Prediction of Baking Characteristics of Hard Winter Wheat Flours Using Computer-Analyzed Mixograph Parameters

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ABSTRACT

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The objective of this research was to determine whether computer-analyzed (objective) mixograph parameters could replace conventional mixograph parameters in the evaluation of flour quality. The 642 hard winter wheat flours, collected from federal regional performance nurseries in 1995 and 1996, were analyzed by a conventional and computerized mixograph. Mixograph bandwidths at 6 min (BW6) showed the most significant linear correlation with subjective mixing tolerance scores ($r = 0.81$, $P < 0.1\%$, $n = 642$). Prediction models of conventional and experimental baking parameters were developed by continuum regression using computer-analyzed mixograph parameters of a calibration set ($n = 282$). The developed models could estimate conventional mixograph mixing time and tolerance scores, baking water absorption and mixing time, and bread loaf volume, showing R^2 values of 0.86, 0.74, 0.68, 0.80, and 0.51, respectively, for a validation set ($n = 380$). These results indicated that computer-analyzed mixograph parameters could be applied to develop prediction models to be used for flour quality evaluation in wheat breeding programs.

The mixograph is a rapid tool used to measure the mixing characteristics of flour. Since Swanson and Working (1933) introduced the basic mixograph system, sample size has been reduced to improve its utilization in breeding programs (Finney and Shogren 1972; Finney 1989; Rath et al 1990; Shogren 1990). Mixograph data have been used to differentiate wheat flours of good and poor baking quality (Finney and Shogren 1972; Bruinsma et al 1978; Finney et al 1987; Buckley et al 1990; Neufeld and Walker 1990; Slaughter et al 1992; Wikström and Bohlin 1996). The 10-g mixograph has been specifically used to evaluate the quality of early generation lines in wheat breeding programs because it utilizes a small sample amount and requires a short analysis time (Finney et al 1987; Gras and O'Brien 1992). Mixograph parameters are very useful in selecting good quality wheat lines in hard wheat breeding programs because they are significantly affected by the genetic effect (Swanson and Kroeker 1932; Larmour et al 1939; Swanson 1941; Harris et al 1944; Finney and Fryer 1957; Johnson et al 1972, Gras and O'Brien 1992; Peterson et al 1992).

Conventional mixograph parameters that have been used in quality evaluation include mixing time, water absorption, and mixing tolerance (Finney 1985). Application of computer technology in the mixograph procedure has improved its control and data processing (Rubenthaler and King 1986; Pon et al 1989; Gras et al 1990; Navickis et al 1990; Sterns and Barta 1990). Some advantages of computerization include facilitation of data handling and processing, and objective interpretation of the mixogram. Computerization also allows calculation of more parameters from the mixogram in a very short time.

The computer-analyzed mixograph parameters had significant correlations with the conventional analysis, suggesting that they could be used to evaluate flour quality instead of the conventional analysis (Pon et al 1989; Gras et al 1990; Ohm and Chung 1999). However, some bias still exists between conventional and computer-analyzed parameters even though linear correlation coefficients were statistically significant between them (Ohm and Chung 1999). Adjustment of the bias would help to improve performance of the computerized mixograph system for quality evaluation.

Computerization of the mixograph gives it more potential for use in quality evaluation than conventional mixogram analysis. One of the potential uses is to develop prediction models of end-use properties using computer-analyzed mixograph parameters. Development of prediction models should be very valuable due to objective testing of flour quality, specifically when the sample amount is limited or the number of samples to be tested is excessive. For example, early generation lines in wheat breeding programs typically require screening of a large number of samples for quality. Multivariate calibration methods have been used to develop prediction models. These methods include ordinary multiple linear regression (MLR), principal component regression (PCR), and partial least squares (PLS). Wikström and Bohlin (1996) reported that the prediction model of bread loaf volume could be developed from mixogram parameters using PLS.

Stone and Brooks (1990) introduced a new multivariate calibration technique, continuum regression (CR) that encompasses MLR, PCR, and PLS. CR appears to have potential to develop a calibration model that can predict more accurately and precisely than other multivariate techniques.

In this study, computer-analyzed mixograph parameters, obtained by a commercial software program called MIXSMART, were used to develop prediction models of conventional mixograph and baking parameters to facilitate quality evaluation in hard wheat breeding programs and industry. The CR was used to develop calibration models with 262 hard winter wheat breeding lines obtained from federal regional performance nurseries. The objective of this study was to investigate whether computer-analyzed mixograph parameters could be used to evaluate flour quality in breeding programs and industry.

