Use of wheat flour analytical characteristics for predicting the Simulator Mixolab measurements

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**Abstract:** - Data describing the flour analytical characteristics (wet gluten content, gluten deformation index, falling number index, ash content, moisture content, protein content) and dough rheological parameters using the Mixolab device with “Simulator” protocol were analyzed by principal component analysis and multivariate prediction models was developed. Principal component analysis (PCA) identifies that the first two principal components account for 99.81 % of the total variance for all the data sets. Significant correlations (p < 0.05 and p < 0.01) between the analytical characteristics of wheat flour and dough rheological parameters were found. The result of backward multiple regressions method related that protein content (PR) and gluten deformation index (GDI) could be used to predict Simulator Mixolab parameters water absorption (CH) and dough weakening (WE), at a 95% confidence interval.

**Key-Words:** - wheat flour, rheological properties, Mixolab, multivariate statistical analysis

**1 Introduction**

The wheat flour dough rheological properties are essential for bread making technology. It gives valuable information regarding the quality of the wheat flour, of the finished bakery products and can describe dough behavior during the technological process of bread making. The most common empirical instruments used to evaluate the rheological wheat flour dough properties are the Farinograph, Mixograph [1 - 4], Extensigraph and Alveograph [4 - 6]. The launched on the market in 2005 of a new empirical rheological instrument by Chopin Technologies Company, the Mixolab device led to new informations regarding the rheological behavior of dough during the bread making process because it allow to determine the mixing and heating properties of the wheat flour dough in one single test [7 - 10] by using its extensive “Chopin” protocol option. This device has also an additional protocol option called “Simulator” less used by researchers, a simplified one whose results are similar to Farinograph values. The difference between Farinograph measurements is that Mixolab flour mass depends on flour water absorption, reported to a fixed parameter the dough mass (75 g) in contrast to Farinograph which works with the constant flour mass (50 or 300 g). Also, another difference is that the Mixolab parameters (dough weakening, dough consistency) are recorded in real SI units (N·m) and not in Brabender arbitrary units [11]. For a better understanding of the Mixolab parameters values different researchers tried to obtain different correlations and predictive models between them and other parameters well known from different rheological devices [7, 9, 12 - 15] or the quality of the finished bakery products [7, 8, 12 - 14]. In their works the researches focused in especially on Mixolab parameters obtained with “Chopin” protocol option and very few with “Simulator” Mixolab parameters [9]. Therefore we consider that is a goal in the international literature regarding this aspect and a study on the correlations between Simulator Mixolab values and wheat flour analytical characteristics are essential for a better understanding of the Mixolab values obtained with “Simulator” protocol.
## 2 Problem Formulation

In Romania, almost all the cereal laboratories from bread making factory are using to evaluate wheat flour quality some analytical parameters like wet gluten content (WG), gluten deformation index (GDI), falling number index (FN), ash content (Ash), moisture content (Mo) and only some of them the protein content (PR). Therefore we choose these wheat flour analytical parameters to establish a series of correlation between them and the wheat flour dough rheological characteristics obtained with the Mixolab device by using the “Simulator” protocol. This fact is more necessary even more as only in Romania from its lunched on the market 12 of these rheological devices have been purchased by different bakery factories [10]. As we mentioned before, if different researchers established some correlations between Mixolab parameters obtained with “Chopin” protocol and flour analytical characteristics from our knowledge only one research study [10] established some correlations between Mixolab parameters obtained with “Simulator” protocol and flour analytical characteristics. To complete the previous research beside those parameters we used in this work and other analytical parameters like gluten deformation index (GDI), moisture content (Mo) and ash content (Ash), parameters that wasn’t used in the previous work. Also, we tried in this manuscript to predict some regression models between Simulator Mixolab parameters and wheat flour analytical characteristics fact that to our knowledge has never done before. For this purpose we used fifty commercial flours purchased from different milling companies. The analytical characteristics of the flours samples was determined according to Romanian or international standard methods: gluten deformation index (SR- No. 90) [15], moisture content (ICC-Standard Method No. 110/1), wet gluten content (ICC-Standard Method No. 106/1), ash content (ICC-Standard Method No. 104/1), falling number index (ICC- Standard Method No. 107/1) [16]. The wheat flour dough rheological properties were determined by Mixolab device (Chopin Technologies, Paris, France) using “Simulator” protocol following the international standard (ICC-Standard Method No. 173, 2008) [16]. The protocol used has the following settings: kneading speed 80 rpm, target torque 1.1 N·m, mixer temperature 30°C, dough weight 75 g, hydration water temperature 30°C, analysis time 30 min. The wheat flour dough rheological parameters obtained from the Mixolab curve using Chopin “Simulator” protocol were: flour water absorption (%) or water required for the dough to produce a torque of 1.1 N·m, mixing stability (min) or elapsed time at which the torque produced is kept at 1.1 N·m, development time (min), maximum consistency during kneading (N·m) and dough weakening (N·m) [17].

