Relationship of Bread Quality to Kernel, Flour, and Dough Properties

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ABSTRACT

This study measured the relationship between bread quality and 49 hard red spring (HRS) or 48 hard red winter (HRW) grain, flour, and dough quality characteristics. The estimated bread quality attributes included loaf volume, bake mix time, bake water absorption, and crumb grain score. The best-fit models for loaf volume, bake mix time, and water absorption had R^2 values of 0.78–0.93 with five to eight variables. Crumb grain score was not well estimated, and had R^2 values ≈0.60. For loaf volume models, grain or flour protein content was the most important parameter included. Bake water absorption was best estimated when using mixograph water absorption, and flour or grain protein content. Bake water absorption models could generally be improved by including farinograph, mixograph, or alveograph measurements. Bake mix time was estimated best when using mixograph mix time, and models could be improved by including glutenin data. When the data set was divided into calibration and prediction sets, the loaf volume and bake mix time models still looked promising for screening samples. When including only variables that could be rapidly measured (protein content, test weight, single kernel moisture content, single kernel diameter, single kernel hardness, bulk moisture content, and dark hard and vitreous kernels), only loaf volume could be predicted with accuracies adequate for screening samples.

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Bread quality is difficult to predict from kernel, flour, or dough characteristics. In many wheat breeding programs, thousands of new lines are tested every year to find high-quality wheat for breadmaking. Most early generation lines are produced in a very limited quantity which does not allow baking tests to be conducted. Therefore, the ability to estimate bread quality using limited sample sizes will be highly beneficial to wheat breeding programs. In addition, if bread quality could be rapidly predicted from grain or flour, millers and bakers could adjust their processes to maximize profits and give consumers a consistently high-quality product.

Various researchers have attempted to predict bread quality by combining measurements made from grain, flour, or dough and combining them into prediction models. Millar (2003) used stepwise regression to develop an equation to predict loaf volume (800-g loaves, n = 181). This equation included glutenin quantity, % gliadins, flour color grade, protein content, glutenin elastic modulus, farinograph water absorption, particle size index, moisture content, and the ratio of HMW glutenins to LMW glutenins. This equation gave a standard error (SE) of 161 cm^3 for loaf volume and a R^2 = 0.39. Their equation showed that glutenin mass, protein content, and the ratio of HMW to LMW glutenins had a positive influence on loaf volume, and that flour color grade and particle size index had a negative influence on loaf volume. In color measurement Millar (2003), a higher color grade indicated more ash in the flour. However, farinograph water absorption, glutenin elastic modulus, and gliadins variables had coefficients that were opposite of what was expected, and including moisture content was difficult to explain. Their results indicate the difficulty in developing a single model to predict baking performance. Parameters not significantly influencing loaf volume were falling number, starch damage, and levels of albumins and globulins.

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Lee et al (2006) predicted loaf volume in a study using blends of the hard white wheat cultivars Betty and Trego and achieved an R^2 = 0.70. The baked loaves were from 100-g flour samples (n = 189). Their prediction equation included grain protein content, hardness index, mixograph water absorption and peak height, and break flour extraction. All variables were positively correlated to loaf volume. Although the prediction equation had a high coefficient of determination, all samples were blends of the two original samples and there was limited variability in the sample set.

Andersson et al (1994) predicted loaf volume using partial least squares regression models that included bulk density, flour and grain protein content, flour and grain falling number, flour and grain moisture content, ash content, flour yield, and farinograph and extensigraph measurements from 100 samples. Andersson et al (1994) baked loaves from 750–950 g of flour and showed that loaf volume was consistently influenced by grain and flour protein content, farinograph dough development, stability, and breakdown, and extensigraph area, peak height, and length. Flour protein content explained ≈50% of the variation in loaf volume, while the addition of all variables explained 65.4% of the variation. The models of Andersson et al (1994) predicted loaf volume with a standard error of prediction of ≈75 cm^3.

Flour protein content was shown by Graybosch et al (1993) to be the primary factor contributing to dough strength and loaf characteristics. However, they noted that no single biochemical component explained >41% of the variation in bread quality and that prediction models would require measurement of numerous components. The canonical analysis by Graybosch et al (1993) showed that loaf volume, bake water absorption, mix time, and texture were influenced by flour protein content, gliadin, glutenin, water-soluble pentosan, LMW residue protein, salt-water soluble protein, total free lipid, and total free polar lipid contents. Their analysis did not combine measurements into prediction models.

Haley et al (1999) developed a relational database where a user could access quality measurements made on samples obtained from the hard winter wheat regional testing program. A baking score could be obtained after the user input the weights assigned to quality measurements such as flour protein, mix time, bake water absorption, and loaf volume. Other researchers (Shuey et al 1975; Dick and Shuey 1976; Nolte et al 1985; Morris and Raykowski 1993) used a similar approach for evaluating the quality of other wheat classes, but databases only allowed samples to be compared with a target or to each other, and quality predictions were not made. The USDA, ARS, Grain Marketing and Production Research Center (GMPRC), Hard Winter Wheat Quality Laboratory, developed an equation to assign a hard winter wheat bake quality score using mixograph water absorption, loaf volume, crumb color, crumb grain, crumb texture, and mixograph mix time using a scale of 0–6 (Anonymous 2005a). A hard spring wheat marketing score was developed to facilitate a better understanding of wheat quality in marketing systems (Anonymous 2005b). The score was determined by using test weight, thousand kernel weight (TKW), falling number, protein content, and ash content. The resulting score was meant to provide information to buyers who are purchasing wheat with a specific end-use in mind.

The three examples mentioned above were not quality prediction systems of the final wheat products, but rather, they compared the quality of a given wheat cultivar to others provided by the same nursery or by the Wheat Quality Council to make decisions on the status of each line for further breeding stages. Some researchers have attempted to explain some variations in bread quality using various grain, flour, or dough traits and have tried to further develop predictive models. The research reported herein utilizes additional grain, flour, and dough properties that are combined into models to estimate bread quality. The specific objective of this research was to estimate bake water absorption, bake mix time, crumb grain score, and loaf volume from best-fit models that were developed using ≈50 measures of grain, flour, and dough quality parameters.

