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# Application of Principal Component Analysis in Assessment of Relation Between the Parameters of Technological Quality of Wheat Grains Treated with Inert Dusts Against Rice Weevil (*Sitophilus oryzae* L.)

**Marija Bodroža-Solarov [1], Petar Kljajić[2], Goran Andrić[2], Bojana Filipčev[1], Olivera Šimurina[1], Marijana Pražić Golić[2] and Milan Adamović[3]**

*[1]Institute of Food Technology, University of Novi Sad, Bulevar cara Lazara 1, 21000 Novi Sad, Serbia*
*[2] Institute of Pesticides and Environmental Protection, Banatska 31b, 11080 Belgrade, Serbia*
*[3]Institute of Technology of Nuclear and Other Mineral Row Materials, Bulevar Franš d'Eperea 86, 11000 Belgrade, Serbia*
*(marija.bodroza@fins.uns.ac.rs)*

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**SUMMARY**

Quality parameters of several wheat grain lots (low vitreous and high vitreous grains, non-infested and infested with rice weevils, (*Sitophilus oryzae* L.) treated with inert dusts (natural zeolite, two diatomaceous earths originating from Serbia and a commercial product Protect-It®) were investigated. Principal component analysis (PCA) was used to investigate the classification of treated grain lots and to assess how attributes of technological quality contribute to this classification. This research showed that vitreousness (0.95) and test weight (0.93) contributed most to the first principal component whereas extensigraph area (-0.76) contributed to the second component. The determined accountability of the total variability by the first component was around 55%, while with the second it was 18%, which means that those two dimensions together account for around 70% of total variability of the observed set of variables. Principal component analysis (PCA) of data set was able to distinguish among the various treatments of wheat lots. It was revealed that inert dust treatments produce different effects depending on the degree of endosperm vitreousness.

**Keywords:** PCA; Inert dusts; Low and high vitreous wheat; Quality parameters

## INTRODUCTION

Infestation of stored grains with rice weevils *Sitophilus oryzae* (L.) (Coleoptera: Curculionidae) is an important quality control problem for food industry due to huge economic losses. Effective insect pest control includes continuous application of chemicals like contact insecticides and fumigants (Hill, 1990; Rees, 2004). Although effective and low-cost, the use of pest-control chemicals exerts many disadvantages such as widespread development of resistance in insects (Korunić et al., 1998; Kljajić and Perić, 2005; Kljajić, 2008) and occurrence of trace residues in food commodities which rises environmental and public health concerns. In order to reduce chemical inputs, investigations and development of alternatives to chemical insecticides have been stimulated.

Interest in suitability of natural zeolite (NZ) and diatomaceous earth (DE) as alternatives to conventional insecticides and fumigants is increasing. Codex Alimentarius Commission (1999) recommends control of insect pests in food commodities and lists zeolite and diatomaceous earth as permitted substances in organic food production and in plant pest and disease control. This has focused efforts on investigating the fumigant action of these materials (commonly designated as inert dusts) for development of a potential new class of safer insect-control agents.

DE is a naturally occurring siliceous mineral compound from marine sediments which consists of microscopic skeletal remains of single-celled algae (phytoplankton) called diatoms. It is composed of amorphous silicon dioxide that is non-toxic to mammals and is registered as a food additive in Canada, the USA, and in many other countries (Korunić et al., 1998). Natural zeolites (NZ) are hydrated aluminosilicates characterized with complex three-dimensional frameworks of silica and alumina tetrahedra linked through shared oxygen atoms. Clusters of tetrahedra form sheetlike or chainlike polyhedral units build up the entire structure by mutual linking (Daković et al., 2007).

There are several research works dealing with the effectiveness of DE (Korunić et al., 1998; Fields and Korunić, 2000; Athanassiou et al., 2005; Vardeman et al., 2007) and NZ (Kljajić et al., 2010) against stored-grain insects. Furthermore, few authors addressed the effects inert dusts treatments exert on the technological quality of grain and flour. It was estimated that around 2% Dryacide (a DE preparation) remains in the flour after treatment (Desmarchelier and Dines, 1987). DE treatments at recommended doses (500-3500 g/t) were found to adversely affect moisture content, flowability, bulk density of treated grains, and hinder handling due to excessive dust formation but were not found to diminish the quality of end-products obtained from the treated flour. Korunić et al. (1996) investigated the effect of another commercial DE **product**, Protect-It® (at 50 and 300 mg/kg doses) and showed no significant differences in the protein content, falling number value, sedimentation value and color of wheat flour, but the flour rheological properties changed which was reflected through increase in farinograph development time and increased extensigraph resistance measured at 45 and 90 min. They also found that baking potential of treated flour was not altered.

