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ARTICLE

Determination of Dry Matter Content in Potato Tubers by Low-Field Nuclear Magnetic Resonance (LF-NMR)

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The objective of this study was to develop a calibration model between time-domain low-field nuclear magnetic resonance (LF-NMR) measurements and dry matter (DM) content in single potatoes. An extensive sampling procedure was used to collect 210 potatoes from eight cultivars with a wide range in DM content, ranging from 16 to 28%. The exponential NMR relaxation curves were resolved into four mono-exponential components using a number of solution diagnostics. Partial least-squares (PLS) regression between NMR parameters (relaxation time constants $T_{2,1-4}$ and magnitudes $M_{0,1-4}$) and DM content resulted in a model with low error (RMSECV, 0.71; RMSEP, 0.60) and high correlation (r_{CV}, 0.97; r_{test}, 0.98) between predicted and actual DM content. Correlation between DM content and each of the proton populations revealed that $M_{0,1}$ ($T_{2,1}$, 3.6 ms; SD, 0.3 ms; r, 0.95) and $M_{0,4}$ ($T_{2,4}$, 508 ms; SD, 53 ms; r, −0.90) were the major contributors to the PLS regression model.

KEYWORDS: Low-field NMR; potato; PLS regression; dry matter content; DoubleSlicing; specific gravity; core consistency

INTRODUCTION

An increased consumer awareness of high-quality potato products increases the interest of the industry in high-technology-grading systems. If uniform good-quality products and high-end gourmet potatoes are to be produced, the industry requires a rapid instrumental method to grade the raw potatoes according to the final sensory and technological qualities. For potatoes, the texture is of great importance for the perception of quality by the consumer, and it is well-established that dry matter (DM) content, starch composition, and cell wall structures significantly affect the final texture of cooked potatoes (*1*−*6*). While starch composition and cell wall structure to a large extent are genetically determined, DM content mainly depends upon the maturity of the potato tuber, the composition of the soil, and fertilization and draft conditions (*7*, *8*). Specific gravity is a reliable measure of DM content, which is determined by weighing potatoes in air and water. This time-consuming and rather cumbersome method is the standard method used for quality control of potato samples in potato industries. Also, the brine grading method with various densities is used for industrial grading of potatoes according to DM content. A simplified, more automated online measurement of DM content could be the first target in obtaining better control on the postharvest potato quality. Two obvious rapid methods exist to determine the DM content of individual tubers: near-infrared spectroscopy (NIR) and low-field nuclear magnetic resonance (LF-NMR) relaxometry. In the case of NIR, the ideal transmission measurements are difficult, if not impossible, to obtain, because the combination of size and high water content of the tubers hinders the transmission of NIR light. The less advantageous NIR reflection measurements are easy to conduct and truly non-destructive but tend to vary strongly with the tuber surface morphology and the soil adhering to the surface. Perhaps most importantly, reflectance measurements will only provide information about the DM content in the outer shell of the tuber, which is likely non-representative for the quality question at hand. These are the main reasons why in the literature NIR assessments of DM content are performed in reflectance mode on a sliced potato (*9*−*11*). On the contrary, LF-NMR considers that the tubers have high water content and that the measurements give information on the entire volume measured. Unfortunately, most current benchtop LF-NMR instruments cannot accommodate a whole potato tuber in the sampling probe. The aim of this study is to characterize the performance and establish if LF-NMR is adequate for determining DM content of individual potato tubers.