MATERIALS AND METHODS

Materials

The 642 hard winter wheats were milled at the USDA-ARS Grain Marketing and Production Research Center, Hard Winter Wheat Quality Laboratory, Manhattan, KS, using a Quadrumat Sr. experimental mill. The wheat samples were collected from breeding lines harvested in Federal Northern, Southern, and Western Plains Regional Performance Nurseries in 1995 and 1996.

Proximate Analyses

Protein content (N × 5.7) was determined by a nitrogen determinator (Leco Corp., St. Joseph, MI) using Approved Method 46-30 (AACC 2000). Ash and moisture content were determined by Approved Methods 08-01 and 44-15A.

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Mixograph Procedure

The mixogram was obtained by using a 10-g bowl mixograph with optimum water absorption according to the procedure of Finney and Shogren (1972). Flour (10 g) was mixed with water for 8 min at 77°F in a mixograph bowl. A mixogram was graded to provide mixing requirement, mixing tolerance, and optimum water absorption. The mixogram was also evaluated using MIXSMART software (v. 3.40, National Mfg. Division, TMCO, Lincoln, NE) (Fig. 1). Computer-analyzed mixograph parameters obtained by MIXSMART included midline peak time (MPT), height (MPH), width (MPW), and area (MPA); midline left and right slope (MLS and MRS, respectively); and envelope right slope (ERS) and envelope peak area (EPA). Other computer-analyzed parameters were band height and width 2 min after MPT (MPH2 and BW2, respectively), and bandwidth at 6 min (BW6). MLS indicates maximum slope of the midline that appears between the starting point and the MPT. ERS indicates slope at the point at which the first inflection appears after envelope peak.

Baking Procedure

The optimized, straight-dough Approved Method 10-10B (AACC 2000) was used for experimental baking. The formula contained 100 g (14% mb) of flour, 6 g of sugar, 3 g of shortening (Vream, Bunge Foods), 1.5 g of NaCl, 1.0 g of dry yeast (Fleischmann), 5 mg of ascorbic acid (50 ppm), and 0.25 g of barley malt (50–60 DU/g, 20°C). Optimum baking water absorption and mix time were determined by the feel and appearance of the dough. After mixing, the dough was fermented at 30°C for 120 min, during which time the dough was punched twice after 69 min of fermentation and then again 34 min later. The fermented dough was proofed at 30°C until the dough of the control flour had risen to 7.6 cm. It was baked at 218.3°C (425°F) for 18 min and weighed immediately after removal from the oven. Loaf volume was then determined by rapeseed displacement. The bread was cooled for 2 hr at room temperature and put into a plastic bag. One-day-old bread was sliced by machine (Oliver, Grand Rapids, MI), and bread crumb grain was evaluated on a 7-point scale of 0–6, where 0 is unsatisfactory and 6 is outstanding crumb grain.

Development of Prediction Model

Among the 642 wheat samples, 262 samples were selected for calibration based on mixing tolerance and the remaining 380 samples, which were considered redundant for calibration, were used for validation. The calibration model was developed by the CR using a chemometrics software, PLS-Toolbox (v. 1.5, Eigenvector Research, Inc., Manson, WA) with the MATLAB software package (v. 5.0, The MathWorks, Inc., Natick, MA). In CR methods, an independent variable matrix X is modified so that PLS could develop a model that is more accurate and precise. Using singular value decomposition, the X can be transformed into $X = USV^T$, where U and V are orthogonal matrices, S is a diagonal matrix, and T means transposed. Modification of S results in a change in the variance in X. In CR, the S is modified to S^m by taking the desired power m. When the power $m > 1$, variables of the modified matrix of X (X^m) have different relative variances. The variables with high variances in X will have higher relative variance in X^m, while the variables with low variances in X will have lower relative variance in X^m. When $m = 1$, no change in variance will occur in X. When $m = 0$, all the variables in X^m will have the same variance. PLS develops a model based on variance along with correlation, when m is very large; therefore, the CR converges to PCR that develops a model based on the variance of independent variables. When $m = 0$, the CR converges to MLR. In continuum regression, the optimum m and number of latent variable for PLS is determined by cross-validation. Prediction model performance was evaluated by coefficient of determination (R^2) and root mean square error (RMSE) between reference and predicted values of calibration and validation sets.