Multivariate analysis is an analysis of a large number of variables, which enables their examination and quantification, as well as identification of their dependence, *i.e.* links between a larger numbers of variables. Principal components analysis (PCA) is one of many multivariate analysis methods. This method enables transformation of a large number of variables into a smaller number of latent variables (principal components, PCs) which are not inter-correlated.

These transformed variables represent linear functions of input variables. PCA is a powerful tool for pattern recognition, classification, modeling, and other aspects of data evaluation (Csomos et al., 2002). Also, PCA is a projection method, and dimension reduction of the data can be achieved using a smaller number of principal components than original variables.

The aim of this research is to apply the PCA on a practical example related to treatment of various wheat lots characterized with different endosperm vitreousness and insect infestation status with inert dust preparations and to reveal which treatment showed statistically significant impact on the variability of technological parameters of wheat quality.

## MATERIAL AND METHODS

### Wheat samples

Two types of wheat (*Triticum aestivum* ssp. *vulgare*) characterized with different degree of endosperm vitreousness: 17.0% (low-vitreous or mealy grains, LVG) and 81.8% (high-vitreous grains, HVG) were used in the investigation. The material was procured from local producers.

### Inert dusts

Various samples of inert dusts were used in the experiment: 1) an inert dust based on natural zeolite (NZ) originating from Serbia and processed at the Institute for Technology of Nuclear and Other Mineral Materials in Belgrade; 2) two dusts based on diatomaceous earth (DE S-1 and DE S-2, originating from Serbia) and 3) registered product Protect-It® (Hedley Technologies Inc., Canada).

The dusts used in tests had the following properties:

- NZ contained: $SiO_2$ (65.7%), $Al_2O_3$ (14.0%), CaO (3.6%), $Fe_2O_3$ (2.3%) and up to 1.5% of MgO, $Na_2O$ and $K_2O$. Particle size <50 μm was predominant.
- DE S-1 contained: $SiO_2$ (78.8%), $Al_2O_3$ (9.4%), $K_2O$ (0.8%), $Na_2O$ (0.08%), MgO (0.1%), CaO (0.6%), $Fe_2O_3$ (1.1%) and $TiO_2$ (0.2%). Particle size <50 μm was predominant.
- DE S-2 contained: $SiO_2$ (63.1%), $Al_2O_3$ (10.3%), $K_2O$ (0.9%), $Na_2O$ (0.08%), MgO (0.3%), CaO (1.0%), $Fe_2O_3$ (1.7%) and $TiO_2$ (0.3%). Particle size <50 μm was predominant.
- Protect-It® is a mixture of 90% marine DE, Celite 209, and 10% silica aerogel. It is a buff colored dust with more than 87% amorphous silicon dioxide. The tested formulation contained about 3% of $Al_2O_3$, about 1% $Fe_2O_3$ and below 1% CaO, MgO, $TiO_3$, and $P_2O_3$. Moisture content of the dust ranged from 3 to 6%. The mean particle size was between 5 and 6 μm, though more than 80% of the particles had a diameter below 12 μm. The specific gravity was 2000 kg/m$^3$ and pH in 10% slurry (with doubled distilled water) was between 5.5 and 5.7 (Korunić et al., 1998).

## Grain treatment with inert dusts

Inert dusts were applied on 0.5 kg wheat samples in five replicates, using doses that were found optimal for efficient storage pest control in preliminary experiments 1) natural zeolite (NZ), 1.0 g/kg, 2) diatomaceous earths (DE S-1 and DE S-2), 0.75 g/kg, and 3) as standard DE product registered worldwide (Protect-It®), 0.2 g/kg.

In separate tests with insect infestation, inert dusts were applied on two types of wheat in the same manner as described above. After 21 days of incubation, the samples were sieved to separate insects. After total seven weeks of incubation, sieving was repeated to remove the progeny in $F_1$ generation. The samples were then placed into plastic bags and put into refrigerator for 24 h. Next day, sieving was repeated again to remove the rest of possibly remained insects. Sieving was conducted using sieves 7/64'' for insect removal only whereas dust was returned to initial grain mass by mixing for one minute. The sieved samples were stored in plastic bags at room temperature until further examination.

