCHA technology is a means to limit the ability of automated spam bots to submit forms on our system. We are currently seeing this activity especially in the User Registration and also sometimes in Leave a Comment. A CAPTCHA library will be added to Leafweb, using the free version of BotDetect CAPTCHA to defeat these bots.

New automated functionality development and data gathering – We are testing codes developed for integrating models of light and C reactions of photosynthesis and the associated parameter estimation algorithms within the Leafweb code system. Models being tested include those for calculating and modeling nonphotochemical quenching (NPQ), fraction of open photosystem II reaction centers under the lake model (qL), the puddle model (qP), and redox reactions of the electron transport chain. The data used for testing these new Leatweb functions came from Prof. Joseph A Berry from the Department of Global Ecology, Carnegie Institution of Washington, Albert Porcar-Castell from Department of Forest Sciences, University of Helsinki, Xinyou Yin from Centre for Crop Systems Analysis, Wageningen University & Research, and Prof Bernard Grodzinski of University of Guelph. Because of the complexity of the new functions, we plan to open them to the general users after we feel confident that the new codes are bugfree and do not crash the existing functions of Leafweb.

Task 8. Deliverable status FY2020 through FY2022

Date	Deliverable	Status	
December 2020	Completion of data search capabilities	Completed	
December 2020	Manuscript on within-canopy variations of PAM parameters	Measurements not conducted due to covid-19	
July 2021	Completion of graphic display capabilities for PAM data	Due to our rapid development in light reaction models, we plan to complete this function as part of new modeling capability implementation in leafweb in the future to avoid interrupting the conventional use of Leafweb	
Oct 2021	Manuscript synthesizing the dynamics of NPQ and qL for modeling photosynthesis	Planned	
May 2022	New website update	Planned	
July 2022	Manuscript on SIF-Vcmax relationship	Planned	

### Task 8 Publications/Manuscripts

Eckert D, Martens HJ, Gu L & Jensen AM (2021) CO<sub>2</sub> rexation is higher in leaves of woody species with high mesophyll and stomatal resistances to CO<sub>2</sub> diffusion. *Tree Physiology* doi:10.1093/treephys/tpab016.

Li J, Zhang Y, Gu L, Li Z, Li J, Zhang Q, Zhang Z, Song L (2020) Seasonally varying relationship between sun-induced chlorophyll fluorescence and photosynthetic capacity from leaf to canopy in a paddy rice field. *Journal of Experimental Botany* 71: 7179-7197.

### TES SFA DATA SYSTEMS, MANAGEMENT, AND ARCHIVING UPDATE

The open sharing of all data and results from the TES SFA research and modeling tasks among researchers, the broader scientific community, and the public is critical to advancing the mission of DOE BER's Earth and Environmental Systems Sciences Division. Active data sharing facilitates delivery of TES 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. Task-specific web sites (e.g., SPRUCE: <a href="https://mnspruce.ornl.gov">https://mnspruce.ornl.gov</a> and FRED: <a href="https://roots.ornl.gov">https://roots.ornl.gov</a>), access to web-based tools (e.g., LeafWeb: <a href="https://leafweb.org">https://leafweb.org</a>) and links to external products (e.g., microbial metagenomes) enable these interactions.

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 data 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 (<a href="https://mnspruce.ornl.gov">https://mnspruce.ornl.gov</a>) and TES SFA (<a href="https://tes-sfa.ornl.gov">https://tes-sfa.ornl.gov</a>) websites.

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. Real-time visual displays of selected monitoring and infrastructure operational control parameters are provided using Campbell Scientific's Real-Time Monitor and Control (RTMC) software. Vista Data Vision (VDV) software has been implemented for performance monitoring, data visualization, and data review by the SPRUCE Team. Data are stored and will be accessible through web-based search and download applications to the project and public.

In addition, ongoing SFA task data products continue to be archived at program-specific archives (e.g., MOFLUX at AmeriFlux). North American Carbon Program (NACP) data synthesis products are archived at the ORNL Distributed Active Archive Center (ORNL DAAC). New SFA task data products are publicly available on the ORNL TES-SFA web site: <a href="https://tes-sfa.ornl.gov">https://tes-sfa.ornl.gov</a>.

See **APPENDIX B** for the list of newly and previously archived datasets and details of data sharing, archiving, and fair use.

#### AFFILIATED TES SFA-SUPPORTED PUBLICATIONS

Staff supported by the TES SFA continue to collaborate and complete work funded by US DOE BER in prior fiscal years that may not explicitly be funded under Tasks 1 through 8. The following listing shows additional manuscripts completed since the June 2020 with some TES SFA support.

- Eckert D, Jensen AM, Gu L (2020) The maximum carboxylation rate of Rubisco affects CO2 refixation in temperate broadleaved forest trees. *Plant Physiology and Biochemistry* 155:330-337. doi:10.1016/j.plaphy.2020.06.052
- Griffis TJ, Roman DT, Wood JD, Deventer MJ, Fachin L, Rengifo J, Castillo DD; Lilleskov E, Kolka R, Chimner RA, del Aguilla J, Wayson C, Hergoualc'h K, Baker JM, Cadillo-Qurroz H, Ricciuto DM (2020) Hydrometeorological sensitivities of net ecosystem carbon dioxide and methane exchange of an Amazonian palm swamp peatland. *Agricultural and Forest Meteorology* 295:108167, doi: https://doi.org/10.1016/j.agrformet.2020.108167.
- Heckman KA, Swanston CW, Torn MS, Hanson PJ, Nave L, Porras RC, Stanovick JS, Mishra U, Bill M (2021) Soil organic matter is principally root derived in an Ultisol under oak forest. *Geoderma* (submitted).
- Jung M, Schwalm C, Migliavacca M, Walther S, Camps-Valls G, Koirala S, Anthoni P, Besnard S, Bodesheim P, Carvalhais N, Chevallier F, Gans F, Goll DS, Haverd V, Köhler P, Ichii K, Jain AK, Liu J, LombardozziD, ... Reichstein M (2020) Scaling carbon fluxes from eddy covariance sites to globe: Synthesis and evaluation of the FLUXCOM approach. *Biogeosciences* 17:1343–1365. <a href="https://doi.org/10.5194/bg-17-1343-2020">https://doi.org/10.5194/bg-17-1343-2020</a>
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- Li J, Zhang Y, Gu L, Li Z, Li J, Zhang Q, Zhang Z, Song L (2020) Seasonally varying relationship between sun-induced chlorophyll fluorescence and photosynthetic capacity from leaf to canopy in a paddy rice field. *Journal of Experimental Botany* 71:7179-7197.