MATERIALS AND METHODS

Wheat Samples

One hundred HRW and 100 HRS wheat samples (1 kg each) from the 2002 and 2003 crop year were selected primarily based on protein content and were expected to result in a wide range of bread quality. Two HRS wheat samples were discarded from the sample set due to insect infestation. Maghirang et al (2006) reported the average and standard deviation of the quality factors for these samples and gave details on their source. Samples were obtained from the USDA Grain Inspection, Packers, and Stockyards Administration (GIPSA), Federal Grain Inspection Service (FGIS), Kansas City, MO.

Wheat Quality Analysis

There were a total of 48 HRW and 49 HRS wheat grain, flour, and dough characteristics measured as described by Maghirang et al (2006). Standard methods were used whenever an approved method was available. Seven whole-grain quality characteristics were measured including test weight (Approved Method 55-10, AACC International 2000), protein content (AACC Approved Method 39-25), moisture content as measured by the DICKEY-john GAC (Auburn, IL), TKW, single-kernel hardness (AACC Approved Method 55-31), single-kernel moisture content, and mean kernel diameter using SKCS. In addition, percentage of dark hard and vitreous kernels was measured on HRS wheat samples.

Milling and flour quality indicators measured (28 total) were flour yield (Approved Method 26-10A, AACC International 2000), wheat and flour ash content (AACC Approved Method 08-01), flour protein content (AACC Approved Method 39-11), L^*, a^*, b^* using a colorimeter (CR-300 Minolta, Osaka, Japan), geometric mean diameters of flour particles and starch granules using a laser light-scattering particle-size instrument (Beckman/Coulter 13 320, Fullerton, CA) equipped with Beckman/Coulter application software (v.4.21), polyphenol oxidase (PPO) content (AACC Approved Method 22-85), falling number (AACC Approved Method 56-81B), SDS sedimentation volume (AACC Approved Method 56-70), total wet gluten content and gluten index (AACC Approved Method 38-12), percentage and mass of insoluble, soluble, and total glutenin proteins, percentage and mass of soluble gliadin proteins, the ratios of insoluble glutenins (%)/soluble glutenins (%), insoluble glutenins (%)/total glutenins (%), and soluble gliadins (%)/total glutenins (%), free lipids (%), polar lipids (%), and nonpolar lipids (%). Protein characterization used the procedure outlined by Bean et al (1998). Lipids were measured as described by Chung et al (1980), Ohm and Chung (1999), and Hubbard et al (2004).

The 13 dough properties were evaluated using the mixograph (Approved Method 54-40A, AACC International 2000), farinograph (AACC Approved Method 54-21), and alveograph (AACC Approved Method 54-30A). Parameters measured by the mixograph were water absorption, mix time, and mixing tolerance. The parameters measured by the farinograph were water absorption, development time, stability, tolerance, and quality number. The parameters measured by the alveograph were peak height, length, swelling index, work, and configuration ratio.

Four breadmaking quality parameters for the pup loaf (100 g of flour) straight-dough procedures were measured: bake water absorption, bake mix time, crumb grain score, and loaf volume (Approved Method 10-10B, AACC International 2000). The determination of optimum mixing time is as described by Finney (1984).

Data Analyses

Maghirang et al (2006) showed that HRS wheat quality was significantly different from HRW wheat, even at similar protein content ranges. The two classes were modeled separately in this research. Regression models were developed using the Statistical Analysis System (SAS Institute, Cary, NC) Proc REG procedure with the MAXR selection. The Mallows Cp statistic (Martens and Naes 1989) was also used to evaluate models. A Cp value larger than the number of variables in the model indicates that the model will have a bias and Cp values should be about equal to the number of variables in the model or be negative. In addition, all combinations of variables that gave predictions with $R^2 > 0.70$ were calculated using the PROC REG procedures with the RSQUARE selection. Four HRW samples had missing data for TKW, two samples had missing alveograph measurements, and one sample had missing flour particle size data. Thus, 93 samples were included in the HRW models. For HRS wheat models, six samples had missing TKW data, one had missing protein quality data, and one had missing alveograph data. Those samples were eliminated from the analyses, resulting in data from 90 HRS wheat samples used in the models.

Additional models were developed using parameters that could be measured rapidly using instrumentation in field locations. These parameters included test weight, grain protein content, single kernel hardness and diameter, moisture content, and TKW for HRW and HRS wheat. The percentage of dark hard and vitreous kernels was included in the HRS wheat models. Dowell et al (2006) attempted to rapidly predict all flour, dough, and bread quality measurements used in this study by NIRS of whole kernels but none of these parameters could be predicted independently of their relationship with protein content.

The HRS samples had higher average protein content than the HRW samples (14.6 vs. 12.6%) (Maghirang et al 2006). In an attempt to remove any bias caused by protein content differences from our analyses, additional models were developed which included only samples in the 11.4–15.8% protein content range. These models included 75 HRS and 73 HRW samples.

The INFLUENCE option in the Proc REG procedure was used to measure the influence of each sample on the prediction models by calculating the studentized residual (RSTUDENT). Samples with an RSTUDENT greater than two were deleted from the analysis and compared with results with all samples included in the models.

Calibration models were developed from 80% of the data and used to predict the remaining samples. The prediction set was selected by removing every fifth sample from the data set. This resulted in 74 calibration set samples and 19 prediction set samples for HRW wheat, and 72 calibration set samples and 18 prediction set samples for HRS wheat.

RESULTS AND DISCUSSION

Loaf Volume of HRW Wheat Flour

When all 48 variables were included in the regression analysis, the best estimate of loaf volume ($R^2 = 0.91$, SE = 27.5 cm^3) was with a seven-variable model. The seven variables that made a significant ($P \leq 0.05$) contribution to the model were grain protein content, farinograph absorption, farinograph stability, flour particle size, test weight, TKW, and falling number (Table I). Some measure of protein quality, as measured by the farinograph or protein composition, was significant in all HRW wheat models containing more than one variable. Farinograph absorption is a measure of the water carrying capacity of the flour and is influenced by protein content (Preston and Kilbom 1984). Farinograph stability is a measure of tolerance to over- or under-mixing and is related to the overall quality of the protein. The farinograph quality number that was used in models with two, three, four, or six variables is a measure of the dough's ability to retain its structure with time during mixing. Other measures of gliadins, insoluble or total glutenins, and total gluten were significant in some models with two or three variables. The falling number, which had a minimum value of 278 sec for HRW and 209 sec for HRS wheat, was also included in some models. The falling number is a measure of α-amylase activity that can be influenced by starch damage. This is the principal enzyme responsible for reducing the long chains of starch in the endosperm into simple sugar units that are useable by the yeast for fermentation. The conversion of starch to maltose and other yeast-fermentable sugars is critical during the breadbaking process. High α-amylase activity results in a decrease in absorption capacity, a slackening of dough consistency, and the development of stickier dough, affecting loaf volume.

