Rapid determination of recalcitrant organic carbon applying Near Infrared Spectroscopy (NIRS) and a Fourier Transform Infrared-Photoacoustic Spectroscopy (FTIR-PAS) for biogas production

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1. Background and Aim

Lignin is an important recalcitrant carbon pool, since it is known to be non-degradable during anaerobic digestion. Wet characterization of lignin analysis is expensive and labor intensive.

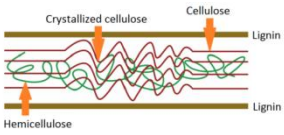


Fig.1 Simplified lignocellulose matrix

Lignin controls enzymatic hydrolysis of cellulose which results in low bio-degradability, and further low biogas yield of lignocellulosic biomass.

The inverse correlation between lignin and biogas production potential has been reported in a number of recent studies, which highlight the importance of lignin analysis with regard to biogas production of lignocellulosic biomass.

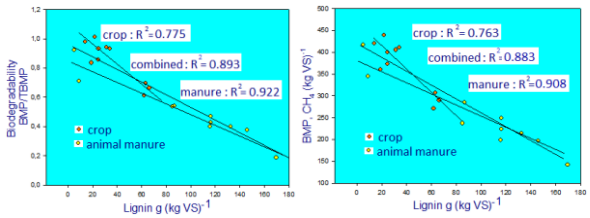


Fig.2 Correlation between lignin, BMP and biodegradability (Triolo et al., 2011)

The aim of this study was to explore potentials of the spectroscopic methods to determine the non-degradable organic pool in plant biomass

2. Methodology

We compare the precision of the lignin concentration assessed by near infrared spectroscopy (NIRS) and a Fourier Transform Infrared-Photoacoustic Spectroscopy (FTIR-PAS).

NIRS

A Bomem QFA Flex Fourier Transform spectrometer, rotating sampler, resolution 32cm^{-1}, Number of scans: 200, NIRS region: 16000 - 0 cm^{-1}.

FTIR-PAS

Nicolet 6700, PA detector: PA-301 (Gasera ltd, Finland), Resolution: 4 cm^{-1}, Number of scans: 32, Mir region: 4000-600 cm^{-1}.

RAW SPECTRA

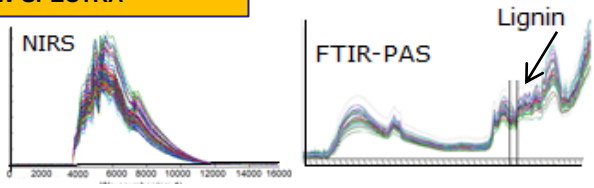


Fig.3 Obtained Spectra of NIRS and FTIR-PAS before preprocessing

3. PLS Modelling Results

We tested the Partial Least Squares (PLS) model by applying a series of pre-processing methods using either PLS Toolbox with Matlab or Unscrambler for data analysis. A total of 54 plant biomass samples were used for model calibration and cross validation was performed for model prediction.

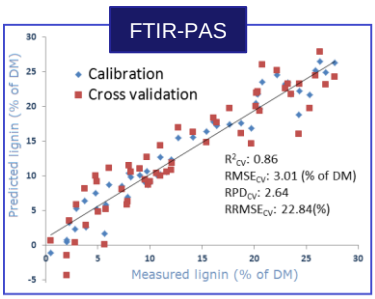
NIRS

	R^2_{Cal}	$RMSE_{Cal}$	R^2_{CV}	$RMSE_{CV}$	F
SNV+Mean center	0.73	4.10	0.59	5.14	6
SNV+DT+Mean center	0.73	4.13	0.57	5.27	6
SNV + DT + SG (15,2,2)	0.88	2.80	0.63	5.14	6
SNV + DT + SG (11,2,2)	0.91	2.41	0.66	4.67	6
SNV + DT + SG (15,2,2)	0.93	2.11	0.81	3.47	5

FTIR-PAS

	R^2_{Cal}	$RMSE_{Cal}$	R^2_{CV}	$RMSE_{CV}$	F
Raw Spectra	0.70	4.32	0.61	5.04	3
SNV	0.83	3.29	0.72	4.28	6
SNV + DT	0.73	4.13	0.68	4.50	2
SNV + DT + SG (7,2,2)	0.92	2.23	0.80	3.56	5
SNV + DT + SG (11,2,2)	0.95	1.79	0.86	3.01	5
SNV + DT + SG (15,2,2)	0.93	2.11	0.81	3.47	5

Lignin predicted versus measured from the best model



The standard error of the best model was 3.01 % of dry matter, where lignin content of the measured value was between 0.46% and 27.7% of dry matter. Coefficient of determination(R^2) and residual prediction deviation (RPD) were 0.86 and 2.64, respectively. Using NIR, the precision of the PLS model was slightly lower than FTIR-PAS, where R^2 in prediction was 0.66, standard error 4.67 % of dry matter and RPD 1.70.

4. Conclusion

The precision of the best PLS model using FTIR- was satisfactory. It is found that FTIR-PAS had better prediction of lignin and the model was moderately successful using it. The study highlights that FTIR-PAS can be applied as an alternative method to assess recalcitrant carbon for biogas production.

5. Reference

Triolo JM, Sommer SG, Møller HB, Weisbjerg MR, Jiang X. A new algorithm to characterize biodegradability of biomass during anaerobic digestion: influence of lignin concentration on methane production potential. Bioresour Technol 2011;102:9395–402.