NMR Relaxometry for the Study of Plants: Faster, Simpler and Sensor-like

Antonia Wörtche[1], Ralf Metzner[1], Robert Koller[1], Carel W. Windt[1]

[1]*Institute for Bio- and Geosciences Plant Sciences (IBG-2), Forschungszentrum Jülich GmbH, Germany*

JÜLICH Forschungszentrum

Member of the Helmholtz Association

Motivation

Fresh weight (FW), **water weight** (WW), **dry weight** (DW) and **water content** (WC) are elementary parameters to quantify plant growth and yield.

However, due to the **lack of suitable measurement techniques** little is known about the dynamics of these traits in living plants.

Time Domain NMR relaxometry has the potential to fill this knowledge gap as it allows to quantify proton pools and distinguish between protons associated with liquids and solid based on differences in proton mobility.

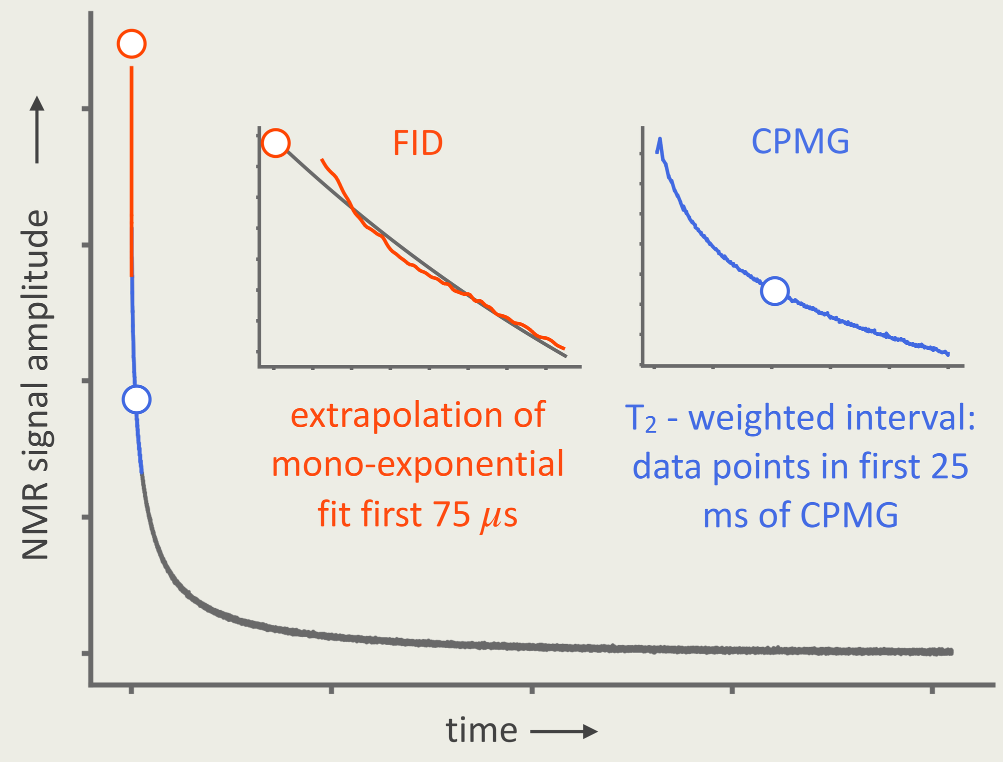
Intact plant organs are **complex systems** with strong spatial heterogeneity in their macro- and micro physicochemical structure. This is reflected in the NMR signal by **species-** and **organ specific** complex **NMR relaxometric signatures**.

Advanced (multidimensional) NMR relaxometric approach can handle the complexity of plant organs but are **time-consuming** and require **expert operators** for acquisition and data analysis.

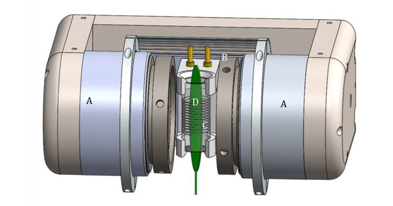
For routine characterization of intact plant organs, a more **straight-forward** and **sensor-like** approach might be applied.

