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# APPLICATION OF MULTI-PARAMETER DATA VISUALIZATION BY MEANS OF MULTIDIMENSIONAL SCALING TO EVALUATE POSSIBILITY OF COAL GASIFICATION

# WYKORZYSTANIE WIZUALIZACJI WIELOWYMIAROWYCH DANYCH PRZY UŻYCIU SKALOWANIA WIELOWYMIAROWEGO DO OCENY MOŻLIWOŚCI ZGAZOWANIA WĘGLA

The application of methods drawing upon multi-parameter visualization of data by transformation of multidimensional space into two-dimensional one allow to show multi-parameter data on computer screen. Thanks to that, it is possible to conduct a qualitative analysis of this data in the most natural way for human being, i.e. by the sense of sight. An example of such method of multi-parameter visualization is multidimensional scaling. This method was used in this paper to present and analyze a set of seven-dimensional data obtained from Janina Mining Plant and Wieczorek Coal Mine. It was decided to examine whether the method of multi-parameter data visualization allows to divide the samples space into areas of various applicability to fluidal gasification process. The "Technological applicability card for coals" was used for this purpose[Sobolewski et al., 2012; 2013], in which the key parameters, important and additional ones affecting the gasification process were described.

**Keywords:** coal gasification, multidimensional visualization, multidimensional scaling, MDS, multidimensional data, jigging

Metody służące do wizualizacji złożonych, wielowymiarowych danych poprzez transformację przestrzeni wielowymiarowej do dwuwymiarowej umożliwiają prezentację tych danych na ekranie komputera. Tym samym są przystępnym instrumentem analizy zbiorów danych, pozwalającym wykorzystać połączenie naszego wzroku z mocą naszej osobistej sieci neuronowej (mózgu) do wyodrębnienia z danych

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cech, których zauważenie przy pomocy innych metod może być bardzo trudne. W artykule zastosowano jedną z takich metod – skalowanie wielowymiarowe – w celu sprawdzenia, skuteczności tej metody do analizy próbek węgla ze względu na jego przydatność do procesu zgazowania w kotle fluidalnym. W tym celu pobrano próbki dwóch węgli, z KWK „Wieczorek" (węgiel typu 32) oraz ZG „Janina" (węgiel typu 31.2), które następnie miały być poddane testom pod względem ich przydatności do zgazowania. Każda z próbek została zbadana ze względu na cechy, których określone poziomy są kluczowe oraz wskazane w kontekście procesu zgazowania według „Karty przydatności węgli do zgazowania" (Sobolewski et al., 2012; 2013).

Każdy z węgli został rozdzielony na osadzarce pierścieniowej (10 pierścieni, uziarnienie węgla 0-18 mm) w wyniku czego powstało pięć warstw (po 2 pierścienie każda). Następnie każda z warstw została rozsiana na 10 klas ziarnowych. Tak otrzymane produkty zostały poddane technicznej oraz chemicznej analizie (ogółem 50 próbek z ZG „Janina" oraz 49 próbek z KWK „Wieczorek" – klasa ziarnowa 16-18 mm w tej drugiej kopalni nie została uzyskana i pomiar był niemożliwy do zrealizowania. Tym samym otrzymano takie parametry do analizy jak: zawartość siarki, zawartość wodoru, zawartość azotu, zawartość chloru, zawartość węgla organicznego, ciepło spalania oraz zawartość popiołu. W wyniku przeprowadzonych badań oraz porównania ich z wymogami prezentowanymi w „Karcie przydatności węgli do zgazowania" okazało się, że tylko 18 próbek spełnia wszystkie wymogi, z czego aż 17 pochodziło z KWK „Wieczorek". Postanowiono poddać ocenie wszystkie próbki bardziej złożonej obserwacji – wielowymiarowej analizie danych za pomocą skalowania wielowymiarowego.

