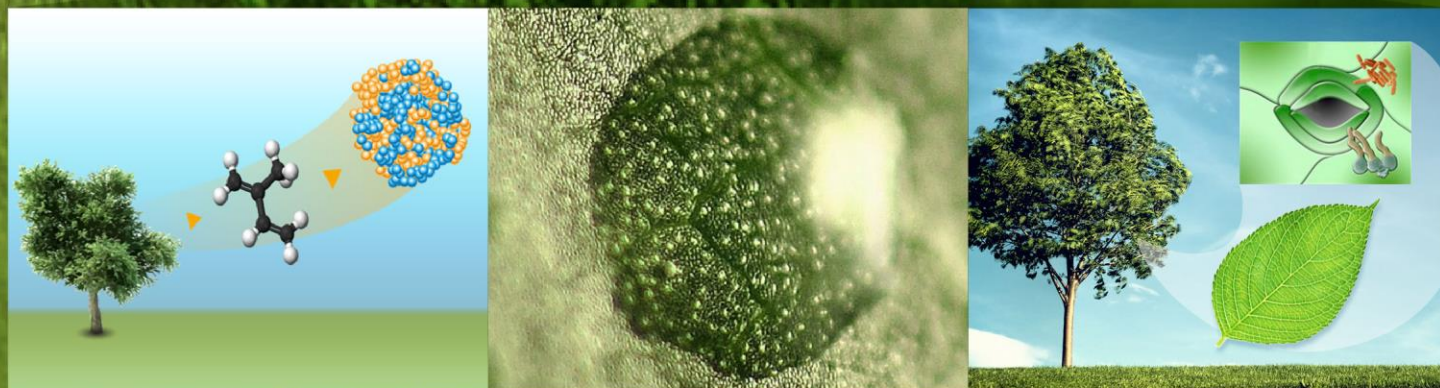


AB Guenther  
June 2015

# LEAP

## Land Ecosystem – Atmosphere Processes Workshop Report

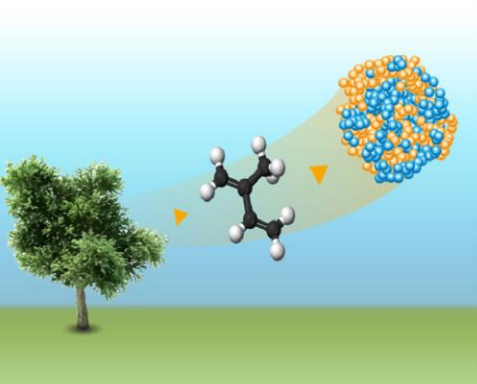
March 9-11, 2015



Prepared for the U.S. Department of Energy's Office of Biological  
and Environmental Research under Contract DE-AC05-76RL01830

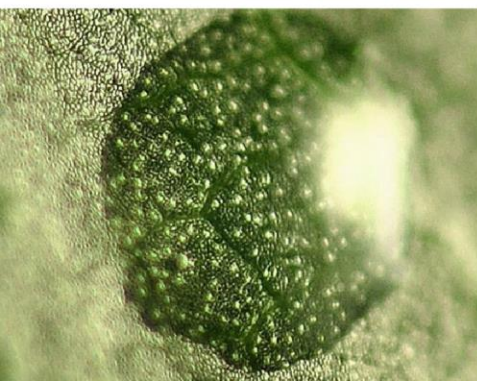
Pacific Northwest National Laboratory  
Richland, Washington 99352

# About the Cover



## Plant biogenic emissions influence the atmosphere.

Biogenic emissions of organic volatiles from plants are a major source of volatile organic compounds in the atmosphere. These compounds are oxidized in the atmosphere forming condensable species that can form new particles and contribute to the growth of existing particles.



## Plant uptake of nanoparticles

The fate of nanoparticles in the atmosphere is not well known, but it needs to be quantified in order to represent the aerosol life cycle in climate models. The deposition of nanoparticles on leaf surfaces could provide a source of nutrients for plants and associated microbes, and the active biological uptake of these particles could influence their atmospheric lifetimes.



## Plant-atmosphere interactions

Biogenic volatiles and biological particles from terrestrial ecosystems are transported through the atmosphere where they are processed. They can then be deposited to leaf surfaces or enter leaves through stomata apertures. The impact of plants on the atmosphere and conversely of the impact of the atmosphere on plants indicates a potential role of organic molecules in biosphere-atmosphere interactions and feedback coupling.

## DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor Battelle Memorial Institute, nor any of their employees, makes **any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.** Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or Battelle Memorial Institute. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

PACIFIC NORTHWEST NATIONAL LABORATORY

*operated by*

BATTELLE

*for the*

UNITED STATES DEPARTMENT OF ENERGY

*under Contract DE-AC05-76RL01830*

Printed in the United States of America

Available to DOE and DOE contractors from the

Office of Scientific and Technical Information,

P.O. Box 62, Oak Ridge, TN 37831-0062;

ph: (865) 576-8401

fax: (865) 576-5728

email: [reports@adonis.osti.gov](mailto:reports@adonis.osti.gov)

Available to the public from the National Technical Information Service,  
U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161

ph: (800) 553-6847

fax: (703) 605-6900

email: [orders@ntis.fedworld.gov](mailto:orders@ntis.fedworld.gov)

online ordering: <http://www.ntis.gov/ordering.htm>



This document was printed on recycled paper.

