Multivariate Analysis as a Tool to Predict Bread Volume from Mixogram Parameters

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ABSTRACT

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We have shown that the baking quality expressed as bread volume of 21 different wheat cultivars can be predicted with 91% explained variance. A 35-g mixograph was instrumented and interfaced to a computer for data acquisition. The obtained mixograms were evaluated with a data processing program extracting 12 parameters from each mixogram. The results were correlated to bread volume with multivariate partial least squares analysis. Five mixogram parameters were found optimal. One parameter, buildup, the difference between the mixing torque at optimum dough development and the mixing torque after the water absorption, was found especially important as it alone explained 77.9% of the variation in bread volume. Including the protein content among the five mixogram parameters resulted in a small increase from 90.9 to 92.8% of explained variation in bread volume. The protein content alone explained 55.0% of the variation in bread volume.

Protein content is used as a quick estimate of wheat quality. Test baking is, however, still the only reliable method for determining the breadmaking performance of wheat flour. Test baking is time consuming and demands rather large amounts of flour so it is of interest to find adequate methods that requires less time and less flour.

Mixing of flour and water, and possibly additives, is necessary when a dough is prepared for breadbaking. This process has three important functions: to achieve a homogeneous dough, to obtain an elastic network of gluten proteins with the ability to retain gas, and to occlude air that forms nuclei for the gas cells.

The mixograph is an instrument that performs measurements on the dough during the mixing action. The mixograph was developed by Swanson and Working (1933) and is still one of the most widely used instruments for physical dough testing. It was accepted in 1961 by the American Association of Cereal Chemists as an official method for dough testing and has only been slightly altered since then (AACC 1995). Parameters from the mixogram are used to classify wheat and to predict properties in the finished product. The mixogram characteristics are dependent on the changes of the plastic, elastic, and viscolelastic properties of the dough during the mixing (Kunerth and D'Appolonia 1985). In the initial phase, water is brought into contact with the flour particles. The mixing action helps to break down the particles by rubbing them against the pins and the walls of the mixer bowl and facilitates water absorption by the starch and protein. In the next phase, the gluten proteins are oriented in the dough by the folding and stretching action of the mixing pins, and the dough begins to develop. The mixing curve then reaches a peak where the dough is fully developed. Further mixing will lead to a breakdown of the dough (Kilborn and Tipples 1972, Kunerth and D'Appolonia 1985, Hoseney 1994).

The evaluation of the mixogram data is done manually from the strip chart, which is a time-consuming and subjective method. A computer-aided data acquisition would certainly shorten this time and improve the evaluation method. There are many examples in the literature of such work (Rubenthaler et al 1986, Gras et al 1990, Navickis et al 1990, Stearns et al 1990). There are also several examples in the literature of attempts to predict dough quality by mixogram evaluations (Johnson et al 1943, Sibbitt et al 1953, Finney et al 1972, Finney 1989, Buckley et al 1990, Gras et al 1992).

In this study, a 35-g mixograph was used to study the mixing characteristics of 21 different wheat cultivars. The mechanical torque measuring device was exchanged for an electronic device, and the mixing torque data were collected by computer. A data processing program extracted 12 different parameters from which most of the features of the mixogram could be reconstructed. Different combinations of these 12 parameters were evaluated by means of multivariate statistical methods to find the parameter combination that best described the variation in bread volume of the 21 wheat cultivars. The bread volume varied between 622 and 1,190 ml, with a mean value of 927 ml. The correlation between the protein content and bread volume for the 21 wheat cultivars was also studied.

MATERIALS AND METHODS

Flours

Twenty-one winter and spring wheat cultivars (1992 and 1994 harvests) differing pronouncedly in protein content and protein quality were supplied by Skånska Lantmännen, Malmö, Sweden, and by Svalöf Weibull AB, Landskrona, Sweden. Wheat kernels were milled and analyzed for protein and moisture contents (ICC 1960). The different cultivars are presented in Table I.

