Characteristics of Fermented Dough Predicted by Using the NIR Technique

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Abstract

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Rheological characteristics of wheat doughs prepared from 179 variety and commercial wheat flour samples (crop years 1999, 2001, 2002, 2003 and 2004) were assessed with SJA fermentograph (Sweden). NIR spectra of the samples were measured on the spectrometer NIRSystem 6500. Calibration equations with cross and independent validations for all rheological characteristics were computed by NIR Software ISI Present WINISI II using mPLS/PLS regression and ANN. The quality of prediction was evaluated by means of coefficients of correlation between the measured and the predicted values from cross and independent validation. A statistically significant dependence (with probability higher than 99%) was determined in all mentioned rheological characteristics in the case of cross-validation. The results suggested the possibility of prediction particularly for the fermentation gas volume parameter, where a high correlation was achieved (r = 0.888). The accuracy of prediction by independent validation was not found on such a satisfactory level. For the sets of ten commercial flours, higher correlation coefficient was calculated for the final dough volume parameter.

Keywords: wheat flour dough; fermentograph; NIRSystem 6500; prediction of rheological characteristics

Wheat flour is able to form a cohesive dough with viscoelastic properties and has the ability to retain gas, which is essential for the production of baked products with a light texture. The factor responsible for the dough formation is gluten protein and its development during mixing (Hrušková *et al.* 2001). During fermentation, a steady gas formation of sufficient amount is needed for the product to obtain desired the loaf volume. Fermentation is a metabolic process serving for some microorganisms to get energy through digestion of simple fermentable sugars, mostly glucose and fructose, forming gas. The amount of CO_2 depends on yeast and flour properties under standard conditions of the dough preparation which have a strong effect on the final product quality (Bloksma 1993).

Important for the technological quality of wheat flour is its strength given by the gluten quality and content, and so are also starch-amylase-complex properties (enzymatic activity, starch particles damage). These properties are observed by means of different methods (Pomeranz 1988).

Rheological characteristics, such as elasticity, viscosity and extensibility, are important for the milling and baking industry in view of the prediction of the processing parameters of dough and the quality of end products. These rheological characteristics change throughout the breadmaking process and are difficult to measure in definitive terms (Hrušková *et al.* 2001).

To assess the fermented dough properties (gas volume, retention capacity) and its behaviour during

maturation, several rheological apparatuses were developed. A common one is SJA fermentograph (Sweden) or advanced type rheofermentometer (Chopin, France). Czuchajowska and Pomeranz (1993) developed a methodology to assess fermentation with the use of rheofermentometer and a shortened baking test on the bread-making machine. The formula of dough also influences the properties of leavened dough. Full-bread-formula is usually used for the dough fermentograph testing (Švec & Hrušková 2004).

Because the baking test and rheological measurements require a lot of time and equipment to be performed, a fast and reliable test is necessary. This problem can be solved by the NIR spectroscopy (Williams & Norris 2001), which is almost well-established to control analytical properties of flour in many industrial mills. The prediction of dough properties by NIR spectra analysis is influenced by many factors, especially errors of rheological methods and the dependence of the results on the protein content of the flours tested. The reliability of the computed characteristics of dough varies according to the calibration sample set, the extent and quality range of flour parameters (Hrušková & Šmejda 2003).

The main goal of this study was to predict dough the rheological properties measured on the fermentograph from NIR flour spectra.

MATERIAL AND METHODS

Samples. Three subsets of commercial and five subsets of variety bakery (fine, bright) flours were used jointly as a calibration set. Commercial flours (53 samples) were mostly obtained from industrial mills (crop years 2001 and 2003). However, twenty of them represented laboratory ground commercial wheat flours (Chopin CD1-auto). Variety flours (126 samples) were supplied by Central Institute for Supervising and Testing in Agriculture in Brno (crop year 1999), SELGEN Stupice (crop years 2002, 2003 and 2004) and Research Institute of Crop Production in Prague-Ruzyně (crop years 2003 and 2004) and all these flours were ground on laboratory mill Chopin CD1-auto (all but samples from Brno) and Bühler MLU 202 (samples only from Brno). Ten samples of flours from retail (crop year 2003) were used as a validation set.

References analysis. The basic flour quality parameters (the ash, moisture, wet gluten, and protein content) were determined using spectrometer Inframatic 8600. Czech standard methods were used for the determination of falling number (ČSN ISO 3093; Falling Number, Perten Instruments, Sweden) and Zeleny sedimentation value (ČSN ISO 5520; Sedi-Test, ZZN Strakonice).

Rheological properties of fermented wheat dough were evaluated by SJA fermentograph (Sweden). As the fermentograph test procedure is not included in any international or Czech standard method, this test was performed according to our internal method. The dough for the fermentograph test was prepared in farinograph (Brabender, Germany) under standard conditions (mixer tempered at 30°C) using the baker test formula (flour 100%, compressed yeast 4.0%, sugar 1.5%, fat 1.0%, salt 0.7%) and the water amount to reach optimal consistency of 600 ± 20 FU (farinograph units). Two pieces of dough (both of 150 g) were then put into two fermentation cylinders, where fermentation proceeded for 160 min at 30°C. Three parameters are extracted from two plots: fermentation gas volume V_G [FeU – fermentograph units], final dough volume V_D [FeU] (the volume at the end of test) and fermentation time T [min] (the time of maximum dough volume).