- Poyatos R, Granda V, Flo V, Mencuccini M, Steppe K, Martínez-Vilalta J, SAPFLUXNET contributors [Hanson PJ, Norby RJ Wullschleger SD] (2020) Global transpiration data from sap flow measurements: the SAPFLUXNET database. *Earth System Science Data* 13:2607-2649, doi:10.5194/essd-13-2607-2021.
- Seward J, Carson MA, Lamit LJ, Basiliko N, Yavitt JB, Lilleskov E, Schadt CW, Smith DS, Mclaughlin J, Mykytczuk N, Willims-Johnson S (2020) Peatland microbial community composition is driven by a natural climate gradient. *Microbial Ecology* doi:10.1007/s00248-020-01510-z.

### **4AII. SCIENCE HIGHLIGHTS SINCE JUNE 2020**

- ORNL TES SFA staff authored 67 papers that have been published or are in press/accepted status since June 2020. Notable papers include the following high impact totals: 1 in *Biological Reviews*, 1 in *Science Advances*, 2 in the *Proceedings of the National Academy of Sciences*, 2 in the *Nature* family of journals. An additional 9 manuscripts are in peer review.
- SPRUCE A summary of C budgets for the SPRUCE treatment plots was published showing linear declining C losses proportionate to warming (Hanson et al. 2020). This article was a cover highlight for the journal AGU Advances (Hanson et al. 2020).
- SPRUCE Wilson et al. (2021) showed that the production of the potent greenhouse gas methane (CH<sub>4</sub>) was shown to increase at a faster rate in comparison to carbon dioxide in response to warming, and evidence indicates that soil respiration and methanogenesis are stimulated by the release of plant-derived metabolites. Results suggest that as peatland vegetation trends towards increasing vascular plant cover with warming, we can expect a concomitant shift towards increasingly methanogenic conditions and amplified climate-peatland feedbacks.
- SPRUCE Using novel, high-resolution minirhizotrons, we found warming increased the abundance of ectomycorrhizal fungal rhizomorphs, especially in deep peat, and extended the belowground active season by 62 days (Defrenne et al., 2021, *PPP*). We also developed an interactive website that allows scientists and the public to peer belowground in the SPRUCE experimental enclosures (https://colleeniversen.ornl.gov/inside-the-spruce-bog).
- SPRUCE Species-specific divergence in tree hydraulic response to warmer, drier conditions was described in two papers (Warren et al. 2021, Dusenge et al. 2022), indicating black spruce was more sensitive to stress, and maintained greater hydraulic safety, but which could lead to reduced growth, relative to larch.
- MOFLUX/SIF Detailed quantification of the climatic dependence of GPP/SIF ratio showed a consistent decrease in GPP/SIF from cold-and-wet climates to hot-and-dry climates (Chen et al., 2020). This article was highlighted by the journal Global Change Biology in a Commentary (Jeong and Park, 2020).
- MOFLUX/SIF The first paper on the application of SIF for partitioning NEE of CO<sub>2</sub> was published in *Geophysical Research Letters* (Okra et al. 2021).
- CC Modeling A new CH<sub>4</sub> model was integrated in ELM-SPRUCE and evaluated against observations (Ricciuto et al., 2021; Yuan et al., 2021). The new model accurately predicts the seasonal cycle of CH<sub>4</sub> fluxes.
- CC Modeling A new model was developed for moss C cycling (Shi et al., 2021) and integrated into ELM-SPRUCE. The model was evaluated against observed NPP and biomass for tree, shrub and moss plant functional types.
- MAAT Multi-Assumption Modeling The first formal model structural (process representation) sensitivity analysis of its kind was published revealing the surprising sensitivity of leaf-scale photosynthesis models to empirical assumptions (Walker et. al., 2021, *Global Change Biology*). The multi-assumption soil organic matter decomposition model in MAAT is in its second phase of development by Matt Craig. Using the first-generation model, Dr. Craig showed that a density-dependence hypothesis of constraints on microbial population growth could lead to saturation of soil organic carbon as input rates increase. Data synthesis provides evidence in support of the density dependence of microbial population growth as soil carbon input rates increase (Craig et al., 2021, *Global Change Biology*).

- Soil C We found that the length of incubations strongly effected the values of all 5 common microbial parameters used in the MEND model (Jian et al. 2020). As length of incubations increased, the values of the microbial parameters decreased, which resulted in predictions of smaller soil carbon loss compared to predictions made with short-term incubations which resulted in predictions of greater soil carbon loss with warming. Both predictions were consistent with meta-analyses of field warming experiments; i.e., short-term field warming experiments observed larger losses of soil carbon, and long-term field warming experiments observed smaller losses of soil carbon.
- Root Traits We released the third version of the Fine-Root Ecology Database (FRED 3.0) in March 2021 (data citation: Iversen et al. 2021) as a searchable database that allows users to filter the observations in FRED according to their scientific needs. The user interface is accessed via <a href="https://roots.ornl.gov/public-release">https://roots.ornl.gov/public-release</a>. We highlighted FRED 3.0 as a community resource for belowground ecologists and modelers alike in an editorial that accompanies a Virtual Special Issue in New Phytologist (Iversen and McCormack, New Phytologist, in press).
- Root Function Neutron imaging of switchgrass roots with and without mycorrhizae indicate differences in water extraction and retention patterns, and a manuscript is in development.

#### **4AIII. ANALYSIS OF PUBLICATIONS**

Through senior and coauthored effort, TES SFA staff produced 67 publications or completed manuscripts since our last summary report. This total includes 58 published/in press/accepted journal articles and 9 working through the review process. This level of 1-year productivity over (67 y<sup>-1</sup>) managed to exceed our average paper production rate from March 2015 through June 2020 of 43 y<sup>-1</sup>. A TES SFA cumulative publication summary since 2015 is provided in **Appendix A** with the most recent publications from the current reporting period listed first. This listing duplicates the Task-specific summaries already provided.