(9/2003)



# LEAP: Land Ecosystem – Atmosphere Processes Workshop Report

March 9-11, 2015

AB Guenther

June 2015

Prepared for the U.S. Department of Energy's Office of Biological and Environmental Research under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory  
Richland, Washington 99352



## Acronyms and Abbreviations

AML	Atmospheric Measurements Laboratory
ASR	Atmospheric Systems Research
BER	Biological and Environmental Research
BSOA	biogenic secondary organic aerosol
BVOC	biogenic volatile organic compound
DOE	Department of Energy
EMSL	Environmental Molecular Sciences Laboratory
EPR	Electron Paramagnetic Resonance
HEP	High Energy Physics
LC	liquid chromatography
LEAP	land ecosystem – atmosphere processes
MS	mass spectrometry
NCAR	National Center for Atmospheric Research
NMR	Nuclear Magnetic Resonance
PNNL	Pacific Northwest National Laboratory
SOA	secondary organic aerosol
U.S.	United States
VOC	volatile organic compound





## Contents

Acronyms and Abbreviations.....	v
1.0 Introduction .....	1.1
2.0 Workshop Overview .....	2.1
2.1 EMSL Science and Capabilities .....	2.1
2.2 Community Research Interests.....	2.1
2.3 Potential EMSL Research Activity .....	2.2
3.0 Plant-Aerosol Interactions Research Activity.....	2.1
3.1 Recommendations .....	3.1
3.1.1 Atmo-metabolomics .....	3.1
3.1.2 Nanoparticle Uptake.....	3.2
3.2 Path Forward .....	3.3
3.2.1 Atmo-metabolomics .....	3.3
3.2.2 Nanoparticle deposition.....	3.4
4.0 EMSL Earth Simulator Facility .....	4.1
Appendix A References .....	A.1
Appendix B Workshop Agendas.....	B.1
Appendix C Workshop Participants.....	C.1



## 1.0 Introduction

The Department of Energy (DOE) Office of Science Biological and Environmental Research (BER) sponsored a workshop on [Molecular Sciences Challenges](#) in May 2014 to identify knowledge gaps and determine tools needed to advance BER molecular research goals. The executive summary of the workshop report emphasizes the importance of land ecosystem-atmosphere chemical exchange and interactions. This includes processes affecting the emission of gases and particles into the atmosphere and their removal from the atmosphere by biological sinks. In addition, processes controlling the formation and growth of atmospheric particles and their impact on climate must be quantified along with feedbacks to terrestrial ecosystems. Research activities addressing the current molecular sciences challenges associated with land ecosystem – atmosphere processes (LEAP) would bridge the gaps between the microbiology, terrestrial ecology and atmospheric sciences research communities. The Environmental Molecular Sciences Laboratory (EMSL), a national scientific user facility funded and sponsored by BER, is well suited for this task with major scientific thrusts in each area.

On March 9-11, 2015, EMSL hosted a workshop on the Pacific Northwest National Laboratory (PNNL) campus in Richland Washington to explore land ecosystem-atmosphere science questions, approaches and research activities that could advance frontiers of climate and environmental science and enhance the unique capabilities of EMSL. Of particular interest was the potential for a multi-disciplinary research activity to address gaps in the current BER program and support research that complements and integrates multiple BER research programs.



## 2.0 Workshop Overview

### 2.1 EMSL Science and Capabilities

The March 9, morning session informed external participants, especially those not familiar with EMSL, about current EMSL scientific research and capabilities. EMSL research activities on soil, plants, and atmosphere were presented by Nancy Hess and Lili Paša-Tolić (soil sciences); Christer Jansson, Abby Ferrieri, and Rodica Lindenmaier (plant sciences); and Alex Guenther (atmospheric sciences). The soil sciences overview included a description of the EMSL “rhizosphere research campaign,” which provided a clear example of a multi-disciplinary, multi-institutional research campaign that is successfully tackling a research challenge at the level appropriate for an EMSL research campaign.

EMSL capability leads for Mass Spectrometry (MS) (Robby Robinson), Nuclear Magnetic Resonance (NMR) and Electron Paramagnetic Resonance (EPR) (Nancy Washton), and Cell Isolation and Systems Analysis (Galya Orr) presented overviews of these capabilities. Participants were informed about EMSL expertise and equipment ranging from high throughput observational techniques to unique measurement approaches. The presentations illustrated ways in which these capabilities are being used for biological and environmental research. The EMSL presentations were followed by a tour of selected EMSL laboratories.

### 2.2 Community Research Interests

During the afternoon session on March 9, a comprehensive view was presented of the current research activities of the external participants with an emphasis on outstanding challenges and questions in LEAP research.

Albert Rivas-Ubach (CREAF, Barcelona, Spain) spoke about the use of ecometabolomic techniques to characterize the metabolomes of aerosols (mainly pollen, spores, and other primary biological particles). He proposed this methodology to understand ecosystem structure and function by characterizing and tracking over space and time molecular compounds that act as biomarkers of ecosystem status.

Jim Smith (National Center for Atmospheric Research (NCAR), Boulder, Colorado) focused his talk on nanoparticle formation in the atmosphere via oxidation of their biogenic volatile precursors. He discussed results from recent field experiments in the Amazon rainforests that are investigating nanoparticle formation in the Amazon, including the sources and fate of these particles.

Russ Monson (University of Arizona) showed results of isoprene emissions from his field experiment in Arizona with transgenic poplar plantations grown under different levels of atmospheric CO<sub>2</sub>. He concluded that the phenotypes of plants are highly dependent on seasonal phenological and environmental context, and that the ecology of plants is crucially important for the interpretation of phenotypic profiling (phenomics).