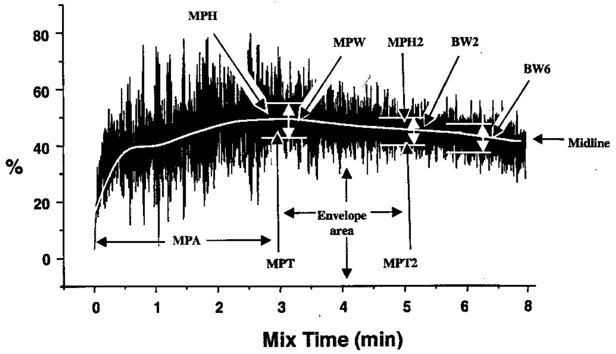

Fig. 1. Computer-analyzed mixograph parameters. MPT = midline peak time, MPH = midline peak height, MPW = midline peak width, MPA = midline peak area, BW6 = bandwidth at 6 min, MPT2 = time 2 min after MPT, MP2 = midline peak height 2 min after MPT, and BW2 = bandwidth 2 min after MPT.

Statistical Analysis

Statistical analysis was performed using SAS (v. 6.11, SAS Institute, Cary, NC).

TABLE I
Ranges and Means (n = 642) of Flour Protein Content, Baking, and Mixograph Parameters

Variables	Mean	SD[a]	Min.	Max.
Protein content (%)[b]	12.0	1.4	8.5	16.1
Conventional mixograph parameters				
Water absorption (%)[b]	65.5	1.8	59.1	72.0
Mix time (min)	3.6	0.7	1.9	6.0
Tolerance score[c]	3.2	1.1	0	5
Computer-analyzed mixograph parameters				
Midline peak				
Time (min, MPT)	4.0	0.8	2.2	6.0
Height	43.0	3.9	29.1	54.3
Width	14.0	2.9	6.1	30.7
Area	135.6	25.4	71.8	211.6
Midline left slope	4.8	2.7	–0.3	14.1
Midline right slope	–1.8	0.9	–11.3	1.0
Band height 2 min after MPT	38.1	7.4	6.5	48.3
Bandwidth 2 min after MPT	10.5	2.9	4.4	28.8
Bandwidth at 6 min	9.9	2.6	3.2	21.7
Envelope right slope	–1.8	0.8	–4.9	0.5
Envelope peak area	23.7	4.4	14.4	40.6
Baking parameters				
Water absorption (%)[b]	66.2	2.0	59.9	72.2
Bake mix time (min)	4.5	1.2	2.1	9.4
Loaf volume (cm^3)	873	95	615	1,122
Crumb grain score[c]	3.1	0.9	0	5

[a] Standard deviation.

[b] On a 14% flour moisture basis.

[c] Score on 7-point scale where 0 = unsatisfactory, 4 = satisfactory, and 6 = outstanding.

TABLE II
Simple Linear Correlation Coefficients Between Conventional and Computer-Analyzed Objective Mixograph Parameters (n = 642)[a]

	Conventional Parameters	
Computer-Analyzed Parameters	Mix Time (min)	Tolerance
Midline peak time (MPT)	0.89	0.64
Midline peak area (MPA)	0.85	0.70
Bandwidth 2 min after MPT (BW2)	0.42	0.65
Bandwidth at 6 min (BW6)	0.63	0.81
Envelope right slope (ERS)	0.59	0.51

[a] Correlation coefficients are significant at $P < 0.1\%$.

RESULTS AND DISCUSSION

Means and Ranges of Mixograph and Baking Parameters

Flour protein content (PC) was 8.5–16.1% with a mean value of 12.0% on a 14% flour mb as shown in Table I. Flour ash content (AC) had a mean value of 0.47% (14% flour mb) with a standard deviation of 0.05. Mixograph water absorption and mix time were 59.1–72.0% and 1.9–6.0 min, respectively. Mixing tolerance score, which indicates stability to overmixing, showed a mean value of 3.2 with a standard deviation of 1.1.

Among computer-analyzed mixograph parameters, MPT is considered to replace the conventional mixograph mixing time. The MPT was 2.2–6.0 min, which was similar to that of conventional mixing time. However, computer-analyzed MPT showed generally higher values than conventional mixing times.

