Tracking of deionised water and deuterated water in wheat by NIR hyperspectral imaging

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Introduction

Conditioning is a step during dry milling that facilitates the best separation of bran from the wheat endosperm. By ensuring optimal separation of bran and endosperm, the baking quality of the resulting flour is improved.[1–5] The conditioning process allows the physical separation of bran and endosperm by softening the endosperm and toughening the bran layers. Toughening of the bran layers prevents powdering of the bran during milling, thus enabling a more thorough separation of bran and endosperm. It also ensures that the flour, after milling, is in optimal condition for sifting and in the desired condition to produce optimal end use qualities.[1,3,5] The conditioning requirements are influenced by kernel hardness, initial moisture content, temperature of the wheat and the condition of the bran coat.[1–3] The harder the wheat, the longer the time required for diffusion of conditioning water to diffuse through the wheat endosperm evenly.

Materials and methods

Samples

Whole wheat kernels of varying degrees of hardness were kindly provided by Sensako (Pty) Ltd, RSA (PO Box 556, Bethlehem, 9700, South Africa). Whole wheat kernels were selected from bread wheat lines used in breeding trails. Selection of wheat lines were based on endosperm hardness as determined by the single kernel characterisation system (SKCS) (AACCI Method 55–31.01).[6] The wheat samples selected consisted of six lines in three hardness categories, i.e. soft, hard and very hard, with two lines in each of these categories. Moisture determination was performed in a vacuum oven (Heraeus Model RVT 360, Henau, Germany) at 130°C until constant weight was achieved.

Wheat conditioning and Image acquisition

Two experiments were performed in parallel with deionised H_2O and D_2O, respectively. Nine wheat kernels, from each sample, were randomly chosen and imaged before conditioning. These kernels were marked and returned to the rest of the corresponding sample. A 50g sub-sample of each sample was then conditioned to 17% moisture with H_2O and D_2O, respectively. Conditioning was done in an airtight container. After water was added the wheat was stirred to distribute water through the wheat sample. The wheat was left to rest to allow the water to equilibrate. NIR hyperspectral images were acquired at 6, 12, 18, 24 and 36 hours after conditioning with the same marked kernel and the same layout was used at each of the time intervals used previously. Nine wheat kernels were randomly selected from each of the samples, and were arranged in a cyclic permutation design on silicon carbide (SiC) sandpaper background. Each higher magnification image consisted of one row in the design. The imaging system consisted of an imaging spectrograph coupled to a 2-D array HgCdTe detector with a 50×100 mm field of view. Images were acquired from 1000 nm to 2498 nm with 6–7 nm intervals and stacked to form a 3D hypercube with the dimensions 320×3225 pixels×239 wavelengths. Internal dark and white reference standards were used for image calibration.

Image analysis

The images acquired using the ChemaDAQ software programme (Specim, Oulu, Finland) were transformed from reflectance to pseudo-absorbance in Evince V2.2.2 (Umbio AB, Umeå, Sweden) multivariate image analysis software. Principal component analysis (PCA) with six components was used on mean-centred data to clean the images. This includes the identification and removal of background, dead pixels, shading errors and edge effects that would interfere with the image analysis. A combination of SNV and Savitzky–Golay smoothing (polynomial order 3, derivative order 0 and 7 right and left points) was applied to the images.

Results and discussion

An increase in intensity could be seen in the score image of PC 3 for the soft kernels (Figure 1a).

It seemed that intensity increased until 18 h conditioning, subsequently no further increase was observed. The loading line plot (Figure 1b) of PC 3 of these kernels indicated a prominent water peak at 1940 nm (O–H stretch and O–H deformation). This indicated that water equilibration into the kernel has been achieved after 18 hours, which corresponds with the time indication as applied in industry. Similar results were obtained for the hard and the very hard kernels. In each case the recommended time for conditioning coincided with the intensity increase in the score images i.e. 24 h for hard and 36+h for very hard). Loading line plots were also analogous. The comparison of average spectra indicated a change in both the free (1910 nm) and the bound water (1940 nm) in the grain. The greatest difference, however, appeared to be in the region of 1940 nm, implying that water added during conditioning was ultimately present as bound water in the kernel.

The intensity of the score image (Figure 2a) portrayed a slight difference between 0 and 6 hours after conditioning for soft kernels, thereafter no definite change was noticeable.