Allison Steiner (University of Michigan) described the possible effects of sub-pollen particles in climate dynamics. She showed experimental evidence that pollen grains can rupture when wet and act as cloud condensation nuclei. Those sub-pollen particles are composed of a variety of macromolecules and elements that may interact with atmospheric processes. She proposed to include pollen emissions and their fate in climate models.

Pawel Misztal (University of California, Berkeley) talked about the interaction of the phyllosphere with the atmosphere, and showed numerous biogenic volatile organic compounds (BVOC) resulting from bacterial emissions. Those BVOC

have multiple functions such as promoting plant growth, and can be important in both outdoor and indoor environments. (Figure 2.1)

Todd Rosenstiel (Portland State University) discussed research activities ranging from bioenergy to bryophytes, linked by a common theme of investigating earth system interactions and feedbacks. The bioenergy plantations of the Pacific Northwest were identified as a nearby potential field site with important implications for energy production. Mosses were noted to be a unique possibility for studying whole ecosystem-atmosphere interactions on small scales.

Jogi Schnitzler (Helmholtz Zentrum Munich, Germany) described novel observational approaches to advance understanding of biosphere-atmosphere interactions. These included studies focused on plant-plant signaling within canopies, beneficial plant-microbe interactions and genetic regulation of BVOC emissions.

### 2.3 Potential EMSL Research Activity

The morning session on March 10, began with discussions summarizing the outstanding challenges in terrestrial ecosystem-atmosphere research, and identifying those that could be uniquely addressed with EMSL scientific expertise and capabilities. This led to a focus on novel aspects of plant-aerosol interactions including the cycling of gases and nanoparticles between plant ecosystems and the atmosphere. Participants identified three main processes involved in this cycling: emission by plants and microbes, transformation in the atmosphere, and deposition/uptake by terrestrial surfaces. A discussion followed on potential research campaign objectives. There was general consensus that the research should focus on novel aspects of plant-aerosol interactions research. The plant component of this interaction was defined to include all associated microbes and fungi. Aerosol particles included biological particles, such as spores and pollen, but the focus was placed on biogenic secondary organic aerosol (BSOA) nanoparticles formed by the oxidation of BVOC. It was recognized that in order to investigate these processes it was also necessary to understand processes that transform BVOC and aerosol in the atmosphere including oxidation, fragmentation, and condensation. While the study of processes controlling SOA particles formation and growth is an active area of research, full understanding of the physiochemical nature of these transitions is limited.

During the morning session, the workshop participants also discussed the possibility that these particles could return to the biosphere and be taken up by plants and microbes, with important implications for both biological systems and the atmosphere. While it is known that atmospheric VOCs and VOC breakdown products can be taken up by plants, where they serve as signaling molecules and/or are catabolized, it was agreed that very little is known about particle deposition, especially BSOA nanoparticle deposition on leaf surfaces, and even less is known about particle uptake and metabolism by plants. Key questions identified by the participants include: Are leaf surfaces repelling or attracting to nanoparticles? How does leaf surface structure influence particle deposition and uptake? Do these particles enter through the stomata and do they reside inside the leaf? What is the impact of these particles on the plant's physiology? Is there any preference for uptake of certain types of particles? Do microbes on or inside the leaf influence the particle uptake? Are there diurnal variations in particle deposition rates driven by changes in stomatal conductance? Is there a plant-microbe competition for nutrients in nanoparticles? How do tropical plants behave compared to temperate zone plants for uptake? How do leaves from the lower canopy compare to leaves at the top of the same tree? Are there differences in urban versus rural environments?

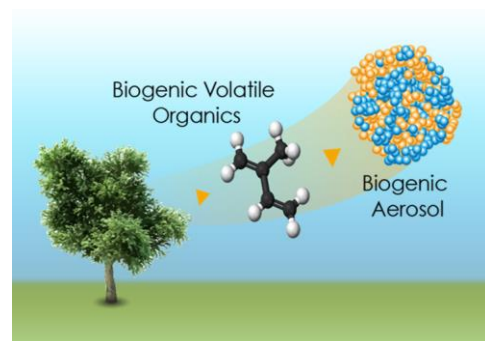


Figure 2.1 Biogenic emissions of organic volatiles from plants are the major source of VOC in the atmosphere. These compounds are oxidized in the atmosphere forming condensable species that can form new particles and contribute to the growth of existing particles.

The afternoon session included discussions on experimental approaches, with the conclusion that a useful approach would investigate three plant-aerosol systems: a very simple system in a controlled laboratory setting, a relatively simple field ecosystem such as a monoculture plantation, and a very complex field ecosystem such as a tropical rainforest. Potential approaches for controlled laboratory ecosystems are described in section 2.4. Poplar (or giant reed) plantations in north central Oregon were discussed as good candidates for the simple field ecosystem. Tropical rainforest sites in French Guiana and Brazil were identified as potential locations for a study of a complex field ecosystem.





## 3.0 Plant-Aerosol Interactions Research Activity

### 3.1 Recommendations

The workshop participants endorsed the goal of developing a multi-disciplinary, multi-institutional EMSL research campaign to fill an important gap in the BER research portfolio and advance the frontiers of climate and environmental sciences. There was also consensus that the proposed research should not just be an incremental advance or integration of existing activities, but should be a novel research project that utilizes unique EMSL capabilities.