Routine Characterization complex plant organs

The Solid Liquid Content (SLC) method - *A simplified T_2-weighted approach*



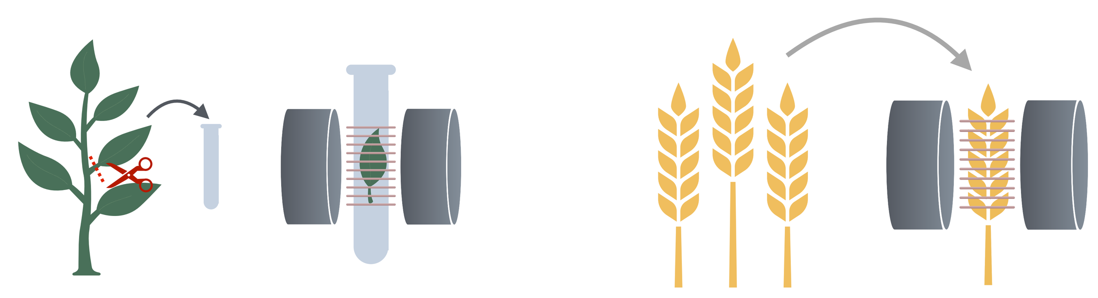
NMR Sensor[1]



○ PD_{tot}: total proton density *Including fast and slow decaying protons*

○ PD_{liq}: liquid proton density *Including slow decaying protons*

Experimental Set Up



Results

So far, the SLC method is based on empirical observations. The following aspects have not been tested:

- ? Sensitivity of results SLC method to changes in the make up of the plant material
- ? Accuracy for predicting FW, WW, DW and WC
- ? Influence of fast decaying proton fraction

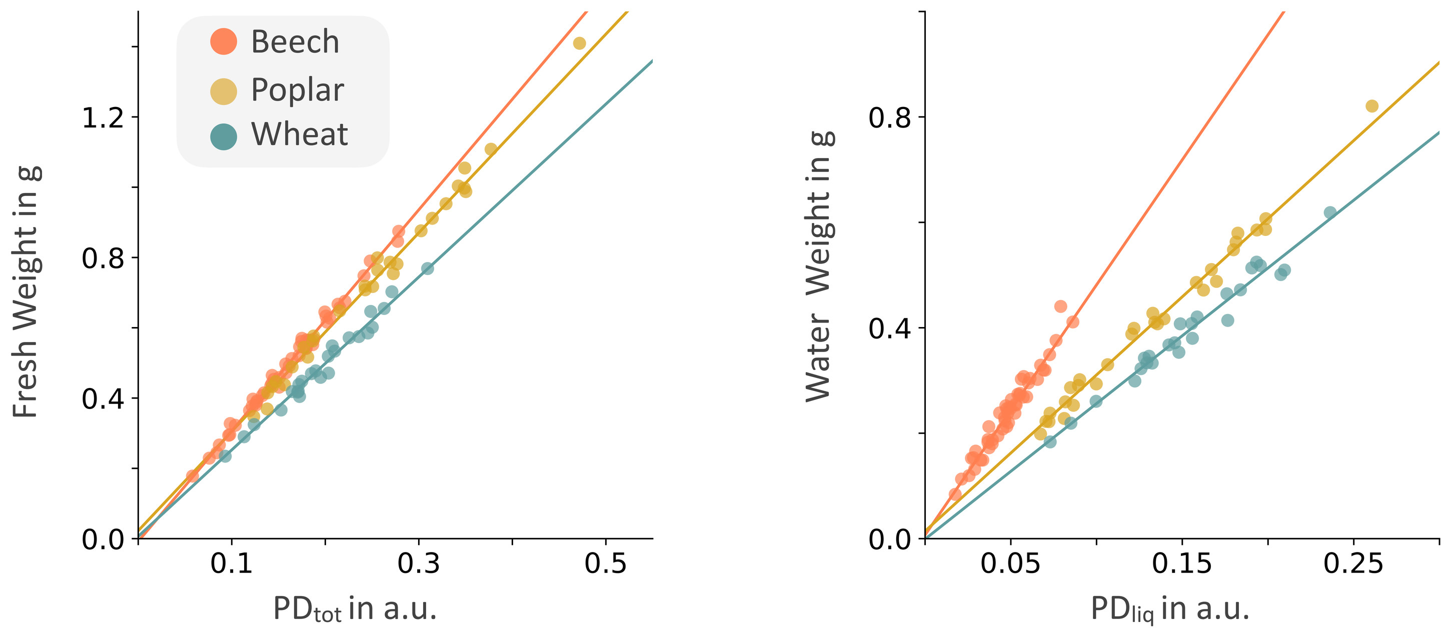


Figure 1: Reference measurements acquired for beech, poplar and wheat leaves to determine the correlation between PD_{tot} and sample FW and PD_{liq} and sampleWW.

