Whole grain prediction of durum wheat yellow pigment by visible/near infrared reflectance spectroscopy

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Introduction

There is a strong international preference for pasta with intense amber colour. Colour is therefore an international specification in durum wheat marketing and is a selection factor in breeding programs. Carotenoid pigments, mainly xanthophyll, present in durum wheat endosperm are the colour source. The amount of pigment varies between cultivars and fluctuates yearly, depending on environmental conditions during kernel development.

The current reference method for yellow pigment requires overnight extraction of samples with water-saturated *n*-butanol, a flammable, noxious chemical which can affect the central nervous system. Durum wheat breeders require a more rapid, small scale and preferably non-destructive test for screening of early generation lines which are of limited sample size. Visible/near infrared spectroscopy could meet these requirements. As well, it could provide a rapid test suitable for conducting surveys of commercial shipments by origin to identify regions of particular pigment levels which meet customer specifications in marketing agreements.

Materials and methods

Sources of durum wheat

A survey during the 1991–92 shipping season, corresponding to the 1991 harvest, provided 532 samples from individual rail carlots as they were moved through terminal elevators. Individual producer deliveries to primary elevators were the source of 2505 samples following the 1992 harvest and 1677 samples following the 1993 harvest. The quality of samples in each year of testing ranged from very good to very poor. Pure cultivars were obtained from the Canadian durum wheat breeding program. There were 22 cultivars grown at 11 locations across western Canada in 1993, to provide a total of 242 samples.

Standard reference

Ground samples were extracted overnight with water-saturated *n*-butanol, then filtered. Absorbance of the filtrate at 435.8 nm was used to estimate yellow pigment content.[1]

Visible/NIR calibrations

Ground grain from the 1991 harvest (n = 159) and whole grain from the 1992 harvest (n = 109) were scanned from 400 to 2500 nm using NIRSystems model 6500. Log 1/R gave the highest degree of accuracy in development of ground grain calibrations (Table 1).

Table 1. Calibrations.

	Ground grain		Whole grain	
	Coefficient	λ	Coefficient	λ
K(0)	17.97		23.16	
K(1)	–112.20	700	866.36	1480
K(2)	–66.16	400	378.36	610
K(3)	–292.48	520	–466.55	2080
K(4)	182.74	670	607.36	1030
K(5)	203.74	460	–553.60	1000
K(6)	–163.96	580	–192.05	520
K(7)	–37.30	2470	460.73	1210
K(8)	24.89	1210	149.46	1360
K(9)	255.15	550	–527.21	790
	$r^2 = 0.865$	$n = 159$	$r^2 = 0.885$	$n = 109$

Whole grain calibrations were most accurate using 1st derivative of log 1/*R* (Table 1). Ground grain calibrations were subsequently used to monitor performance of whole grain analyses, with random checks being tested by the standard reference method.

Results

Samples from the 1991 carlot survey, predicted by visible/NIR ground grain calibration, demonstrated a wide variation in pigment content across western Canada (Figure 1). A similar degree of variation was evident in the 1992 (Figure 2) and in the 1993 (Figure 3) harvest surveys, predicted by visible/NIR whole grain calibration. It was also obvious that there was a large variation in pigment content from year to year and distribution of pigment across loactions.

Durum wheat cultivars vary inherently in pigment content and because of agronomic characteristics tend to be grown in specific areas. In order to determine the effect of cultivar and location, plant breeder lines (22 lines grown at each of 11 locations) were tested against the calibrations. Estimation of pigment content in ground samples by visible/NIR is already being used in the Canadian durum wheat breeding program.[2] Our ground grain calibration was approximately equal to that of McCaig and co-workers in prediction of pigment content relative to the reference method ($r^2 \approx 0.9$). Whole grain prediction was also highly correlated with the reference method ($r^2 \approx 0.86$), with the added advantage of being non-destructive. The range in pigment content across cultivars was 7.8 to 12.1 ppm and average values across locations varied from 6.9 to 12.2 ppm. Robustness of the calibrations was demonstrated by the fact that bias of whole grain predicted values to reference method values across cultivars ranged from –1.0 to 0.5 ppm and across locations varied from –1.0 to 0.8 ppm.

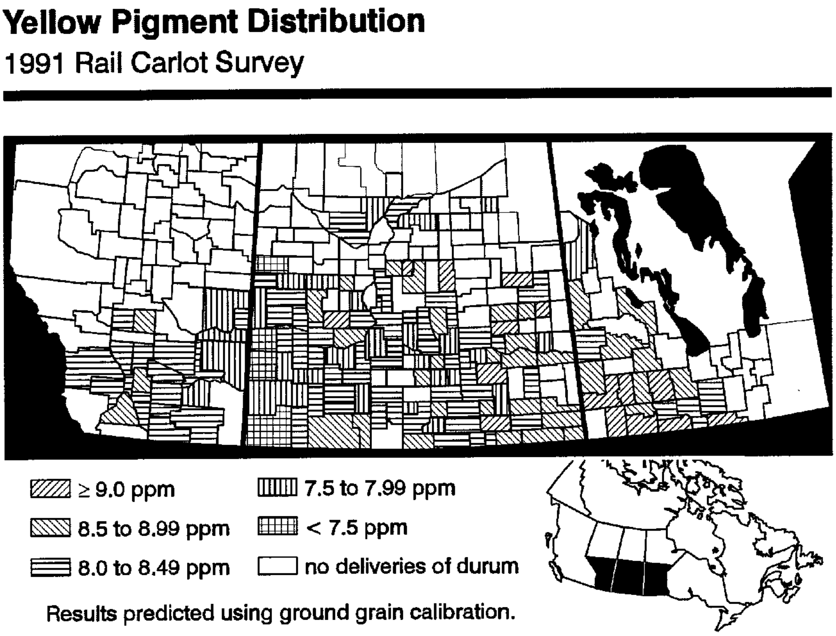

Figure 1. Yellow pigment distribution from 1991 rail carlot survey. Results predicted using ground grain calibration.