When only one variable was used, equations that used grain or flour protein content each predicted loaf volumes with an $R^2 \approx 0.84$ and an SE ≈ 35 cm^3 (Table I). This similarity between flour and grain protein content was expected because flour and grain protein content were highly correlated ($r = 0.99$). For all subsequent multivariable models, models containing grain protein content generally had R^2 values ≈0.01 greater and SE values ≈1 cm^3 less than those achieved when models containing flour protein content. Equations that used other characteristics such as total wet gluten content, mixograph water absorption, and quantities of

TABLE I
Hard Red Winter Wheat Loaf Volume Models

No. Variables[a]	Variables Selected	R^2	SE (cm^3)
1	Grain protein content	0.84	34.4
1	Flour protein content	0.84	34.8
2	Grain protein content + either farinograph absorption, farinograph development time, or farinograph quality number	0.86	33.0
2	Insoluble or total glutenins (mg) + either insoluble glutenins (%), gliadins (%), gliadins/total glutenins, or farinograph absorption	0.85	34.0
2	Grain protein content + test weight or total gluten	0.85	33.8
3	Grain protein content + farinograph absorption + either farinograph stability, farinograph quality number, farinograph development time, or (–) flour geometric mean diameter, alveograph configuration ratio, gluten index, or test weight	0.88	31.0
3	Farinograph absorption + insoluble or total glutenins (mg) + farinograph stability, alveograph configuration ratio, farinograph quality number, or gliadins (%).	0.87	32.0
4	Grain protein content + farinograph absorption + either (–) flour geometric diameter or test weight + either farinograph stability, farinograph quality number, or farinograph development time	0.89	30.0
5	Grain protein content + farinograph absorption + farinograph stability + test weight – flour geometric mean diameter	0.90	28.8
6	Grain protein content + farinograph absorption + farinograph stability + test weight – flour geometric mean diameter – either single kernel diameter or thousand kernel weight	0.90	27.9
6	Grain protein content + farinograph absorption + farinograph stability – flour geometric mean diameter + falling number + either PPO, test weight, or single kernel moisture content	0.90	28.3
6	Grain protein content + farinograph absorption – flour geometric mean diameter + test weight – thousand kernel weight + farinograph quality number	0.90	28.5
7	Grain protein content + farinograph absorption + farinograph stability + test weight – flour geometric mean diameter – thousand kernel weight + falling number	0.91	27.5

[a] All variables in models reported were significant at $P < 0.05$.

TABLE II
Correlations (r) between Breadmaking Quality Parameters of Hard Red Winter Wheat and Flour and Dough Characteristics

Variables[a]	Bake Water Absorption	Bake Mix Time	Loaf Volume
Loaf volume	0.75	. . .	. . .
Grain protein content, %	0.72	. . .	0.92
Flour protein content, %	0.73	. . .	0.91
SDS volume, cm^3	. . .	. . .	0.76
Total gluten content, %	0.75	. . .	0.90
Insoluble glutenins, mg	. . .	. . .	0.86
Soluble glutenins, mg	. . .	. . .	0.79
Total glutenins, mg	. . .	. . .	0.90
Gliadins, mg	. . .	. . .	0.86
Mixograph water absorption, %	0.75	. . .	0.89
Mixograph mix time, min	. . .	0.83	. . .
Farinograph absorption, %	. . .	. . .	0.77
Alveograph length	0.71	. . .	0.77
Alveograph swelling index	0.70	. . .	0.78
Alveograph work	0.75	. . .	0.80

[a] Only variables with $r > 0.7$ are included.

gliadins, total glutenins, or insoluble glutenins each predicted loaf volumes with an $r^2 > 0.73$ ($r > 0.85$) (Table II). The ability of these equations to predict loaf volume was likely due to the high correlation ($r \geq 0.93$) of the variables to grain and flour protein content.

When two-, three-, four-, five-, or six-variable models were used, many combinations of the seven-variable model (which usually included grain protein content and farinograph measurements) resulted in models with R^2 values ranging from 0.85 to 0.90 (Table I). For two-variable models, grain protein content could be combined with test weight or dough quality measurements as determined by farinograph absorption, development time, and quality number, or total gluten content. The quantity of insoluble or total glutenins could replace protein content in these models, probably because of its high correlation ($r \geq 0.93$) to protein content. Loaf volume could generally be predicted from an equation that combined protein content with measurements of the water-carrying capacity of the flour (farinograph absorption), dough strength (farinograph development time or quality number, or glutenin content), gliadin content or total wet gluten content. Test weight was not correlated to any r factor > 0.59, but the significance of including the test weight into a two-variable model could perhaps be best explained by the correlations of test weight to kernel size and protein content. Test weight was negatively correlated to protein content ($r = -0.58$). Kernel size was positively correlated to test weight ($r = 0.57$) and to TKW ($r = 0.59$). However, Table I shows that when test weight and protein content both increased, the combination appeared to be an important predictor of loaf volume.

For three-variable models, farinograph absorption, along with either grain protein content or the mass of insoluble or total glutenins, were picked to be the first two variables in all models. The third variable was chosen from other farinograph measurements, alveograph configuration ratio, flour particle size, test weight or gluten index. Measures of protein content, absorption, and dough strength or quality were generally useful for three-variable equations. Models with four to seven variables showed little increase in prediction statistics even though variables made statistically significant contributions to the models (Table I).