The TES SFA group published in 38 different peer-reviewed publications in this reporting period including one in *Science Advances* (Bergmann et al. 2020), two in *The Proceedings of the National Academy of Sciences* (Malhotra et al. 2020; Wilson et al. 2021), and 2 in the *Nature* family of journals. We also published 9 papers in *Global Change Biology*, 6 papers in *Journal of Geophysical Research – Biogeosciences*, 5 in *New Phytologist*, and 4 in *Agriculture and Forest Meteorology*.

Journal selection for publication of TES SFA work is at the discretion of the author team. Journals are selected to achieve maximum exposure of the research results for the science community. We focus on journals having high impact factors, but that is not necessarily the primary criteria for the selection of a journal for publication of a given research result. High-profile journals (e.g., *Science*, *Nature* family of journals, *PNAS*) are pursued for the publication of results anticipated to be of general interest to a wide audience. We find that solid and well-presented scientific results are well received and cited in all of our chosen journals.

We also continue to place significant and sustained effort on the production of archived data sets based on TES SFA work. A complete and cumulative summary of TES SFA data sets is provided in **Appendix B**.

#### 4B. FUTURE SCIENCE GOALS AND PLANS

Future science plans for the TES SFA were detailed in the quadrennial review document submitted to DOE BER in February 2019. Plans have been made to add additional high-temporal resolution CO<sub>2</sub> and CH<sub>4</sub> flux observations for all SPRUCE treatments.

The TES SFA plans to enhance efforts to leverage knowledge gained from past and ongoing process studies, manipulative experiments, and ecosystem observations (e.g., SPRUCE, PiTS, belowground fundamentals, landscape fluxes, EBIS, and TDE) to improve ecosystem models. Future, experimental studies will be used to test key mechanistic processes in ELM. To improve the modeling of gross primary production, we will apply new understanding of canopy processes enabled through the development of the SIF instrument and use to improve the modeling of gross primary production in ELM.

<u>Improved Sphagnum modeling</u> – Within the ELM framework we will continue to improve a mechanistic model of *Sphagnum* photosynthesis based on in situ assessment of GPP, *Sphagnum* production, capitula water content and environmental conditions. The data and modeling results will also provide critical information for latent heat and energy balance calculations.

<u>Heterotrophic versus autotrophic respiration</u> – Tasks 6 and 5 are using the measured soil chamber respiration data and SIF information from MOFLUX over the last 3 years to examine how seasonal and diurnal patterns and responses to drought influence the proportions of heterotrophic versus autotrophic respiration. Of particular interest is the sensitivity of diurnal time lags between autotrophic and heterotrophic respiration to environmental conditions. This work will eventually lead to improvements in conceptual understanding and quantitative modeling of soil and ecosystem respiration.

### 4C. NEW SCIENCE FOCUS AND IDENTIFIED KNOWLEDGE GAPS

We have clearly seen warming induced changes in the phenology of the bog vegetation with the expected acceleration of spring growth activities, but also a clear extension of the autumn growing season. In many current ecosystem models including SPRUCE-ELM, the predominant driver for fall senescence based on the interpretation of observational interannual variation is day length. The SPRUCE data show that algorithms will need to be modified to include warming influences on fall phenology changes. We have added new phenology cameras to better capture dynamics of ground layer vegetation.

Carbon cycle analysis clearly shows major losses of C from the SPRUCE ecosystem proportionate to the level of warming. At this time models are overestimating the influence of eCO<sub>2</sub> on C uptake and may not be adequately accounting for nutrient and water limitations.

Early year results from the SPRUCE study suggest further investment in the biogeochemical cycling of both nitrogen and phosphorus are needed to adequately capture long-term nutrient feedbacks within the bog with warming. Several key areas identified include N and P mineralization, nutrient resorption during fall senescence, and the availability of organic N and P in soils. Field measurements investigating the temperature response of N and P mineralization, as well as organic nutrient availability were originally planned for the summer of 2020 but we are considering making these observations on laboratory incubations instead because of COVID-19 – related travel restrictions. Resorption of N and P during fall senesce is being quantified for litter samples collected in the fall of 2019. Models are being used to evaluate the potential feedback magnitudes from P limitations and N<sub>2</sub> fixation inputs to better define the need for future measurements.

Identified knowledge gaps also drive model developments for land surface development of the E3SM model, and within NGEE project tasks that are complementary to efforts within the TES SFA. The TES SFA will continue to contribute new science to E3SM code base, including new algorithms for phenology and responses to extremes, and *Sphagnum* processes described above. TES SFA modeling efforts will benefit from developments in the other projects, such as improved hydrology through the ELM-PFLOTRAN coupling in NGEE-Arctic and the inclusion of a global phosphorus cycling model in E3SM.

### 4D. COLLABORATIVE RESEARCH

We continue to encourage key external groups to develop complementary research tasks for the benefit of TES SFA research tasks. Support for the following independently funded research groups is being provided through the use of SPRUCE leased office/lab facilities and access to the SPRUCE experimental site on the S1 Bog:

- Dr. Joel Kostka (Georgia Tech), Jeff Chanton (Florida State) and colleagues have received support from DOE BER for their ongoing studies of microbial ecology at SPRUCE, and the TES SFA took on management of that funding via subcontract for FY2018, FY2019 and FY2020.
- Dr. Andrew Richardson (Northern Arizona University) leads the task on phenology with his funding for the PhenoCam network and made this a funded subtask in FY2018 and beyond.
- Drs. Brandy Toner, Ed Nater and colleagues from the University of Minnesota, are examining mercury and sulfur dynamics in the SPRUCE experiment using funding provided through the USDA Forest Service.
- Dr. Karis McFarlane and colleagues at LLNL-CAMS provide measurement support for <sup>14</sup>C isotopic composition of air, plant tissues and peat from the S1-Bog and SPRUCE experimental plots.