Bake water absorption, bake mixing time, and loaf volume ranges were 59.9–72.2% (14% flour mb), 2.1–9.4 (min), and 615–1,122 cm^3, respectively (Table I). The loaf volumes showed a larger variation than that of hard winter wheat cultivars studied by Ohm et al (1998), probably because of the inclusion of breeding lines grown in wider regions in this sample set.

Correlations Between Mixograph and Baking Parameters

The correlation coefficients (r) between conventional and computer-analyzed mixograph parameters are summarized in Table II. Conventional mixograph mixing time showed significant correlation with MPT. Linear regression analysis showed $R^2 = 0.79$ ($r = 0.89$, $n = 642$) with RMSE = 0.31 between MPT and conventional mixograph mixing time. Conventional mixograph mixing time also significantly correlated to MPA, BW2, and BW6. Mixing tolerance score, obtained subjectively by human expert, showed the highest correlation with BW6 among computer-analyzed mixograph parameters, with $r = 0.81$ ($P < 0.1\%$, $n = 642$). Mixing tolerance score also had significant correlations with MPT, MPA, BW2, and ERS (Table II). This result supports Ohm and Chung (1999), who reported that BW6 could be a good parameter to evaluate mixing tolerance.

TABLE III
Simple Linear Correlation Coefficients (r) Between Mixograph and Baking Parameters ($n = 642$)

Quality Parameters[a]	r[b]
Flour protein content (%) versus	
Midline peak height (MPH)	0.74
Midline peak width (MPW)	0.58
Midline left slope (MLS)	0.56
Envelope right slope (ERS)	–0.56
Envelope peak area (EPA)	0.56
Bake absorption (%) versus	
Mixograph water absorption	0.69
Bake mix time (min) vs.	
Conventional mixograph mix time	0.81
Conventional mixing tolerance	0.72
Bandwidth at 6 min (BW6)	0.77
Midline peak area (MPA)	0.74
Midline peak time (MPT)	0.73
Bandwidth at 2 min after MPT (BW2)	0.58
Loaf volume (cm^3) vs.	
Envelope peak area (EPA)	0.58
Midline peak width (MPW)	0.54
Midline peak height (MPH)	0.53

[a] Flour protein content and bake absorption on a 14% flour moisture basis.
[b] All correlation coefficients are significant at $P < 0.1\%$.

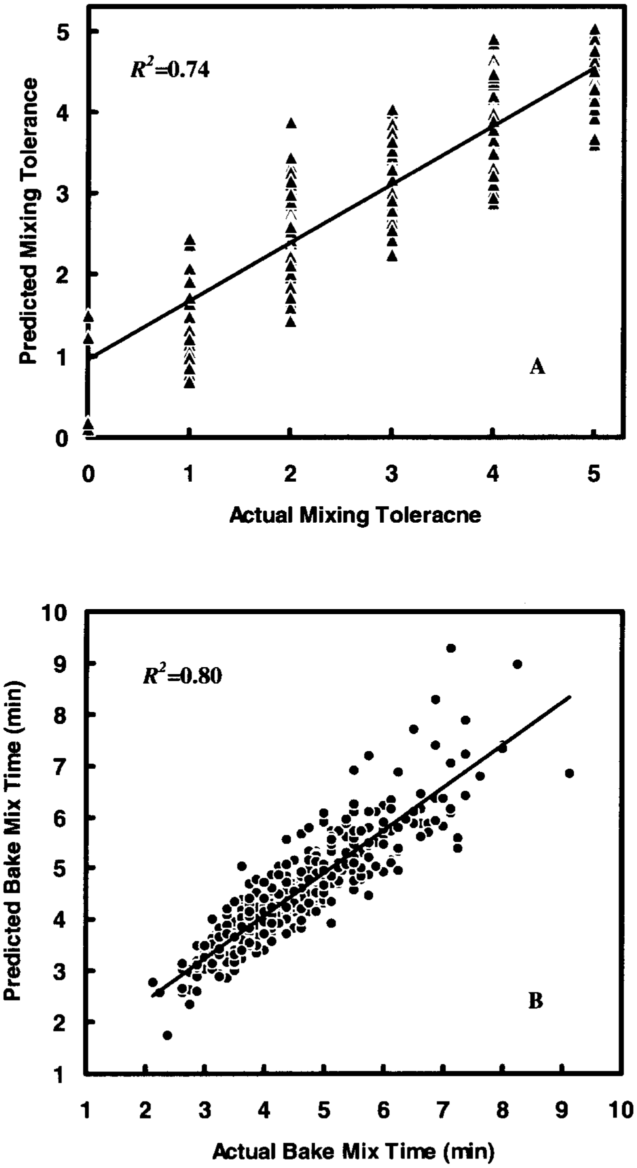

Fig. 2. Comparison of actual mixograph mixing tolerance values (**A**) and baking mixing time (**B**) with predicted values by models developed by continuum regression using computer-analyzed mixograph parameters on a validation set ($n = 380$).