Generally model variables agreed with those reported by Millar (2003), although the statistics reported herein were better than those reported by Millar (2003). The range in protein content and loaf volume reported by Millar (2003) was slightly narrower than that of the samples used herein, as reported by Maghirang et al (2006). However, the standard deviation for protein content was less than that reported herein (0.08% vs. 1.6%), and loaf volume coefficient of variation was also much less than the one reported herein (2% vs. 10%). Data used to develop our models were bet-

TABLE III
Hard Red Spring Wheat Loaf Volume Models

No. Variables[a]	Variables Selected	R^2	SE (cm^3)
1	Flour protein content	0.85	34.8
1	Grain protein content	0.83	37.0
1	Mixograph water absorption	0.78	41.3
1	Total glutenins (mg)	0.77	43.1
1	Gliadins (mg)	0.70	49.1
2	Flour protein content + gluten index	0.89	30.0
2	Flour protein content + alveograph work	0.88	31.6
2	Flour protein content + mixograph mixing tolerance	0.87	32.2
2	Insoluble glutenins (mg) or total glutenins (mg) – insoluble glutenins (%)	0.86	33.0
2	Flour protein content – total gluten	0.86	33.1
2	Flour protein content + either insoluble glutenins (mg), (–) soluble glutenins (mg or %), insoluble/total glutenins, (–) gliadins (mg), SDS sedimentation volume, farinograph stability, farinograph development time, farinograph quality number, (–) mixograph mix time, or alveograph peak height	0.85	34.0
3	Flour protein content + flour geometric mean diameter + gluten index	0.89	29.3
3	Flour protein content + gluten index + mixograph mix time	0.89	29.4
3	Gluten index – total glutenins (%) + total glutenins (mg)	0.89	29.7
4	Gluten index – insoluble glutenins (%) + insoluble glutenins (mg) – mixograph mix time	0.90	28.4
4	Gluten index – total glutenins (%) + total glutenins (mg) – mixograph mix time	0.90	28.5
4	Gluten index – total glutenins (%) + total glutenins (mg) + flour geometric mean diameter	0.90	28.8
5	Gluten index – insoluble glutenins (%) + insoluble glutenins (mg) – mixograph mix time + mixograph mixing tolerance	0.91	27.8
5	Flour protein content + flour geometric mean diameter + gluten index – mixograph mix time + mixograph mixing tolerance	0.90	28.3

[a] All variables in models reported were significant at $P < 0.05$.

TABLE IV
Correlations (r) between Breadmaking Quality Parameters of Hard Red Spring Wheat and Flour and Dough Characteristics

Variables[a]	Bake Water Absorption	Bake Mix Time	Loaf Volume
Loaf volume	0.82	· · ·	· · ·
Grain protein content, %	0.81	· · ·	0.91
Flour protein content, %	0.82	· · ·	0.92
Total gluten content, %	0.71	· · ·	0.83
Total glutenins, mg	0.82	· · ·	0.88
Insoluble glutenins, mg	0.75	· · ·	0.80
Gliadins, mg	0.70	· · ·	0.84
Mixograph water absorption, %	0.83	· · ·	0.89
Mixograph mix time, min	· · ·	0.93	· · ·
Mixograph tolerance	· · ·	0.81	· · ·
Farinograph absorption, %	0.73	· · ·	0.71
Farinograph development time, min	0.75	0.80	0.71
Farinograph stability, min	· · ·	0.73	· · ·
Alveograph work, J	· · ·	· · ·	0.76

[a] Only variables with $r > 0.7$ are included.

ter distributed across the protein content range and probably contributed to better model statistics.

When samples with RSTUDENT values >2 were deleted from the analysis, R^2 value (n = 88) increased to 0.94 and the SE was reduced to 22.8 cm^3 (data not shown). PPO content and alveograph configuration ratios replaced the test weight and the TKW in the seven-variable model in Table I to give the maximum R^2 value. However, a model forced to include test weight and TKW resulted in essentially the same prediction statistics. Eliminating samples that strongly influenced residual errors in the model did not affect variables selected in the prediction models but eliminating those samples improved model statistics. Because eliminating these samples had little influence on variables selected for the HRW model, the RSTUDENT was not calculated for HRS wheat.

When the six parameters that can be measured rapidly (test weight, single kernel hardness, single kernel diameter, grain protein content, TKW, and grain moisture content) were used in prediction models using all data, R^2 = 0.85 and SE = 34.3 cm^3. Test weight and protein content were the only significant variables in the model, and prediction statistics were about the same as when using only protein content (Table I).

Loaf Volume of HRS Wheat Flour

The best HRS wheat loaf volume models used five of the 49 variables resulting in an $R^2 \approx 0.90$ and an SE = 28 cm^3 (Table III). These models included gluten index, mixograph mix time, and mixing tolerance, and either flour protein content and geometric mean diameter of flour particles, or the mass and percentage of insoluble glutenins. Generally grain protein content could be substituted for flour protein content with a reduction in R^2 values ≈ 0.02 and an increase in the standard error of ≈2.0 cm^3. Gluten index and mixograph mix time are measures of dough strength but were measured using different techniques and were not correlated. Mixograph mix time is the time to reach optimum dough development, whereas gluten index depends on the amount of wet gluten that passes through a sieve under centrifugal force, with the stronger gluten components remaining on the sieve. Mixograph mixing tolerance is related to dough extensibility and its resistance to breakdown. Geometric mean diameter of flour particles may be related to the kernel hardness, starch damage, and amount of water that flour can absorb. Loaf volume of HRS wheat flour was predicted using variables that measure dough strength, protein quality, and flour particle size.

TABLE V
Predicting End-Use Quality When Using Only Variables That Can Be Rapidly Measured

			Calibration Set		Prediction Set	
Predicted Trait	**Class**	**Variables Selected**	**R²**	**SE**	**R²**	**SE**
Loaf volume, cm³	HRW	48.5 × grain protein content + 7.6 × test weight – 241	0.83	34.1	0.90	34.2
	HRS	49.7 × grain protein content – 4.4 × single kernel moisture content + 271.8	0.83	37.8	0.85	40.5
Bake absorption, %	HRW	0.86 × grain protein content + 0.12 × thousand kernel weight + 48.0	0.59	1.14	0.39	1.44
	HRS	0.84 × grain protein content + 53.0	0.69	1.0	0.45	1.11
Bake mix time, min	HRW	0.15 × grain protein content – 0.11 × thousand kernel weight – 0.039 × single kernel hardness + 8.0	0.29	0.69	0.31	0.82
	HRS	–0.012 × dark hard vitreous kernels (%) – 0.36 × test weight + 0.33 × single kernel moisture content – 2.4 × single kernel diameter + 30	0.64	0.88	0.43	0.95

[a] Regression coefficients are calculated using all data (HRW n = 93; HRS n = 90). Regression statistics are calculated from the calibration set model (HRW n = 74; HRS n = 72) and prediction set (HRW n = 19; HRS n = 18). Only variables that can be measured rapidly were included in models. These variables were grain protein content, test weight, thousand kernel weight, single kernel moisture content, single kernel diameter, single kernel hardness, and bulk moisture content. Additionally, dark hard and vitreous kernels were measured on HRS samples.