LF-NMR as an analytical method is abundantly present in the food industry and food science research because of its unique capability to provide information about the mobility and distribution of water and fat protons in food products (*12*, *13*). These in turn are known to be critical to the perceived texture. Numerous studies have documented that LF-NMR is an excellent method for characterization of water mobility and water distribution in food items, such as meat, fish, cheese, cereals, fruits, and vegetables, including potatoes (*11*, *14*, *15*). Moreover, LF-NMR is capable of monitoring dynamic changes during processing, because

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measurements can be performed non-destructively for example during cooking of potatoes with different levels of DM (*16*). In previous studies, LF-NMR has demonstrated a high correlation to DM content because of the inverse relationship between the water content in the raw potatoes with the starch and DM content. However, these studies were performed on limited sample sets with few different cultivars, using only a small range in DM content (*11*, *14*, *15*). One challenge when determining DM content in potatoes is the large biological variation between cultivars, within cultivars, and within each potato tuber.

To establish a rapid and reliable method for the determination of DM content by LF-NMR, we will use a large sample set using an extensive sampling procedure. The variation in DM content was obtained using eight different potato cultivars grown under different conditions and harvested at variable maturity to expand the natural biological variation and variation in DM content. The establishment of a general rapid method can have practical use in the potato industry for grading high-end gourmet potatoes.

MATERIALS AND METHODS

Potato Samples. Eight different potato cultivars ('Ballerina', 'Bintje', 'Inova', 'Fakse', 'Sava', 'Jutlandia', 'Estima', and 'Gunda') were selected to represent a large variation in DM content. The cultivars were received from the Danish Potato Breeding Station, the Danish Institute of Agricultural Sciences, and commercial growers. The potatoes were grown and harvested at different conditions to obtain a large variation in DM content. After harvest, the potatoes were stored at 4 °C and 95% relative humidity up until the day before analysis. All cultivars were subcategorized in 1−6 groups by a non-destructive grading using specific gravity (SG), which is highly correlated to DM content (eq 1)

$$\mathrm{SG} = \left(\frac{w}{w - w_{\mathrm{w}}}\right) \tag{1}$$

where w is the weight in air and w_{w} is the weight in water, i.e., with the scale immerged in water. Using the SG value, DM estimates ($\mathrm{DM_{est}}$) were calculated by the following equation (*17*, *18*):

$$\mathrm{DM_{est}} = (214\mathrm{SG}) - 211.44 \tag{2}$$

Accordingly, 21 cultivar/subcategories were obtained, each of which will be called DM bin in the remainder of the paper (**Table 1**). For each of the 21 DM bins, 10 potato tubers were collected, giving a total of 210 samples. This extensive sampling procedure ensured that the material represented a large and relevant variation in DM, cultivars, and texture quality of potatoes.

For determination of LF-NMR and DM content, a cylindrical sample (diameter, 11.5 mm; length, 45.0 mm) was taken from the storage parenchyma tissue in the bud end of the tuber with a cork borer, avoiding tissue from the center. The cylinder was first used for LF-NMR measurement and then for determination of DM content. The sample was placed in a glass tube with a plastic lid and placed in a measurement glass tube. The temperature of the sample was adjusted to 25 °C in a water bath for 10−15 min before LF-NMR measurements.

LF-NMR Relaxometry. The LF-NMR relaxation measurements were performed on a Maran benchtop pulsed NMR analyzer (Oxford Instruments, Witney, U.K.) with a magnetic field strength of 0.47 T corresponding to a resonance frequency for protons of 23.2 MHz. The NMR instrument was equipped with an 18 mm temperature-controlled probe; the temperature was set to 25 °C. The transverse relaxation time constant, T_2, was measured using the Carr−Purcell−Meiboom−Gill (CPMG) sequence (*19*, *20*). The T_2 measurements were performed with a τ value of 150 μs. The repetition time between two consecutive scans was 6 s. The dwell time was 0.5 μs, and the receiver gain was 5.0%. Data from 4096 echoes were acquired; they were obtained as a 16 scan repetition, with 1 dummy scan in front to ensure that a spin system is in a steady state before data are collected. Inaccuracy in the 180° pulse setting was compensated for using only even-numbered echo, resulting in 2048 data acquisition points per measurement.