The recommended research focus was on plant-aerosol interactions, with an ecosystem-level view of these interactions including soil and microbial activity. Figure 3.1 shows hypotheses that were developed to guide the project:

The participants noted that plant-aerosol interactions should be investigated in different seasons (spring, summer), locations (tropical forest versus temperate forest/plantation, urban environment and agricultural systems), and plant types (with different leaf surface structure).

#### 3.1.1 Atmo-metabolomics

The application of metabolomics to atmospheric samples, i.e., the combination of atmospheric sampling and metabolomic analysis, hereinafter referred to as “atmo-metabolomics,” is a novel approach that could provide a useful tool for both ecologists and atmospheric scientists. Ecologists would benefit from this approach to investigate the response of whole ecosystems to environmental change. Atmospheric scientists would acquire an innovative tool for quantifying the immense diversity of biogenic contributions to the composition of the atmosphere, potentially improving model simulations of biogenic emissions and their air quality, and climate impacts. Metabolomics approaches analyze the metabolome of an organism, the total set of thousands of small (typically less than 1000 Da) molecular weight compounds (metabolites) present in an organism at a given time (Fiehn 2002). Such molecules include substrates and products of cellular primary metabolism such as sugars, amino acids, and nucleotides as well as the secondary metabolism compounds such as terpenoids, all involved in a great variety of complex physiological processes to maintain the organisms’ homeostasis, growth, and responses to biotic and abiotic stressors (Peñuelas and Sardans 2009). The metabolome can thus be considered as the chemical phenotype of the organism (Fiehn 2002).

The metabolome of the atmosphere includes molecular compounds present in gas-phase volatile species known as Volatile Organic Compounds (VOC) and aerosols, including primary biological particles (e.g., pollen, fungi, bacteria, and detritus from plants and animals) and secondary aerosols formed during the oxidation of primary emissions. Atmo-metabolomics could be a useful approach for investigating ecological status using changes in the metabolic composition of the air. It may also become a key tool to follow the dynamics of ecological status in response to natural and anthropic

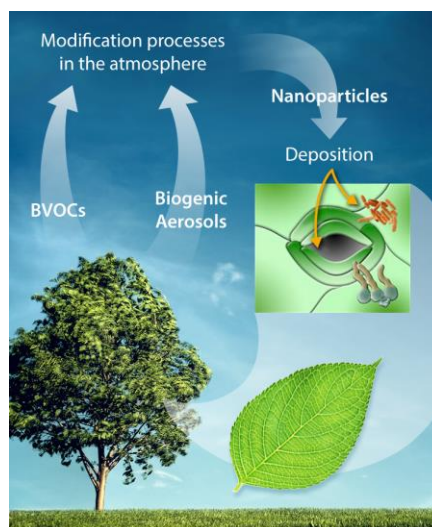


Figure 3.1. Hypotheses for the project

Hypothesis 1: Emissions of atmospheric biogenic aerosol and volatile precursors are controlled by ecosystem responses to environmental conditions, resulting in variations that can be explained using metabolomic (and other omics) approaches.

Hypothesis 2: Deposition of aerosol particles to ecosystem surfaces result in molecular uptake by plants, impacting the structure and function of the phyllosphere microbial community and plant metabolism.

environmental changes. Clearly, it will be necessary to recognize that some of the compounds observed in the atmosphere are not emitted from the ecosystem and instead are either produced by anthropogenic sources or are the oxidation products of biogenic compounds, which could be addressed with experiment design.

Only a small fraction of the enormous diversity of organic constituents in the atmosphere has been identified and quantified in atmospheric studies (Nozierre et al., 2015). Comprehensive characterization of changes in the metabolome of individual organisms has led to a better understanding of how an organism responds to the environment. Ecologists have recently extended this approach to develop ecometabolomics techniques for investigating the functioning of whole ecosystems and their response to environmental change (Peñuelas and Sardans 2009). Ecometabolomics have been used to study strategies for allocating resources and to understand coupling between cellular metabolism, ecosystem structure and nutrient cycling (Sardans et al., 2011; Rivas-Ubach et al., 2012; Rivas-Ubach et al., 2013; Sardans et al., 2011; Rivas-Ubach et al., 2014; Gargallo-Garriga et al., 2014). We propose to extend this approach to the atmosphere, using atmospheric measurements of VOC and particles in conjunction with analytical and statistical approaches that have been successfully applied for ecometabolomic studies of plant tissues. Measurements of genomics and other omics techniques should be included in the project to provide complementary information on origins of the organic material. We expect that this approach for investigating the unexplored organic constituents in the earth's atmosphere could lead to an improved representation of the aerosol life cycle, a major uncertainty in climate models.

### 3.1.2 Nanoparticle Uptake

Nanoparticles are formed in the atmosphere when condensable gases form clusters that grow to become small particles. The potential fates of nanoparticles include deposition to surfaces, coagulation with other particles, or growth to larger particles that can influence climate. The workshop participants from the atmospheric science community noted that very little is known about the deposition of nanoparticles, but their uptake on leaves could be an important loss mechanism. Participants from the biological sciences community noted that nanoparticles are composed of molecules that could be biologically active sources of carbon and nutrients for phyllosphere microbes living on the surface (epiphytes) and in the mesophyll space (endophytes) of leaves. In addition, the carbon and nutrients in nanoparticles that enter the leaf through the stomata could be available for plants. Some of the key processes that should be investigated are the importance of leaf surface structure in determining nanoparticle deposition and particle uptake, nanoparticle uptake through stomata, the fate of nanoparticles on leaf surfaces or inside leaves, and the impact of nanoparticles on plant physiology and the phyllosphere.