TABLE VI
Predicting End-Use Quality from Grain, Flour, and Dough Properties

			Calibration Set		Prediction Set	
Predicted Trait	**Class**	**Variables Selected**	***R*²**	**SE**	***R*²**	**SE**
Loaf volume, cm³	HRW	27.8 × grain protein content + 15.5 × farinograph absorption + 3.3 × farinograph stability + 10.1 × test weight – 4.5 × flour geometric mean diameter – 3.9 × thousand kernel weight + 0.06 × falling number – 681	0.90	26.7	0.91	25.9
	HRS	57.1 × flour protein content + 3.4 × flour geometric mean diameter + 5.0 × gluten index – 17.1 × mixograph time + 13.4 × mixograph tolerance - 568	0.91	27.8	0.87	28.9
Bake absorption, %	HRW	0.39 × farinograph absorption + 0.025 × alveograph length + .085 × farinograph stability + 0.092 × polar lipids – 0.47 × gliadins (mg) + 0.11 × gluten index + 2.1 × total gluten + 0.14 × starch particle size + 19.7	0.81	0.77	0.63	1.12
	HRS	0.23 × farinograph absorption + 0.10 × farinograph stability – 0.029 × farinograph tolerance + 0.71 × glutenins (mg) – 22.3 × insoluble glutenins/total glutenins – 0.06 × nonpolar lipids + 0.06 × gluten index + 0.07 × thousand kernel weight + 52.2	0.89	0.62	0.70	0.76
Bake mix time, min	HRW	0.62 × mixograph mix time + .035 × farinograph stability + 0.085 × glutenins (%) + 0.060 × gluten index + 0.20 × color *L** + 0.10 × flour protein content – 1.2 × single kernel diameter – 24.1	0.81	0.36	0.86	0.40
	HRS	0.88 × mixograph mix time + 0.0047 × farinograph quality number + 0.019 × free lipids + 0.037 × total glutenins (%) + 0.028*gluten index + 0.19 × single kernel moisture content – 0.023 × single kernel hardness – 5.7	0.95	0.35	0.87	0.42

[a] Regression coefficients are calculated using all data (HRW n = 93; HRS n = 90). Regression statistics are calculated from the calibration set model (HRW n = 74; HRS n = 72) and prediction set (HRW n = 19; HRS n = 18).

When only one variable was used to estimate the loaf volume of HRS wheat flour, then flour protein content, grain protein content, or mixograph water absorption resulted in R^2 = 0.85, 0.83, and 0.78, respectively, with SE = 34.8, 37.0, and 41.3 cm^3, respectively.

When a two-variable regression was used, along with the variables of flour protein content combined with dough strength indicators such as gluten index, total gluten content, alveograph work, mixograph mixing tolerance, and the total amount of glutenins (mg), or insoluble glutenins (mg), loaf volume was predicted with R^2 = 0.86–0.89 and with an SE of 30–33 cm^3. There were many other protein quality or dough strength measurements such as SDS sedimentation volume, farinograph, mixograph, or alveograph methods that contributed significantly to two-variable models, resulting in slightly lower R^2 and higher SE values of ≈0.85 and 34 cm^3, respectively (Table III).

For a three-variable model, gluten index could be combined with various combinations of flour protein content, geometric-mean diameter of flour particles, mixograph mix time, percentage of glutenins, or mass of glutenins, to give R^2 and SE values of

TABLE VII
Hard Red Winter Wheat Baking Water Absorption Models

No. Variables[a]	Variables Selected	R^2	SE (%)
1	Mixograph water absorption or total gluten	0.59	1.16
1	Alveograph work	0.58	1.16
1	Flour protein content	0.56	1.19
2	Farinograph absorption + alveograph length or work	0.68	1.01
3	Farinograph absorption + alveograph length + either farinograph stability, mixograph mixing tolerance, or gluten index	0.71	0.98
4	Farinograph absorption + farinograph stability + alveograph length + either mixograph mixing tolerance, polar lipids, gluten index, or – gliadins (mg)	0.73	0.94
5	Farinograph absorption + farinograph stability + alveograph length – flour protein content + color *a**	0.75	0.93
5	Farinograph absorption + farinograph stability + alveograph length + polar or nonpolar lipids + mixograph mixing tolerance or – gliadins (%)	0.75	0.93
6	Farinograph absorption + farinograph stability + alveograph length + mixograph mixing tolerance + polar lipids + starch GMD	0.76	0.91
6	Farinograph absorption + farinograph stability + alveograph length + polar lipids + color *a** – gliadins (mg)	0.76	0.91
6	Farinograph absorption + farinograph stability + alveograph length + mixograph mixing tolerance + mixograph water absorption – flour protein content	0.75	0.92
7	Farinograph absorption + farinograph stability + alveograph length + color *a** + starch GMD – gliadins (mg) + polar lipids	0.77	0.90
7	Farinograph absorption + farinograph stability + alveograph length + mixograph mixing tolerance – nonpolar lipids + free lipids + starch GMD	0.77	0.90
7	Farinograph absorption + farinograph stability + alveograph length + mixograph mixing tolerance + polar lipds – gliadins (mg) + total gluten	0.77	0.90
8	Farinograph absorption + farinograph stability + alveograph length + starch GMD + total gluten + gliadins (mg) + polar lipids + either gluten index, – color *b**, or – gliadins (mg)	0.78	0.88

[a] All variables in models reported were significant at $P < 0.05$.