Baking Procedure

The flours were test baked by Svenska Cereallaboratoriet AB, Svalöv, Sweden. The test baking was performed (Olered 1979) in triplicates with a standard deviation of <3.5%. The ingredients were 230 g of flour, 125 g of dough liquid, 4% yeast, 0.95% NaCl, 1.25% sugar, 1% fat, and ascorbic acid (100 ppm to winter wheats and 200 ppm to spring wheats). A farinograph with a 300-g bowl was used as dough mixer. Flour (180 g) of was poured into the bowl and mixed for a few seconds before the dough liquid (including all additives) was added. Then within the first 2 min, more flour was added until a consistency of 400 BU was reached. The doughs were mixed for 5 min at 90 rpm and 30°C. After mixing, the dough was fermented for 60 min at 60% rh and 35°C. The dough was then divided and weighed into three 100-g pieces which were rounded, placed in pans, and proofed for 80 min at 85% rh and 35°C. The breads were baked at 220°C for 20 min and were then allowed to rest for 2 hr. Volume was measured with rapeseed displacement.

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Mixograph

Mixing of the doughs. The doughs were mixed according to approved mixograph standards (AACC 1995) for 10 min at 25°C. Water absorption was estimated according to farinograph standards for seven of the flours (AACC 1995). Single mixograph measurements were made for these seven flours due to limited amounts of flour. Water absorption for the other 14 were estimated according to Table II. Mixograph measurements were made in duplicates for these latter 14 cultivars, which resulted in a total of 35 mixograms.

Modification of the mixograph. The standard 35-g mixograph design (National Manufacturing Division, TMCO, Lincoln, NE) uses a soft spring to counterbalance the mixing torque, which results in a rather large angular deflection of the lever arm. This provides a direct pen recording on a strip chart.

We modified the mixograph with all the mechanical parts, electronics, and Windows software that were needed. (Bohlin Reologi AB, Öved 19,S-275 94 Sjöbo, Sweden). The lever was attached to a stiff double spring at its end (Fig. 1). The stiffness of the spring was such that a torque corresponding to a full-scale reading on the strip chart recorder now produced a deflection of 1 mm at the position of a linear variable differential transformer. This small deflection resulted in the mixing bowl being virtually fixed during the mixing process. Because this system was nearly undamped, it showed pronounced resonance at frequencies that were excited by the mixing transients. This was addressed by introducing a damping element, consisting of a metal plate on the lever immersed in a stationary rectangular slit filled with 10 P silicone oil.

TABLE I
Protein Content, Water Absorption, and Baking Results for the Flours

Flour[a–d]	Abbreviation	Protein (%)[e]	Water Absorption[f,g]	Bread Volume (ml)
Kosack[b]	Kos	11.1	58.2[f]	814
Feeding[b]	Feed	8.8	55.9[f]	654
Rouquin[d]	Rouq	12.8	52.9[f]	884
Sport[a]	Spo92	12.3	64.2[f]	1,124
Prairie[b]	Pra	12.5	65.2[f]	897
Prego[c]	Pre	9.0	53.7[f]	622
Dragon[a]	Dra92	12.5	57.0[f]	1,066
Nova[b]	No	11.4	56.0[g]	662
Mp[b]	Mp	12.4	58.0[g]	884
Hp[b]	Hp	13.4	60.0[g]	846
Dragon[a]	Dra94	14.4	64.0[g]	1,024
Sport[a]	Spo94	16.8	64.0[g]	1,190
Tjalve[a]	Tja	13.8	64.0[g]	930
Thasos[a]	Tha	13.7	64.0[g]	851
Curry[a]	Cu	13.1	64.0[g]	1,019
Avans[a]	Av	13.7	64.0[g]	965
SW 32470[a]	SW32	13.3	64.0[g]	948
SW 33177[a]	SW331	13.5	64.0[g]	1,095
SW 33294[a]	SW332	13.1	64.0[g]	1,043
SW 34254[a]	SW34	13.2	64.0[g]	1,090
St 902016[a]	St90	12.5	62.0[g]	856

[a] Spring wheat.
[b] Winter wheat.
[c] Triticale.
[d] Cross between a spelt wheat (*Triticum spelta*) and an ordinary wheat.
[e] N × 5.7.
[f] Farinograph standard according to approved Method 54-21. (AACC 1995).
[g] Based on protein content (see Table II).