After multiple transformations following primary emissions of biogenic VOC and biological particles, some secondary and primary particles return to the biosphere and are deposited to leaves. Given the large areal extent of leaf surfaces (Sexton et al., 2013), their contribution to particle sink is of primary importance (Andreae and Crutzen, 1997). While some studies have investigated the leaf size effect on particle collection efficiency (Huang et al., 2015) or the deposition of polycyclic aromatic hydrocarbons or lead uptake by vegetation from the atmosphere (Simonich and Hites, 2004; Uzu et al., 2010), they emphasize that the mechanisms responsible for foliar uptake are still unclear. Terrestrial plants have the ability to absorb nutrients through the leaves (Mengel, 2002), and nanoparticles may follow the same pathway. Nutrients and particles have to cross several physical barriers before entering cytosol of epidermal cells, this penetration being strongly dependent on weather conditions, plant species, physiological status, and speciation of the element (Schönherr and Luber, 2001).

Potential techniques recommended for investigating these processes include the following:

- Use plant enclosures coupled with an aerosol generator to create nanoparticles of various composition and study uptake by plants (based on composition, size, shape, content).

- Use marker aerosol compounds to easily detect particles (for example, metallic or other composite particles are detected well by spectroscopy).
- Identify biomarkers and genetic material within nanoparticles including micro RNAs.
- Characterize microbial communities on leaf surfaces.
- Use imaging techniques (e.g., SEM) to follow nanoparticles in different tissues of plant leaves.

### 3.2 Path Forward

An initial scoping study is recommended for May-September 2015 to assess the importance and feasibility of a full plant-aerosol interaction research campaign and develop a specific plan, if warranted. The plan for future work would include a project team made up of some workshop participants as well as other members of the scientific community. The scoping study would include efforts on the two major research themes of the project: atmo-metabolomics and nanoparticle deposition. PNNL postdoctoral scientists Albert Rivas-Ubach (for atmo-metabolomics) and Rodica Lindenmaier (for nanoparticle deposition) could serve as project coordinators for these two components of the project. The first task for each research theme would be a thorough literature review on each topic. This would primarily be the responsibility of the project coordinator with input from all interested participants. A second task would be to develop measurement protocols and conduct initial observations to guide the development of a research campaign proposal.

#### 3.2.1 Atmo-metabolomics

A protocol for conducting the atmo-metabolomic analyses will be developed during the scoping study. The protocol will include both liquid chromatography (LC) and MS (for particles), and gas chromatography-mass spectrometry (GC-MS) (for volatiles) techniques. Aerosol samplers will be installed for several months in two different locations near the PNNL campus in late spring and summer.

Sample sets will be simultaneously collected from each site. Each set will include a particle filter sample and several VOC cartridge samples. Each particle sample will be collected on a quartz filter for an 18 hour period with air pulled at a constant flow rate of approximately 100 L per minute. Samples will be collected weekly and stored at -20°C until analyzed. Several extractions will be performed on those samples, including blank filters to optimize the extraction of metabolites. This will include methanol/water extractions at different proportions. Sonication and centrifuge steps will be also performed with different parameters. Final extracts will be processed with LC-MS and GC-MS systems in EMSL. The objective is to optimize a protocol to identify and quantify as many molecular species as possible.

Once the protocol is optimized, we will apply the methodology using filter samples from ongoing international research programs including the GoAmazon project (Manaus, Brazil 2014-2015) and the IMBALANCE-P research program in French Guiana (2015-2017). Both studies are investigating the impact of environmental change on ecosystem-atmosphere interactions and provide a comprehensive database of ancillary measurements for interpreting these atmo-metabolomic observations. The fingerprints and metabolome profiling of the aerosol samples will be analyzed by different modern statistical methods for the preparation of a manuscript describing the approach and potential applications.

### 3.2.2 Nanoparticle Deposition

To assess the potential importance of this research theme, a preliminary study will be conducted to quantify nanoparticle deposition to leaves and determine if the rates are sensitive to changes in stomatal conductance. A controlled environment (e.g., temperature, humidity, light levels) glass cuvette system will be used to measure nanoparticle deposition rates to foliage by enclosing leaves of several representative plant species and exposing them to an air stream containing artificially produced nanoparticles of various compositions. The physiological status (photosynthesis, transpiration) and stress level (chlorophyll fluorescence) of each plant will be measured using a LICOR 6400XT. This initial study will be conducted using potted plants growing in a growth chamber. Selected plant species will include poplars to complement potential field measurements in Pacific Northwest poplar plantations and tropical plants to complement future tropical forest studies.

## 4.0 EMSL Earth Simulator Facility

The 2014 EMSL Atmospheric Aerosol Systems Science Theme Advisory Panel identified three high priority science focus areas and recommended potential capabilities that EMSL should consider that would build on existing EMSL strengths and leverage its measurement capabilities and computational resources to develop innovative methods for investigating atmospheric aerosols. One of these high priority science focus areas was on plant-aerosol-climate interactions. The panel concluded that EMSL strengths in laboratory-based measurements could be effectively applied to climate and earth system studies by developing a multi-chamber earth simulator facility that minimized wall effects and artifacts and enabled investigations of interactions between key earth system components (e.g., plants, soil, aerosol, and clouds).