TABLE IV
Results of Calibration and Validation

Parameters	No. of Latent Variables	Continuum Power (m)	Calibration ($n = 262$)		Validation ($n = 380$)	
			R^2	RMSE[a]	R^2	RMSE
Conventional mixograph parameters						
Mix time (min)	10	0.9	0.92	0.2	0.86	0.3
Tolerance	9	1.2	0.84	0.5	0.74	0.6
Bake parameters						
Water absorption (%)[b]	10	0.6	0.74	1.1	0.68	1.2
Mix time (min)	9	1.2	0.86	0.5	0.80	0.5
Loaf volume (cm^3)	5	0.4	0.65	65	0.51	61

[a] Root mean square of error.
[b] On a 14% flour moisture basis.

Baking parameters had significant correlations with both conventional and computer-analyzed mixograph parameters. Flour PC had a significant but low correlation with mixograph water absorption ($r = 0.14$, $P < 0.1\%$, $n = 642$). Flour PC had significant correlations with many computer-analyzed parameters including MPH, MPW, MLS, ERS, and EPA (Table III). The significant correlation of flour PC with MLS and ERS suggests that flour PC could influence the rate of dough developing and weakening rate, as reported previously (Johnson et al 1943; Swanson and Johnson 1943; Ohm and Chung 1999). Also, simple linear regression indicated that mixograph water absorption was not good enough to predict bake water absorption because of low R^2 value of 0.48 ($r = 0.69$) and RMSE of 1.5 ($n = 642$). Bake mix time had significant correlations with conventional mixograph mixing time and mixing tolerance as well as with some computer-analyzed parameters including BW6, MPA, MPT, and BW2. Loaf volume had a significant but low correlation with conventional mixing tolerance ($r = 0.26$, $P < 0.1\%$, $n = 642$) (data not shown) but was significantly correlated with EPA, MPW, and MPH among computerized mixograph parameters. Significant correlation of loaf volume with these computer-analyzed mixograph parameters might be influenced by PC because mixograph parameters that had significant correlations with loaf volume were also significantly correlated to flour PC. The PC has a large influence on variation in mixograph parameters within a cultivar (Swanson 1941).

Crumb grain score of bread had a significant but low correlation with flour PC ($r = 0.23$, $P < 0.1\%$, $n = 642$) EPA ($r = 0.42$, $P < 0.1\%$, $n = 642$), and mixing tolerance ($r = 0.34$, $P < 0.1\%$, $n = 642$). The r values are too low to be used for prediction.

Development of Prediction Models

Computer-analyzed mixograph parameters were used by CR to develop prediction models of mixograph mixing time, mixing tolerance, bake water absorption, bake mixing time, and bread loaf volume. The 642 flour samples were separated into calibration ($n = 262$) and validation ($n = 380$) sample sets. Calibration and validation results are summarized in Table IV.

The MPT was biased from mixograph mixing time as previously mentioned. The prediction model of mixograph mixing time was developed to adjust the bias. The ranges of mixograph mixing time for calibration and validation samples, respectively, were 1.9–6.0 min with a mean value of 3.5 min and 1.9–5.5 min with a mean value of 3.6 min. Among computer-analyzed mixograph parameters, MPT, $(\text{MPT})^2$, MLS, $(\text{MLS})^2$, MRS, $(\text{MRS})^2$, MPA, MPH2, BW2, BW6, $(\text{BW6})^2$, EPA, and ERS were used to develop prediction models. The optimum power m and number of latent variables used to develop a model by CR were 0.9 and 10, respectively (Table IV). The m value of 0.9 indicates that the prediction model is nearly a PLS model. The calibration set ($n = 262$) showed R^2 of 0.92 with RMSE of 0.2, and the validation set ($n = 380$) showed R^2 of 0.86 with RMSE of 0.3. The validation set showed a slightly lower R^2 value, because of its larger sample number and more redundant sample structure than the calibration set. The square of some parameters such as MPT, MLS, MRS, and BW6 improved performance of the prediction model.