TABLE II
Water Absorption (14% mc) Based on Protein Content for Scandinavian Wheat Cultivars

	Protein (%)				
	<8.6	8.6–10.0	10.1–11.5	11.6–13.0	>13.0
Winter wheats	52.0	54.0	56.0	58.0	60.0
Spring wheats	56.0	58.0	60.0	62.0	64.0

Data Processing

The first step in obtaining the mixing torque data is to sample the mixing torque 50 times per second and to calculate an average value and a root mean square value of the torque at 1-sec intervals. These two values of mixing torque correspond to the center and the width of the mixing curve. For a mixing time of 10 min, for example, we obtain 600 values for center and width of the mixing curve as stored data.

When the torque data are entered into the data processing plot, they are plotted in analogy with the pen recorder as a vertical line for each sampled data set, running from the lowest value (center height minus half width) to the highest value (center height plus half width).

We refer to these endpoints of the vertical line as max and min. Next, a moving average is calculated on the max and min values, respectively. Each moving average is taken over 40 points (sec) and then shifted backwards 20 points. We now have smoothed data for the upper and lower bounds of the mixing curve running from 20 sec to 580 sec (a 600-sec run).The drag and drop boxes (DDB) are then placed on the max and min moving averages. T1 is put on 30 sec. The maximum of the max moving average is located, and T3 is put on that time. T2 is put on (T1+T3)/2. T5 is put on the last moving average data point. T4 is put on T3+(T5+T3)/3.

With these time settings as initial values, the DDB (A1–A5, B1–B5) are placed on the max and min moving averages, respectively (Fig. 2). Thereafter, they are dragged to the natural breakpoints and dropped. These final DDB positions are used to calculate 12 parameters from each mixogram. 1) initslope = A1/T1: the initial slope of the curve calculated for the max curve; 2) initwidth = A1–B1: the width of the curve at T1; 3) initbuildup = A2–A1: a period of slow development may be observed

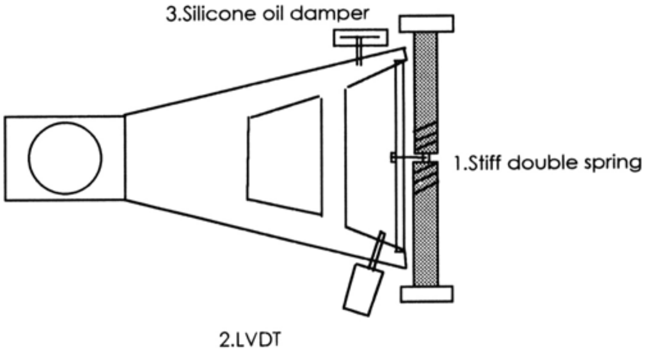

Fig. 1. Top view of the modified mixograph. LVDT = linear variable differential transducer.

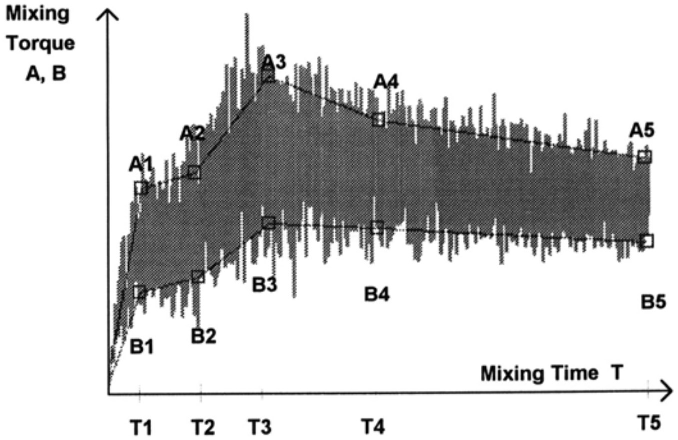

Fig. 2. Example of computer mixogram with drag and drop boxes and corresponding time settings.