**Table 1.** Experimental design and sample designation

| | Inert dust treatment with and without insect | Sample |
|---|---|---|
| Low vitreous wheat without insect | LVG Control | 1 |
| | LVG NZ | 2 |
| | LVG DS-1 | 3 |
| | LVG DS-2 | 4 |
| | LVG Protect-It® | 5 |
| Low vitreous wheat with insect | I LVG Control | 6 |
| | I LVG NZ | 7 |
| | I LVG DS-1 | 8 |
| | I LVG DS-2 | 9 |
| | I LVG Protect-It® | 10 |
| High vitreous wheat without insect | HVG Control | 11 |
| | HVG NZ | 12 |
| | HVG DS-1 | 13 |
| | HVG DS-2 | 14 |
| | HVG Protect-It® | 15 |
| High vitreous wheat with insect | I HVG Control | 16 |
| | I HVG NZ | 17 |
| | I HVG DS-1 | 18 |
| | I HVG DS-2 | 19 |
| | I HVG Protect-It® | 20 |

Kernel vitreousness was determined by visual inspection where vitreous kernels appear glassy and translucent whereas non-vitreous kernels appear starchy and opaque (ICC, No 129). Test weight was determined using Schopper scale. Measurement of test weight was repeated five times for each sample. Protein contents were determined according to ICC approved methods No 105/2. Content of $SiO_2$ in wheat was determined gravimetrically according to official methods (31, 1972). Rheological properties of wheat flour samples were analyzed in a Brabender farinograph according to method ICC No 115/1, and Brabender extensigraph according to method No ICC 114/1.

## Statistical analysis (Principal Component Analysis – PCA)

The algorithm of PCA can be found in standard chemometric material (Oto, 1999). Descriptive analysis of the data and the PCA were performed using the software package STATISTICA 10.0. In summary, PCA decom-

**Table 2.** Technological quality parameters of wheat grain lots

| Sample | Test weight (kg/hl) | Vitreousnes (%) | Insect-damaged kernels (%) | Protein content (%, d.m) | Content of $SiO_2$ (g/kg) | Water absorption value (%) | 15-minute drop | FQN | Extensigraph area (cm$^2$) | Extensibility (mm) | Resistance to extension BU |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 75.4 | 17.0 | 0.0 | 11.60 | 0.00 | 52.0 | 75 | 53.3 | 67 | 310 | 125 |
| 2 | 71.6 | 18.0 | 0.0 | 11.70 | 0.02 | 53.0 | 80 | 51.4 | 68 | 320 | 130 |
| 3 | 71.2 | 16.7 | 0.0 | 11.60 | 0.04 | 53.0 | 78 | 51.2 | 67 | 305 | 131 |
| 4 | 71.3 | 17.0 | 0.0 | 11.50 | 0.02 | 53.2 | 79 | 49.4 | 69 | 330 | 126 |
| 5 | 71.6 | 18.7 | 0.0 | 11.70 | 0.04 | 53.2 | 80 | 51.6 | 66 | 290 | 130 |
| 6 | 69.6 | 17.0 | 25.7 | 12.80 | 0.00 | 56.7 | 175 | 38.8 | 56 | 270 | 127 |
| 7 | 70.3 | 18.0 | 9.6 | 11.80 | 0.14 | 55.0 | 60 | 59.2 | 74 | 280 | 142 |
| 8 | 70.6 | 16.7 | 8.8 | 11.70 | 0.06 | 53.6 | 85 | 55.6 | 80 | 330 | 136 |
| 9 | 70.4 | 17.0 | 7.8 | 11.70 | 0.06 | 55.0 | 120 | 51.0 | 74 | 380 | 124 |
| 10 | 69.9 | 18.7 | 10.2 | 11.80 | 0.12 | 55.5 | 140 | 45.5 | 71 | 370 | 120 |
| 11 | 79.3 | 81.8 | 0.0 | 13.70 | 0.00 | 59.7 | 65 | 65.9 | 69 | 240 | 146 |
| 12 | 78.6 | 82.0 | 0.0 | 13.70 | 0.06 | 61.6 | 60 | 66.2 | 70 | 230 | 150 |
| 13 | 77.6 | 79.0 | 0.0 | 13.80 | 0.02 | 61. | 60 | 68.3 | 69 | 220 | 149 |
| 14 | 77.7 | 79.3 | 0.0 | 13.80 | 0.02 | 59.9 | 61 | 67.4 | 65 | 230 | 142 |
| 15 | 77.7 | 82.5 | 0.0 | 13.80 | 0.02 | 61.9 | 61 | 68.2 | 65 | 220 | 143 |
| 16 | 77.2 | 81.8 | 15.7 | 14.30 | 0.00 | 63.5 | 150 | 49.6 | 62 | 280 | 133 |
| 17 | 77.2 | 82.0 | 9.5 | 14.10 | 0.12 | 61.1 | 65 | 59.4 | 74 | 270 | 146 |
| 18 | 77.0 | 79.0 | 6.5 | 13.90 | 0.05 | 62.3 | 55 | 62.9 | 82 | 270 | 156 |
| 19 | 76.9 | 79.3 | 6.1 | 13.90 | 0.05 | 62.4 | 80 | 62.4 | 79 | 290 | 146 |
| 20 | 77.0 | 82.5 | 7.0 | 14.10 | 0.10 | 61.9 | 78 | 67.8 | 90 | 330 | 146 |