- Dr. Nancy Glenn (Boise State) is contracted through SPRUCE to provide ground-level LIDAR observations as a supplement to our destructive woody harvests and *Sphagnum* production estimates. Jake Graham is executing the onsite work.
- Dr. Yiqi Luo's group (Northern Arizona University) is utilizing new high-temporal-resolution, model-data iterative analyses to better define measured ecosystem responses with the intention of helping the research group apply measurement efforts to critical processes.
- Dr. Xiaofeng Xu (San Diego State University) continues work with the modeling group on improved biogeochemical cycling models for methane flux.
- Dr. Danielle Way (University of Western Ontario) is an unfunded collaborator who has been providing expertise and multiple PhD students to assist with seasonal assessment of Picea and Larix photosynthetic and respiratory thermal and CO<sub>2</sub> acclimation.
- Dr. Jalene M. LaMontagne (DePaul University) joined the SPRUCE group in 2017 to study mast seeding patterns in response to climate change.
- Dr. Bruce McCune (Oregon State University) and Sarah Jovan (USDA Forest Service) have their own support to study lichen responses to warming and eCO<sub>2</sub> within the SPRUCE experimental infrastructure.
- Dr. M. Luke McCormack (Morton Arboretum) is making new observations across a phylogenetically and ecologically diverse suite of tree species from mature forestry plots at The Morton Arboretum, Lisle, IL to advance our framework of root trait understanding gained from FRED.
- Dr. Al Kovaleski (University of Wisconsin) is an unfunded collaborator that plans to evaluate how cold hardiness changes in the tree and shrub species due to warming treatments, and the interaction with a longer growing season and warmer winters, and how different chilling models perform in predicting dormancy stage in woody perennials.
- Dr. Anping Chen (Colorado State University) continues work with the modeling group on the global SIF analysis and the use of observational SIF to constrain the ELM GPP.
- Prof. Mingzhou Jin (University of Tennessee at Knoxville) and his PhD student, Rongyun Tang, continue work with the modeling group on the wildfire analysis and modeling for ELM.

# CITED REFERENCES (NOT IN THE TES SFA APPENDIX LISTS)

BERAC (2017) Grand Challenges for Biological and Environmental Research: Progress and Future Vision; A Report from the Biological and Environmental Research Advisory Committee, DOE/SC-0190, BERAC Subcommittee on Grand Research Challenges for Biological and Environmental Research (science.energy.gov/~/media/ber/berac/pdf/Reports/ BERAC-2017-Grand-Challenges-Report.pdf).

US DOE (2018) Climate and Environmental Science Division Strategic Plan 2018-2023, U.S. Department of Energy, Office of Science, DOE/SC-0151,

https://science.energy.gov/~/media/ber/pdf/workshop%20reports/2018 CESD Strategic Plan.pdf

#### 5. STAFFING AND BUDGET SUMMARY

### 5A. FY2021 FUNDING ALLOCATION BY PROGRAM ELEMENT

Total expected available funding for ORNL's TES SFA in FY2021 included \$5,463K carryover from FY2020 (including \$544K for external commitments) and \$8,300K of new budget authorization. FY2021 spending is summarized in the following table.

FY2021 Budget expenditures by TES SFA Program Element through 16 June 2021. The data include prior year carryover amounts.

Task	Cost Through 16 June 2021 (\$K)	Commitments Through 16 June 2021 (\$K)	Remaining Funds 16 June 2021 (\$K)
T1: SPRUCE Science	\$2,330K	\$407K	\$1,574K
T6: MOFLUX, etc.	479	102	247
T3ab: Carbon Cycle Modeling	817	79	436
T3d: MAAT	179	0	173
T4c: Process Study - Root Func.	104	24	43
T5: Soil C Studies	91	6	192
T4b: Process Study - Root traits	198	0	202
T8: LeafWeb	55	0	85
T1.1: SPRUCE – Operations	820	409	891
T1.2: SPRUCE – Materials	132	126	75
T1.3: SPRUCE – Reserve	4	0	964
SFA Contingency	17	0	1,959
SFA Totals	\$5,226K	\$1,153K	\$6,841K

We are currently spending at rates consistent with the spending plans outlined in the February 2019 TES SFA renewal proposal budgets for FY2021. We anticipate unspent carry over funds to be approximately \$2,500K across all TES SFA tasks and external SFA commitments.

A total of \$247K carry-over provide through the TES SFA are for closely related activities managed as independent efforts and not detailed in the analysis above.

## 5B. FUNDING ALLOCATION TO EXTERNAL COLLABORATORS

A variety of collaborations are maintained and funded by the TES SFA to provide necessary commodities, and disciplinary expertise and effort in areas critical to the completion of research tasks. In FY2021 we directly funded the following individuals or groups.

The University of Missouri (\$196K) is subcontracted to provide MOFLUX on site execution of the following measurements: stand-level eddy covariance, soil CO<sub>2</sub> efflux, belowground production via repeated minirhizotron image collections, stem allometric increment data, and litter basket net primary production. Since June 2016, J.D. Wood serves as Missouri site-PI of the MOFLUX site.

**Yiqi Luo- Northern Arizona University (\$150K)** – Dr. Luo's research group at NAU is developing an ecological forecasting capability at SPRUCE. Using the TECO model as a demonstration, data assimilation capabilities are being developed and applied using SPRUCE observations, and forecasts were

made for the 10 experimental plots using a range of future scenarios. A methane model was also added to TECO.

**Xiaofeng Xu - San Diego State University (\$38K)** - In a joint subcontract with NGEE-Arctic, Dr. Xu is developing and testing a CH<sub>4</sub> modeling capability for the CLM and ELM-SPRUCE modeling efforts. This work has contributed to two manuscripts. Work to refine and optimize the model with SPRUCE observations is continuing.

**John Latimer (\$57K)** – We have subcontracted John part-time through XCEL Engineering since 2014 to collect weekly minirhizotron images from the SPRUCE experimental plots, and to collect and exchange ion-exchange resin capsules every 28 days from the SPRUCE experimental plots.

**M.** Luke McCormack – The Morton Arboretum (\$70K) – Dr. McCormack has been subcontracted to analyze global patterns in root traits compiled in the Fine-Root Ecology Database (*FRED*) and develop a manuscript on this topic. In addition, Luke is working with an interdisciplinary team of empiricists, modelers, and database managers to improve the conceptual representation of root traits and their associated functions in terrestrial biosphere models.

Richard J. Norby (\$40K) – Dr. Norby provides expertise in the evaluation of Sphagnum communities and their growth and contributions to community net primary production. He works directly with David Weston on the field measurement collections and the analysis and interpretation of results.

RhizoSystems, LLC (\$28K) – The company who designed and built the automated minirhizotrons (AMRs) is being subcontracted for support and maintenance of these systems. This includes off-site repair and maintenance of all AMR and RhizoSystems-installed equipment and remote assistance with field repair on-site. It also includes assistance with and support of the RV3n software as well as AMR-related software updates to and routine maintenance of RhizoSystems-installed computers.