Table 1. Overview of DM Grading Bins and Range and Mean DM Determined by Specific Gravity ($\mathrm{DM_{SG}}$) on Intact Potatoes and Oven Drying on Sample Cylinders ($\mathrm{DM_{oven}}$)

DM grading bins	DM range (%)	mean $\mathrm{DM_{SG}}$ (%)	mean $\mathrm{DM_{oven}}$ (%)
Bintje_16.2	16.2−17.2	17.0	17.9
Bintje_18.5	18.5−20.5	19.0	19.5
Bintje_20.5	20.5−22.5	21.4	22.4
Bintje_22.5	22.5−23.5	23.0	23.9
Bintje_23.5	23.5−25.0	24.5	25.7
Bintje_25.0	25.0−28.0	26.2	27.8
Ballerina_16.4	16.4−17.4	16.9	16.6
Ballerina _17.4	17.4−18.4	17.7	18.8
Ballerina _18.4	18.4−19.4	18.9	19.7
Estima_19.0	19.0−21.0	20.3	19.9
Faxe_18.2	18.2−20.2	18.7	20.4
Faxe_20.2	20.2−22.2	21.8	23.5
Inova_16.0	16.0−17.5	16.6	17.7
Inova_17.5	17.5−18.5	18.1	19.1
Inova_18.5	18.5−20.0	19.6	19.6
Jutlandia_19.5	19.5−20.5	20.1	20.3
Jutlandia_20.5	20.5−21.5	20.9	20.0
Sava_18.0	18.0−19.5	18.3	17.7
Sava_19.5	19.5−20.5	19.9	19.6
Sava_20.5	20.5−22.2	22.0	22.4
Gunda_19.2	18.5−19.8	19.4	19.0

DM Content. The cylinder from the LF-NMR measurements was cut transversely and longitudinal and dried in an oven at 80−85 °C for 16−18 h, where after DM content, $\mathrm{DM_{oven}}$ was calculated.

Data Analysis. Regression analysis between LF-NMR data and the DM content was performed by partial least-squares (PLS) regression (*21*). To perform a comprehensive and comparative correlation analysis between the LF-NMR data and the DM content, a number of different data analytical models were applied to the LF-NMR data prior to PLS regression: (1) Raw relaxation data in the time domain. (2) Distributed exponential fitting analysis uses a regularization approach to the inverse Laplace transform, which results in a continuous distribution of relaxation time constants T_2 (*22*). Mathematically, the distributed exponential fitting problem is ill-defined, because it is very sensitive to the constraints used. (3) Discrete multi-exponential fitting by curve resolution of the relaxation curves into characteristic relaxation time constants $T_{2,n}$ and corresponding magnitudes $M_{0,n}$ (eq 3) (*23*, *24*)

$$M(t) = \sum_{n=1}^{N} M_{0,n} \exp\left(\frac{-t}{T_{2,n}}\right) + e(t) \tag{3}$$

where $M(t)$ is the residual magnetization at time t, $M_{0,n}$ is the concentration or magnitude parameter of the nth exponential, $T_{2,n}$ is the corresponding transverse relaxation time constant, and $e(t)$ is the residual error. After deconvolution of the relaxation curve into n exponential components, inspection of the residuals will reveal whether the curve has been modeled by too few, too many, or the correct number of components. Appropriate loss in fit and χ^2 misfit tests can also be used to validate if the right number of components have been used. (4) Multi-exponential fitting by "matrix fit" (*24*, *25*) of the relaxation curves into common characteristic relaxation time constants T_2 and corresponding magnitudes M_0. Matrix fit is the two-dimensional analogue to discrete exponential fitting and is generally less prone to overfitting compared to discrete exponential fitting. The disadvantage is that the T_2 values in samples might be more correctly described as a distribution of T_2 values. It should be emphasized that the matrix fit method represents the same underlying model as single Slicing (*25*) and PowerSlicing (*26*), which are not included in this paper. (5) Multiexponential fitting by "DoubleSlicing" (*27*) of the relaxation curves into transverse relaxation time constants T_2 and corresponding magnitudes M_0. The DoubleSlicing technique uses the fact that in every part of a multi-exponential decay curve each of the mono-exponentials are present but in different amounts. The technique pseudo-upgrades a single relaxation curve to become trilinear data, by cutting the relaxation curve into slices. When parts of the signal curve are selectively removed (slicing) and the remaining curve is used, the relaxation curve can be transformed from

