APPLICATION OF PRINCIPAL COMPONENT ANALYSIS IN COMMODITY SCIENCE

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1. Introduction

The research activity in the Division of General and Analytical Chemistry during more than two decades was strongly associated with various aspects of steroid chemistry. Prof. A. Smoczkiewicz was first who implemented research on qualitative and quantitative analysis of steroids *in vivo* and *in vitro* material [1]. In addition some analytical problems of fats and lipids were studied. Later on research on steroids turned into direction of physical organic chemistry namely investigation of weak basic properties of steroid enones. This activity has been reviewed recently [2]. Those studies required more advanced data treatment: Linear Free Energy Relationship, similarity models and multivariate methods. The main results achieved by application of those methods including Principal Component Analysis are reviewed by Zalewski [3] and were presented during the IV European Conference on Correlation Analysis in Organic Chemistry organized in Poznań in 1988 by our Division.

The purpose of this paper is to present our recent results on application of Principal Component Analysis (PCA) in the field of commodity science.

Principal Component Analysis (PCA) was first established by Pearson [4] and developed [5] to meet requirements in psychology in explaining the large amount of experimental data. The possibilities of PCA has been rediscovered in various scientific fields apart from psychology. PCA was introduced to chemistry in the nineteen sixties by Malinowski [6] and the number of its application has been growing since then very dynamically. Many good text books [7-12] and review articles [3, 13] have been published. The method of PCA explore other fields related to chemistry, food chemistry [14, 15] being a good example. Martens and Harries [15] collected and classified more than 200 references on the application of multivariate statistical techniques to the investigation of food contaminants, foodstuff properties and sensory responses, PCA being dominating in the period 1945-1982. Recently Zalewski has reviewed [16] applications of PCA and similar methods in food chemistry for the period 1980-1988.

PCA is ideally suited to deal with large data matrices and look for 'hidden' regularities. The large table of data is very difficult for the human mind to comprehend.

The routine is to compare two rows or two columns at a time using linear regression or plots. The graphical examination of data is useless beyond three dimensions (lines, curves, planes and surfaces are thus available). An assumption of orthogonality of variables is automatically accepted, but frequently is not true.

The main results of PCA of the data matrix are summarized as follows:

a) examination of the relationship between columns and rows,
b) finding the 'true' dimensionality of data matrix,
c) finding the new orthogonal system of variables, called principal components,
d) reduction of dimensionality,
e) calculation of principal components scores and loadings,

and may be used by the researcher for:

(i) simplification of the data matrix by elimination of redundant information,
(ii) detection of outliers among objects or variables,
(iii) selection of a better set of objects or variables,
(iv) reconstitution of data matrix with one, two ... principal components,
(v) classification of variables or objects,
(vi) discrimination of variables or objects,
(vii) modelling and prediction of data,
(viii) explanation of principal components in terms of given branch of science.

Despite of such broad possibilities, PCA is not very much used in commodity science. The aim of this paper is to present some recent applications of this powerful statistical tool to solve the problems of commodities investigation in this laboratory. In addition some applications to solve general analytical problems are described. The mathematical background of PCA was given previously [3, 16] and will not be repeated now.

2. Application in Commodity Science

2.1. *Quantitative analysis of two, three and four component mixtures*

A quantitative analysis of multicomponent mixture is a common task in many laboratories. Absorbance spectroscopy in various regions of electromagnetic radiation is used assuming Beer-Lambert law. Data matrix of absorbances measured at k wavelength and r mixtures, $A_{k,r}$ equals to the summation of components's 1 ... n absorbances (Equation 1):

$$A_{k,r} = a_{k,1}c_{1,r} + a_{k,2}c_{2,r} + \ldots \varepsilon \tag{1}$$

from one side, and may be represented by PCA model on the other:

$$A_{k,r} = A_k + p_{1,k}l_{r,1} + p_{2,k}l_{r,2} + \ldots \varepsilon \tag{2}$$

Principal components $p_{n,k}$ and loadings $l_{n,r}$ contain all information concerning the shape of spectra and relative concentration of all components. The PC model in a form of equation (2) is convenient for quantitative analysis. However, for elucidation of real absorption spectra of both compounds in mixture of two it is better to apply the following equation [3]:

$$A_{k,r} = p_{1,k} l_{r,1} + p_{2,k} l_{r,2} \tag{3}$$

If the total concentration in a set of mixtures is constant, numerical values of loadings are linearly related to the concentration of the first component and second component, according to Equation 4:

$$c_{1,r} = 1 - c_{2,r} = b\, l_{1,r} + d \tag{4}$$

in which b and d are slope and intercept, respectively.

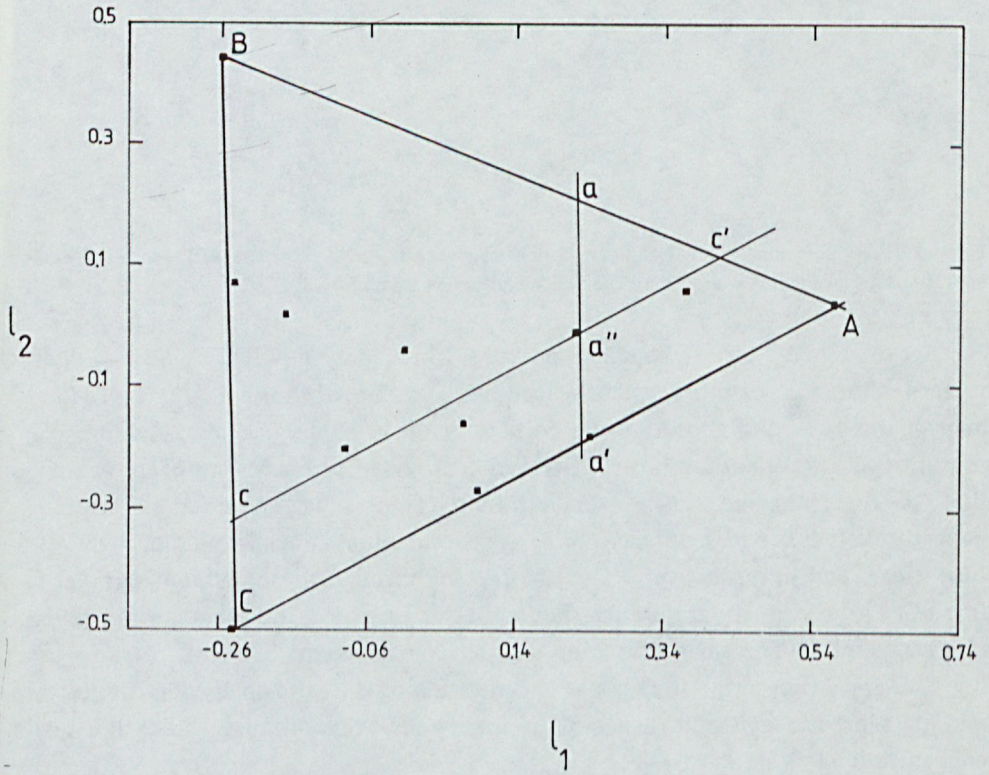


Figure 1. Plot of loadings for three component mixture: A — ∝-hexylcinnamic aldehyde, B — ∝-jonone, C — eugenol. For explanation see text