Interagency Agreement with the USDA Forest Service (\$40K) – This agreement allows Forest Service employees to help with the operation, planning and execution of the SPRUCE experimental infrastructure and science tasks. It also provides some coverage for the use of the USDA FS bunk house on the Marcell Experimental Forest.

**Keith Oleheiser (\$90K)** - Keith Oleheiser is based in Minnesota and collects water samples (porewater, outflow, precipitation) and hydrology measurements and analyzes all SPRUCE water samples at the USFS research lab in Grand Rapids, MN for pH, specific conductivity, alkalinity, anions, cations, nutrients, and total organic C. Keith transitioned to a full-time ORNL technician in June 2021.

**Kyle Pearson (\$95K)** – A technical contractor with XCEL Engineering to help W. Robert Nettles with the day-to-day operation of SPRUCE treatments and the calibration and upkeep of automated data collections systems (prior to his transition to an ORNL technical professional staff position in June 2021).

**Andrew Richardson – Northern Arizona University (\$98K)** – This contract allows Dr. Andrew Richardson's group to maintain the automated phenology observations and greenness calculations for all treatment and ambient plots on the SPRUCE site. Dr. Richardson also leads the phenology task for the SPRUCE project.

Nancy Glenn – Boise State University (\$60K) This contract provides twice annual terrestrial lidar scans of the SPRUCE experimental plots to help assess vegetation growth and microform elevation change (hummock and hollow distributions).

**Karis McFarlane – Lawrence Livermore National Laboratory (\$136K)** – We contract with LLNL to provide isotopic analyses (<sup>14</sup>C and <sup>13</sup>C) for air (x5 events per year) and tissue analyses (x1 per year) to provide a record of the application and accumulation of unique isotopic tracers into the SPRUCE ecosystem. Funding is also provided in for her group to return to the site to evaluate the isotopic composition of emitted CO<sub>2</sub> and CH<sub>4</sub>.

Nate McDowell – Pacific Northwest National Laboratory (\$53K) – We contract with PNNL for FY 21 to provide non-structural carbohydrate analysis for the woody plant species at SPRUCE to improve understanding of carbon availability and storage in context of shifts in growth and respiration rates, regrowth after damage from freezing, heat/drought or insect events.

Infrastructure subcontracts in support of the SPRUCE project in FY2020 include funds and funding for site maintenance (Pokegama Electric \$55K), electrical service (Lake Country Power \$130K), propane supply (Lakes Gas Co. \$360K), eCO<sub>2</sub> supply (PRAXAIR Inc. \$120K), fiber internet

connections (\$10K), and leased space in Minnesota (\$41K). The amounts required for each of these operational contracts are reevaluated annually as actual usage rates and prices change.

## 5c. Personnel Actions and Procedures

<u>New Hires and Promotions</u> – Subcontracted SPRUCE support staff were transitioned to full-time ORNL offsite positions in FY2021. In June, Kyle Pearson was hired to take the place of W. Robert Nettles and Keith Oleheiser was transitioned to full time technical support. We anticipate one more technical staff hire to participate in the routine operations of the SPRUCE site in support of Kyle Pearson. Dr. Bin Wang was hired as a post-doctoral researcher funded partly through the Root Traits task (4b). Geoff Schwaner was hired in 2021 as a full-time ORNL technical staff person to primarily conduct laboratory operations in Oak Ridge.

<u>Anticipated Future Hires</u> – Looking ahead to FY2022, the TES SFA plans to pursue hiring or replacing postdoctoral fellows to sustain effort and to supplement full time staff positions and as the budget allows.

Retirements and Releases – Anthony King and Deanne Brice retired in FY2021.

<u>Procedures for advancing new and developing investigators</u> - New TES SFA staff members are commonly first 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 and are hired as staff into leadership roles as appropriate for our needs.

Where identified disciplinary needs are established (and for which adequate funding is available) the TES SFA also has the capacity to hire established staff persons directly into a task leadership role. When a need for new staff is identified but funding is insufficient to initiate a new hire, ORNL internal funds may be requested through a strategic hire program to bring individuals on board. This internal program allows for a 1 to 2-year transitional period to enable the TES SFA group to establish an appropriate, stable, and fully funded position.

Within the TES SFA, task accomplishments and budget management is executed at an overarching level by the Principal Investigator with feedback from all Task leads. Individual Task leads are given the responsibility to track scientific progress and the responsibility for managing their fiscal resources within an annual cycle. Training to allow new staff to understand ORNL procedures, accounting systems, and managerial activities is available and provided when appropriate. Such training, in addition to one-on-one mentoring with established staff, provides developing staff with the information and skill sets required to transition into leadership roles. At the institutional level, ORNL has formal programs for mentoring high-potential early career staff, and we use informal mentoring at the personal level to ensure that staff with potential leadership qualities are identified and helped with career development.

### 5D. NATIONAL LABORATORY INVESTMENT IN THE PROGRAM IN FY2021

Concepts for the belowground warming technologies used for the SPRUCE Experiment (Task R1) were initiated with ORNL LDRD funds totaling \$480K in FY2008 and FY2009. In FY2014, ORNL provided the equivalent of \$1000K staff support from internal funds to allow completion of the SPRUCE warming aboveground infrastructure. No ORNL funds were requested or have been needed in FY2021.

The Climate Change Science Institute brings together all ORNL Climate Change staff including members of the TES SFA to foster day-to-day interactions among modelers, experimentalists and data management specialists. 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. We continue to be engaged with neutron sciences through cutting-edge root and rhizosphere imaging research at the High Flux Isotope Reactor (HFIR) and active participating in science development teams for the future VENUS beamline at SNS and proposed beamlines at the potential Second Target Station. We work with the DOE BER data center ESS-DIVE as our primary permanent data repository (see also Appendix B).

We also use other facilities at collaborating DOE National Laboratories. The Lawrence Livermore National Laboratory – Center for Accelerator Mass Spectrometry (LLNL-CAMS) provides large volume, high precision <sup>14</sup>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.

# **5E. CAPITAL EQUIPMENT**

Since the threshold amount of funds needed to define a capital expenditure is high, no ORNL TES SFA funds have been used to acquire capital equipment in FY2021. Funding for SPRUCE experimental infrastructure maintenance and development at the S1 Bog are not classified as capital expenditures but represent an analogous investment for the decadal duration of the experiment.