TABLE VIII
Hard Red Spring Wheat Baking Water Absorption Models

No. Variables[a]	Variables Selected	R^2	SE (%)
1	Mixograph water absorption or total glutenins (mg)	0.68	0.98
1	Flour or grain protein content	0.65	1.02
2	Mixograph water absorption + either farinograph development time, farinograph quality number, or mixograph mixing tolerance	0.73–0.75	0.87–0.91
2	Farinograph absorption + either mixograph mix time or mixograph mixing tolerance	0.73	0.91
3	Farinograph absorption + mixograph mixing tolerance + either flour protein content, grain protein content, total glutenins (mg), or mixograph water absorption	0.78–0.79	0.80–0.82
3	Farinograph absorption + farinograph stability + either grain protein content or total glutenins (mg)	0.78	0.82
4	Farinograph absorption + farinograph stability + insoluble or total glutenins (mg) + either (–) insoluble/soluble glutenins, (–) insoluble/total glutenins, or soluble glutenins (%)	0.81–0.82	0.76–0.77
5	Farinograph absorption + polar lipids + gluten index + single kernel moisture content + either flour or grain protein content	0.83	0.72
5	Farinograph absorption + farinograph stability + polar or (–) nonpolar lipids + insoluble or total glutenins (mg) – insoluble/total glutenins or insoluble/soluble glutenins	0.83	0.73
6	Farinograph absorption + farinograph stability – farinograph tolerance – nonpolar lipids + insoluble glutenins (mg) – either insoluble glutenins/total glutenins or insoluble glutenins/soluble glutenins	0.85	0.70
6	Farinograph absorption + farinograph stability + polar lipids – insoluble glutenins/total glutenins + insoluble glutenins (mg) + (–) dark hard and vitreous kernels or gluten index	0.85	0.70
6	Farinograph absorption + polar lipids + gluten index + single kernel moisture content + either (–) insoluble glutenins (%) and total glutenins (mg) or grain protein content and farinograph tolerance	0.84	0.70
7	Farinograph absorption + farinograph stability + polar or (–) nonpolar lipids – insoluble glutenins/total glutenins or insoluble glutenins/soluble glutenins + insoluble glutenins (mg) or total glutenins (mg) + gluten index + either single kernel moisture content, (–) dark hard and vitreous kernels, or (–) farinograph tolerance	0.86	0.67
8	Farinograph absorption + farinograph stability + farinograph tolerance – nonpolar lipids – insoluble glutenins/total glutenins + insoluble glutenins (mg) + gluten index + thousand kernel weight	0.87	0.66
8	Farinograph stability + polar lipids – insoluble glutenins/soluble glutenins + total glutenins (mg) + gluten index + flour geometric mean diameter – flour yield + single kernel moisture content	0.87	0.66

[a] All variables in models reported were significant at $P < 0.05$.

≈0.89 and 29 cm^3, respectively. Measures of flour strength and absorption were included in these three-variable models. Glutenins are related to the dough mixing requirements (Hoseney and Finney 1971). The equation that includes the total percentage and mass of glutenins indicates that both measurements of glutenins gave useful information for predicting loaf volume, in agreement with the correlations reported by Orth and Bushuk (1972). These two variables (percentage and mass of glutenins) are independent because the percentage of glutenin is the portion of total protein comprising glutenins. Four-variable models are shown in Table III but show little improvement over three-variable models.

Flour protein content and gluten index were significant variables in most models. Protein content was well correlated to loaf volume ($r > 0.90$, Table IV), so it is reasonable that it would be included in models. However, gluten index with a range of 78–99% had no significant correlation to any parameter measured in this study. When used alone, the gluten index predicted loaf volume with an $R^2 = 0.006$. But when combined with other measures of grain and flour quality, the gluten index significantly improved prediction accuracies.

When the seven parameters that can be measured rapidly (test weight, dark, hard and vitreous kernels, single kernel hardness, single kernel diameter, grain protein content, TKW, and grain moisture content) were used in prediction models, they resulted in $R^2 = 0.83$ and SE = 37.5 cm^3. Protein content was the only significant variable in the model when using all samples but single kernel moisture content was significant in the calibration model developed from 80% of the data (Table V).

When a calibration was developed with 80% of the HRW or HRS wheat samples and was used to predict the remaining 20% of the respective class, the prediction statistics were very similar to the statistics calculated from the calibration set (Tables V and

TABLE IX
Hard Red Winter Wheat Baking Mix Times Models

No. Variables [a]	Variables Selected	R^2	SE (min)
1	Mixograph mix time	0.69	0.48
2	Mixograph mix time + either insoluble glutenins (%), insoluble glutenins/soluble or total glutenins, farinograph stability, or (–) single kernel moisture content	0.72–0.75	0.43–0.45
3	Mixograph mix time + farinograph stability + either insoluble glutenins (%) or insoluble glutenins/soluble glutenins, or insoluble glutenins/total glutenins	0.77–0.79	0.40–0.42
3	Mixograph mix time + insoluble glutenins (mg) + either total gluten or gluten index	0.76	0.42
4	Mixograph mix time + farinograph stability – total gluten + insoluble glutenin (mg)	0.80	0.39
4	Mixograph mix time + farinograph stability – soluble glutenins (%) + insoluble glutenin/soluble glutenin	0.79	0.40
5	Mixograph mix time + farinograph stability + insoluble glutenins (mg) + color *L** – total gluten	0.81	0.38
5	Mixograph mix time + farinograph stability + insoluble glutenins (%) – single kernel diameter + either gluten index or color *L**	0.81	0.39
6	Mixograph mix time – farinograph absorption – single kernel moisture content + flour ash + gluten index + insoluble glutenins (mg)	0.82	0.38
5	Mixograph mix time + farinograph stability + insoluble glutenins (mg) + gluten index – total gluten – either thousand kernel weight or single kernel diameter	0.82	0.38
7	Mixograph mix time + farinograph stability + insoluble glutenins (mg or %) – either total gluten, grain protein content, or flour protein content + gluten index + color *L** – either single kernel diameter or test weight	0.83	0.37

[a] All variables in models reported were significant at $P < 0.05$.