poses the original matrix into several products of multiplication into loading (parameters of quality) and score (different treatment with inert dusts) matrices. Parameters of grain quality are taken as variables (column of the input matrix) and different treatment with inert dust as mathematical-statistical cases (rows of the matrix).

## RESULTS AND DISCUSSION

The ranges of average values for wheat sample quality were as follows: test weight, 69.65-79.30 kg/hl; vitreousness, 16.70-82.50%; insect-damaged kernels, 0-25.7%; protein content, 11.50-14.30%; content of $SiO_2$, 0-0.14%; water absorption value, 52-63.5%; 15-minute drop 55-175 BU; FQN,38.80-68.30; extensigraph area, 56-90 cm$^2$; extensibility 220-380 mm; resistance to extension 120-156 BU (Table 2).

The number of factors retained in the model for proper classification of the data from Table 2 was determined by application of Kaiser's and Rice's rule (1974). Therefore, two components having eigenvalues >1 were used for further analysis. PCA yields two PCs explaining 74.2% of the total variance in the data. Loading values (i.e. correlation coefficients) higher than 0.700 were marked throughout Table 3 in boldface type.

Projection of the variables in the factorial plane (Table 3) indicates that the variables vitreousness (0.948); test weight (0.932); resistance to extension (0.920); FQN (0.913) most contributed to the first PC indicator (which accounted for 55.61% of the variability), and thus to the total variability of the basic set. The second PC indicator (which accounted for 18.93% of the variability) is contributed most by the content of $SiO_2$ (-0.653) and extensigraph area (-0.762).

The loadings plot of components in factorial 2D plane shows that the highest contribution to the description of the second PC indicator was due to $SiO_2$ content as it forms the smallest angle with PC2 loading axis. The content of $SiO_2$ was higher in those samples treated with inert dusts but more damaged by insects (Figure 1).

Factor coordinates of individual observations (Figure 2) indicate that the total variability of the first component is influenced mostly by the non-treated low vitreous samples without insect infestation (Control) (-3.64) and those infested and treated with Protect-It® (-3.51).

Factor coordinates also indicate that the total variability of the second component was influenced mostly by the low vitreous samples without insect infestation (3.68) and high vitreous non-treated samples (3.41).

**Table 3.** Results of Principal Component Analysis for wheat quality parameters in Grain sample treated with different inert dusts: Varimax Rotated Principal Component Loadings

| Parameters | PC1 | PC2 |
|---|---|---|
| Test weight | **0.932** | 0.184 |
| Vitreousness | **0.948** | 0.207 |
| Insect-damaged kernels | -0.329 | 0.444 |
| Protein content | **0.917** | 0.231 |
| Content $SiO_2$ | -0.021 | **-0.653** |
| Water absorption value | **0.846** | 0.309 |
| 15-minute drop | **-0.616** | 0.593 |
| Flour Quality Number (FQN) | **0.913** | -0.298 |
| Extensigraph area | 0.304 | **-0.762** |
| Extensibility | **-0.729** | -0.404 |
| Resistance to extension | **0.920** | -0.146 |
| **Explained variance** | **6.621** | **2.26** |
| **Proportion of total variance %** | **55.61** | **18.61** |

Figure 2 shows that according to the first two PCs, the grain lots of low vitreous wheat (infested and non-infested) treated with the preparations are similar to each other. Also, there is similarity within the treated wheat lots of high vitreous wheat (infested and non-infested). The first PC distinguishes between the lots of low and high vitreous wheat grains which suggest that the inert dust treatments produce different effect regarding test weight, FQN and resistance to extension in dependence to endosperm vitreousness. Two points (sample 6 and 16) appeared as outliers: control samples of low and high vitreous wheat infested with insects (non-treated with inert dusts). These samples were characterized with the poorest technological quality as they were most damaged by insects.