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### APPENDIX A: COMPLETE PUBLICATION LIST – ORNL TES SFA

## Published, accepted and in review papers since the June 2020 annual Report

- Ardón, M., L.H. Zeglin, R.M. Utz, S.D. Cooper, W.K. Dodds, R.J. Bixby, A.S. Burdett, J.J. Follstad Shah, N.A. Griffiths, T.K. Harms, S.L. Johnson, J.B. Jones, J.S. Kominoski, W.H. McDowell, A.D. Rosemond, M.T. Trentman, D.J. Van Horn, and A.K. Ward. (2021) Experimental nitrogen and phosphorus enrichment stimulates multiple trophic levels of algal and detrital-based food webs: A global meta-analysis from streams and rivers. *Biological Reviews* 96:692-715
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- Chang CY, Zhou R, Kira O, Marri S, Skovira J, Gu L, Sun Y (2020) An Unmanned Aerial System (UAS) for concurrent measurements of solar-induced chlorophyll fluorescence and hyperspectral reflectance toward improving crop monitoring. *Agricultural and Forest Meteorology* 294. <a href="https://doi.org/10.1016/j.agrformet.2020.108145">https://doi.org/10.1016/j.agrformet.2020.108145</a>
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- Chen A, Mao J, Ricciuto D, Xiao J, Frankenberg C, Li X, Thornton PE, Gu L, Knapp AK (2021b) Moisture availability mediates the relationship between terrestrial gross primary production and solar-induced fluorescence: Insights from global scale variations. *Global Change biology* 27:1144-1156.
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- 9. Curtinrich HJ, Sebestyen SD, Griffiths NA, Hall SJ (2021) Warming stimulates iron-mediated carbon and nutrient cycling in mineral-poor peatlands. *Ecosystems* doi: 10.1007/s10021-021-00639-3
- 10. DeCarlo KF, Bilheux JC, Bilheux H, Caylor K, Warren JM (2020b) RootProcessing: An open-source python package for root/soil analysis at the neutron imaging beamline at ORNL. *Plant and Soil* (in revision).
- 11. DeCarlo KF, Caylor K, Bilheux H, Warren JM (2019) Integrating fine root morphology and soil distance mapping to characterize the plant-soil interface. *New Phytologist* (in revision)
- 12. Defrenne CE, Childs J, Fernandez CW, Taggart M, Nettles WR, Allen MF, Hanson PJ, Iversen CM (2021) High-resolution minirhizotrons advance our understanding of root-fungal dynamics in an experimentally warmed peatland. *Plants People Planet* https://doi.org/10.1002/ppp3.10172.
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- 30. Hu C, Griffis TJ, Baker JM, Wood JD, Millet DB, Yu Z, Lee X (2020) Modeling the sources and transport processes during extreme ammonia episodes in the U.S. Corn Belt, *Journal of Geophysical Research: Atmospheres* 125:e2019JD031207, doi: 10.1029/2019JD031207.
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#### APPENDIX B: TES SFA DATA SETS AND POLICIES

## Data Policy for 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 BER's Earth and Environmental Systems Sciences Division. 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 BER Earth and Environmental Systems Sciences Division. A complete copy of our data policy may be found at:

https://mnspruce.ornl.gov/sites/default/files/ORNL\_TES-SFA\_Policy\_2090515.pdf
TES-SFA data management plans and policies align with the most recent DOE policies for "Public Access to the Results of DOE-Funded Scientific Research"

<u>https://mnspruce.ornl.gov/sites/default/files/DOE\_Public\_Access%20Plan\_FINAL.pdf</u> and the "Statement on Digital Data Management"

https://science.osti.gov/Funding-Opportunities/Digital-Data-Management

#### **Data Products Archived**

SPRUCE has archived and shared with the public 79 data products. There are currently 5 products, available to the project only, that are awaiting publication of a paper and a few others in a development queue at any one time.

For ongoing TES-SFA tasks, 28 products are available to the public. 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 3.0), and characterization of SPRUCE plots (e.g., elevation).

Persistent identifiers (digital object identifiers, DOIs) for all products are registered through 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 facilitate the transfer of metadata, documentation, and data to the DOE's Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) archive.

### **Transfer of Data Products to DOE ESS-DIVE Archive**

Data management staff of the TES SFA are working with archive staff to continue transferring copies of selected TES-SFA and SPRUCE data products to the ESS-DIVE Archive. The first set of transferred datasets included those currently publicly accessible and considered final, that is, they will not be updated with periodic new data additions. Product data and metadata are reviewed and updated as needed to meet archive requirements and to ensure efficacious data search and discovery. To date, copies of 19 SPRUCE and 9 TES-SFA data products have been transferred to ESS-DIVE.

### **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 (<a href="https://e3sm.org/resources/policies/">https://e3sm.org/resources/policies/</a>). Development branches of the E3SM code for research purposes will also be available through <a href="https://github.com/E3SM-Project/E3SM/">https://github.com/E3SM-Project/E3SM/</a>. 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.

# **Websites Upgrades**

The FRED, SPRUCE and TES SFA Websites have been 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. The FRED Website and TES SFA Websites have been upgraded. The SPRUCE website will be upgraded by the end of FY 2021.