between the initial fast increase in the curve due to water absorption and the main development of the dough where the increase in max torque during this period is calculated; 4) time1–2 = T2–T1: the time elapsed during initbuildup. 5) buildup = A3–A2: the increase of the max curve calculated from the end of initbuildup to the maximum height of the curve; 6) maxtime = T3: the time elapsed from the start to the time of maximum height of the curve; 7) maxwidth = A3-B3: the width of the curve at maxtime; 8) maxcenter = (A3+B3)/2: the height from the base line to the center of the curve at maxtime; 9) breakdown = A3–A4: at times beyond maxtime the curve starts to descend, often with an initially steeper slope that later levels off, breakdown is calculated for the max curve from maxtime to the point were the curve levels off; 10) residual = (A4–B4)/(A3–B3): the ratio between the width of the curve at T4 and the width of the curve at maxtime, T3; 11) areabelow = area enclosed by the baseline and the min curve (0,B1,..,B5); 12) areawithin = the area enclosed by the max curve (0,A1,..,A5) and the min curve (0,B1,..,B5).

The mixing process can be divided in three stages: 1) water absorption (parameters 1–4), 2) dough development (parameters 5–8), and 3) breakdown of the dough (parameters 9–10). The last two parameters (parameters 11–12) reflect the mixing curve as a whole.

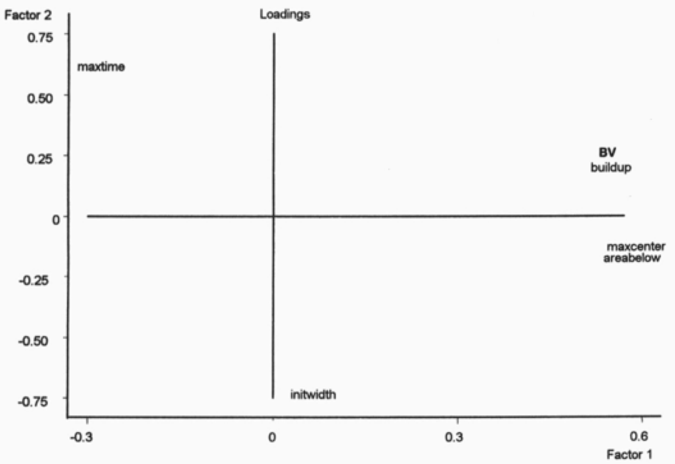

Fig. 3. Loading plot of two partial least squares factors describing the relationships between five mixogram variables and the bread volume. Object name is centered on the actual point.

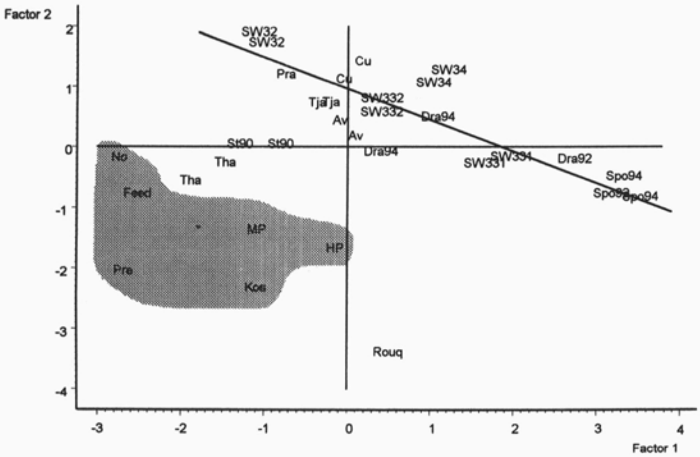

Fig. 4. Score plot of two partial least squares factors showing the distribution of different wheat varieties. Object name is centered on the actual point.