NIR apparatus. NIR spectra were collected on the wavelenght scanning instrument NIRSystem 6500 (Foss NIRSystems, Inc., USA) using a small ring cup. Scanning range from 400 to 2500 nm and wavelenght increments of 2 nm were used. Diffuse reflectance was recorded as $\log(1/R)$. Each sample was measured once (five scans) and was used for calibration.

Statistics. NIR Software ISI Presents WINISI II (Infrasoft Int., USA) was used to evaluate the data and to develop chemometric models. No-scatter correction and four-scatter correction methods (SNV, detrend, SNV + detrend, standard MSC) were applied. The data were treated by the first derivative (math setting 1, 4, 4, 1, and 1, 8, 8, 1). Calibration was carried out by Modified Partial Least Square (mPLS), and Partial Least Square (PLS) regression. In addition, Artificial Neural Network (ANN) was used. The number of terms was limited to four. In the case of mPLS/PLS, no samples were eliminated on account of their higher deviation and "one-out" cross-validation was used. In the case of ANN, the outliers were eliminated and the starting set was divided into the calibration and the validation parts in the ratio of 75:25. The best calibration equations for mPLS/PLS and ANN were selected according to

their highest coefficient of correlation (*r*) or minimum standard error of cross-validation (SECV) or standard error of validation (SEV; for ANN). These equations were consequently validated by the set of flours from retail.

RESULTS AND DISCUSSION

Analytical characteristics

Analytical characteristics describing flour quality of the sets tested (crop years 1999, 2001–2004) are given in Table 1. The quality of wheat flours corresponded to Czech standard for the mill products of fine type. The analytical ranges were from 8.6 to 16.1% for protein, from 20 to 72 ml for Zeleny sedimentation value, and from 164 to 572 s for falling number. The commercial and the variety flour subsets (data not shown) are comparable according to the mean analytical values. However, wider range of qualitative characteristics was observed in the variety subset (e.g. 5.7% contra 2.2% for protein). A feature of most flours is a high falling number indicating a low activity of amylases. The samples used for the validation belong to flours with a higher protein content representing average wheat quality of this crop year (2003).

Rheological characteristics

The results with doughs as obtained on fermentograph are summarised in Table 2. The param-

Table 1. Flour analytical parameters

| Parameters | Mean | Range | | Coefficient of variation (%) |
		min.	max.	
Calibration set (179 samples)				
Ash[a] (%)	0.59	0.48	0.75	9.9
Wet gluten[a] (%)	31.42	18.4	46.9	10.6
Protein[a] (%)	11.76	8.6	16.1	7.3
Falling number (s)	362	164	572	21.1
Zeleny sedimentation value (ml)	40	20	72	28.4
Validation set (10 samples)				
Ash[a] (%)	0.6	0.55	0.65	4.5
Wet gluten[a] (%)	34.16	29.1	39.5	8.3
Protein[a] (%)	13.59	12.5	14.7	5.5
Falling number (s)	352	265	388	9.2
Zeleny sedimentation value (ml)	51	42	62	13.9

[a]dry matter basis

Table 2. Flour fermentograph parameters

| Parameters | Mean | Range | | Coefficient of variation (%) |
		min.	max.	
Calibration set (179 samples)				
Final dough volume (FeU)	68	29	95	21.8
Optimal fermentation time (min)	64	25	126	33.8
Fermentation gas volume (FeU)	108	54	147	22.6
Validation set (10 samples)				
Final dough volume (FeU)	79	60	89	9.7
Optimal fermentation time (min)	54	48	59	5.7
Fermentation gas volume (FeU)	134	126	145	4.2

Table 3. Prediction of flour fermentograph characteristics

Parameters	Calibration					Cross-validation			
	n	Terms	SEC	CV	*r*	*n*	SEP	CV	*r*
mPLS/PLS									
Final dough volume (FeU)	172	12	5.98	8.89	0.831	172	8.17	12.14	0.687
Optimal fermentation time (min)	174	9	9.89	16.57	0.769	174	11.75	19.70	0.676
Fermentation gas volume (FeU)	177	12	4.68	4.23	0.963	177	8.19	7.41	0.888
ANN									
Final dough volume (FeU)	140	8	4.82	.	0.895	35	6.08	.	0.818
Optimal fermentation time (min)	136	8	11.55	.	0.707	40	9.80	.	0.815
Fermentation gas volume (FeU)	134	8	8.00	.	0.895	42	8.51	.	0.872

SEC – standard error of calibration; *r* – coefficient of correlation; $r_{(\alpha = 0.01, df = 100)} = 0.254$; $r_{(\alpha = 0.01, df = 35)} = 0.418$; $r_{(\alpha = 0.05, df = 25)} = 0.487$; df – degree of freedom; CV – coefficient of variation (%), SEP – standard error of prediction; mPLS/PLS – modified partial least square/partial least square regression; ANN – artificial neural network

eter values ranges from 29 to 95 FeU for the final dough volume, from 25 to 126 min for the optimal fermentation time and from 54 to 147 FeU for the fermentation gas volume. The optimal fermentation time parameter is characterised by the highest variation (33.8%). The greater uniformity of commercial flours in the case of fermentograph properties (data not shown) was revealed only by a lower variance of the final dough volume (11.2% beside 26.9%). Higher and considerably more uniform values of the fermentation gas volume parameter were observed in the case of the variety flours subset (mean 122 FeU beside 93 FeU). The flours used for the validation had rather higher values of the final dough volume and the fermentation gas volume and shorter fermentation times. In the bakery process, this means a lower resistance to the mechanical stress and good gas evolution and retention.