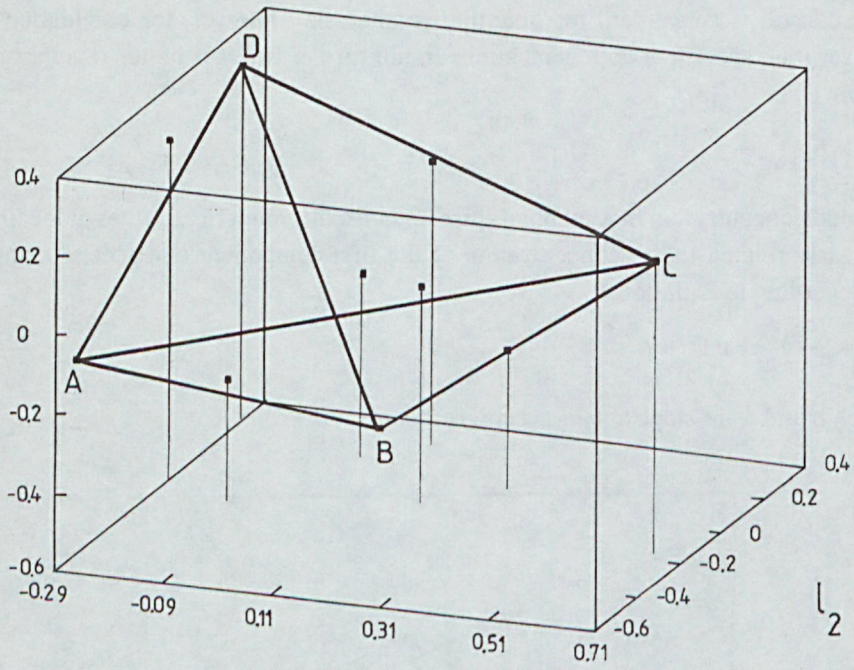


Figure 2. Three dimensional plot of loadings for four component mixture: A — ∝-jonone, B — anetol, C — ∝-amylcinnamic aldehyd, D — cinnamic alcohol. For explanation see text

The solution of a three component mixture, which is exemplified by a simple perfumery mixture is possible by plotting loadings $l_{2,r}$ vs $l_{1,r}$ as shown in Figure 1. Pure components A, B and C occupy the corners of the triangle. Connecting lines represent two-component mixtures. The Euclidean distance decreasing from A along line AC represents decreasing concentration of this component and increasing concentration of C. The points a′ and a″ represent equal concentration of A in mixture with C and B, respectively. The line passing through those points is parallel to line BC. Three component mixtures falling in this line have the same concentration of component A. The same reasoning is true for component C. Points c and c′ on lines BC and AC describe the equal concentration of C in two-component mixtures, and a″ represent concentration of C in three-component mixture. Since the total concentration was set 1,

$$c_B = 1 - (c_A + c_C) \tag{5}$$

the computer program faciliating this problem is now under preparation [17].

With a four-component mixture, three dimensions are necessary to represent concentrations of components, and the appropriate plot of loadings is shown in Figure 2. All informations for quantitative analysis are present in a tetrahedron. Corners A through D represent four components, edges (eg. AB, CD) represent two-component mixtures, and sides (eg. ABC, BCD) represent three-component mixtures. All volume inside the tetrahedron is the domain of four component mixtures. The calculation of component concentrations is more laborious and will be achieved by a more advanced program.

The method is general and might be used to other families of curves given by multicomponent mixture (IR, GC for example) and profiles, and to more complex mixture. With n components, (n−1) principal loadings are necessary to gain quantitative information. Theoretically, with n components, n principal components will contain all necessary information to calculate spectra of each component. This was done for a set of spectra of a very weak basic compound which was only half-protonated in concentrated sulphuric acid [18]. Work is in progress to extend it beyond n=2 [17].

2.2. *Substituent and conformation effects on ^{13}C NMR substituent chemical shifts of cyclohexanes and steroids*

The increasing applicability of ^{13}C NMR spectroscopy requires a better understanding of the shielding mechanism in terms of the experimental shift caused by a change of a substituent and its conformation, and the structure of the molecular frame. This approach has been begun by Dalling and Grant [19]. The other approach relies on PCA calculations. For example a family of 2-substituted norbornanes (7*exo* and 7*endo* isomers) shows three principal components [20], the nature of which has been partly explained. Similar calculations were done in our laboratory and reported in the literature. Monosubstituted cyclohexanes [21], t-butyl-4-substituted cyclohexanes [22] and various steroids [3] behave similarly.

Three principal components explained almost all data variability. In all systems, the $p_{1,k}$ describes more than 94% of total data variability and the second adds from 2.2 to 5.5%. The small third (0.1-0.5%) brings the total data variability to at least 99.9%. The three component model describes the data in satisfactory agreement with the experiment. Figure 3 shows a typical projection of the three principal components exemplified by 3 substituted cholestanes. The numerical values of $p_{1,k}$ are distributed over a 60 unit range, and values of $p_{2,k}$ over a 17 unit range, with a tendency to linearity with negative slope. All compounds fall into two clusters: upper with positive $p_{3,k}$ consists of axial susbtituents, and the lower groups together equatorial substituents.