Statistical Analysis

Multivariate data analysis was used as a tool for the statistical evaluation. The point of multivariate analysis is to consider several related variables simultaneously, each considered to be equally important at the beginning of the analysis (Manly 1994). If there are correlations between the variables, it is possible to reduce the number of original variables to a small number of transformed variables. Each variable may be described as a dimension in a coordinate system. The transformation is achieved by projecting all variables onto a coordinate system with fewer dimensions.

Terminology. An object is a set of corresponding values of all measured variables. The transformed variables are called factors. The coordinates of the objects related to the factors are called scores. The coordinates of the original variables related to the factors are called loadings. Data decomposition means to extract information from one data set to make a projection model. Calibration is to make a model of the relationships between two sets of data, *X* and *Y*. Calibration set is the objects used to make a calibration model. Prediction is to use a calibration model and new *X* values to predict new *Y* values, respectively. Validation is a procedure for assessing quantitatively how well a model will work on future *X* samples or give an estimate of the modeling error. Cross-validation is a series of calibration runs using different segments of calibration objects as validation objects in each run. The size of the segments has to be specified. Test set (validation set) is the data set used to test how good the calculated model is. It may consist of entirely new objects or may be extracted from the calibration set before validation. The residual variance is a measure of how much of the variation of data that is unexplained. Leverage is a measure of how much an object or a variable influences the model, with a certain numbers of factors used in the model. The root mean square error of prediction (RMSEP) is an expression for the expected error as an absolute value, which can be directly compared to predicted *Y* values in original units. Principal component analysis (PCA) is a simple method to use for extraction of the systematic variations in a data set. When a mathematical relation between two data sets (*X* and *Y*) is needed, multivariate regression analysis is used. Partial least squares regression (PLS) performs a simultaneous and interdependent PCA decomposition in both *X* and *Y* matrices, in such a way that the information in the *Y* matrix is used directly as a guide for optimal decomposition of the *X* matrix, and then performs regression of *Y*. The algorithms used for PCA and PLS are described in Martens and Næs (1991).

To study the relationship between the mixogram parameters and the bread volume (BV) for the 21 wheat cultivars, a multivariate regression method called PLS1 in the Unscrambler program (CAMO A/S, N-7011 Trondheim, Norway) was used. Each set of mixogram parameters, referred to as the *X* variables, together with the corresponding BV, referred to as the *Y* variable, is considered as an object, resulting in 35 objects. Three of the 35 objects were considered as outliers and were excluded from the calibration set. Every single piece of data corresponding to a certain variable was divided by the standard deviation for that variable to achieve the same variance for all the variables. All variables thus had an equal participation in the modeling. The PLS model was validated by cross-validation and root mean square error of prediction (RMSEP) to verify the prediction quality of the model and to avoid overfitting.

We have described how the mixogram was processed to give 12 parameters from which the most of the features of the mixogram could be reconstructed. The aim, however, was to find only those parameters that best describe the baking quality (expressed as BV) of the 21 wheat cultivars used. This was done by reducing the number of parameters one-by-one, removing the parameter with a combination of high variance and low leverage that seemed to contribute the least to the model at hand. After each reduction, a new calibration model was made with the parameters remaining.

RESULTS AND DISCUSSION

This procedure resulted in 12 calibration models that were evaluated and compared (Bohlin et al 1985).

By comparing the 12 calibration models, we found that 1) the parameter buildup in itself explained 77.9% of the BV; 2) the calibration model including five parameters (buildup, maxtime, initwidth, areabelow, and maxcenter) was optimal and explained 90.9% of the variation in BV with two PLS factors as significant. The two factors together explained 87.7% of the total variance in the *X* variables.

The loading plot in Figure 3 shows the relationship between the five parameters and the BV, and their positions along the axis of factor 1 and 2. Factor 1 (73.2% of the total variance in the *X* variables) is interpreted as a dimension of strength, closely related to buildup, areabelow and maxcenter, which all describe the dough development. High values for these variables are related to a strong dough.

