Biomass Compositional Analysis: NIR Rapid Methods

Developing rapid calibration models to predict the composition of biomass

Scientists at NREL use near-infrared spectroscopy to predict the composition of a variety of biomass types.
Photo by Dennis Schroeder, NREL 26528

NREL biomass analysis scientists use near-infrared (NIR) spectroscopy correlated with compositional data, produced using traditional wet chemical techniques, to develop rapid calibration models. These models dramatically decrease the time required for (and the cost of) routine compositional analyses. NREL has models to predict the composition of a variety of biomass types.

Instrumentation

- Foss XDS Rapid Content Analyzer NIR
- Thermo Antaris II FT-NIR Analyzer

The Biomass Compositional Analysis Laboratory at NREL houses one Foss dispersive NIR and two Thermo FT-NIR spectrometers. All three instruments have reflectance, transmission, and transflectance capabilities as well as flexible sample presentation accessories.

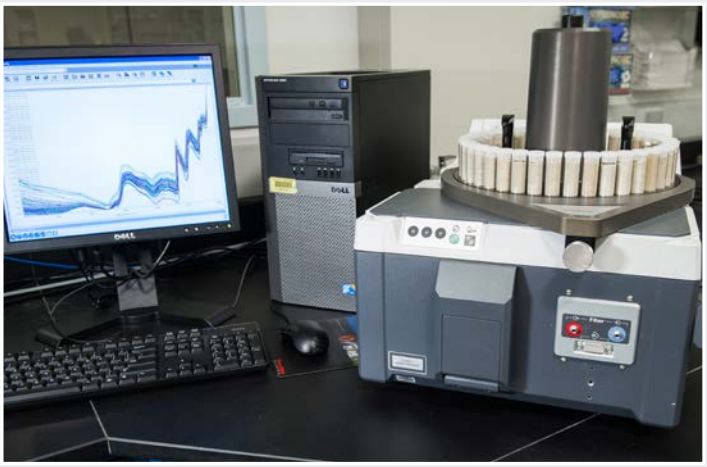
Quality Assurance and Quality Control

NREL scientists have developed a robust quality assurance and quality control program for NIR analytical instrumentation, calibration models, and sample prediction.

- NIR instrument stability is tracked daily using multiple internal and external standards.
- Calibration models are regularly updated with new samples to expand the population and capabilities of the model. Modeling statistics are also monitored for alignment with published wet chemical uncertainties.
- Sample predictions are assessed by spectral outlier detection and prediction uncertainty thresholds. These thresholds are determined by the calibration model and published wet chemical analysis uncertainties.

Available Models

Model	Particle Size	Description
Corn Stover	2mm	Contains whole stover and anatomical fractions from stover.
Mixed Herbaceous	2mm	Includes six different herbaceous feedstocks.
Sorghum	2mm	Includes a variety of sorghum types and maturities.
Pretreated Corn Stover Solids	2mm	Includes a variety of pretreatment conditions and severities. Solids composition is determined from solids washed free of soluble components and air dried.
Pretreated Corn Stover Slurry	variable	Includes a variety of pretreatment conditions and severities. Solids composition is determined *in situ* on whole slurry.



The Biomass Compositional Analysis Laboratory at NREL houses two Thermo FT-NIR spectrometers (one is shown here) and a Foss XDS NIR (see photo page 1). *Photo by Dennis Schroeder, NREL 26530*

Service Capabilities

- NREL scientists can provide predictions of chemical composition of client samples using an existing model (see table).
- NREL licenses the spectra and constituent values from these existing models. Each model has approximately 100–300 samples for license.
- NREL scientists can work with clients to develop, implement, and support custom NIR calibration methods for specific applications.

Licensing and Levels of Support

- Clients interested in licensing NREL models can provide 5–10 samples for NIR scanning. This allows NREL to determine if the client samples fit into our model population and the ability to incorporate these samples into a new combined model, if desired.
- NREL offers a tiered system for model transfer.
  - Clients can license the spectra and constituent values, and build their own models.
  - Clients can license the spectra and constituent values, and NREL scientists can help clients establish working models on the clients' instruments.
  - NREL can build custom models tailored to the client's needs.

Associated Publications

Sluiter, A.; Wolfrum, E. (2013). "Near infrared calibration models for pretreated corn stover slurry solids, isolated and *in situ." J. Near Infrared Spectrosc.* (21); pp. 249-257.

Laurens, L.M.L.; Wolfrum, E. J. (2012). "Rapid Compositional Analysis of Microalgae by NIR Spectroscopy." *NIR News* (23:2); pp. 9-11.

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Wolfrum, E.; Sluiter, A. (2009). "Improved Multivariate Calibration Models for Corn Stover Feedstock and Dilute-Acid Pretreated Corn Stover." *Cellulose* (16:5); pp. 567-576. www.nrel.gov/docs/fy13osti/56838.pdf

Kelley, S.; Rials, T.; Snell, R.; Groom, L.; Sluiter, A. (2004). "Use of near infrared spectroscopy to measure the chemical and mechanical properties of solid wood." *Wood Science and Technology* (38:4); pp. 257-276.

Hames, B. R.; Thomas, S.R.; Sluiter, A.D.; Roth, C.J.; Templeton, D.W. (2003). "Rapid Biomass Analysis: New Tools for Compositional Analysis of Corn Stover Feedstocks and Process Intermediates from Ethanol Production." *Applied Biochemistry and Biotechnology* (105[1-3]); pp. 5-16.

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