a one-dimensional signal (a vector x) into two-dimensional data (a tensor X). When this procedure is repeated on the matrix, the data are transformed to three-dimensional data (a cube X) and three-way mathematical methods can now be used. The technique has been shown to be extremely rapid and have improved solution diagnostics. Andrade et al. (*27*) tested the performance of DoubleSlicing against existing methods and found that it was accurate in estimating relaxation times and that it outperformed exponential fitting by a factor of 4 with regards to computation time. These different data analytical approaches all have known advantages and disadvantages, but in this work, they are primarily applied to determine the correct rank of the data, i.e., the number of underlying exponential components extractable from the data. While the number of components in the PLS model under (1) is statistically validated, the approach adopted under (5) is accompanied by rigorous diagnostics of the number exponential components (*28*). The number of components in the curve fitting model under (3) and (4) can only be evaluated by the decrease in the residual error of the fit and visual inspection of residuals.

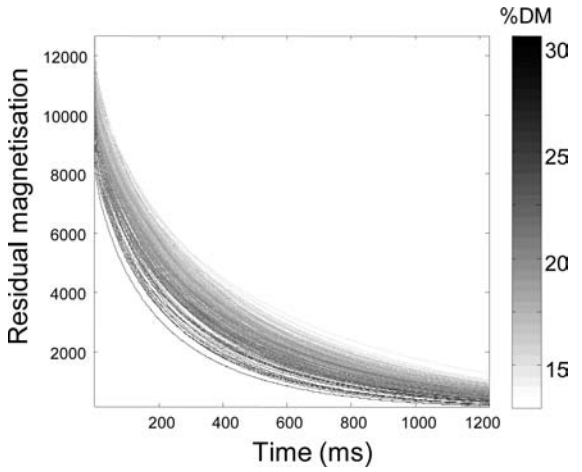

Figure 1. Raw LF-NMR relaxation data for 210 potato samples. The curves are gray-scale-colored according DM content.

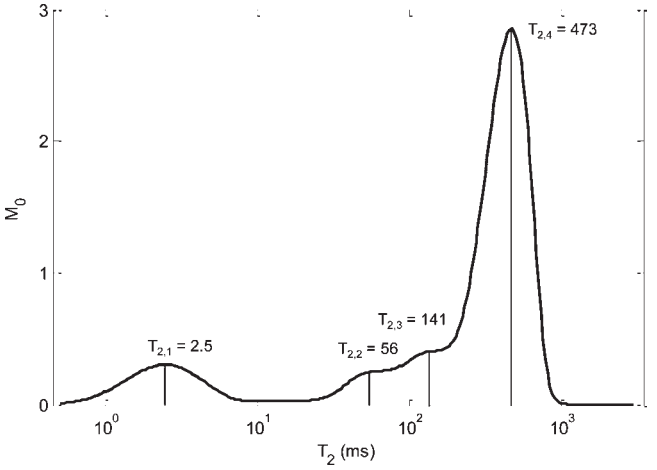

Figure 2. Mean distribution of T_2 relaxation times of 210 potatoes estimated by distributed exponential fitting of LF-NMR CPMG relaxation curves.

PLS Model Validation. For the PLS modeling, the sample set was divided into a calibration set and an independent test set. Of the 210 samples, 4 samples were chosen randomly from each of the 8 cultivars, giving a total of 32 samples in the independent test set. The test set was not used for PLS modeling but was only used to predict DM content from the generated PLS model. The PLS modeling was performed on the remaining 178 samples using segmented cross-validation, leaving out one cultivar at the time. The generated PLS models were compared by a correlation coefficient (r) and root-mean-square error of cross-validation (RMSECV) for the calibration set and root-mean-square error of prediction (RMSEP) for the independent test set.

