NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Molecular Beam Mass Spectrometry

Enabling fundamental understanding of thermochemical biomass conversion and biomass composition recalcitrance

The MBMS can be used by industrial partners to analyze high-temperature vapors in thermochemical processes. *Photo by Bryan Bechtold, NREL/PIX 17382*

NREL has six molecular beam mass spectrometers (MBMS): two stationary systems; two field-deployable systems, customized for use in industrial environments; and two additional high-throughput stationary systems with autosamplers.

NREL's custom-built molecular beam mass spectrometers provide:

- Rapid quantitation of reactive species in high temperature environments
- Online, real-time measurements of industrial pyrolysis and gasification processes
- Mass spectra with high information content that is easily data mined and integrable
- Rapid characterization of plant and plant-derived materials, including soil carbon and chars.

MBMS applications include:

- Analytical pyrolysis
- Transportable MBMS
- Catalyst characterization
- Fundamental studies of thermoconversion
- Carbon management.

MBMS Specifications

Systems	Transportable (2 units): axial ionizer, single quadrupole Stationary (1 custom unit and 2 commercial units): crossed-beam ionizer, single quadrupole Stationary (1 unit): crossed-beam ionizer, triple quadrupole for MS/MS
Mass Range	1–1,000 amu
Sampling Conditions	Sub-ambient to 30 psig 500°C (typical) to 2,000°C with cooling of sample nozzle
Detection Limits	1 ppmv typical (lower with special tuning)

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Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.**

Applications

Plant cell wall chemistry characterization by analytical pyrolysis

- Rapid estimates of plant cell wall constituents and lignin structure
- Analysis complements traditional wet chemical methods that are time consuming and expensive.

Onsite monitoring of thermochemical processes using transportable MBMS

- Real-time, continuous monitoring with near-universal detection of chemical compounds
- Direct, robust sampling preserves condensable/reactive species, including high-temperature, high-pressure, wet, and particulate-laden gases and vapors.

Catalyst characterization using real pyrolysis and gasification process streams

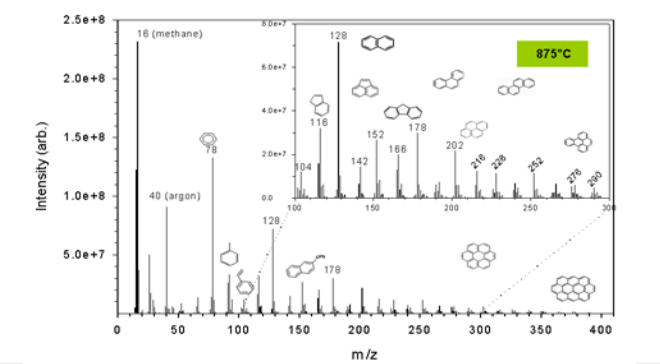
- Heterogeneous catalyst screening and product yield estimates
- Modeling of catalyst deactivation.

Fundamental studies of thermochemical reactions and kinetics

- Identification of thermal degradation pathways
- Investigation of pyrolysis and gasification mechanisms and kinetics
- Reaction parameter screening for engineering scale-up.

Soil carbon measurement and modeling

- Measurement of soil carbon changes as a function of time, depth, and geographic location
- The results can be used as inputs for soil carbon models to predict how soil carbon will be affected by land use.



Typical mass spectrum observed during gasification of mixed wood at 875°C. *Figure by NREL*

Associated publications

Carpenter, D., et al. (2007) "Quantitative Measurement of Biomass Gasifier Tars Using a Molecular-Beam Mass Spectrometer: Comparison with Traditional Impinger Sampling." *Energy Fuels* (21); pp. 3036-3043.

French, R.; Czernik, S. (2010). "Catalytic Pyrolysis of Biomass for Biofuels Production." *Fuel Proc. Technol.* (91); pp. 25-32.

Magrini, K., et al. (2007). "Using Pyrolysis Molecular Beam Mass Spectrometry to Characterize Soil Carbon in Native Prairie Soils." *Soil Sci.* (172:9); pp. 659-672.

Sykes, R., et al. (2009). "High-Throughput Screening of Plant Cell-Wall Composition Using Pyrolysis Molecular Beam Mass Spectroscopy." Biofuels: Methods and Protocols. *Methods in Molecular Biology* (581); pp. 169-183.

Evans, R.J.; Milne, T.A. (1987). "Molecular Characterization of the Pyrolysis of Biomass: I. Fundamentals." *Energy Fuels* (1); pp. 123-137.

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