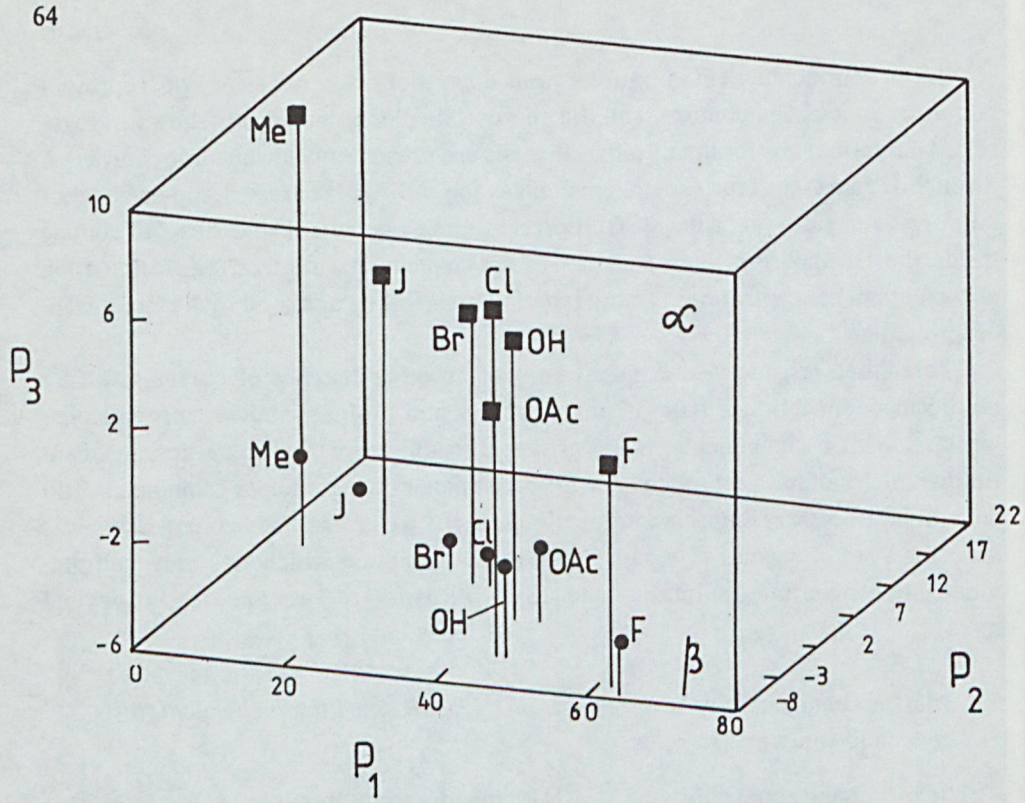


Figure 3. Three dimensional plot of loadings for 3-substituted cholestanes. 3β (Δ) and 3α (0) form separate clouds along $l_{3,k}$ axis

The examination of the relationships between principal components for various investigated structural varietes, loadings and substituent parameters for various electronic effects leads to the following conclusions:

(i) the first principal component characterizes electronegativity contribution of the substituent on the electron distribution in the cyclohexane ring through polarization of X-C_{ipso} ∂ bond,

(ii) the second principal component describes the inductive power of substituent through field effect, which is non-proportional to the electronegativity effect [23],

(iii) the third principal component discriminated between axial and equatorial substituents, perhaps on the basis of γ-gauche interactions and the deformation of the cyclohexane skeleton by axial groups.

In addition, it was also possible to detect specific long-range effects of substituents in steroid molecules. PCA indicates the field-inductive nature of this phenomenon which is stronger in 3β isomers (axial).

2.3. *Analysis of soaps, washing powders and toothpastes*

Those commodities are of general importance to maintain hygiene of people and their clothes and houses. From a chemical point of view they are more or less complex mixtures of various components such as surfactants, soaps, protectors, alkali, salts, fillers, colorants, fragrances. The appearence, shape, colour and smell given to those commodities seem to be very important factors for consumers opinion. The properties of soaps, washing powders and toothpaste to be tested (according to national standards) are numerous, including physical, chemical, and physico-chemical parameters, usefulness and sensoric descriptors. It is a common procedure to examine 20-30 such descriptors of various kind for each product. At the level of the producer it is difficult, if possible at all, to observe relations between various descriptors and decide whether they are mutually correlated or not. It is also difficult to see the relationship between the global property (usefulness and quality) of a product and its individual composition. The action of particular component (chemical species) is 'hidden' and may be screened or enhanced by other components present. It is also difficult to judge the quality of a product from the results of the analysis itself.

The Polish Standards overestimate the meaning of physical and chemical measurements of mentioned products, and neglect to a large extent the examination of sensoric and usefulness descriptors. The effective approach to the above problems is analyzing all possible descriptors for a large amount of similar products. The resulting table of data is a matrix, and the correlation between descriptors (in columns of data matrix) or between the objects (in rows of data matrix) may be calculated, assuming linear relationship. The matrix of correlation coefficients is a starting source in Principal Component Analysis [3-5].

a) toilet soaps

Eighteen toilet soaps of different quality grade made in Poland, England, Spain, DDR and Hungary were analyzed [24] according to the Polish Standard [25]. Twenty two descriptors were measured, including: D1 – fatty and resin acids, D2 – non-saponificable fat and substances, D3 – non-saponificable substances only, D4 – resin acids, D5 – sodium hydroxide, D6 – chlorides, D7 – carbonates, D8 – melting point of fatty acids, D9 – iodine number, D10 – titration number, D11 – water and volatile compounds, D12 – water, D13 – substancs insoluble in ethyl alcohol, D14 – substances insoluble in water, D15 – soaking number, D16 – foaming ability, D17 – foam lasting, D18 – silica oxide, D19 – appearence, D20 – homogenity, D21 – smell and D22 – colour.

The data matrix of format 18 x 22 was processed using PCA and SIMCA program. The plot of principal component loadings for 18 soaps is shown in Figure 4. Two soaps: Knight Castille (No 9, England) and Tessa (No 14, Spain) were rejected, as outliers. The remaining soaps tend to form a cluster as indicated. The principal

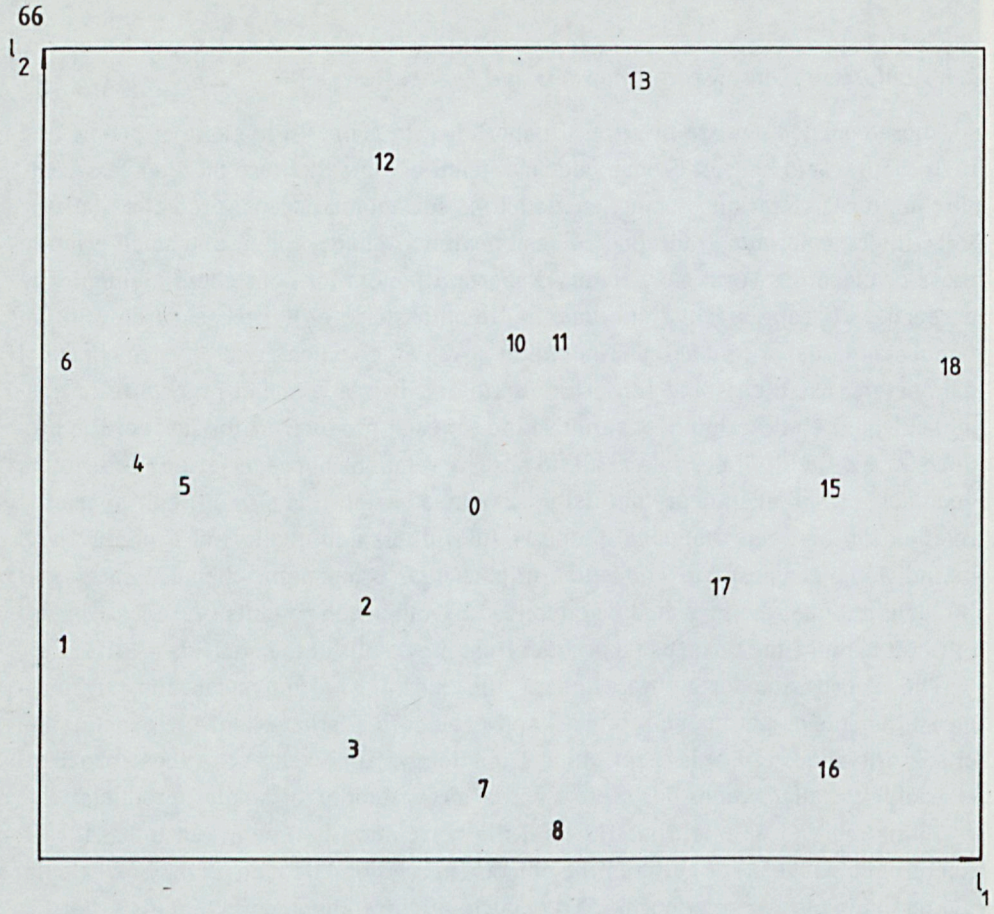


Figure 4. Plot of principal component loadings for toilet soaps tend to show clusters

component scores for 22 descriptors are shown in Figure 5. The first principal component after rotation is strongly connected with sensory parameters D19 – D21, concentration of fatty acids and saponificable – nonsaponificable compounds D1 – D3, and some other descriptors. The second principal component is much less important, and connected with the content of water and volatile compounds D12, and resine acids D4. Other descriptors are of very little importance.