TABLE X
Hard Red Spring Wheat Baking Mix Time Models

No. Variables[a]	Variables Selected	R^2	SE (min)
1	Mixograph mix time	0.87	0.48
2	Mixograph mix time + farinograph quality number	0.90	0.43
2	Mixograph mix time + either farinograph stability, (–) tolerance or development time, single kernel moisture content, SDS volume, free lipids, total glutenins (%), insoluble glutenins (mg)	0.88–0.89	0.45–0.47
3	Mixograph mix time + farinograph quality number + either single kernel moisture content, (–) mixograph water absorption, (–) gliadins (mg), (–) total gluten, (–) gliadins/total glutenins, (–) flour geometric mean diameter, (–) flour protein content or (–) grain protein content	0.91	0.42
4	Mixograph mix time + farinograph quality number + single kernel moisture content + either (–) mixograph water absorption, (–) gliadins (mg), (–) total gluten, (–) gliadins/total glutenins, (–) flour geometric mean diameter, (–) flour protein content or (–) grain protein content, gluten index, or free lipids	0.92	0.39
5	Mixograph mix time + farinograph quality number + single kernel moisture content + gluten index + either (–) single kernel hardness, free lipids, or (–) flour geometric mean diameter	0.92	0.38
6	Mixograph mix time + farinograph quality number + single kernel moisture content – single kernel hardness + free lipids + either gluten index, total glutenins (%), (–) gliadins (mg), (–) gliadins (%), or (–) gliadins/total glutenins	0.93	0.37
6	Mixograph mix time + farinograph quality number – flour protein content – flour geometric mean diameter + total glutenins (mg) + gliadins (%)	0.93	0.37
6	Mixograph mix time + farinograph quality number – grain protein content – single kernel hardness + single kernel moisture content + total glutenins (mg)	0.93	0.37
7	Mixograph mix time + farinograph quality number + free lipids + gluten index + single kernel moisture content – single kernel hardness + total glutenins (%) or gliadins/total glutenins	0.93	0.36
7	Mixograph mix time + farinograph quality number + free lipids + single kernel moisture content – single kernel hardness + gliadins/total glutenins – thousand kernel weight	0.93	0.36
7	Mixograph mix time + farinograph quality number + free lipids + single kernel moisture content – single kernel hardness + total gluten + total glutenins (mg)	0.93	0.36
7	Mixograph mix time + farinograph quality number + single kernel moisture content + total glutenins (mg) – flour protein content + gliadins (mg or %) + either (–) flour geometric mean diameter or gluten index	0.93	0.37

[a] All variables in models reported were significant at $P < 0.05$.

VI) and to the entire data set (Tables I and III) when using all variables, or when using only variables that can be rapidly measured.

Comparing Loaf-Volume Models of HRW and HRS Wheat Flours

Many of the variables identified in the loaf-volume models of HRS and HRW wheat flours did not appear to be interchangeable. For example, when the five variables identified for the best HRS wheat model were forced into an HRW wheat model, R^2 was reduced from 0.91 to 0.85 and SE increased from 27.5 to 34.7 cm^3 when compared with the best HRW wheat models. Similarly, when the best seven variables identified in the HRW wheat analysis were forced into an HRS wheat model, R^2 decreased from 0.90 to 0.85 and the SE increased from 28.3 to 35.5 cm^3. The variables identified in the HRS wheat models do not interchange well with the HRW wheat model variables, and vice versa. One reason for this lack of similarity between the models may be due to the protein content range of the two sample sets, which was 9–16% and 11–19% for HRW and HRS wheat, respectively.

For samples within a common protein content range (11.4–15.8%), only four variables were needed for both models. These variables were farinograph absorption, gluten index, the amount (mg) of total glutenins, and total glutenin composition (% of total proteins). The HRW wheat model predicted loaf volume with R^2 = 0.75 and SE = 30.9, and the HRS wheat model predicted loaf volume with R^2 = 0.85 and SE = 24.7 cm^3. A comparison of these statistics to Tables I and III shows that R^2 values decreased for models developed using the narrower protein content range when compared with models developed using the entire range. As with other models, variables that were highly correlated to those in these models could be substituted with little effect on model performance. When comparing these results to models developed using the entire protein content range, it appeared that the higher protein content of the HRS wheat samples caused different variables to be selected to predict loaf volume.

All samples were milled using common roll gaps, which resulted in a significant difference in flour yield (HRW = 65.9% vs. HRS = 67.0%) for this sample set, as reported by Maghirang et al (2006). This may have affected variables selected in the models because milling can affect dough and baking characteristics. An analysis was conducted that included only 51 HRW and 51 HRS wheat samples with flour yields of 66.5 ± 1%. Resulting loaf volume prediction models had poor Mallows Cp statistics (HRW Cp = 458 for five variables, HRS Cp = 149 for three variables), which indicate a large bias because the Cp value should be equal to or less than the number of variables in the model, probably because too few samples were included in the analyses. Although not investigated further, milling to optimal yield should be included as a variable in future tests. In addition, a measure of starch damage as described by Farrand (1969) should be included in future tests.

Bake Water Absorption

An eight-variable HRW wheat model that included farinograph absorption and stability, alveograph length, geometric mean diameter of starch granules, total gluten content, gluten index, gliadin content (mg), and polar lipid content estimated bake water absorption with R^2 = 0.78 and SE = 0.88% (Table VII). All models with less than eight variables included either mixograph or farinograph absorption, and either alveograph work or length. Mixograph water absorption was the best single variable to select and resulted in R^2 = 0.59 and SE = 1.16%. Flour protein content could estimate bake water absorption with R^2 = 0.56 and SE = 1.19%. Most other models included some combination of farinograph, alveograph, and mixograph measurements. Chung et al (1982) showed that polar lipid contents were positively correlated to loaf volume, and nonpolar lipid contents were negatively correlated to loaf volume. Because loaf volume and bake water absorption were well correlated (Table II), it is reasonable to include lipid contents in the absorption prediction models. Unfractionated total free lipid contents and fractionated polar lipid contents had a positive influence on water absorption models, whereas the nonpolar lipid contents had a negative influence on the absorption requirement (Table VII).

Eight significant variables were included in a HRS wheat model that predicted bake water absorption with R^2 = 0.87 and SE = 0.66% (Table VIII). The model included farinograph absorption, stability and tolerance values, gluten index, TKW, insoluble glutenin content (mg), the ratio of insoluble glutenins/total glutenins, and nonpolar lipid content for a negative response and polar lipid content for a positive response. For single-variable models, mixograph water absorption, flour protein content, or grain protein content predicted bake water absorption with R^2 = 0.68, 0.65, and 0.65, respectively. For two-variable models, mixograph water absorption combined with farinograph development time or quality number predicted bake water absorption with R^2 = 0.73–0.75. Most other models with up to eight variables included some combination of protein content, gluten index, some measures of lipids, farinograph stability, absorbance, and tolerance, and mixograph mixing tolerance, water absorption, or mix time.