## **TES SFA Software:**

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

# SPRUCE Public Data Sets (\*\*New since June 2020):

- \*\*Childs J, Defrenne CE, Brice DJ, Woodward J, Holbrook KN, Nettles WR, Taggart M, Iversen CM (2020D) SPRUCE High-Resolution Minirhizotrons in an Experimentally-Warmed Peatland Provide an Unprecedented Glimpse at Fine Roots and their Fungal Partners: Supporting Data. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.25581/spruce.081/1637336
- \*\*Dusenge ME, Ward EJ, Warren JM, McLennan DA, Stinziano JR, Murphy BK, King AW, ChildsJ, Brice DJ, Phillips JR, Stefanski A, Villanueva R, Wullschleger SD, Cruz M, Reich PB, Way DA (2020D) SPRUCE Photosynthesis and Respiration of *Picea mariana* and *Larix laricina* in SPRUCE Experimental Plots, 2016-2017. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.25581/spruce.056/1455138">https://doi.org/10.25581/spruce.056/1455138</a>
- Dusenge ME, Stinziano RJ, Warren JM, Ward EJ, Wullschleger SD, Hanson PJ, Way DA (2018D)
   SPRUCE Whole Ecosystem Warming (WEW) Photosynthesis and Respiration of *Picea* and *Larix* in Experimental Plots, 2016. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.25581/spruce.056/1455138">https://doi.org/10.25581/spruce.056/1455138</a>
- 4. Fernandez CW, Heckman K, Kolka R, Kennedy PG (2019D) **SPRUCE Fungal Necromass Litter Bag Decomposition Study in SPRUCE Experimental Plots, 2016-2018.** Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.25581/spruce.063/1503589">https://doi.org/10.25581/spruce.063/1503589</a>
- Finzi AF, Giasson MA, Gill AL (2016D) SPRUCE Autochamber CO<sub>2</sub> and CH<sub>4</sub> 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
- Furze ME, Jensen AM, Warren JM, Richardson AD (2018D) SPRUCE S1 Bog Seasonal Patterns of Nonstructural Carbohydrates in Larix, Picea, Rhododendron, and Chamaedaphne, 2013. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.25581/spruce.037/1473917
- 7. Graham JD, Glenn NF, Spaete LP (2019Da) **SPRUCE Terrestrial Laser Scanning of Experimental Plots Beginning in 2015.** Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.25581/spruce.067/1515552">https://doi.org/10.25581/spruce.067/1515552</a>
- 8. Graham JD, Glenn NF, Spaete LP (2019Db) **SPRUCE Microtopography of Experimental Plots Derived from Terrestrial Laser Scans Beginning in 2016.** Oak Ridge National Laboratory, TES

- SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.25581/spruce.068/1515553
- 9. Griffiths NA, Hook LA, Hanson PJ (2016Da) SPRUCE S1 Bog and SPRUCE Experiment Location Survey Results, 2015 and 2020. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.3334/CDIAC/spruce.015
- Griffiths NA, Sebestyen SD (2016Db) SPRUCE S1 Bog Porewater, Groundwater, and Stream Chemistry Data: 2011-2013. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. http://dx.doi.org/10.3334/CDIAC/spruce.018
- 11. Griffiths, N. A., Sebestyen, S. D., Oleheiser, K. C., Stelling, J. M., Pierce, C. E., Nater, E. A., Toner, B. M., & Kolka, R. K. (2016Dc) **SPRUCE Porewater Chemistry Data for Experimental Plots Beginning in 2013 (Version 3).** Oak Ridge National Laboratory, TES SFA, US Department of Energy, Oak Ridge, Tennessee, USA. <a href="https://doi.org/10.3334/CDIAC/spruce.028">https://doi.org/10.3334/CDIAC/spruce.028</a>
- Griffiths NA, Sebestyen SD (2017D) SPRUCE Hollow Elevation Data for Experimental Plots Beginning in 2015. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="http://dx.doi.org/10.3334/CDIAC/spruce.035">http://dx.doi.org/10.3334/CDIAC/spruce.035</a>
- 13. Gutknecht J, Kluber LA, Hanson PJ, Schadt CW (2017D) SPRUCE Whole Ecosystem Warming (WEW) Peat Water Content and Temperature Profiles for Experimental Plot Cores Beginning June 2016. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="http://dx.doi.org/10.3334/CDIAC/spruce.041">http://dx.doi.org/10.3334/CDIAC/spruce.041</a>
- 14. Hanson PJ, U.S. Forest Service Staff, and SPRUCE Team (2012D) SPRUCE S1-Bog Vegetation Survey and Peat Depth Data: 2009. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="http://dx.doi.org/10.3334/CDIAC/spruce.003">http://dx.doi.org/10.3334/CDIAC/spruce.003</a>.
- 15. 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. <a href="http://dx.doi.org/10.3334/CDIAC/spruce.004">http://dx.doi.org/10.3334/CDIAC/spruce.004</a>.
- 16. Hanson PJ, Krassovski MB, Hook LA (2015D) SPRUCE S1 Bog and SPRUCE Experiment Aerial Photographs. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.3334/CDIAC/spruce.012
- 17. \*\*Hanson PJ, Nettles WR, Riggs JS, Krassovski MB, Hook LA (2021D) **SPRUCE CO<sub>2</sub> and H<sub>2</sub>O Data Beginning In 2015**. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.25581/spruce.092/1784060">https://doi.org/10.25581/spruce.092/1784060</a>
- 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. <a href="https://doi.org/10.25581/spruce.052/1433837">https://doi.org/10.25581/spruce.052/1433837</a>
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   U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A.
   https://doi.org/10.25581/spruce.055/1455014
- 20. Hanson, PJ, Phillips JR, Riggs JS, Nettles WR (2017D) SPRUCE Large-Collar in Situ CO<sub>2</sub> and CH<sub>4</sub> Flux Data for the SPRUCE Experimental Plots: Whole-Ecosystem-Warming. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.3334/CDIAC/spruce.034">https://doi.org/10.3334/CDIAC/spruce.034</a>
- 21. Hanson PJ, Phillips JR, Riggs JS, Nettles WR, Todd DE (2014D) **SPRUCE Large-Collar in Situ CO<sub>2</sub> and CH<sub>4</sub> 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. <a href="http://dx.doi.org/10.3334/CDIAC/spruce.006">http://dx.doi.org/10.3334/CDIAC/spruce.006</a>.