Factor 2 (14.5% of the total variance in the *X* variables) is interpreted as a water absorption dimension. The initwidt variable describes the water absorption phase and is closely related to factor 2. The maxtime variable is related to both factor 1 and factor 2, which suggests that time until maximum dough development is dependent on the water content but also on the strength of the flour.

The score plot in Figure 4 expresses the relationship between the 32 objects and the PLS factors 1 and 2. The winter wheats No, Feed, Pre, MP, Kos, and HP have negative scores for both factors 1 and 2 and are placed in the lower left in the plot. The spring wheats seem to be distributed along factor 1, from the upper left to the lower right in the plot.

The score plot and the loading plot can also be interpreted together. The objects with high scores for one particular factor also have high values on the variables with high loadings for the corresponding factor. If the score plot in Figure 4 is studied together with the loading plot in Figure 3, it can be seen that the winter wheats, along with the Triticale (Pre), are characterized by a low value of buildup and, correspondingly, a low BV. A study of the spring wheats distributed from left to right along factor 1 shows increasing values for areabelow and maxcenter together with decreasing values of maxtime, which all correspond to increasing BV.

Rouquin appears as an outlier with a high value for initwidth. It should be mentioned that Rouquin is a cross between an ordinary wheat and a line of spelt wheat. Spelt wheats have been shown to give much weaker doughs than modern wheats do (Leife 1995). To estimate the modeling error, the calibration model was evaluated with cross-validation. This resulted in an explained variance of 90.9% (as stated above) and a RMSEP of 40. The result of the prediction is shown in Figure 5, where the predicted BV is plotted against the corresponding reference value of BV.

To further evaluate the capacity of the five mixogram parameters to predict BV, eight objects were chosen and withdrawn from the calibration set by carefully studying the score plot. The eight objects were sited as far apart as possible in the score plot with the intention of covering most of the variation in as many of the variables as possible (Andersson 1993). A new PLS calibration was performed on the remaining 24 objects. Cross-validation of this new calibration model gave an explained variance in BV of 88.6%, with two factors as significant and a RMSEP of 44. A prediction was then made using the eight objects as a test set. The result of this prediction is shown in Figure 6, where BV predicted by the model are plotted against measured BV. The RMSEP value was 31 for the test set.

Because protein content is used as a quick estimate of wheat quality, it is of interest here to see how well the protein content was correlated to BV for the 21 cultivars. The BV is plotted against protein content in Figure 7. It can be seen that there are several wheats with approximately the same protein content but with large differences in BV. The obvious conclusion is that the prediction capability should be rather low. This was confirmed by

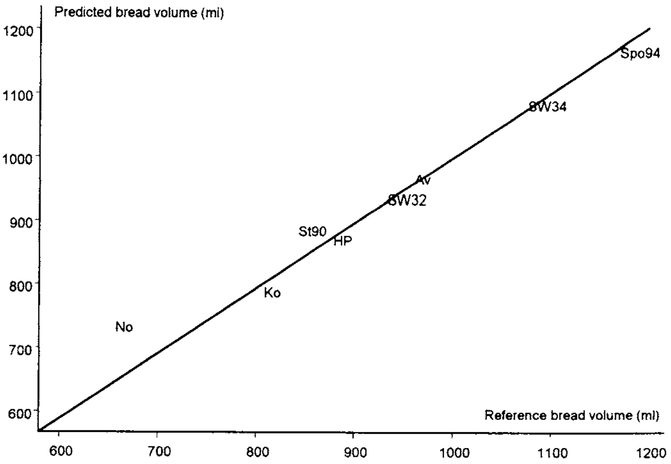

Fig. 6. Validation of 24-object model with a test set of eight objects. Estimated bread volume plotted vs. real bread volume. Object name is centered on the actual point.