When a calibration was developed using 80% of the HRW or HRS wheat samples and used to predict the remaining samples from their respective class, R^2 decreased from 0.78 to 0.63 for HRW and 0.87 to 0.70 for HRS wheat, and the SE increased for both classes (Tables VI, VII, and VIII). When the parameters that can be measured rapidly were used in the water absorption prediction model of HRS wheat, the result was R^2 = 0.36 and SE = 0.71% for HRW and R^2 = 0.67 and SE = 1.02% for HRS wheat when using all samples. When a calibration was developed from 80% of the samples and used to predict the remaining samples R^2 = 0.39 and SE increase to 1.44% for HRW and R^2 = 0.45 and the SE increased to 1.11% for HRS wheat (Table V).

The water absorption models of both HRW and HRS wheat flours included dough and protein quality measurements such as farinograph absorption and stability, measures of gliadins and glutenins, gluten index, and lipids. However, when the eight variables selected in the HRS wheat model were used in the HRW wheat model, R^2 = 0.68 and SE = 1.06%, which was similar to a HRW wheat model with only two variables. When the eight variables selected in the HRW wheat model were used in the HRS wheat model, R^2 = 0.80 and SE = 0.81%, which was similar to a HRS wheat model with only three variables.

When the protein content range was restricted to a common range for both HRS and HRW wheat (11.4–15.8%), little change in the variables selected for either the HRW wheat or HRS wheat models was seen (data not shown). Higher protein content range in the HRS wheat did not affect the variables selected to predict water absorption.

Crumb Grain

The crumb grain score of bread from HRW wheat flour was predicted only with R^2 = 0.65 and SE = 0.42. Some measure of flour color (L^*, a^*, or b^*) was included in most models, regardless of the number of factors but further results were not reported due to the poor R^2 values. A crumb grain score model of HRS wheat flour bread with eight significant variables predicted crumb grain score with R^2 = 0.56 and SE = 0.45. The model included grain moisture, flour protein, PPO, total gluten, and free lipid contents, mixograph time and tolerance, and alveograph configuration ratio. Because these models were very poor, no further analysis is reported.

Bake Mix Time

For the HRW wheat flour breads, a seven-variable model that included mixograph mix time, farinograph stability, insoluble glutenin content or composition (mg or %), gluten index, color L^*, either single kernel diameter or test weight, and either total gluten content, grain protein content, or flour protein content, predicted the bake mix time with an $R^2 = 0.83$ and SE = 0.37 min (Table IX). Mixograph mix time alone predicted bake mix time with $R^2 = 0.69$ and SE = 0.48 min and was selected in all models.

For the HRS wheat flour breads, bake mix time was predicted with $R^2 = 0.93$ and SE = 0.36 min when using seven significant variables (Table X). The variables selected were mixograph mix time, farinograph quality number, free lipid content, gluten index, and single kernel moisture content, single kernel hardness, and either total glutenin composition (%) or the ratio of gliadins to total glutenins as the positive variables and single kernel hardness as a negative variable. When only one variable was selected, mixograph mix time predicted bake mix time with $R^2 = 0.88$ and SE = 0.48 min, and mixograph mix time was important in all models. Mixograph mixing tolerance and water absorption and flour particle size were important in some models.

When the seven variables identified in the HRS wheat model were forced into the HRW wheat model, R^2 decreased from 0.83 to 0.77 and SE increased from 0.37 to 0.43 min. When the seven variables identified in the HRW wheat model were forced into the HRS wheat model, R^2 reduced from 0.93 to 0.89 and SE increased from 0.37 to 0.46 min.

When the protein content range was restricted to a common range for HRS and HRW wheat (11.4–15.8%), there was little change in variables selected for the models (data not shown). HRS wheat flour with higher protein content did not affect the variables selected for estimating bake mix time.

When a calibration developed using 80% of the samples was used to predict the remaining HRS or HRW samples, R^2 and SE were similar to the statistics when all samples were used (Tables VI, IX, and X). When the six HRW and seven HRS parameters that can be measured rapidly were used in bake mix time models, R^2 values decreased ≈50% and SE values increased about twofold (Table V vs. Tables VI, IX, and X).

CONCLUSIONS

Forty-nine HRS and 48 HRW grain, flour, and dough quality measurements were combined into models to predict bread quality. Loaf volume and baking mix time, and water absorption could be predicted with R^2 of 0.78–0.93, and almost all quality measurements significantly contributed to one or more of these models. The measurements that were not significant in any models were wheat ash content, alveograph swelling index, and the ratio of soluble glutenins to total glutenins. The measurements that were common in at least one model each for HRW and HRS wheat loaf volume, bake water-absorption, and mix-time models were grain and flour protein contents and gluten index. Other measurements that were common in many models were total gluten content, insoluble and total glutenin contents, and farinograph stability. Crumb grain was not predicted well using any model.

For loaf volume prediction models, grain or flour protein content was the most important term to be included but the model could be improved slightly by adding measures of dough strength, absorption, protein quality, or viscoelastic properties. Bake water absorption was predicted best when using mixograph absorption, flour protein content, or grain protein content. Bake water absorption models could generally be improved by including farinograph, mixograph, or alveograph measurements. Bake mix time was predicted best when using mixograph mix time, and models could be improved with glutenin measurements. Many other grain, flour, and dough quality measurements could be added to these models, but with only slight improvement in prediction statistics.

When the sample set was divided into calibration and prediction sets and using calibration equations with five to seven terms, loaf volume and bake mix time models showed promise for predicting end-use quality factors with accuracies adequate for screening samples for breeding programs. Bake absorption models did not perform well when divided into calibration and prediction sets.

When only variables that can be rapidly measured were included in calibration models and used to predict end-use quality, only loaf volume could be predicted with accuracies adequate for screening when using models that included protein content and test weight for HRW wheat, or protein content and single kernel moisture content for HRS wheat.

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