



Contribution ID: 448

Type: **Poster Presentation**

## NMR relaxometry characterization of water adsorption in corn stover anatomical fractions

*Tuesday, 23 May 2023 10:30 (1h 30m)*

Despite being major contributors to global CO<sub>2</sub> emissions, fossil feedstocks are finite natural resources frequently used to produce high value goods including fuels and plastics. One alternative is to replace fossil feedstocks with renewable agricultural feedstocks due to their ability to sequester carbon during growth. While a promising alternative, the use of food crops as feedstocks brings its own set of challenges. Recent emphasis has been placed on deconstruction of agricultural residues, such as corn stover, into fuels and chemicals. Polysaccharides from lignocellulosic plant cell walls can be converted to glucose, but biomass recalcitrance to enzymatic hydrolysis presents a practical challenge to this pathway. Pretreatment steps help improve enzymatic access to plant cell walls and once optimized, allow for these processes to be scaled. Nuclear magnetic resonance (NMR) relaxometry is applied to corn stover to gain a better understanding of these systems and the impacts of pretreatment. These measurements directly measure water adsorption in anatomical fractions of corn stover. NMR transverse  $T_2$  relaxation time distribution measurements indicate multiple water populations, which vary with anatomical fraction and water adsorption. Measured  $T_2$  data are used to calculate thermodynamic properties of Brunauer-Emmet-Teller (BET) adsorption theory using a model to estimate mono and bilayer relaxation.  $T_2$  data are used directly to determine rotational diffusion correlation times indicating adsorption interaction strength.  $T_1 - T_2$  longitudinal-transverse relaxation time correlation measurements quantify differences in the molecular level structural order of the adsorbate surface water as a function of water activity, i.e. relative humidity or water vapor partial pressure. The  $T_1/T_2$  ratio provides a measure of the surface energy related to the adsorption strength and surface diffusive mobility of the water adsorbate, and differentiates the anatomical fractions. The results indicate that direct measurement of NMR relaxation times can be used to characterize corn stover biomass water adsorption, which are data relevant to biomass processing and handling. These procedures may be extended to pretreated lignocellulosic materials to study how morphological changes impact adsorption, and applied to monitor enzymatic hydrolysis progress *in situ*.

Figure 1. Corn Stalk MRI. A 1 mm thick transverse slice taken of a hydrated corn stalk with a 25x25 mm field of view over 128x128 pixels for a resolution of 195  $\mu\text{m}/\text{pixel}$ .

### Participation

In-Person

### References

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**Session Classification:** Poster

**Track Classification:** (MS02) Porous Media for a Green World: Water & Agriculture