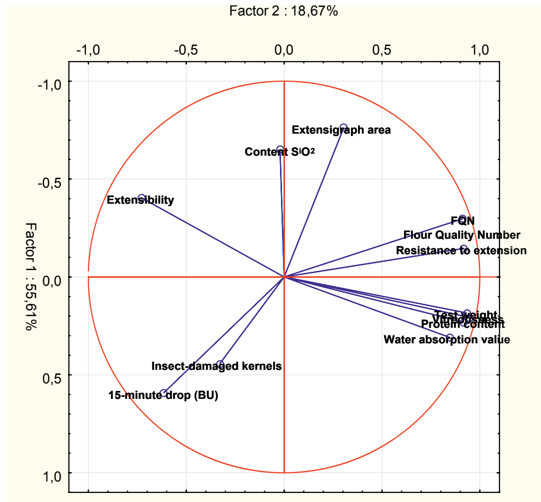


**Figure 1.** Rotated principal componential loadings (similarities among wheat quality parameters)

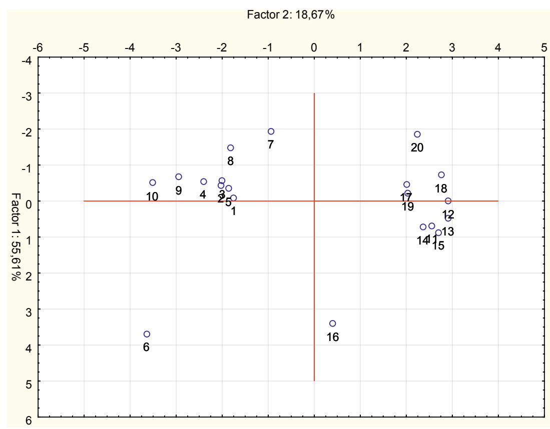


**Figure 2.** Rotated principal componential scores (similarities between inert dust treatments with and without insect infestation)

Principal component analysis (PCA) of data set was able to distinguish among the various treatments of wheat lots. It was revealed that inert dust treatments produce different effects depending on the degree of endosperm vitreousness. The best predictor of technological quality is endosperm vitreousness and the most affected parameters of technological quality are test weight, resistance to extension, flour quality number, and extensigraph area.

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# Analiza tretmana pšenice inertnim prašivima sa ciljem zaštite od pirinčanog žiška (*Sitophilus oryzae* L.) kroz promenu parametara tehnološkog kvaliteta primenom metode glavnih komponenti

**REZIME**

Cilj istraživanja je ispitivanje uticaja tretmana inertnih prašiva (prirodni zeolit i dve dijatomejske zemlje poreklom iz Srbije, kao i komercijalni preparat Protect-It®) na brašnavu i staklavu pšenicu, infestiranu i neinfestiranu pirinčanim žiškom (*Sitophilus oryzae* L.), kroz parametre tehnološkog kvaliteta.

Primenom metoda analize glavnih komponenti (PCA) zaključeno je da se ukupna varijabilnost (preko 73%) posmatranog skupa može dovoljno objasniti pomoću prve dve dimenzije, ili glavne komponente. Najveći uticaj na formiranje prve glavne komponente imali su procenat staklavosti (0,95) i hektolitarska masa (0,93), dok je druga glavna komponenta najbolje objašnjena kroz parametar tehnološkog kvaliteta, energije na ekstenzogramu (-0,76).

Primenjen metod je ukazao na značajan uticaj staklavosti pšenice na efekat inertnih prašiva. Istovremeno, potvrđen je uticaj praširva na smanjenje stepena infestiranosti i poboljšanje parametara kvaliteta. Takođe, pokazano je da različita inertna praširva daju slične efekte pri istoj staklavosti endosperma pšenice.

**Ključne reči:** PCA; inertna prašiva; brašnava i staklava pšenica; kvalitet