The inspection of the correlation matrix calculated from the data matrix indicated a number of essential correlations ($r > 0.54$) [26]. For example descriptor D3 is linearly related to D2 ($r = 0.88$) and may be delated in future analysis. The content of water D12 investigated by the xylene method is linearly related to D13 and as more precise should be recommended for future use. The high correlation coefficient 0.86 between the fraction insoluble in water and in alcohol, allows to reject one descriptor. The number of high correlations seem to be random, e.g. those including the content of silica oxide with the melting point of fatty acids, iodine number and soaking

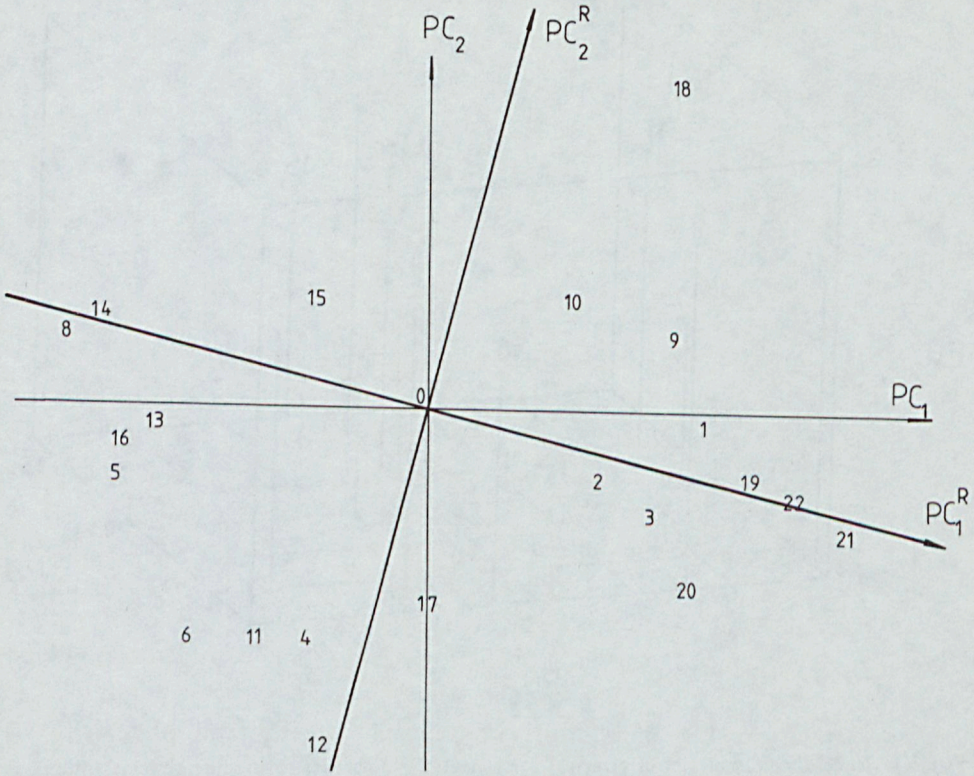


Figure 5. Plot of principal components for twenty two descriptors of toilet soaps. Abstract solution (PC) and real solution (PC^R) after rotation. For explanation see text

number or between the melting point of fatty acids and sensory parameters D20 – D22.

b) washing powders

Fifteen varietes of washing powders produced in Poland and imported were analyzed [24] on their agreement with the National Standards [27]. The following chemical and usefulness parameters were measured: D1 – solubility in ethyl alcohol, D2 – content of P_2O_5, D3 – content of anion-active surfactants, D4 – content of carboxymethyl cellulose, D5 – content of silica oxide, D6 – pH, D7 – solubility in water, D8 – content of sulphates, D9 – content of perborates, D10 – washing power, D11 – specific gravity, D12 – fabrics protecting ability, D13 – organic incrustation, D14 – inorganic incrustation and D15 – fabrics strength after 20 washings in standard conditions.

Washing powder, among other things must fulfill the following usefulness parameters: protecting ability better than 72%, total incrustation no more than 2.5%, washing

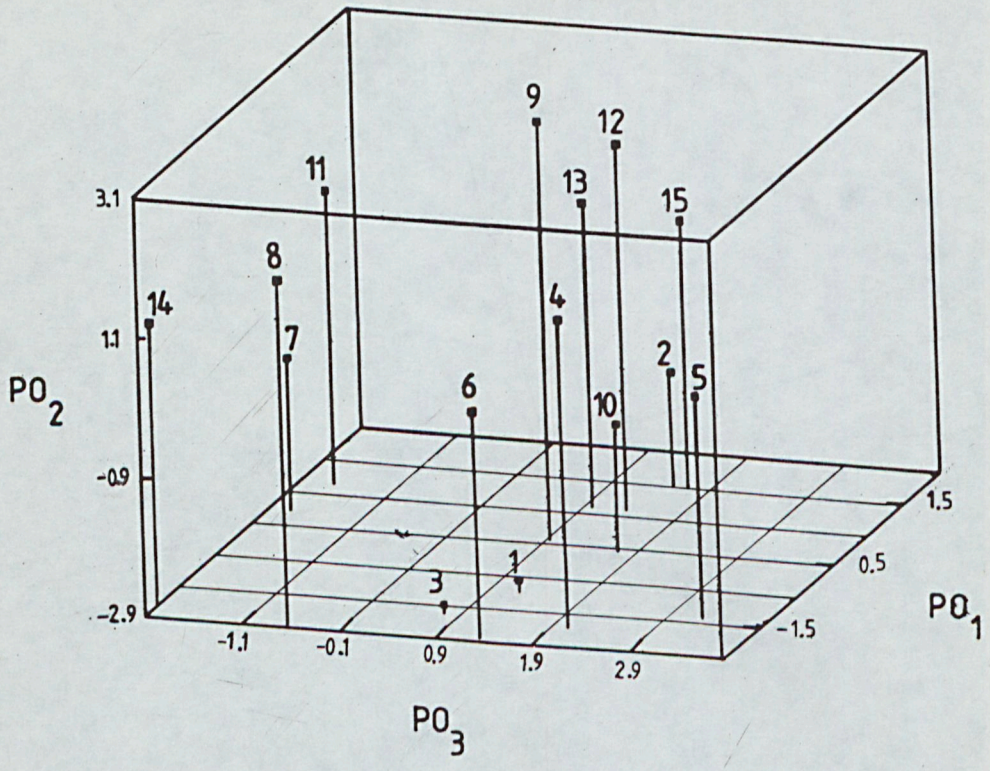


Figure 6. Three dimensional plot of principal components for properties of washing powders with three clusters indicated

power at least 110% and decrease of fiber strength not higher than 25%. Biodegradation, not investigated here, is also very important.