? Calibration constants not generic for all species and susceptible to sample water content - *Leaf Samples*

1. Calibration function varies between different species, especially if they exhibit strongly varying physicochemical properties
2. Estimation of PD_{tot} and PD_{liq} can be susceptible to sample water content

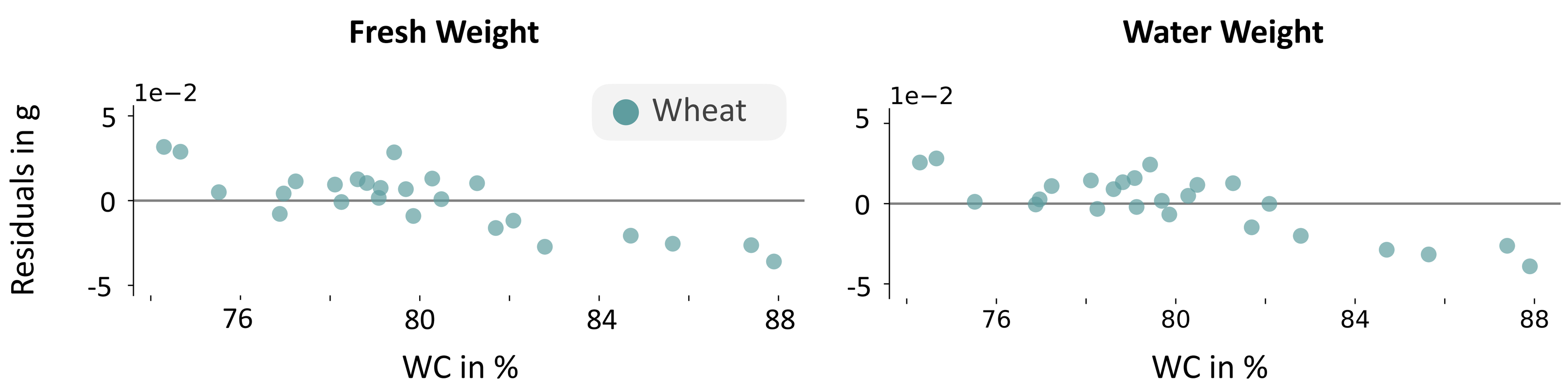


Figure 2: Residuals of linear regression between total PD_{tot} and FW and PD_{liq} and WW. Residuals are shown in dependence of sample water content.

? Applicability of SLC method in terms of predictive performance depends on species and biological process to be measured- *Leaf samples*

Root Mean Squared Error (RMSE) and Normed Root Mean Squared Error (NRMSE) used as measure for accuracy of results SLC method.

