Application of ASCA to characterise effects of roasting temperature, -time and milling method on SWIR spectral data of whole and milled wheat

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INTRODUCTION

0.15

Perten

Quadrumat

- Dry thermal treatment to modify wheat starch has been increasingly investigated (Ma et al., 2021).
- Structural changes of starch in heat treated wheat affects the molecular order, pasting properties, and retrogradation (Van Rooyen et al., 2022).
- Analysis of variance simultaneous component analysis (ASCA) partitions variation and interprets these partitions with SCA (Smilde et al., 2005).

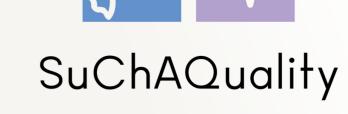


Characterisation of wheat modification during roasting and milling of wheat kernels using SWIR spectroscopy and multivariate data analysis







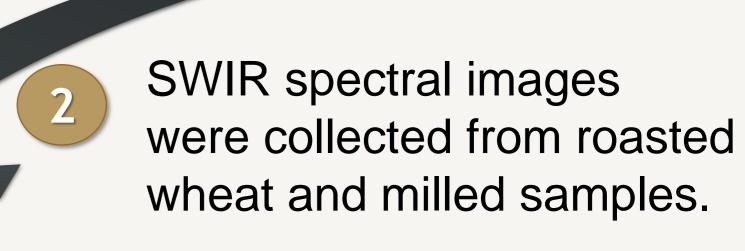


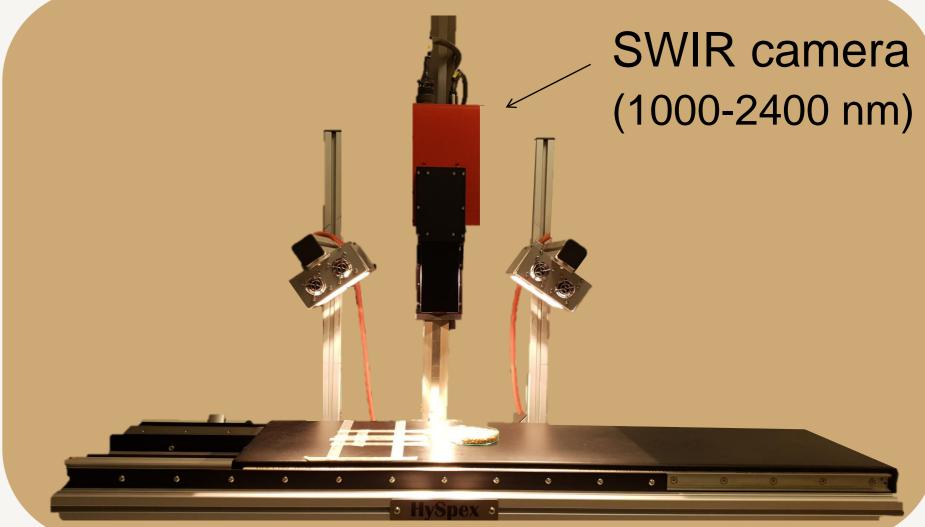


The experimental design included three roasting temperatures (90°C, 115°C, 140°C), three roasting speeds (47 Hz, 65 Hz, 83 Hz) and two milling methods (Perten and Quadrumat).



ASCA was used to assess statistical significance and characterisation of the contributing spectral features.







protein &

starch

starch &

protein

fibre

moisture

Figure 1 Loadings plot showing

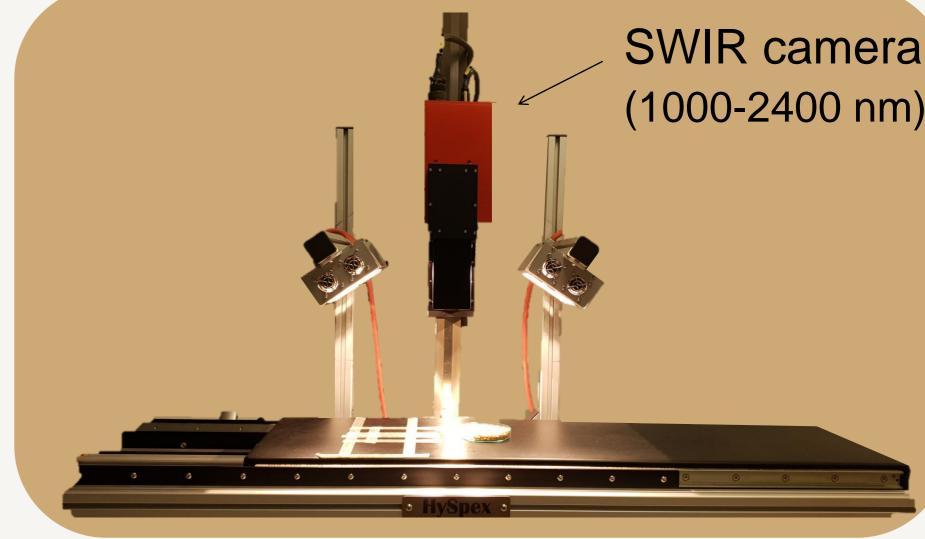
significant effects of milling method on

SWIR spectral data

& DISCUSSION

Table 1: 'Roasting temperature' and 'milling method' had significant effects (p<0.05) on the samples. High temperature significantly affected starch (i.e. partial gelatinisation) and protein (i.e. denaturation). Intermediate temperature affected starch and moisture more compared to low temperature. 'Roasting time' could have notable effect in practice (p=0.06). Figure 1: The most prominent difference between the two milling methods was observed as changes in starch, protein, moisture

(Quadrumat) and fibre (Perten).