The comparison of results achieved with the Standard [27] indicated pronounced deviations, especially for imported goods. For example OMO fails in five analysis, DIXAN, BIOMIX and TOMI in four. OMO and also AVA, LANZA and TOMI contain 30-40% of sulphates, eg. several times more than allowed, less soluble in ethanol surfactants and very little phosphates. The protecting ability of all washing powders does not reach the minimum value of 72%, and most of them are charakterized by higher total incrustation. Only AVA follows the Polish Standard.

The essential deviations of imported washing powders of world reputation from the Polish Standard mean that our regulations are not acceptable outside the country.

The data matrix of format 15 x 15 was standardized prior to PCA calculations. Only following pairs of descriptors show an essential correlation: D15 – D12, D2 –D14 and D4 – D5. Washing power D10 does not correlate with the content of substances soluble in ethyl alcohol D1 nor the content of phosphates D2, however the dual parameter equation $D10 = a\,D_1 + b\,D2 + c$ gives a correlation coefficient of regresion

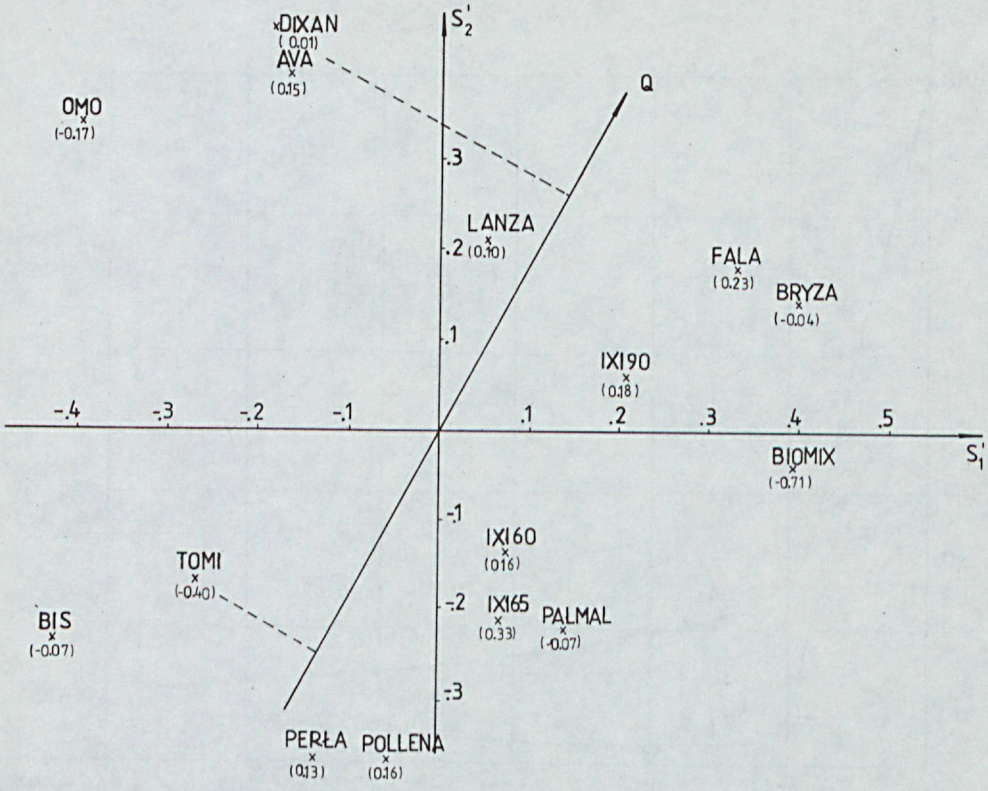


Figure 7. Plot of loadings for washing powders. Axis Q denotes firstappriximation of general quality index. Dotted lines show projection of products on axis Q

r = 0.993. The relation between the content of both active components and washing power is thus obvious.

Three principal components describe 65.29% of total data variability and their three-dimensional image is presented in Figure 6. Three clusters are visible. One can be labeled as the cluster of the chemical properties connected with the washing process (D1, D2, D3, D6 and D10), the cluster of physical properties (D7, D8, D11 and D14) and the cluster of protecting ability (D4, D5, D12, D13 and D15). The content of perborates D9 is an outlier. Those clusters are well separated in the property space, however, they are not exactly parallel to principal component axes.

The first principal component (after rotation) is significantly correlated with descriptors D2, D4, D8 and D14, and the second principal component is correlated with D3, D12 and D13. Loadings of principal components for 15 investigated washing powders are plotted as shown in Figure 7. The results of PCA calculations were utilized for computation of general the quality index [24] Q:

$$Q = l_{r,1} \Sigma(p_{1,k})^2 + l_{r,2} \Sigma(p_{2,k})^2 + \ldots \qquad (6)$$

