

Methods

This is an abbreviated description of the methods used to produce this data set. More information can be found in the publications listed below. The use of trade or firm names in this publication is for reader information and does not imply endorsement by the US Department of Agriculture of any product or service.

Step 1.

These steps are identical up to FTIR analysis as those found in the "Pyrolysis Gases Measured by Gas Chromatography and Mass Spectrometry from Fires in a Wind Tunnel and at Ft. Jackson, SC" data set. Eighty-eight fuel beds 2.4 m long and approximately 0.8 m wide composed of longleaf pine needles and various combinations of fetterbush, sparkleberry, blueberry and inkberry plants were burned in an open-topped low-speed wind tunnel with environmental controls under 0 and 1 m s⁻¹ wind conditions November 8-18, 2017, February 23-March 1, 2018 and October 30 - November 2, 2018. Fuel beds were constructed by uniformly distributing 1000 g (wet weight) of needles over the entire fuel bed in sections and then placing the plants in predetermined locations. A complete randomized design was used, but it was modified as we sought to maximize the production of pyrolyzates by increasing the number of plants in a fuel bed. In the wind tunnel, environmental conditions simulated growing season (Nov. 2017, 2018) (dead fuel moisture 9.6%, air temperature 297 K, relative humidity 35%) and dormant season (Feb-March 2018) (dead fuel moisture 10.6%, air temperature 280.6 K, relative humidity 63%) conditions.

Step 2.

Measured fuel and environmental conditions included air temperature and relative humidity, fuel temperature (measured by long wave infrared camera), fuel moisture content, and fuel mass.

Step 3.

Mass loss, total and radiant heat fluxes from the flame were measured. Convective heat flux estimated using background-oriented schlieren imagery. Flame height ocularly estimated.

Step 4.

Gases were extracted from the wind tunnel burns via 3/8" stainless-steel tubing, HEPA-filtered to eliminate tar and char contamination, and pumped into an 8 m White cell (Bruker A136, 2.2 L volume) housed inside a Bruker Tensor 37 spectrometer. The extractive probe was placed directly above a plant as close as possible to the foliage. To prevent analyte and tar condensation, both the transfer tubing and the gas cell were heated to ~ 55 °C using heating tape (and a voltage regulator) and a cell heating shroud, respectively. A thermocouple was suspended into the White cell to record the gas temperature for subsequent spectral analysis, with a pressure gauge mounted atop the cell. Prior to data collection, the White cell was aligned using the FTIR's Ge / CaF₂ beamsplitter and tungsten lamp source. Once aligned, these were replaced with a Ge / KBr beamsplitter and mid-IR globar source, along with a mercury cadmium telluride detector, thereby

configuring the Tensor 37 to record spectral data from 7500 to 500 cm^{-1} . Details of determining composition of background gases and calibration of spectrometers provided in publications.

Step 5.

Two data acquisition modes were used to analyze the gases: an extractive (or static) mode and a dynamic mode. In the extractive mode the gas flowing through the White cell was isolated for analysis; the inlet–outlet valves were simultaneously closed such that the emitted gases were isolated in the cell at a desired pressure of ca. 740–700 Torr (990–930 hPa) for high pressures and 430–400 Torr (570–530 hPa) for lower pressure measurements.

Step 6.

A combination of software was used for the post-acquisition spectral analysis and confirmation of the species observed during the campaign. The MALT5 software utilizing both HITRAN line-by-line data and the PNNL 50 °C gas-phase reference spectra as input libraries, was used to identify and quantify vapor-phase chemicals in the spectra. Spectra were compiled into parameter files and analyzed by the MALT5 software using parameters including pressure, temperature, path length, resolution, and estimated initial values for chemical mixing ratios. The software generates a spectrum to simulate the measured spectrum by adjusting mixing ratios until the residual between the simulated and measured spectra is minimized. To confirm the species were actually present, each spectrum generated by MALT5 was input to OPUS and subtracted from the measured spectrum; the target compound was purposefully omitted from the subtraction process to visually inspect if the omitted compound was in fact present.

Step 7.

Five 0.1 ha experimental plots located at Fort Jackson near Columbia, SC, in longleaf pine–slash pine forests (*P. elliottii* Engelm.) were burned in May 2018.