As an initial step towards assessing existing capabilities and community interest in an EMSL earth simulator facility, a half-day session was held on March 11, 2015 that included the LEAP workshop participants and additional PNNL participants. Earth simulator facilities with various physical chambers that enclose earth system components (e.g., atmosphere, hydrosphere, rhizosphere, phyllosphere) have been used by the scientific community to investigate the response of specific earth system components and/or interactions under controlled laboratory conditions. Simulators that include multiple components have been used for studies of interactions. The session provided an overview of existing earth system simulators that are currently being used for at least some aspect of plant-aerosol interactions research. The participants were also asked to consider the need for a new facility to advance LEAP research.

Jim Smith described potential interest in the BER Atmospheric Systems Research (ASR) community in simulation chambers and summarized discussions from past ASR meetings. The BER and ASR community has made extensive use of existing atmospheric reaction chambers, but it has been recognized that the existing facilities are not ideal. David Asner described DOE High Energy Physics (HEP) interests in a chamber facility and summarized past meetings and relevant discussions on this topic that indicate a willingness of the HEP community to collaborate with the ASR community in the development of an atmosphere and/or cloud chamber.

Todd Rosenstiel (Portland State University) described the need for flexible, adaptable earth simulator platform that can accommodate a diversity of plant forms and support authentic plant-atmosphere/plant-rhizosphere interactions. The need to provide infrastructure support for growth in functional ecological genomics was emphasized along with the need to support growth in rational design/selection/creation of genotypes for green infrastructure and sustainable solutions. There was also a recommendation for including field portability. Russ Monson (University of Arizona) described capabilities and research activities at Biosphere2, which covers an area of 1.27 ha and is the largest earth simulator in the world. Current focus includes a Landscape Evolution Observatory to investigate how landscapes and ecosystems develop. The development and application of ecosystem omics capabilities within earth system simulators is of mutual interest and there is potential for a complementary partnership. Jogi Schnitzler (Helmholtz Zentrum Munich, Germany) described custom designed chamber systems at Helmholtz Zentrum that are used to investigate plant VOC emissions and aerosol interactions.

While there are similarities with EMSL capabilities, there is also good potential for complementary facilities and collaboration in areas including plant-plant signaling, plant-microbe interactions and VOC phenotyping. Jim Smith described biosphere-atmosphere interaction chambers at NCAR that are used to study new particle formation as part of the DOE ASR program. While this facility has been successful in providing insights, it was concluded that a new community facility could further advance this science. John Shilling described the PNNL Atmospheric Measurements Laboratory (AML) aerosol chamber for conducting research focused on BER and ASR research priorities. The frequent community studies held at the AML chamber demonstrate the strong potential for interest by the ASR community that would likely be

increased by a facility with more flexibility and capabilities. Christer Jansson described EMSL and community interests in a national phenomics facility. The phenomics facility was the focus of an EMSL workshop held March 12-13, 2015 and will be described in detail in another report. The proposed phenomics facility would complement an earth system simulator capability with joint development of plant growth, biological systems modeling, and omics capabilities.

Considerable progress has been made in identifying and investigating the individual processes controlling atmospheric composition and climate change. There has been less advancement on quantifying complex interactions that determine earth system responses to environmental change. For example, interactions of anthropogenic pollution and biogenic volatile organic compound emissions may be a major source of atmospheric aerosol leading to a strong feedback with the climate system. If this is the case, then investigating anthropogenic pollutants or biogenic compounds separately is insufficient for representing aerosol production in numerical climate models. A laboratory chamber facility for investigating and quantifying individual processes and their interactions under controlled environmental conditions could serve multiple purposes including the development of new analytical approaches and reconciling disparities between theoretical, laboratory, and field investigations of biosphere-atmosphere interactions. The presenters in this session described chamber facilities for investigating biogenic emissions and aerosol production that have been built in the United States (U.S.) and Europe. While they have successfully demonstrated the utility of chamber approaches, they do not cover the entire scope of biogenic aerosol and earth system research and do not fully solve key experimental concerns, such as avoiding wall effects. There is no adequate facility in the U.S. for investigating the full range of biosphere-atmosphere interactions including biogenic emissions and uptake, aerosol production and growth, and feedbacks to biogenic emissions. Thus, an opportunity exists to build a novel EMSL facility that would complement and integrate EMSL capabilities with DOE BER field study approaches. The participants in this session encouraged EMSL to move forward with a process to consider the development of a highly instrumented plant and aerosol chamber system, one that would include high quality core measurements (e.g., primary VOC, ozone, NO and particle concentrations and fluxes), as well as provide innovative aerosol and gas measurement using both on-line monitoring capability and off-line analysis. In addition, the proposed user facility would enable researchers to bring unique instruments to the chamber for specific, tailored experiments. This user facility can be fully integrated with the infrastructure for a plant phenotyping platform discussed in the ensuing Workshop on PhytoPhenomics that was held on March 12-13. The next steps in assessing the need and feasibility of an EMSL aerosol chamber facility include:

- Compile a description of existing earth simulator (e.g., atmospheric aerosol, terrestrial ecology, biogenic emissions) chamber facilities.
- Investigate user community interest in using the facility.
- With community input, develop an initial design of the major features of the facility.