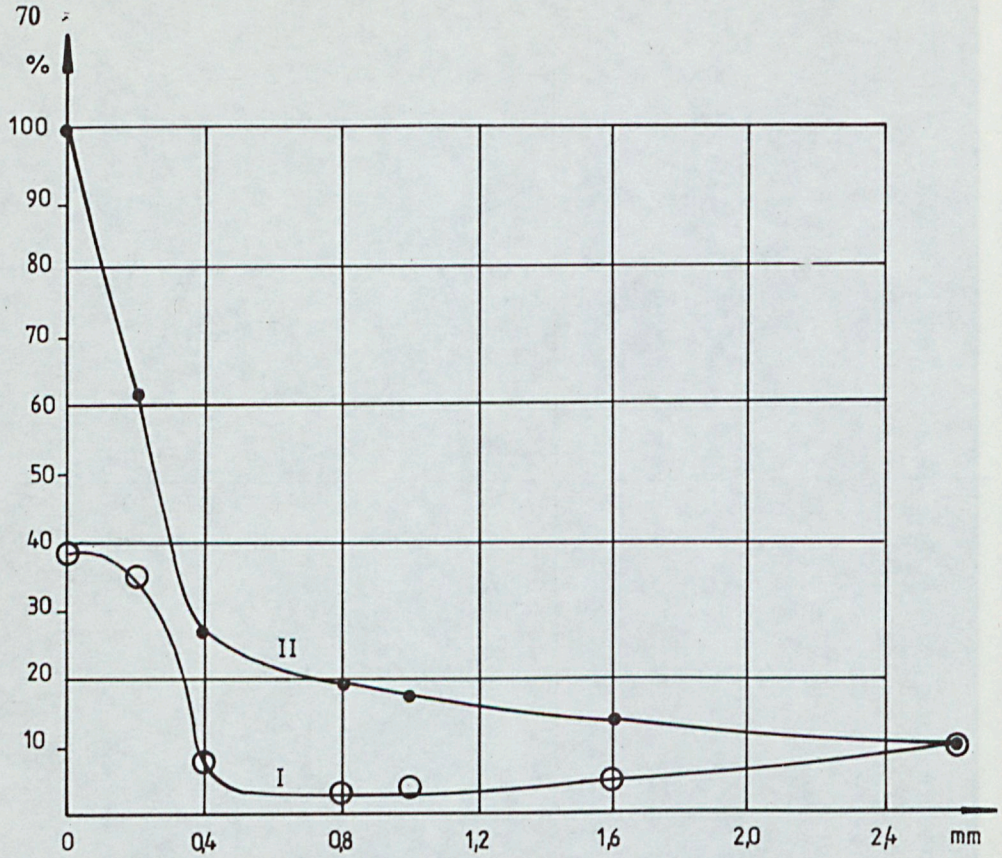


Figure 8. Particle size distribution in OPAL En washing powder

Its value decreases in a first approximation along the axis Q shown in Figure 7. Further work on the general quality index is now in progress.

c) granulometric distribution and technology of washing powders

A particle size distribution in washing powders is connected with their quality. It is preferable to use washing powders with a small amount of large – and small – size particles. The first are not well soluble in cold water, the next may give alergic symptomes. As a rule, the fraction 0.2-2.0 mm is preferable and should amount to not less than 90% of total product gravity. The particle size distribution in washing powders depends on the chemical constitution and method of production.

The effect of technology in the production of washing powders in Poland on the particle size distribution has been investigated recently [28]. Twenty washing powders produced by means of Ballestra tower, Niro tower, cold tower or mixing device were compared with five imported items (DIXAN, MERFIX, HIT, LOTOS, COLON). The particle size distribution was measured in ranges (mm) >2.5, 2.5-1.6, 1.6-1.0, 1.0-0.8, 0.8-0.4, 0.4-0.2 and <0.2. Figure 8 shows a profile of OPAL En washing powder as an example. In addition, friability and lumpiness were investigated.

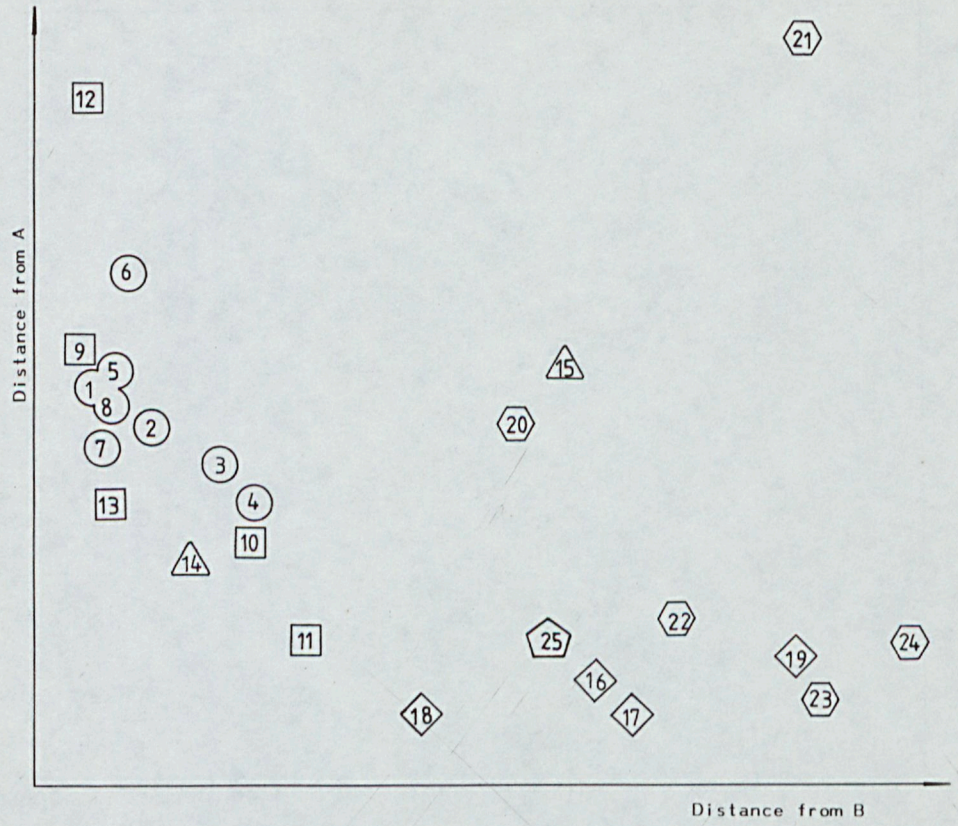


Figure 9. Distance of washing powders (denoted by numbers) from class A and class B PC model. Technology used: ○ – Ballestra tower, △ – Niro tower, ◇ – cold tower, ⬡ – mixing device, ⬠ – vibrofluidal, □ – imported washing powders

We used data matrix [28] without a prior standardization for PCA and SIMCA calculations. Two principal components explain 85% of the total data variability, and the third adds approximately 10%. The plot of two largest loadings allow to distinguish three classes. Two of them group home products and the third test class was composed of form imported washing powders.

Polish washing powders produced in Ballestra tower were placed in class B and PCA model has been calculated by SIMCA. Two principal components were significant according to crossvalidation. Dusty fraction, friability and lumpiness were rejected because of their very low modeling power.

Class A groups products manufactured in cold tower and mixing device. Class A principal component model has only one significant component. The modelling power of 1.0-0.8 mm and dust fractions and again lumpiness was very low, and these variables were rejected.