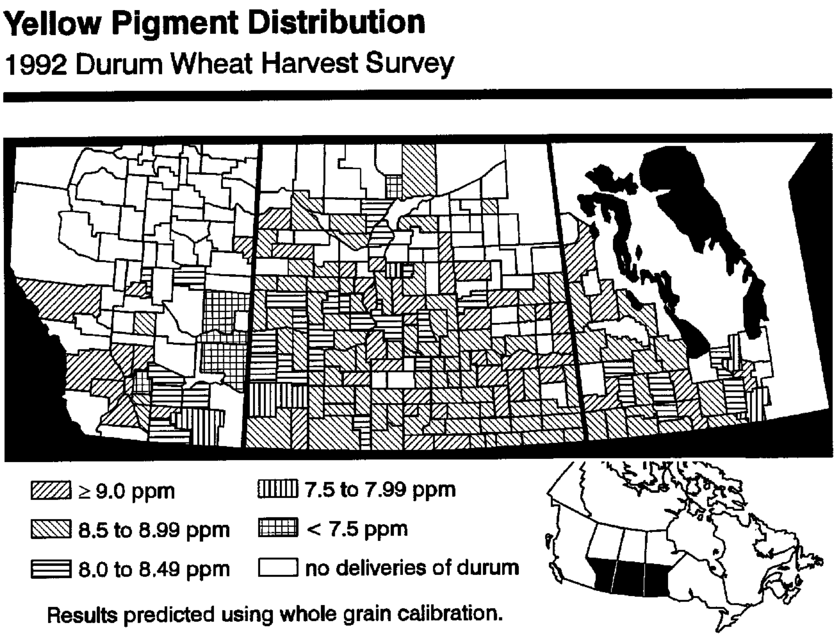

Figure 2. Yellow pigment distribution from 1992 durum wheat harvest survey. Results predicted using whole grain calibration.

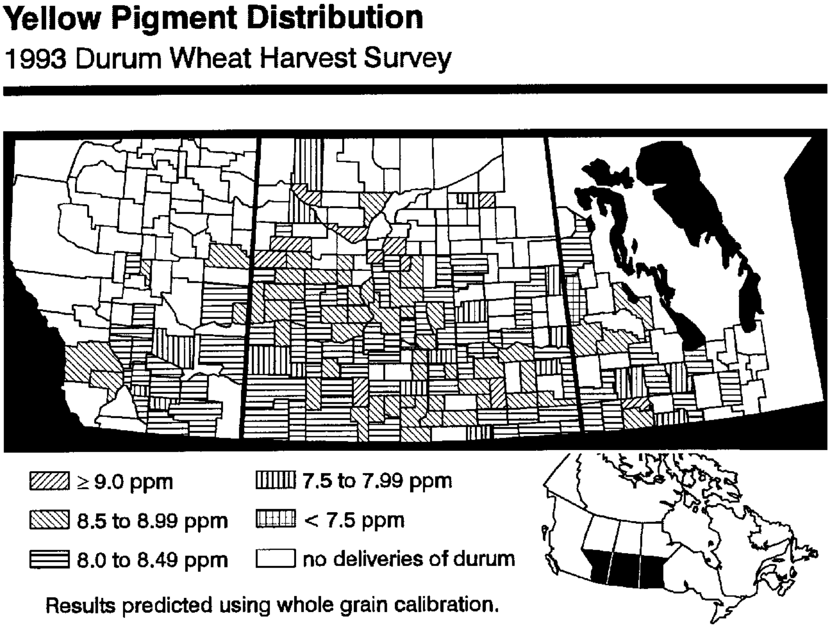

Figure 3. Yellow pigment distribution from 1993 durum wheat harvest survey. Results predicted using whole grain calibration.

Conclusions

Ground grain calibrations were so strongly related to values obtained by reference method ($r^2 \approx 0.9$) under all conditions studied that ground grain calibrations could be used to verify whole grain results. Effectiveness of the calibrations to predict yellow pigment was unaffected by the physical condition of the wheat, which ranged from very good to very poor. Ability to predict pigment appeared robust across environmental factors and genetic diversity as determined by the testing of 22 pure cultivars grown at 11 different locations. Whole grain calibrations should prove valuable to durum breeding programs because of the ability to discriminate differences in pigment levels without any sample loss. Annual variation in pigment level as a result of environmental factors associated with location was at least equal to variability resulting from cultivar differences.

References

1. American Association of Cereal Chemists, *Approved Methods of the AACC*. Method 14–50, approved April 1961, revised Oct. 1982 and Oct. 1984. The American Association of Cereal Chemists, St Paul, MN (1983).
2. T.N. McCaig, J.G. McLeod, J.M. Clarke and R.M. DePauw, *Cereal Chem.* **69,** 671 (1992).