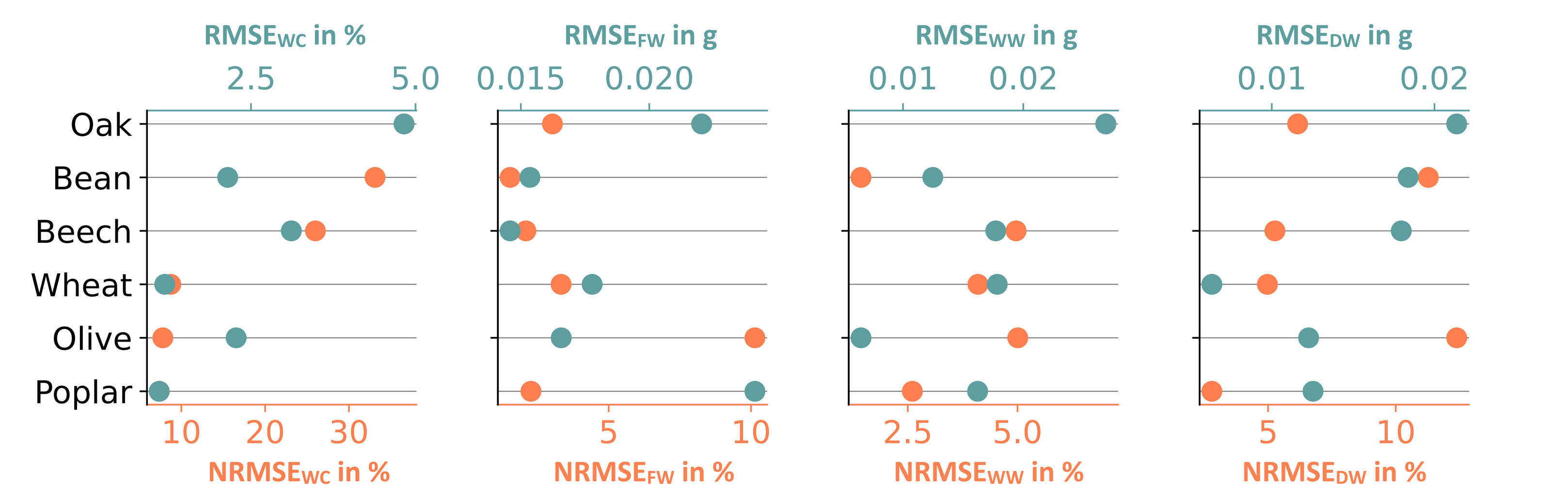


Figure 3: RMSE (blue dots) and NRMSE (red dots) for prediction of WC, FW, WW and DW for leaf samples of different species.

? Below 40% Water Content presence of fast decaying proton fraction results in underestimation of total Proton Density - *Intact wheat ears*

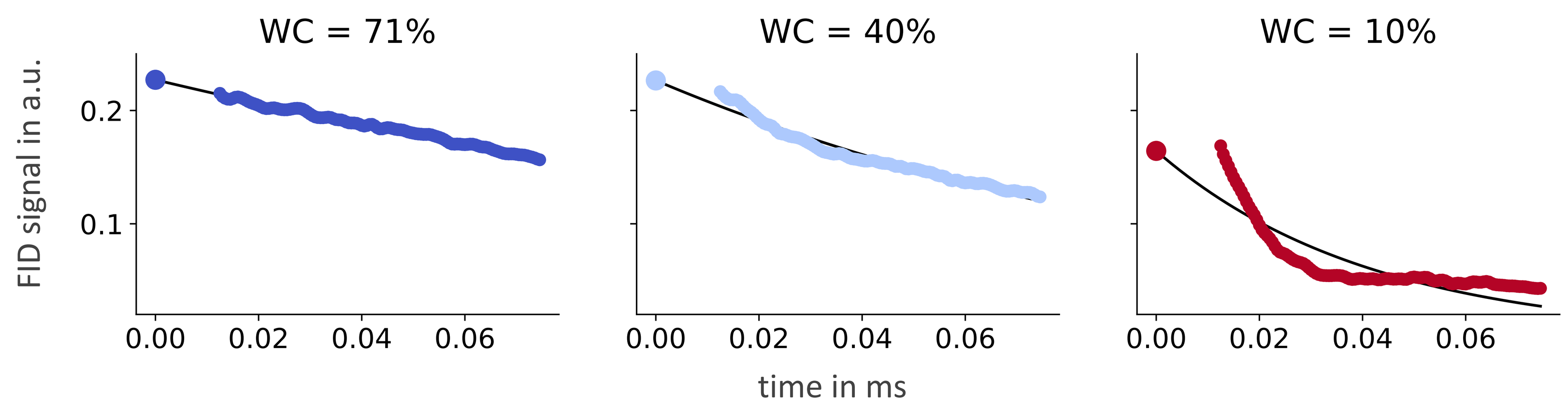


Figure 4: Appearance of deviations from mono-exponential decay (solid line) of FID for three different wheat ear samples with WC 71%, 40% and 10%.

Accumulation of dry matter in wheat seeds during development results in a large fast decaying proton fractions.

For samples with high dry matter content (WC ≦ 40%) the fast decaying proton fraction gives rise to deviations from mono-exponential decay in the FID and underestimation of the total proton density.

This is reflected in the correlation between PD_{liq}/PD_{tot} and sample water content.

Deviations from the fit are quantified by the sum of residual squares (RSS) normed by the maximum signal amplitude of the FID.