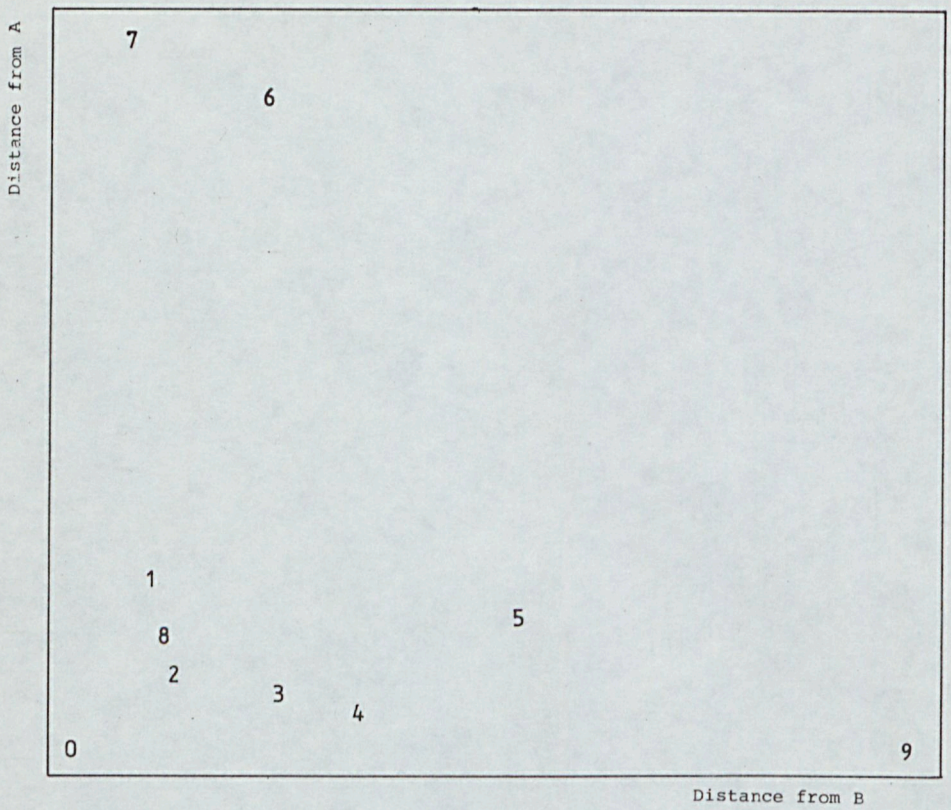


Figure 10. Scatter of fraction distribution data for washing powder OPAL En (class A) and LOTOS (class B)

PC models for class A and B were used for all washing powders population to measure the distance of each object from both models. The results achieved are shown in Figure 9. Washing powders produced by Ballestra tower technology and part of imported ones are very close to class B. Products manufactured by cold tower or mixing device (in part) are close to class A. However, two enzymatic washing powders 'E' and 'E automat' are placed exactly in the middle of both classes. Also two washing powders from Niro tower, occupy position between both defined classes. POLAR produced by vibrofluidal technology falls into class A.

The most representative washing powders for each class are these, which are close to their own class, and apart from the other. In our case 'Lotos' is most characteristic in class B, and 'Opal En' is a good representant of class A. This is also shown by a scatter of points in Figure 10, with no trace of correlation between the particle size distribution.

d) toothpastes

Sixteen toothpastes produced in Poland and imported were analyzed [24] using methods provided by the Polish Standards [29]. In addition consumer tests were performed (D13 – D25) assigning values in range 0 – 5. Totally twenty five descriptors were evaluated, including: D1 – water and volatile substances, D2 – pH, D3 – phosphates, D4 – chlorides, D5 – stampness, D6 – sweeteners (yes no), D7 – stability at 35°C, D8 – stability at –10°C, D9 – taste and smell, D10 – non disease bacteria, D11 – mould, D12 – heavy metals, D13 – 15 appearence, D16 – 17 odour, D18 – consystency, D19 – yield, D20 – 21 taste, D22 – foam, D23 – freshness, D24 – suitability for children and D25 – polishing property.

Data matrix of format 16 x 25 after standardization has been used in PCA calculations. The correlation coefficient matrix contains numerous significant appearing mainly between customer descriptors and only very few between descriptors provided by the Polish Standard, for example D3 – D4 (r = 0.73), D5 – D9 (r = 0.71) and D6 – D12 (r = 1.00). The last correlation between the content of heavy metals and sweeteners seems to be an effect of a very raw method of estimation (present – absent, trace).

Three principal components describe more than 71% of total data variability. The first principal component is strongly associated with the content of water and volatile substances D1, and various consumer's descriptors such as colour – D15, yield – D19, polishing property – D25, typical smell – D17 and typical taste – D21. The second one is associated with pH – D2 and both content of heavy metals and sweeteners – D6 and D12, and the third is connected with the content of phosphates and chlorides – D3, D4, respectively.

Three dimensional image of principal components loadings is presented in Figure 11. FRESHPEPSODENT 1 and PEPSODENT 2, the best toothpastes form a cluster apart from the others. All products from Bulgaria 4-8 are close in the space of loadings. NIVEA 10 and SALODENT 9 may be treated as outliers of low quality in accordance to the consumer opinion. The remaining home products form two clusters of similar quality. The classification on the basis of loading image has been prooved by the non-hierarchical classification.

2.4. *Analysis and differentiation of honeys*

A chemical composition of bee-honey is complex and diverse, depending on various factors. Values of physical and chemical parameters describing various properties vary within wide ranges [30], reducing the possibility of identifying the origin of honey sample. However, the set of data on over hundred samples of various honeys of different geographical location (rape – *Brassica*, linden – *Tilia* and floral from nectars of different flowers as well as honeydew honeys) collected in our Institute [31]

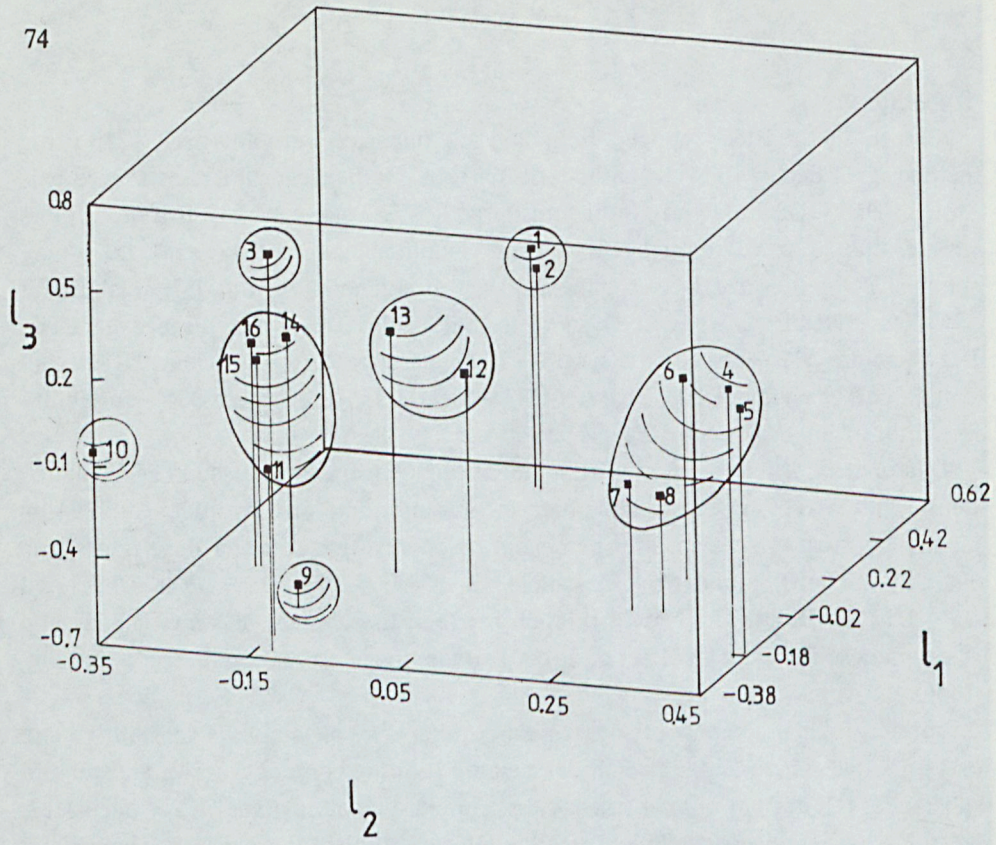


Figure 11. Three dimensional image of toothpaste loadings indicate outliersa and classes

was suitable for PCA. For each sample the following descriptors were evaluated: moisture, reducing sugars, sucrose, ash, free acids, lactone, pH, diastaze number and electrical conductivity. The data matrix of format 104 x 10 (in addition to those mentioned above, the sum of acids and lactone was used) has been performed. Three principal components describe 76.6% of the total data variability, the following next three increase this number to 95.2%. The interpretation of all components is not possible. The first one is strongly associated with diastaze number, pH, ash content and electrical conductivity; the second – with lactone content. The content of the third principal component of the third principal component is not clear. The correlation coefficients between ash and electrical conductivity is very high (r = 0.93) and for other descriptors influencing PC1 is less than 0.63.