## Appendix A References





## Appendix A

- Andreae, M.O. and P. Crutzen 1997, “Atmospheric Aerosols: Biogeochemical Sources and Role in Atmospheric Chemistry”. *Science* 276 (5315), 6.
- Fiehn O. 2002, "Metabolomics — the link between genotypes and phenotypes." in *Functional Genomics*, ed. C Town, pp. 155-171. Springer Netherlands. doi: 10.1007/978-94-010-0448-0\_11
- Gargallo-Garriga A, J Sardans, M Perez-Trujillo, A Rivas-Ubach, M Oravec, K Vecerova, O Urban, A Jentsch, J Kreyling, C Beierkuhnlein, T Parella, and J Peñuelas. 2014. "Opposite metabolic responses of shoots and roots to drought." *Scientific Reports* 4:6829. doi:10.1038/srep06829
- Huang, C.W., M. Lin, A. Khlystov, and G. Katul, 2015 “The effects of leaf size and microroughness on the branch-scale collection efficiency of ultrafine particles”. *Journal of Geophysical Research: Atmospheres* 120(8), 2014JD022458.
- Mengel K. 2002. "Alternative or Complementary Role of Foliar Supply in Mineral Nutrition." *Acta Horticulturae* 594:33-47.
- Peñuelas J, and J Sardans. 2009. "Ecological metabolomics." *Chemistry and Ecology* 25:305-309. doi:10.1080/02757540903062517
- Rivas-Ubach A, A Gargallo-Garriga, J Sardans, M Oravec, L Mateu-Castell, M Pérez-Trujillo, T Parella, R Ogaya, O Urban, and J Peñuelas. 2014. "Drought enhances folivory by shifting foliar metabolomes in *Quercus ilex* trees." *New Phytologist* 202:874-885. doi:10.1111/nph.12687
- Rivas-Ubach A, M Pérez-Trujillo, J Sardans, A Gargallo-Garriga, T Parella, and J Peñuelas. 2013. "Ecometabolomics: optimized NMR-based method." *Methods in Ecology and Evolution* 4:464-473. doi:10.1111/2041-210X.1202
- Rivas-Ubach A, J Sardans, M Pérez-Trujillo, M Estiarte, and J Peñuelas. 2012. "Strong relationship between elemental stoichiometry and metabolome in plants." *Proceedings of the National Academy of Sciences* 109:4181-4186. doi:10.1073/pnas.1116092109
- Sardans J, J Peñuelas, and A Rivas-Ubach. 2011. "Ecological metabolomics: overview of current developments and future challenges." *Chemoecology* 21:191-225. doi:10.1007/s00049-011-0083-5
- Schönherr J, and M Luber. 2001. "Cuticular penetration of potassium salts: Effects of humidity, anions, and temperature." *Plant and Soil* 236:117-122. doi:10.1023/A:1011976727078
- Simonich, S.L., R. Hites, 1994. “Vegetation-Atmosphere Partitioning of Polycyclic Aromatic Hydrocarbons”, *Environ. Sci. Technol.*, 28, 939-943.
- Sexton, J. O. et al., 2013. “Global, 30-m resolution continuous fields of tree cover: Landsat-based rescaling of modis vegetation continuous fields with lidar-based estimates of error”, *International Journal of Digital Earth*, 6 (5), 427–448.
- Uzu, G., S. Sobanska, G. Sarret, M. Muñoz, and C. Dumat, 2010. “Foliar lead uptake by lettuce exposed to atmospheric fallouts”, *Environ. Sci. Technol.*, 44, 1036-1042.



## Appendix B Workshop Agendas



## Appendix B

### Contacts:

Alex Guenther  
Julie Barriball

## AGENDA

### Monday, March 9:

#### *Morning Session: Introduction to EMSL*

8:30 am	<b>Welcome, Introductions, Agenda and Objectives</b> Alex Guenther
9:00 am	<b>EMSL Overview</b> Allison Campbell and Karl Mueller
9:30 am	<b>Mass Spectrometry at EMSL</b> Robby Robinson
9:45 am	<b>NMR and EPR at EMSL</b> Nancy Washton
10:00 am	<b>CISA at EMSL</b> Galya Orr
10:15 am	<b>Break</b>
10:30 am	<b>Soil Science at EMSL</b> Nancy Hess, Lili Paša-Tolić, Vanesa Bailey
10:45 am	<b>Plant Science at EMSL</b> Christer Jansson, Rodica Lindenmaier, Abby Ferrieri
11:00 am	<b>Atmospheric Science at EMSL</b> Alex Guenther
11:15 am	<b>EMSL Tour</b> External visitors only
12:15 pm	<b>Lunch Break</b> Please note that lunch is <u>on your own</u>

**Afternoon Session: Synergistic Activities**

1:30 pm	<b>Developing an EMSL Research Campaign</b> Alex Guenther
2:00 pm	<b>Research Activities</b> Albert Rivas and Josep Penuelas (CREAF Barcelona)
2:30 pm	<b>Research Activities</b> Jim Smith (NCAR)
3:00 pm	<b>Research Activities</b> Russ Monson (University of Arizona)
3:30 pm	<b>Break</b>
3:45 pm	<b>Research Activities</b> Toss Rosenstiel (Portland State University)
4:15 pm	<b>Research Activities</b> Jogi Schnitzler (Helmholtz Zentrum Munich)
4:45 pm	<b>Research Activities</b> Allison Steiner (University of Michigan)
5:15 pm	<b>Research Activities</b> Pawel Misztal and Allen Goldstein (University of California, Berkeley)
5:45 pm	<b>Adjourn</b>