All data analysis steps were performed by Matlab, version 7.6 (MathWorks, Inc., Natick, MA), using in-house algorithms (www.models.life.ku.dk).

RESULTS AND DISCUSSION

Table 1 shows the range of cultivars and DM grading bins used in the study, which ensures a large DM variation when modeling against LF-NMR relaxation data. DM content determination using SG data on a whole tuber and oven-drying data on cylinder samples gives similar results and is highly correlated (r = 0.96, albeit with a bias of ~1%). The small discrepancy between DM determinations by the two methods could be explained by sample heterogeneity because the SG method gives a DM estimate of the entire potato tube, while the oven-drying method was only carried out on a cylinder taken from a specific part of the tubers.

The LF-NMR CPMG relaxation curves are shown in **Figure 1**, gray-scaled colored according to DM content. It is observed that potatoes exhibiting slow relaxation have low DM content; i.e., an inverse relation is observed between T_2 and DM. **Figure 2** shows the mean distribution of T_2 relaxation times of 210 potatoes estimated by distributed exponential fitting of the relaxation data. The mean T_2 distributed curve shows the presence of four populations (**Figure 2**). Even though the three most slow-relaxing populations are overlapped, the distributed T_2 data indicate the presence of four proton components in the potato tubers. The development in residuals when using 1−5 components for discrete exponential fitting and DoubleSlicing is shown in the Supporting Information. It is observed that, after calculations using four components, both fitting approaches show residuals that are randomly distributed around zero and contain only noise. The minimal improvement in RMSE after 5 components contributes to the validation of a 4-component system. The determination of the correct number of components is a major challenge and often requires data inspection and subjective decision making; the main advantages for the DoubleSlicing method is calculation speed and improved solution diagnostics. The core consistency will drop dramatically from positive to negative values when the appropriate number of components is exceeded. This is shown on one representative NMR relaxation curve in the Supporting Information. By comparison, the drop in fit (e.g., RMSE) between consecutive components is more gradual and less obvious when an overfitted model is used.

Table 2. Effect of Different Modeling Approaches Resolving LF-NMR Relaxation Data Curves[a]

	T_2 (ms)				population size (%)			
fitting method	$T_{2,1}$	$T_{2,2}$	$T_{2,3}$	$T_{2,4}$	$M_{0,1}$	$M_{0,2}$	$M_{0,3}$	$M_{0,4}$
discrete	2.8 (0.2)	45 (2.7)	197 (18)	500 (53)	10 (2.0)	7.6 (1.3)	25 (3.7)	57 (6.1)
DoubleSlicing	3.6 (0.3)	53 (3.5)	213 (18)	508 (53)	9.4 (2.0)	8.4 (1.8)	27 (3.9)	56 (6.5)
distributed[b]	2.5	56	141	473	7.9	6.6	11	75
matrix fit	3.9	84	336	625	10 (1.9)	14 (4.4)	48 (10)	28 (13)

[a] Mean T_2 and population size for 210 potatoes are given with standard deviation in parentheses. [b] The population size for the distributed exponentials was calculated from the intensities of the peak maxima.