$$RSS = \sum_i (y_i - y_{i,fit})^2$$

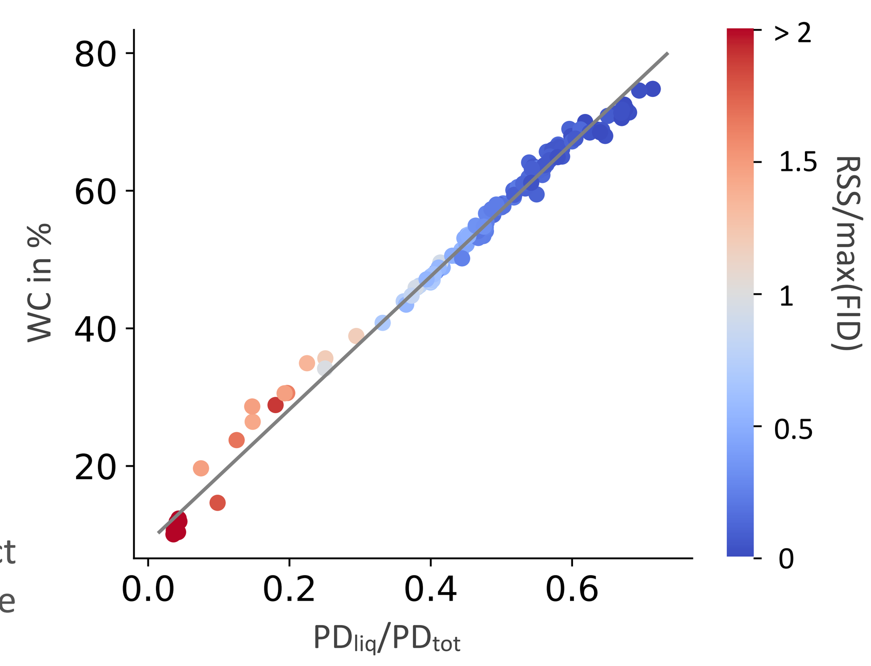


Figure 5: Reference measurement acquired for intact wheat ears. The color quantifies the deviation of the FID from mono-exponential decay

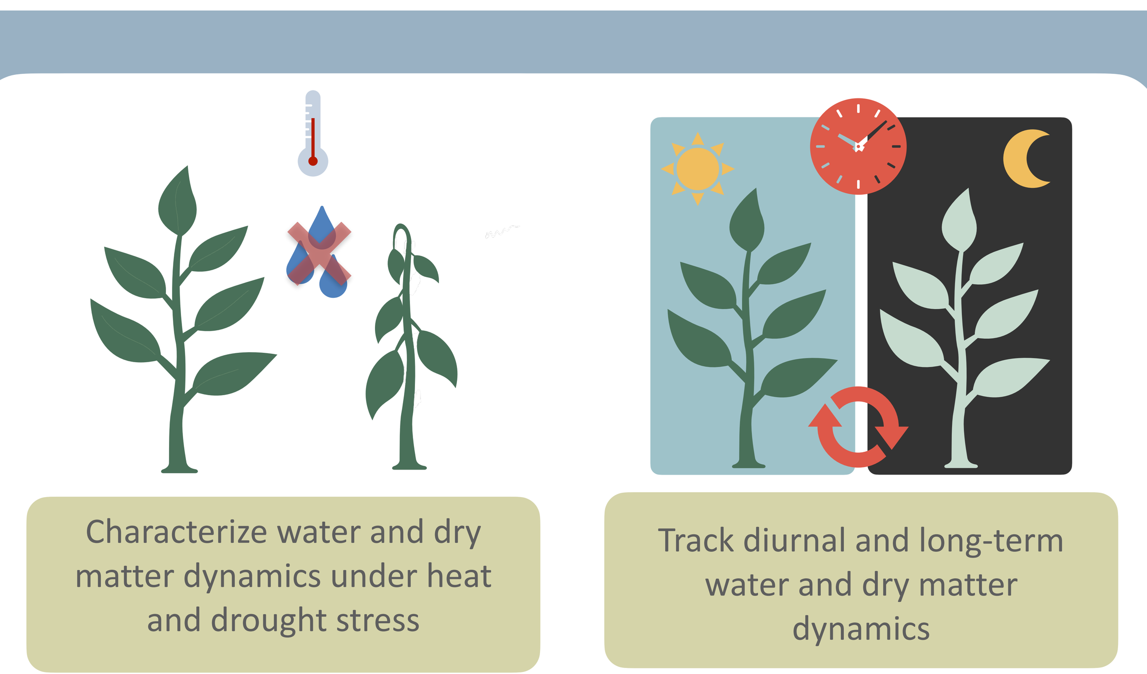
Conclusion

The SLC method gives linear correlations between the proton densities and weight parameters of interest (FW and WW)

The calibration function and the accuracy of the method vary for different species.

For samples with WC ≦ 40% deviations in estimation of PD_{tot} occur due to presence of a fast-decaying proton fraction.

Outlook



Characterize water and dry matter dynamics under heat and drought stress

Track diurnal and long-term water and dry matter dynamics

References

[1] C.W. Windt, et al. A mobile NMR sensor and relaxometric method to non-destructively monitor water and dry matter content in plants, Frontiers in Plant Science, 12 (2021)