**Tuesday, March 10:**

**Morning Session: Research Campaign Objectives**

8:30 am	<b>Identify Potential Research Focus and Scientific Questions</b>
10:30 am	<b>Break</b>
10:45 am	<b>Prioritize and Select Specific Objectives</b>
12:15 pm	<b>Lunch Break</b> Please note that lunch is <u>on your own</u>

### ***Afternoon Session: Research Campaign Approach***

1:00 pm	<b>Identify Research Sites</b>
1:30 pm	<b>Develop Approaches</b>
3:00 pm	<b>Break</b>
3:15 pm	<b>Continue to Develop Approaches</b>
4:30 pm	<b>Identify Participants, Roles, Next Steps</b>
5:30 pm	<b>Adjourn</b>

### **Earth System Simulation – Environmental Chamber Facility Discussion**

March 11, 2015

EMSL Boardroom

## **AGENDA**

8:00 am	<b>Welcome, Introductions, Agenda and Objectives</b> Alex Guenther
8:15 am	<b>EMSL Process for Developing Major Capabilities</b> Dave Koppenaal and Scott Tingey
8:30 am	<b>DOE interest in Environmental Chambers</b> Jim Smith and Alex Guenther
8:45 am	<b>PNNL AML Aerosol Chamber</b> John Shilling
9:00 am	<b>EMSL Phenomics and Plant Sciences Program</b> Christer Jansson
9:15 am	<b>NCAR environmental chambers</b> Jim Smith and Peter Harley
9:30 am	<b>Biosphere 2 Environmental Chambers</b> Russ Monson
9:45 am	<b>Break</b>

## LEAP: Land Ecosystem – Atmosphere Processes Workshop Report

---

10:00 am	<b>Portland State Environmental Chambers</b> Todd Rosenstiel
10:15 am	<b>Helmholtz Zentrum Environmental Chambers</b> Jogi Schnitzler
10:30 am 10:45 am	<b>HEP David Asner</b> <b>Summary, Discussion, Next Steps</b> Alex Guenther
11:30 am	<b>Adjourn</b>



## Appendix C Workshop Participants



## Appendix C

### External participants

Allen Goldstein, UC Berkeley (via videoconference)

[ahg@berkeley.edu](mailto:ahg@berkeley.edu)

Peter Harley, NCAR (Retired)

[harleypc@forethought.net](mailto:harleypc@forethought.net)

Pawel Misztal, UC Berkeley

[pkm@berkeley.edu](mailto:pkm@berkeley.edu)

Russ Monson, University of Arizona

[russmonson@email.arizona.edu](mailto:russmonson@email.arizona.edu)

Josep Penuelas, CREAM Barcelona (via videoconference)

[josep.penuelas@uab.cat](mailto:josep.penuelas@uab.cat)

Todd Rosenstiel, Portland State University

[rosensti@pdx.edu](mailto:rosensti@pdx.edu)

Jogi Schnitzler, Helmholtz Zentrum Munich

[jp.schnitzler@helmholtz-muenchen.de](mailto:jp.schnitzler@helmholtz-muenchen.de)

Jim Smith, NCAR

[jimsmith@ucar.edu](mailto:jimsmith@ucar.edu)

Allison Steiner, University of Michigan

[alsteine@umich.edu](mailto:alsteine@umich.edu)

### PNNL participants

David Asner, Radiation Detection and Nuclear Sciences

[david.asner@pnnl.gov](mailto:david.asner@pnnl.gov)

Vanessa Bailey, Microbiology

[Vanessa.Bailey@pnnl.gov](mailto:Vanessa.Bailey@pnnl.gov)

Abigail Ferrieri, Post-Doc, Mass Spectrometry

[abigail.ferrieri@pnnl.gov](mailto:abigail.ferrieri@pnnl.gov)

Alex Guenther, Science Theme Lead, Atmospheric Aerosol Systems

[alex.guenther@pnnl.gov](mailto:alex.guenther@pnnl.gov)

Nancy Hess, Science Theme Lead for Terrestrial and Subsurface Ecosystems

[nancy.hess@pnnl.gov](mailto:nancy.hess@pnnl.gov)

## LEAP: Land Ecosystem – Atmosphere Processes Workshop Report

---

Christer Jansson, Director of Plant Sciences  
[georg.jansson@pnnl.gov](mailto:georg.jansson@pnnl.gov)

Rodica Lindenmaier, Post-Doc, Atmospheric Sciences  
[rodica.lindenmaier@pnnl.gov](mailto:rodica.lindenmaier@pnnl.gov)

Galya Orr, CISA  
[Galya.Orr@pnnl.gov](mailto:Galya.Orr@pnnl.gov)

Paša-Tolić, Lead Scientist for Mass Spectrometry  
[ljiljana.pasatolic@pnnl.gov](mailto:ljiljana.pasatolic@pnnl.gov)

Albert Rivas, CREAM Barcelona  
[albert.rivas.ubach@pnnl.gov](mailto:albert.rivas.ubach@pnnl.gov)

Robby Robinson, Mass Spectrometry  
[Errol.Robinson@pnnl.gov](mailto:Errol.Robinson@pnnl.gov)

John Shilling, Atmospheric Sciences  
[john.shilling@pnnl.gov](mailto:john.shilling@pnnl.gov)

Scott Tingey, EMSL Chief Operating Officer  
[scott.tingey@pnnl.gov](mailto:scott.tingey@pnnl.gov)

Nancy Washton, NMR/EPR  
[Nancy.Washton@pnnl.gov](mailto:Nancy.Washton@pnnl.gov)