Step 8.

Our approach to sampling used an extractive collection device whose tube inlet sampled air and emissions directly ahead of the flame. This simple solution is similar to other canister methods often used with gas chromatographic analysis and also conceptually similar to the land-based FTIR used to sample emissions. The canister sampling package, mounted on a metal frame, contained a set of evacuated canisters that were carried to the individual burn plots. The sampling package consisted of a 12 V swing-piston KNF Neuberger pump plumbed with stainless-steel tubing and a pressure-relief valve to regulate the pressure of the system and ultimately the fill pressure of the canisters. The flow rate to fill the canisters was 15 L min^{-1} . A sampling probe (2.5 m of 6 mm stainless-steel tubing plus 2 m of flexible stainless-steel line) was attached to the inlet of the package to collect pyrolysis gases from point sources of vegetation within the burning plots. To capture a pyrolysis sample, the probe was placed near the base of the flame, immediately above the fuel where the pyrolysis gases should be emitted at maximal levels. A total of 7 to 10 aliquots of gas sample were added to a single canister as the device was moved in front of the flame to capture pyrolysis gases. Each 3 L Summa canister was filled to approximately 138 kPa (20 psia) for the FTIR analysis.

Step 9.

The canisters were analyzed using a Bruker T37 spectrometer in a similar fashion to the wind tunnel samples within 24 hours of collection in laboratory space made available by a colleague at the University of South Carolina. Details are described in the articles listed in file FTIR_Methods_Intro.txt.

Step 10. Publication references

Banach, Catherine A., Ashley M. Bradley, Russell G. Tonkyn, Olivia N. Williams, Joey Chong, David R. Weise, Tanya L. Myers, and Timothy J. Johnson. 2021. “Dynamic Infrared Gas Analysis from Longleaf Pine Fuel Beds Burned in a Wind Tunnel: Observation of Phenol in Pyrolysis and Combustion Phases.” *Atmospheric Measurement Techniques* 14 (3): 2359–76. <https://doi.org/10.5194/amt-14-2359-2021>.

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Phillips, M. C., T. L. Myers, T. J. Johnson, and D. R. Weise. 2020. “In-Situ Measurement of Pyrolysis and Combustion Gases from Biomass Burning Using Swept Wavelength External Cavity Quantum Cascade Lasers.” *Optics Express* 28 (6): 8680. <https://doi.org/10.1364/OE.386072>. Available at <https://www.fs.usda.gov/research/treesearch/60023>

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Scharko, Nicole K., Ashley M. Oeck, Tanya L. Myers, Russell G. Tonkyn, Catherine A. Banach, Stephen P. Baker, Emily N. Lincoln, et al. 2019. “Gas-Phase Pyrolysis Products Emitted by Prescribed Fires in Pine Forests with a Shrub Understory in the Southeastern United States.” *Atmospheric Chemistry and Physics* 19 (15): 9681–98. <https://doi.org/10.5194/acp-19-9681-2019>.

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Weise, David R., Wei Min Hao, Stephen Baker, Marko Princevac, Amir-Hessam Aminfar, Javier Palarea-Albaladejo, Roger D. Ottmar, Andrew T. Hudak, Joseph Restaino, and Joseph J. O'Brien. 2022. "Comparison of Fire-Produced Gases from Wind Tunnel and Small Field Experimental Burns." *International Journal of Wildland Fire* 31 (4): 409–34. <https://doi.org/10.1071/WF21141>. Available at <https://www.fs.usda.gov/research/treesearch/64276>

Weise, David R., Timothy J. Johnson, Tanya L. Myers, Wei Min Hao, Stephen Baker, Javier Palarea-Albaladejo, Nicole K. Scharko, Ashley M. Bradley, Catherine A. Banach, and Russell G. Tonkyn. 2023. "Comparing Two Methods to Measure Oxidative Pyrolysis Gases in a Wind Tunnel and in Prescribed Burns." *International Journal of Wildland Fire* 32 (1): 56–77. <https://doi.org/10.1071/WF22079>. Available at <https://www.fs.usda.gov/research/treesearch/65732>

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