All the measurements were done in triplicates. Values of the parameters are expressed as the mean ± standard deviation to a confidence interval of 95%. Pearson’s correlation analysis and multivariate statistics techniques (principal component analysis, PCA and multiple regression analysis, MRA) were carried out using Statistical Package for Social Sciences (v.13.0, SPSS Inc., Chicago, IL, USA).

In order to analyze the interdependence among all variables (analytical characteristics of flours samples and Simulator Mixolab rheological parameters) the Principal Component Analysis (PCA) was applied. PCA is a multivariate statistical technique that can be applied to primary data to reduce the number of variables by preserving as much as possible the variance of the primary data obtained, resulting in a smaller set of variables non-correlated. The new variables, called principal components or PCs are determined, expressed as linear combinations of the primary data and it’s arranged in decreasing order of importance: the first principal component has maximum variance, while the second principal component has a variance as high as possible but less than that of the first principal component.

The method selected to test the effects of independent variables (predictor) on a single dependent variable (criterion) was multiple regression analysis (MRA). The MRA was used to determine whether the Simulator Mixolab rheological parameters of dough were functionally related to wheat flour analytical characteristics.

To build the regression model, the backward method from SPSS software was selected. By this method, building the model begins with all variables being considered in the model, and at each step the value of independent variable with the least importance is eliminated, the value that determines the smallest reduction in the Fisher test, F. Variables are eliminated step by step up to a previously established level of significance of 0.05.

The equation of multiple regression contains independent variables (Simulator Mixolab rheological parameters) and coefficients $b_i$ $(i = 0–5)$, which are calculated based on the correlation coefficient between each independent variables and the dependent variable (wheat flour analytical characteristics), their values expressing the contribution of each independent variable in estimating the dependent variable:
\[ Y = B_0 + B_1 \cdot X_1 + B_2 \cdot X_2 + \ldots + B_n \cdot X_n \] (1)

where \( B_0 \) is a constant value, \( B_i, i = 1, \ldots, n \), are the regression coefficients of the predictive model (Table 3) and \( X_1 \ldots X_n \) are the values of the independent variables. Student's t-test was used to determine the significance of each coefficient in the regression model. Fisher’s test was performed on experimental data in order to evaluate the statistical significance of the predictive models.

### 3 Problem Solution

The analytical characteristics of the wheat flours samples set the mean and range with abbreviated names are given in Table 1. The wheat flours set cover a wide range of bread making quality ranging from poor to very good.

#### Table 1. Flour analytical characteristics

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Abbreviated name</th>
<th>Mean</th>
<th>Range min.</th>
<th>Range max.</th>
<th>Std. dev.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Moisture content (%)</td>
<td>Mo</td>
<td>14.30</td>
<td>13.20</td>
<td>15.20</td>
<td>0.49</td>
</tr>
<tr>
<td>Protein content (%)</td>
<td>PR</td>
<td>14.04</td>
<td>9.30</td>
<td>16.30</td>
<td>1.86</td>
</tr>
<tr>
<td>Wet gluten content (%)</td>
<td>WG</td>
<td>26.60</td>
<td>21.60</td>
<td>30.00</td>
<td>1.92</td>
</tr>
<tr>
<td>Gluten deformation index (mm)</td>
<td>GDI</td>
<td>5.68</td>
<td>2.00</td>
<td>11.00</td>
<td>2.30</td>
</tr>
<tr>
<td>Falling Number index (s)</td>
<td>FN</td>
<td>393.45</td>
<td>198.00</td>
<td>499.00</td>
<td>89.17</td>
</tr>
<tr>
<td>Ash content (%)</td>
<td>Ash</td>
<td>0.58</td>
<td>0.50</td>
<td>0.68</td>
<td>0.04</td>
</tr>
</tbody>
</table>

The values obtained with the Chopin “Simulator” protocol are shown in Table 2.