The classification of honeys is based on loadings of principal components and may be seen in Figure 12. Three groups are well distinguishable: rape honeys, linden and floral honeys and honeydew honeys. Rape honeys occupied a separate position (except two samples) on the left side of the plot, linden and floral honeys occupied the middle, and honeydew honeys are located to the right. Unfortunatelly there is no clear distinction between linden and floral honeys. The main descriptors influencing

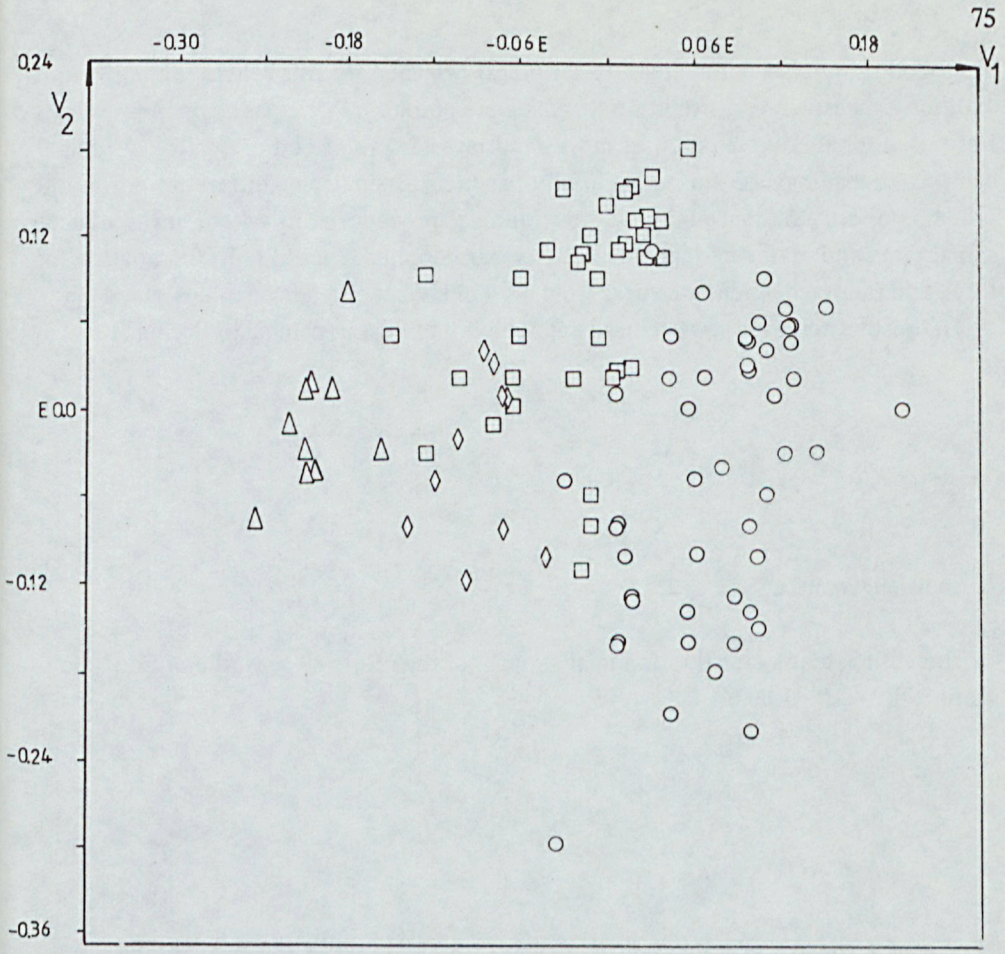


Figure 12. Differentiation of honeys: △ – ape honeys, ◇ – linden and multifloralhoneys and ○ – honeydew honeys on two dimensional plot of 103 samples

the classification are electrical conductivity (in ranges 1.5-2.3, 5-7 and 10-12·10^{-4} s·cm^{-1} for rape, floral and honeydew honeys) and ash content. The acidity of samples determines their location in the horizontal direction.

It may be concluded now, that the classification of honey samples by PCA [32] agree in principle with the sensoric classification. The points of interest are samples located on the borders between classes or incorrectly placed and the possibility of breaking the class of floral honeys into more definite classes.

3. Conclusions

PCA has been used to analyze the large data matrices (tables) on various commodities: washing powders, toilet soaps, toothpastes and honeys. Each product was

described by typical parameters (descriptors) provided by the Polish Standards and additional measures (eg. usefulness, consumers opinion). Principal component scores were used for the explanation of most important factors affecting quality. Principal component loadings were used to classify products as similar or different and to find products of outstanding quality. Both graphical procedures in two or three dimensional plots and mathematical calculations were applied. In addition, the analysis of three and four component mixtures from a set of UV spectra has been described.

The results achieved show a large applicability of PCA in commodity science.

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ZASTOSOWANIE ANALIZY GŁÓWNYCH KOMPONENTÓW W TOWAROZNAWSTWIE

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Streszczenie

Przedstawiono zastoşowanie Analizy Głównych Komponentów do analizy doświadczalnych danych zgromadzonych dla różnych grup towarów (proszki do prania, mydła toaletowe, pasty do zębów, miody). Opisano zastosowanie tej metody do rozwiązania mieszanin dwu- i trójskładnikowych i do analizy profili rozkładu cząsteczek w analizie sitowej. Z reguły 2 lub 3 komponenty opisują większą część całkowitej zmienności danych. Wskazano na możliwość klasyfikowania zmiennych i wyrobów. Opisano obliczanie ogólnego wskaźnika jakości z uzyskanych wyników AGK.

ПРИМЕНЕНИЕ АНАЛИЗА ГЛАВНЫХ КОМПОНЕНТОВ В ТОВАРОВЕДЕНИИ

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Резюме

Представлено применение Анализа Главных Компонентов для рассмотрения экспериментальных данных разных групп товаров (стиральный порошок, туалетное мыло, зубная паста, мёд). Описано применение этого метода для определения концентрации двух- и трёхкомпонентных смесей и для анализа профиля распада молекул в ситовом анализе. Как правило, 2 или 3 компонента характеризуют большую часть переменности данных. Показана возможность классификации переменных и изделий. Описано вычисление общего показателя качества на основе полученных результатов АГК.