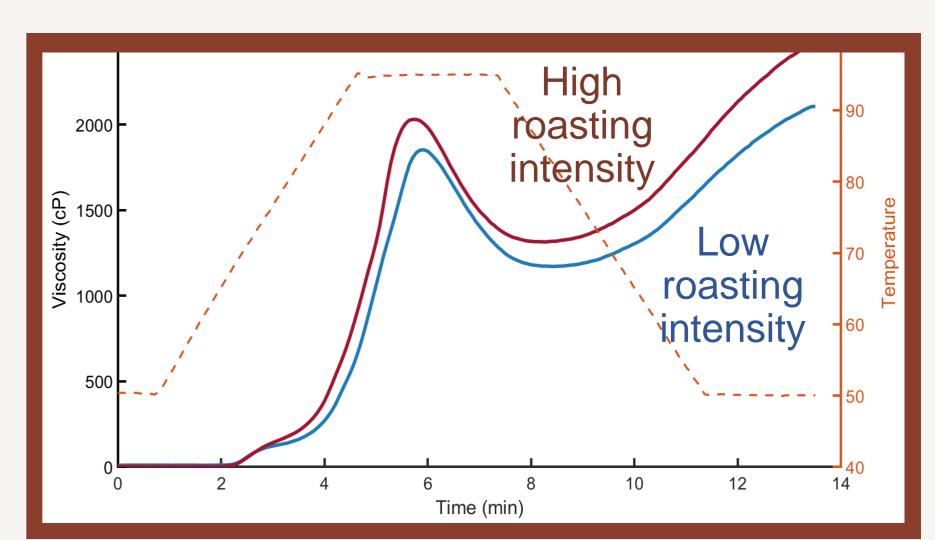


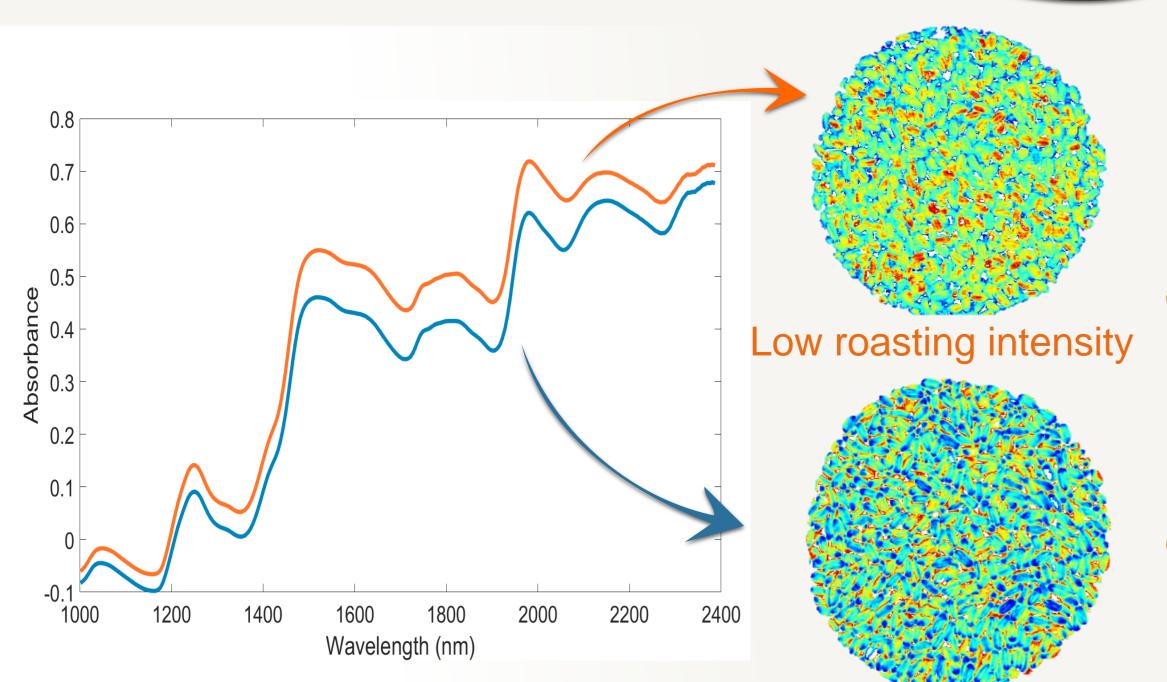
temperature on SWIR spectra Wavelength Bond Chemical vibration (nm) structure

Table 1 Significant effect of roasting

()		
High temperature		
2000	C-O	Starch
2242	N-H, NH ₃ +	Protein
2252, 2276	O-H, C-C	Starch
2294	N-H, C=O	Protein
Intermediate temperature		
1450, 1480,	O-H str. 1 st	Starch,
1528, 1540	overtone	water

Confirmed protein denaturation and starch gelatinisation by increased **RVA** viscosities





High roasting intensity

CONCLUSION

- ASCA applied to SWIR whole wheat and flour spectral data effectively characterised the effect of roasting on wheat properties.
- Significant differences in wheat starch and protein structures were observed.

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REFERENCES:

- Ma, Y., Xu, D., Sang, S., Jin, Y., Xu, X. & Cui, B. (2021). Food hydrocolloids, 112, pp. 1-9.
- Smilde, A.G., Jansen, J.J., Hoefsloot, H.C.J., Lamers, R-J.A.N., Van der Greef, J. & Timmerman, M.E. (2005). Bioinformatics, 21(13), pp. 3043-3048.
- Van Rooyen, J., Simsek, S., Oyeyinka, S.A. & Manley, M. (2022). Foods, 11(2), pp. 1–19.

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