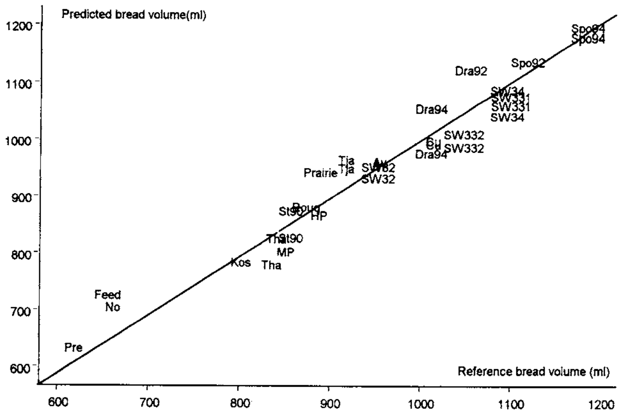

Fig. 5. Result of cross-validation of the 32-object model. Estimated bread volume plotted vs. real bread volume. Object name is centered on the actual point.

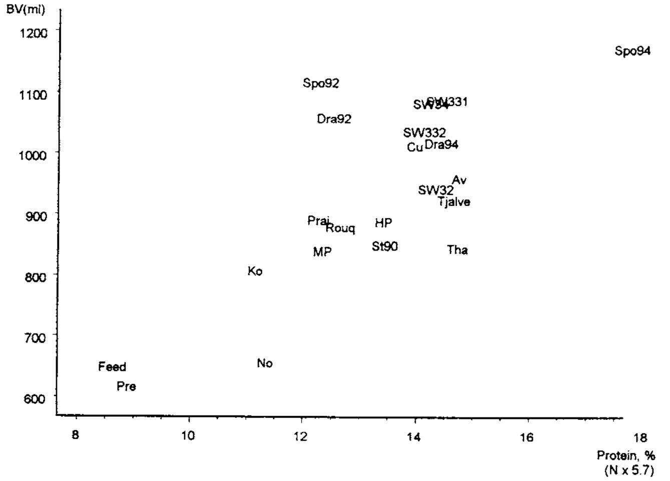

Fig. 7. Bread volume plotted vs. protein content for 21 wheat cultivars. Wheat name is centered on the actual point.

the results achieved from a PLS model, where protein alone explained only 55.0% of the variation in BV. This should be compared with the mixogram parameter buildup, which alone explained 77.9%. If a new PLS calibration was made where protein was included as an *X* variable together with the five mixogram parameters, the explained variation in BV increased from 90.9 to 92.8%.

CONCLUSIONS

Twenty-one different wheat cultivars with protein contents varying between 8.8 and 17.8 % were mixed in a 35-g mixograph interfaced to a computer for data acquisition. Twelve parameters, from which the most of the features of the mixogram could be reconstructed, were initially extracted from each mixogram. Different combinations of these 12 parameters were evaluated by means of multivariate PLS to find the parameter combination that best described the BV variation of the 21 wheat cultivars. One parameter alone, buildup, explained 77.9% of the variation in BV. Five of the mixogram parameters (buildup, maxtime, initwidth, areabelow, and maxcenter) were found optimal for the final evaluation, explaining 90.0% of the variance in BV.

Because protein content is used as a quick estimate of wheat quality, we correlated the protein content to the BV for the 21 different wheat cultivars and found 55.0% of the variation to be explained. A calibration model with the protein content added to the five mixogram parameters explained 92.8% of the variation in bread volume.

This work has shown the usefulness of multivariate analysis in visualizing differences and relationships among many different cultivars of wheat using mixogram data only. It also has shown that several parameters extracted from the mixogram can be used simultaneously in a model to predict important quality properties such as BV. The method can certainly be most useful for bakers, millers, and plant breeders. A test bakery for example, where thousands of bakings are made each year, could establish their own calibration model by running mixogram evaluations against baking tests. A calibration can either be made for each class of wheat (winter wheats, spring wheats, durum wheats, feeding wheats) or be made for a mixture of classes. The calibration model can continuously be revised and improved to make predictions increasingly adequate by including new flours in the model. With a satisfactory prediction ability, test bakings can be largely replaced by a prediction from a mixogram.

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