#### Table 2. Mixolab parameters of flours samples using “Simulator” test

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Abbreviated name</th>
<th>Mean</th>
<th>Range min.</th>
<th>Range max.</th>
<th>Std. dev.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water absorption (%)</td>
<td>CH</td>
<td>58.60</td>
<td>53.80</td>
<td>64.70</td>
<td>2.33</td>
</tr>
<tr>
<td>Development time (min)</td>
<td>DT</td>
<td>2.91</td>
<td>1.08</td>
<td>8.07</td>
<td>1.84</td>
</tr>
<tr>
<td>Weakening (N·m)</td>
<td>WE</td>
<td>0.22</td>
<td>0.10</td>
<td>0.42</td>
<td>0.08</td>
</tr>
<tr>
<td>Stability (min)</td>
<td>ST</td>
<td>9.10</td>
<td>2.50</td>
<td>15.06</td>
<td>3.37</td>
</tr>
<tr>
<td>Maximum consistency during</td>
<td>CM</td>
<td>1.11</td>
<td>0.96</td>
<td>1.25</td>
<td>0.07</td>
</tr>
</tbody>
</table>

The interdependence among analytical characteristics of wheat flour dough and the Simulator Mixolab parameters curve was analyzed using Principal Component Analysis (PCA). The first two principal components (PCs) (Fig. 1) explain 99.81% of the total variance (PC1 = 99.65% and PC2 = 0.16%).

In respect to the first principal component PC1, the flour analytical parameters protein content (PR), wet gluten content (WG) and falling number (FN) are placed at the right of the graph showing the fact that between them are positive correlations. Protein content parameter is significant correlated with parameters wet gluten content and falling number with correlation coefficients values of \( r = 0.458 \) and \( r = 0.726 \), respectively at a level of significance of \( p = 0.01 \). This fact is explainable because in cereals rich in proteins (and therefore in wet gluten content) the amylolytic activity decreases due to the deactivation of \( \alpha \)-amylase which is retained by glutenin in quantities that become larger as glutenin becomes larger [9].

![Fig. 1 PCA loadings plot for flour analytical characteristics and Simulator Mixolab parameters.](image)

Symbols and definitions: \( \Delta \) - analytical characteristics of flours; \( \bigcirc \) - Simulator Mixolab rheological parameters

According to the PCA graph along to the PC1 axe we can see that parameter protein content (PR) is positive correlated with parameter stability (ST) \( (r = 0.445, p = 0.01) \), the second high placed parameter on the graph and negative correlated with parameter dough weakening (WE) \( (r = -0.296, p = 0.05) \). This fact is explainable because flour with a good quality for bread making must have a certain amount of protein content to form a uniform and stable network in wheat flour dough. Flour with a poor quality for bread making has low protein / wet gluten content with a poor quality that will form...
wheat flour dough with weak rheological properties becoming at the end of the mixing stage sticky, with a weak consistency, less elastic.

Regarding dough stability (ST) parameter we noticed that it increases simultaneously with an increase of falling number (FN) value between these parameters being a significant correlation value \( r = 0.488 \) at a level of significance \( p = 0.01 \). This can probably be attributed to the fact that the high level of \( \alpha \)-amylose to wheat flour leads to an intensification of the starch degradation process and thus of the flour maltose level \([18]\) that will exerts a hydrolytic release of water from the gluten substrate, which reduces the dough stability.

The second principal component, PC2 is correlated to the Mixolab parameters: dough stability (ST), dough development time (DT) and water absorption (CH). The parameters: CH and ST indicated a very well correlation \( (r = 0.754) \) and a moderate correlation with DT \( (r = 0.387) \), significant correlations at a level of 0.01.

The closeness of the moisture content (Mo) variable to the centre of PC shows that this parameter has an insignificant importance on wheat flour rheological properties between this parameter and the rest of the parameters taking into account in this study. Also, the Mixolab parameter maximum consistency during kneading (CM) is the second variable relatively closed to the centre of PC axes its correlations with the rest of the variables being as well insignificant.

Direct significant correlation \( (r = 0.318) \) was obtained at level of significance \( p = 0.05 \), between the parameter GDI and the Mixolab parameter curve dough weakening (WE). This fact is explainable because the gluten deformation index (given by wet gluten capacity to extend when it is left in a rest time period) is lower when the proteolytic activity of the flour decreases \([19]\) and therefore dough weakening increases.

As regards the second principal component PC2, this axe underlines the opposition between Mixolab parameter dough weakening (WE) and analytical parameters direct correlated: protein content (PR), falling number (FN), wet gluten content (WG), with which is in a negative correlations. The second principal component opposes the parameter dough weakening (WE) to the Mixolab parameters dough stability (ST), dough development time (DT) and water absorption (CH) with which also it present negative correlations. Also, we can noticed that along PC2 axe the parameters dough weakening (WE) is placed the lowest while the parameters water absorption (CH) is placed the highest. The highest placed parameter on PCA graph, water absorption (CH) is generally recognized as affected by two major factors, protein content and damaged starch \([20]\). Therefore, the increase of protein/wet gluten content will conduct to an increase of water absorption values between protein content and flour water absorption being a significant correlation value \( r = 0.330 \). Starch absorbs water even more if it is previously hydrolyzed by flour amylases especially \( \alpha \)-amylose between falling number index and water absorption being a significant correlation of \( r = 0.323 \) at a level of significance of \( p = 0.05 \). Also, a great influence on wheat flour water absorption has the quality of gluten proteins given by the wet gluten content and gluten deformation index. A flour of a poor quality for bread making which contains protein of an inferior quality will have a lower water absorption capacity than strong flour with superior rheological properties. Therefore we obtained a negative significant correlation value of \( r = -0.312 \) between Mixolab parameter water absorption and analytical parameter gluten deformation index. As well, the wheat flour dough development time is influenced by wheat flour water absorption and flour mineral content, flours of a high ash values requiring higher water absorption than the flours with a lower mineral content. A direct significant correlation was found between water absorption and parameters ash content \( (r = 0.367, \ p = 0.05) \) and development time \( (r = 0.387, \ p = 0.01) \).