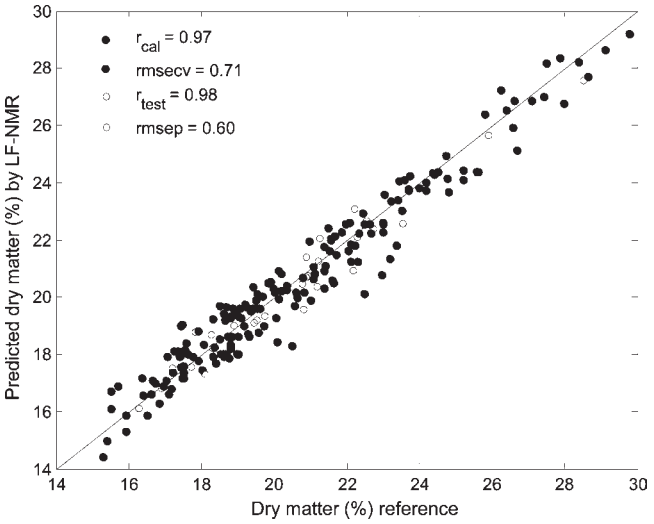

Figure 3. PLS regression (4 latent variables) of LF-NMR parameters (T_2 and M_0) resolved using DoubleSlicing and DM content as the response variable (●, calibration set; ○, test set).

Table 3. Prediction Error Performance for DM Content in Potatoes for Different Modeling Approaches Using LF-NMR Relaxation Curves

PLS modeling input	number of variables	number of LV	r_{cv}	RMSECV	R_{test}	RMSEP
raw NMR data	2048	5	0.96	0.89	0.97	0.65
$T_2 + M_0$ from discrete fitting	8	4	0.98	0.71	0.97	0.62
$T_2 + M_0$ from DoubleSlicing	8	4	0.97	0.71	0.98	0.60
M_0 from matrix fit	4	4	0.94	1.08	0.95	0.83

Table 2 describes the T_2 and M_0 distributions in the potato tubers as found by the four data analysis approaches: distributed exponential fitting, discrete exponential fitting, matrix fit, and DoubleSlicing. The four data analytical approaches give T_2 values that are in the same order of magnitude. It is observed that the classical discrete exponential fitting gives very similar T_2 relaxation time constants as DoubleSlicing, although the latter results in slightly higher values for all components. The magnitudes are also very similar for discrete exponential fitting and DoubleSlicing. The largest population $M_{0,4}$ represents more than half of the total proton population in the potato and is characterized by a $T_{2,4}$ of ~500 ms, representing the most mobile water in the sample. In previous studies, only two water components have been found, representing compartments with 20 and 80% water (*11*, *15*, *16*). The results of PLS regression of LF-NMR data and DM content are given in **Figure 3** and **Table 3**, which also include the model evaluation for LF-NMR data features from discrete exponential fitting, DoubleSlicing, and matrix fit. The table shows that the RMSECV and RMSEP are of similar size for all models, indicating that none of the models are overfitted. PLS regression using raw NMR data gives surprisingly good results with a high correlation ($r = 0.96$) and low error (RMSECV = 0.89) compared to previous observations in studies with less potato samples [r, 0.78 (*14*); *r*, 0.88 (*15*)]. Using the T_2 values and population sizes $M_{0,1-4}$ determined by exponential fitting (*r*, 0.98; RMSECV, 0.71) and DoubleSlicing (*r*, 0.97; RMSECV, 0.71) as variables in a PLS regression to DM content gives slightly better performance than using the raw NMR data. NMR parameter estimation from exponential fitting and DoubleSlicing gives nearly the same results for PLS model performance (**Table 3**).