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- Hanson PJ, Riggs JS, Hook LA, Nettles WR, Dorrance C (2015D) SPRUCE S1-Bog Phenology Movies, 2010-2106. 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.011.
- 26. 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. <a href="http://dx.doi.org/10.3334/CDIAC/spruce.013">http://dx.doi.org/10.3334/CDIAC/spruce.013</a>
- 27. Hanson, P.J., Riggs, J.S., Nettles, W.R., Krassovski, M.B., Hook, L.A. (2016D) SPRUCE Whole Ecosystems Warming (WEW) Environmental Data Beginning August 2015. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.3334/CDIAC/spruce.032">https://doi.org/10.3334/CDIAC/spruce.032</a>
- Haynes KM, Mitchell CPJ, Kolka RK (2019D) SPRUCE Total Gaseous Mercury Fluxes and Peat Mercury Concentrations, 2014-2015. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.25581/spruce.066/1512288
- 29. Hofmockel KS, Chen, J, Hobbie EA (2016D) SPRUCE S1 Bog Pretreatment Fungal Hyphae Carbon and Nitrogen Concentrations and Stable Isotope Composition from In-growth Cores, 2013-2014. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. http://dx.doi.org/10.3334/CDIAC/spruce.025
- 30. Hopple AM, Pfeifer-Meister L, Zalman CA, Keller JK, Tfaily MM, Wilson RM, Chanton JP, Bridgham SD (2019D) **SPRUCE Does dissolved organic matter or solid peat fuel anaerobic respiration in peatlands?: Supporting Data.** Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.25581/spruce.062/1500027">https://doi.org/10.25581/spruce.062/1500027</a>
- 31. Iversen CM, Hanson PJ, Brice DJ, Phillips JR, McFarlane KJ, Hobbie EA, Kolka RK (2014D) SPRUCE Peat Physical and Chemical Characteristics from Experimental Plot Cores, 2012. 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.005.
- 32. \*\*Iversen CM, Brice DJ, Childs J, Vander Stel HM, Salmon VG (2021D) **SPRUCE S1 Bog Production of Newly-Grown Fine Roots Assessed Using Root Ingrowth Cores in 2013**. Oak
  Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A.
  <a href="https://doi.org/10.25581/spruce.091/1782483">https://doi.org/10.25581/spruce.091/1782483</a>
- 33. Iversen CM, Childs J, Norby RJ, Garrett A, Martin A, Spence J, Ontl TA, Burnham A, Latimer J. (2017D) SPRUCE S1 Bog fine-root production and standing crop assessed using with minirhizotrons in the Southern and Northern ends of the S1 Bog. 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.019.
- 34. Iversen CM, Garrett A, Martin A, Turetsky MR, Norby RJ, Childs J, Ontl TA (2017D) **SPRUCE S1 Bog tree basal area and understory community composition assessed in the Southern and Northern ends of the S1 Bog.** 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.024.
- 35. Iversen CM, Latimer J, Burnham A, Brice DJ, Childs J, Vander Stel HM (2017D) **SPRUCE plant-available nutrients assessed with ion-exchange resins in experimental plots, beginning in 2013**. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="http://dx.doi.org/10.3334/CDIAC/spruce.036">http://dx.doi.org/10.3334/CDIAC/spruce.036</a>.
- 36. Iversen CM, Ontl TA, Brice DJ, Childs J (2017D) **SPRUCE S1 Bog plant-available nutrients assessed with ion-exchange resins from 2011-2012 in the Southern end of the S1 Bog.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="http://dx.doi.org/10.3334/CDIAC/spruce.022">http://dx.doi.org/10.3334/CDIAC/spruce.022</a>.
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- 38. Jensen AM, Warren JM, Hook LA, Wullschleger SD, Brice DJ, Childs J, Vander Stel HM (2018D) SPRUCE S1 Bog Pretreatment Seasonal Photosynthesis and Respiration of Trees, Shrubs, and Herbaceous Plants, 2010-2015. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.3334/CDIAC/spruce.008">https://doi.org/10.3334/CDIAC/spruce.008</a>
- 39. Kluber LA, Allen SA, Hendershot JN, Hanson PJ, Schadt CW (2017D) SPRUCE Deep Peat Microbial Diversity, CO<sub>2</sub> and CH<sub>4</sub> Production in Response to Nutrient, Temperature, and pH Treatments during Incubation Studies. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="http://dx.doi.org/10.3334/CDIAC/spruce.040">http://dx.doi.org/10.3334/CDIAC/spruce.040</a>
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- 41. Kluber LA, Phillips JR, Singh S, Jagadamma S, Wang G, Schadt CW, Mayes MA (2020D) **Soil** respiration and microbial biomass from soil incubations with <sup>13</sup>C labeled additions. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.3334/CDIAC/ornlsfa.010">https://doi.org/10.3334/CDIAC/ornlsfa.010</a>
- 42. Kluber LA, Yang ZK, Schadt CW (2016D) **SPRUCE Deep Peat Heat (DPH) Metagenomes for Peat Samples Collected June 2015.** Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="http://dx.doi.org/10.3334/CDIAC/spruce.033">http://dx.doi.org/10.3334/CDIAC/spruce.033</a>
- 43. <u>Kl</u>uber LA, Yip DZ, Yang ZK, Schadt CW (2018D) **SPRUCE Deep Peat Heating (DPH) to Whole Ecosystem Warming (WEW) Metagenomes for Peat Samples Collected June 2016**. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. <a href="https://doi.org/10.25581/spruce.053/1444071">https://doi.org/10.25581/spruce.053/1444071</a>
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- 47. McPartland MY, Kane ES, Falkowski MJ, Kolka R, Turetsky MR, Palik B, Montgomery RA (2019Db) **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
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- 14. **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 <a href="http://leafweb.ornl.gov/">http://leafweb.ornl.gov/</a>.
- 15. **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 <a href="http://ameriflux.ornl.gov/fullsiteinfo.php?sid=64">http://ameriflux.ornl.gov/fullsiteinfo.php?sid=64</a>.
- 16. 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. <a href="http://dx.doi.org/10.3334/CDIAC/ornlsfa.006">http://dx.doi.org/10.3334/CDIAC/ornlsfa.006</a>
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- 24. Shi X, Wang D (2014D) **GSOD Based Daily Global Mean Surface Temperature and Mean Sea** Level Air Pressure (1982-2011)", doi:10.15149/1130373.
- 25. **Tool for Evaluating Mesophyll Impact on Predicting Photosynthesis** (<u>TEMIPP</u>). 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<sub>2</sub> 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<sub>2</sub> fertilization. *Proceedings of the National Academy of Sciences of the United States of America* 15774–15779, doi: 10.1073/pnas.1418075111. Download TEMIPP at <a href="http://tes-sfa.ornl.gov/node/80">http://tes-sfa.ornl.gov/node/80</a>.
- 26. **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 <a href="http://walkerbranch.ornl.gov/">http://walkerbranch.ornl.gov/</a>.
- 27. 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 <sup>13</sup>C Labeling and Shade Treatments. Oak Ridge National Laboratory, TES SFA, U.S. Department of Energy, Oak Ridge, Tennessee, U.S.A. https://doi.org/10.3334/CDIAC/ornlsfa.001.
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- 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 (2016D) 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 (2013D)

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