Mixograph mixing tolerance is one of the most important parameters used by a breeder for screening early generation lines, and yet is graded subjectively by an expert. The mean values of mixing tolerance for calibration and validation samples were 2.9 with a standard deviation of 1.4, and 3.4 with a standard deviation of 0.9, respectively. When compared with the calibration set, the validation sample set showed a higher mean value but a lower standard deviation because it was more redundant. Computer-analyzed mixograph parameters used to develop the prediction model included BW6, MPT, MPA, $(\text{MRS})^2$, MLS, MPW, $(\text{MPW})^2$, BW2, ERS, and EPA. Nine latent variables and a continuum power of 1.2 were selected as optimum values to develop the model by CR. The results for the calibration set ($n = 262$) showed R^2 of 0.84 and RMSE of 0.5 (Table IV). The estimation of mixing tolerance using objective computer-analyzed mixograph parameters appears possible from model validation, which showed a lower R^2 of 0.74 and RMSE of 0.6 ($n = 380$) as shown in Fig. 2A. In comparison with the calibration set, the lower R^2 of the validation set for mixograph mixing time was also caused by a more redundant sample structure of the validation set, as pointed out in the prediction model for mixograph mixing time. At a given tolerance value, there are wide ranges of variations (Fig. 2A), due to the tolerance value scaled by a whole number. In spite of wide ranges of variations, the prediction model is very useful for wheat breeders because of screening the lines with tolerance values of 0 or 1 from those of 3 or higher.

Range of bake water absorption was 59.9–71.8% for the calibration set, and 61.3–72.2% for the validation set. Parameters used to develop a model included mixograph water absorption (MWA), $(\text{MWA})^2$, flour PC, MPA, $(\text{MPW})^2$, $(\text{MPH})^2$, $(\text{MRS})^2$, BW2, BW6, ERS, and EPA. Ten latent variables with a continuum power of 0.6 were used to develop prediction models by the CR. The R^2 values for the calibration ($n = 262$) and validation ($n = 380$) sets were 0.74 and 0.68, with RMSE of 1.1 and 1.2, respectively (Table IV).

The range of bake mixing time was 2.1–9.4 min for the calibration set, and 2.4–9.1 min for the validation set. The parameters used to develop a prediction model included MPT, MPA, MLS, $(\text{MLS})^2$, MPH2, $(\text{MPW})^2$, $(\text{MRS})^2$, BW2, $(\text{BW2})^2$, BW6, EPA, ERS, and $(\text{ERS})^2$. CR used nine latent variables with a continuum power of 1.2 to develop the prediction model. The R^2 values of the calibration ($n = 262$) and validation ($n = 380$) sets were 0.86 and 0.80, and RMSE values were 0.5 and 0.5, respectively. This result suggested baking mixing time could be predicted using computer-analyzed mixograph parameters (Fig. 2B).

The prediction model for loaf volume was developed using flour PC, MPH, $(\text{MPH})^2$, MPW, EPA, and $(\text{EPA})^2$. Optimum m value and number of latent parameters were 0.4 and 5, respectively. The R^2 and RMSE values for the calibration set ($n = 262$) were 0.65 and 65, respectively. The validation set ($n = 380$) showed an R^2 value of 0.51 and RMSE of 61 between reference and predicted values. The lower RMSE value for the validation set indicated that the model performed good enough to be used in quality evaluation of breeding lines even though the R^2 value was lower than that of the calibration set. The lower R^2 value of the validation set could be caused by its redundant sample structure.

SUMMARY

Mixograph parameters obtained from computer analysis can be used in quality evaluation of wheat breeding lines. Significant correlations occurred between conventional and computer-analyzed mixograph parameters, suggesting that computer-analyzed mixograph parameters can replace conventional parameters to eliminate human subjectivity. MPT was significantly correlated with mixograph mixing time, even though some bias existed between them. BW6 had a significant and positive correlation with mixing tolerance. Computer-analyzed mixograph parameters were also significantly correlated with baking parameters. The prediction models of mixograph and bake mixing time, bake water absorption, and bread loaf volume were developed using computer-analyzed mixograph parameters by the CR method. The models performed well enough to use in quality evaluation in wheat breeding programs and industry. CR is considered a good calibration method to develop models for wheat quality evaluation. CR showed better performance than other multivariate statistical methods such as stepwise MLR, PCR, and PLS (data not shown).

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