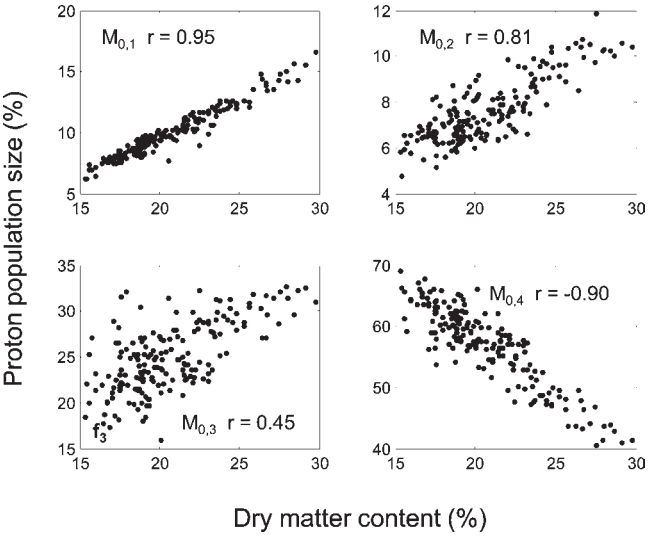

Figure 4. Scatter plot between the population concentration $M_{0,1-4}$ and DM. The correlation coefficients are given in each subplot. T_2 description of the relaxation components is given in **Table 2**.

Inspection of PLS loading and regression coefficients (not shown) revealed that the population sizes $M_{0,1-4}$ (not the T_2 values) were the dominating contributor to the PLS model. This is expected because the population size contains the quantitative information about the proton populations, which, in turn, are expected to be correlated to the DM content. To investigate why there is a high correlation between LF-NMR and DM, the population sizes ($M_{0,1-4}$) are plotted against the DM content (**Figure 4**). $M_{0,1}$ and $M_{0,4}$ are highly correlated to the DM content with $r = 0.95$ and -0.90, respectively. The strong positive correlation between $M_{0,1}$ and the DM content is in agreement with the fact that this population previously has been assigned to water on the surface or inside starch granules (*29*, *30*). The short T_2 relaxation time constant (~3 ms) of $M_{0,1}$ also indicates that this population of protons is strongly associated to potato constituents. In this context, the size of the $M_{0,1}$ proton population is an indirect marker for DM content. The negative correlation between $M_{0,4}$ and DM content is in agreement with the previous finding that this proton population represents extracellular water and water located in the cytoplasm (*29*). The negative correlation to DM content can be explained simply by the cytoplasmatic and extracellular water replacing DM. It is noteworthy that the PLS models in **Table 3** and shown in **Figure 3** give better correlation between predicted versus actual than each individual $M_{0,1-4}$. Thus, the exclusion of DM ($T_{2,4}$) and the proximity to DM ($T_{2,1}$) combined provide a better quantitative description of DM in potato.

With this study, we have confirmed a high correlation between LF-NMR data and DM content of single potatoes using a much larger sample material than previously investigated, including eight cultivars. A new decomposition method of the NMR relaxation curves into mono-exponentials unambiguously revealed that four components were required. The decomposition also revealed why LF-NMR data correlate well to DM. The proportion of the fastest relaxing proton population ($M_{0,1}$) is an indirect marker for DM content, because this population represent water on the surface or inside starch granules. The concentration of the most slowly relaxing protons ($M_{0,4}$) contributes information about DM because high amounts of cytoplasmatic and extracellular water are inversely related to DM content. When the two parameters describing the proportion of the two water pools are combined, $M_{0,1}$ and $M_{0,4}$, the correlation to DM content is further improved. The results show that LF-NMR is the most

precise and direct probe for DM content in potatoes. Because no online potato methods for grading potatoes according to DM content are available yet, there will be several advantages of using LF-NMR methods in the future. An online LF-NMR method can replace measurements of specific gravity of samples of potato bulks and gives more precise quality control data on the individual tuber level.

ABBREVIATIONS USED

LF-NMR, low-field nuclear magnetic resonance; DM, dry matter; UC, ultracentrifugation; NMR, nuclear magnetic resonance; PCA, principal component analysis; PLS, partial least squares; CPMG, Carr−Purcell−Meiboom−Gill; RMSECV, root-mean-square error of cross-validation.

Supporting Information Available: Residuals versus time for 1−5 components when using discrete exponential fitting and DoubleSlicing (Supplementary Figure 1) and solution diagnostic core consistency for 1−5 fitted exponentials using DoubleSlicing (Supplementary Figure 2). This material is available free of charge via the Internet at http://pubs.acs.org.

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