Prediction according cross-validation

The prediction of rheological properties in the calibration flours set is show in Table 3. Statistically significant dependence between the predicted and the reference values with probability higher than 99% was found for all three parameters in using both methods. However, in view of high coefficient of variation (> 10%), the mPLS/PLS calibrations obtained cannot be thought reliable (variation coefficient for ANN was not computed). The highest statistical correlation (*r* = 0.888) in all samples set was achieved for the fermentation

gas volume parameter, and can be considered as medium strong. Weaker statistical dependencies were found for the final dough volume and the optimal fermentation time (statistical level 99%). In the case of ANN, the results were similar, but moderate correlations for all parameters were achieved. This may be due to some numbers selection from the calibration/validation samples. The validation subset seems not to be representative for the optimal fermentation time, since SEV attained is lower than SEC.

Prediction according independent validation

The correlation coefficient (*r*) and the standard error of prediction (SEP) for rheological parameters are shown in Table 4. Using calibration equations for the prediction of the measured properties of independent samples, quality of which will be within the range of the calibration set, a satisfactory accuracy resulting from SEP (SECV) of the appropriate characteristic can be suggested (Pekárková *et al.* 2000). The best calibration equations (selected according to SECV/SEV) were verified by independent validation, for which the independent set of ten flours from retail was used. For all three parameter observed, lower coefficients of correlation and high biases were found. With bias corrected, the volume change of the dough sample was predicted the most precisely (bias-corrected standard error of prediction SEP(C) = 5.78 FeU). A less reliable prediction was found

Table 4. Independent validation of calibration equations

Parameters	Calibration				Independent validation				
	n	Terms	SEC	*r*	*n*	SEP(C)	bias	CV	*r*
mPLS/PLS									
Final dough volume (FeU)	172	12	5.98	0.831	10	5.78	5.24	8.59	0.506
Optimal fermentation time (min)	174	9	9.89	0.769	10	5.90	−20.03	9.89	0.333
Fermentation gas volume (FeU)	177	12	4.68	0.963	10	11.70	31.73	10.59	0.007
ANN									
Final dough volume (FeU)	140	8	4.82	0.895	10	4.99	7.53	7.41	0.620
Optimal fermentation time (min)	136	8	11.55	0.707	10	5.95	−16.60	9.97	0.254
Fermentation gas volume (FeU)	134	8	8.00	0.895	10	9.41	30.70	8.52	0.018

SEC – standard error of calibration; *r* – coefficient of correlation; $r_{(\alpha = 0.01, df = 100)} = 0.254$; $r_{(\alpha = 0.01, df = 8)} = 0.765$; $r_{(\alpha = 0.05, df = 8)} = 0.632$; df – degree of freedom; SEP(C) – standard error of prediction corected for bias; CV – coefficient of variation (%); mPLS/PLS – modified partial least square/partial least square regression; ANN – artificial neural network

for the fermentation gas volume parameter; the optimal fermentation time was predicted with a higher error. ANN in comparison with mPLS/PLS regression provided comparable results for all three parameters and only minor differences could be observed. The prediction of wheat dough behaviour with commercial flour samples was calculated usually with a lower accuracy than assessed in our previous work (Hrušková *et al.* 2004).

CONCLUSIONS

NIR technique was used to predict the dough baking quality of both commercial and variety flours. A statistically significant dependence between the predicted and the reference values with probability higher than 99% was found during calibration for all three parameters with both mPLS/PLS and ANN methods. The fermentation gas volume parameter was revealed as the best predicted parameter in the calibration set, suggesting the possibility of NIR evaluation. Since the extent of the calibration parts differs for mPLS/PLS and ANN, one must be careful when comparing the parameters of the calibration equations. Using ANN, standard errors attained were slightly lower or equal. However, in predicting properties of ten flours from retail, the accuracy was not achieved on such a satisfactory level. Probably because the validation set was represented by specific flour type (well-balanced end-user flours from different mills) with characteristics not included

in calibration set. Thus, the prediction of the gas production seems to be rather more prospective then the prediction of other parameters of fermented dough. The calibration and the validation sets of samples, come from five year crops, seem to be satisfactory for the estimate of rheological parameters of fermented dough using flour from laboratory milling process. Higher number of samples must be tested in the case of rheological behavior prediction of commercial flour. Similar results of mathematical prediction of farinograph, extensigraph, and alveograph characteristics by independent validation were documented in our previous work (Hrušková *et al.* 2004).

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