The regression equations obtained with the backward method included significant coefficients \( (p < 0.05) \) only, and an independent Mixolab parameter curve using the “Simulator” protocol with coefficient of determination \( (R^2) \) of the fitting model is showed in Table 3.

The regression model for water absorption (CH) containing two analytical characteristics of flours as independent variables: protein content (PR) and gluten deformation index (GDI). The coefficients of all variables are statistically significant. Semi-partial correlation coefficient values indicate that variables PR \( (r_{sp} = 0.351) \) and GDI \( (r_{sp} = -0.334) \) have a medium effect on the dependent variable CH. The conjunct action of independent variables PR and GDI on the dependent variable CH has a medium level \( (R^2 = 0.220) \).

The model for weakening (WE) includes GDI and PR independent variables, whose regression coefficients are significant (Table 3). The value of determination coefficient \( (R^2 = 0.202) \) shows that the model explains 20.2% of the variation of the WE dependent variable, the global effect having a medium level. Regarding the effect dimension for each of the two independent variables contained in
the model, both have an medium contribution to the variability of the dependent variable WE, the variable GDI ($r_{sp} = 0.338$) being a positive predictor and PR ($r_{sp} = -0.317$), a negative predictor.

As the value of the statistical significance of Fisher’s test is small ($p < 0.008$), it can be concluded that the models presented in Table 3 are significant.

Table 3 Significant coefficients (95 % confidence interval) of the backward regression fitting model for Mixolab parameters using “Simulator” protocol on wheat flour analytical characteristics

<table>
<thead>
<tr>
<th>Factor</th>
<th>CH (%) Value</th>
<th>SE</th>
<th>WE (N·m) Value</th>
<th>SE</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTE</td>
<td>54.351</td>
<td>2.469</td>
<td>0.362</td>
<td>0.094</td>
</tr>
<tr>
<td>PR (%)</td>
<td>0.440</td>
<td>0.169</td>
<td>-0.015</td>
<td>0.006</td>
</tr>
<tr>
<td>GDI (mm)</td>
<td>-0.339</td>
<td>0.137</td>
<td>0.013</td>
<td>0.005</td>
</tr>
<tr>
<td>$R^2$</td>
<td>0.470</td>
<td></td>
<td>0.449</td>
<td></td>
</tr>
<tr>
<td>$R^2$ of estimate</td>
<td>0.220</td>
<td></td>
<td>0.202</td>
<td></td>
</tr>
<tr>
<td>SE of estimate</td>
<td>2.109</td>
<td></td>
<td>0.080</td>
<td></td>
</tr>
</tbody>
</table>

Independent variables were Protein content (PR) and Gluten deformation index (GDI). NS, no significant effect at $p < 0.05$; CTE constant of the fitted equation; $R$, correlation coefficient; $R^2$, coefficient of determination.

Among different wheat flour analytical characteristics, protein content (PR) and gluten deformation index (GDI) were found to be the best indicators of water absorption (CH) and dough weakening (WE) evaluation.

**4 Conclusions**

The methodology of principal component analysis accompanied by the graphical presentation of bi-plots provides information about association between wheat flour analytical characteristics and dough rheological parameters determined using the Mixolab device with “Simulator” protocol. A close positive relationship between protein content (PR), falling number (FN) and stability (ST) was found. Dough weakening (WE) was inversely associated with analytical characteristics of flours, PR and FN.

A multivariate regression model obtained indicated that wheat flour analytical characteristics could be used to predict dough rheological parameters. The results indicated that protein content (PR) and gluten deformation index (GDI) could be used to predict water absorption (CH) and dough weakening (WE). The models obtained explained more than 20% of the variability of the dough rheological parameters: water absorption and dough weakening.

The analytical characteristics of the wheat flour: protein content (PR) and gluten deformation index (GDI) offer the explanation of the variation of dough rheological parameters: water absorption (CH) and dough weakening (WE) determined using the Mixolab device with “Simulator” protocol.

**References:**