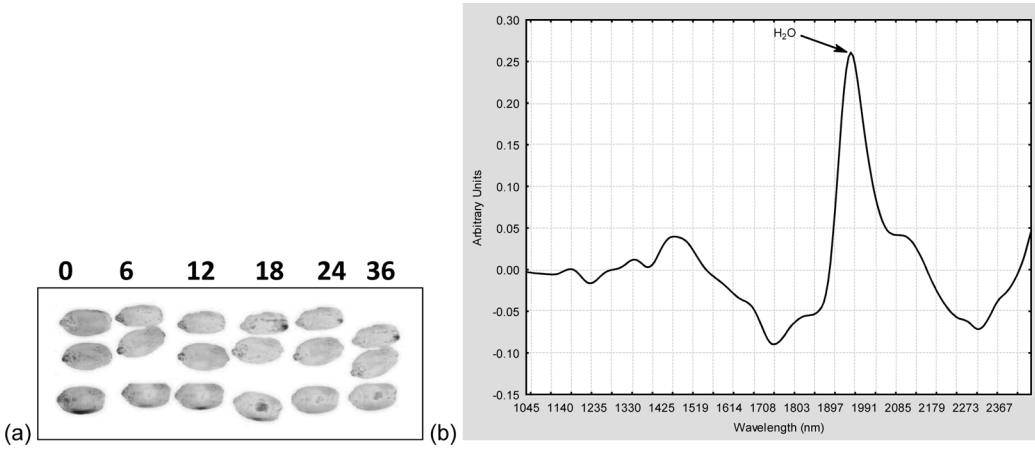

Figure 1. (a) Score image of PC 3 for the soft sample and (b) the corresponding loading line plot.

The loading line (Figure 2b) of PC 5 for soft wheat conditioned with D_2O portrayed an absorbance peak at 1954 nm (O–D stretch and O–D deformation)[7] which indicated that the variation in PC 5 was attributed to D_2O. This most likely indicates absorption of D_2O into the wheat kernel directly after addition of conditioning water, but no further diffusion of the water into the wheat endosperm. Similarly, the loading line plots for hard and very hard samples showed prominent absorption peaks at 1954 nm (O–D stretch and O–D deformation) due to D_2O. As with the soft sample only minor intensity differences between 0 and 6 hours after conditioning were apparent in the score image of hard and very hard wheat, indicating that diffusion of D_2O did not occur between 6 h and 36 h.

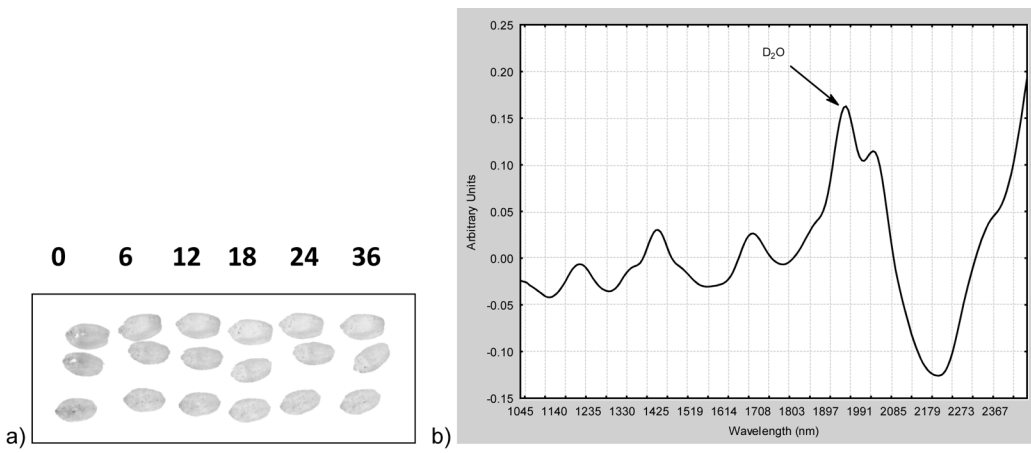

Figure 2. (a) Score image of PC 5 for the soft sample and (b) the corresponding loading line plot.

Conclusion

Conditioning with H_2O, rather than that with D_2O, gave an indication of the time required for water to diffuse into the wheat kernel. Estimated conditioning times from score images seem to agree with those obtained in literature and those currently used in industry. It would be interesting to further study the interaction of bound and free water during conditioning. This would improve the understanding of the interaction of water with wheat starch and protein during conditioning.

References

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