W rozdziale 3 przedstawiono szczegółowo zastosowaną metodologię analizy wraz z opisem algorytmu. Następnie, w rozdziale 4 przedstawiono wyniki obserwacji przeprowadzonych za pomocą opracowanego w tym celu programu komputerowego, napisanego w języku C++. Rysunki 1-3 przedstawiają sytuację, gdzie dane reprezentujące próbki węgla mniej lub bardziej przydatne do zgazowania zaczynają tworzyć podgrupy. Proces grupowania został przedstawiony etapowo, tzn. rys. 1 prezentuje sytuację wyjściową, Rys. 2 sytuację przy bardzo małej wartości parametru ITER = 5, zaś Rys. 3 najlepszy możliwy widok, otrzymany przy wartości parametru ITER = 340. Widać na tym rysunku, że obrazy punktów reprezentujących próbki węgla bardziej oraz mniej podatnego na zgazowanie zajmują osobne podobszary. Widać, że na całym obszarze rysunku, podobszary te można łatwo od siebie odseparować. Przez to możemy na podstawie tego rysunku stwierdzić, że skalowanie wielowymiarowe pozwala podzielić przestrzeń próbek na obszary o różnej przydatności do procesu zgazowania fluidalnego. Dzięki temu analizując następne, nieznane próbki możemy poprzez ich wizualizację zakwalifikować je do grupy bardziej podatnych na zgazowanie lub mniej podatnych na zgazowanie. Ważne jest to szczególnie dlatego, ponieważ w analizowanej sytuacji próbki węgla bardziej podatnego na zgazowanie zajmują wnętrze siedmiowymiarowego prostopadłościanu – co jest znacznym uproszczeniem. Wynika to bezpośrednio z faktu, iż przyjęte warunki określające przynależność do tej grupy („Karta przydatności Technologicznej węgla") to proste nierówności przy pomocy których łatwo można sprawdzić taką przynależność. W rzeczywistości, może się jednak okazać, że obszar przynależności może mieć znacznie bardziej skomplikowany kształt. Wtedy na podstawie większej ilości próbek, których przynależność do klasy węgla bardziej podatnego na zgazowanie zostanie stwierdzona empirycznie, można będzie próbować przy pomocy skalowania wielowymiarowego uzyskać podział przestrzeni na obszary reprezentujące próbki węgla bardziej oraz mniej podatnego na zgazowanie. Rys. 4 przedstawia podobny podział, ale bez wzięcia pod uwagę parametru „zawartość chloru". Również i w tym przypadku próbki węgla mniej lub bardziej podatnego na zgazowanie tworzą wyraźne podgrupy. Przy pominięciu parametru „zawartość chloru" już 78 próbek (37 z ZG „Janina" oraz 41 z KWK „Wieczorek") z analizowanych 99-ciu spełniałoby wymogi zawarte w „Karcie przydatności węgla do zgazowania".

Rys. 5 przedstawia inne podejście do analizowanych próbek węgla. Tym razem za kryterium podziału przyjęto pochodzenie węgla z KWK „Wieczorek" lub ZG „Janina", bez rozpatrywania ich w kontekście przydatności do zgazowania. Również i tym razem okazało się, że zastosowana metodologia pozwala stwierdzić możliwość efektywnego rozdzielenia, a tym samym prawidłowego rozpoznania analizowanych próbek węgla. Tym samym dowiedziono, że metoda skalowania wielowymiarowego może być bardzo przydatnym narzędziem podczas wieloparametrycznej analizy próbek różnego typu węgli.

**Słowa kluczowe:** zgazowanie węgla, wizualizacja wielowymiarowa, skalowanie wielowymiarowe, MDS, wielowymiarowe dane, wzbogacanie w osadzarkach

# 1. Introduction

In the article, coal samples obtained from two coal mines, Janina Mining Plant and Wieczorek Coal Mine, were analysed. The above mentioned samples were taken in order to evaluate their suitability for on-surface gasification in fluidised bed. The properties of coals directed to gasification must comply with the limits (Agrawal, 2011; Blaschke, 2009; Borowiecki et al., 2008; Chmielniak & Tomaszewicz, 2012; Kosminski et al., 2006; Lee et al., 2007; Marciniak-Kowalska, 2012-13; Strugała et al., 2011; Strugała & Czerski, 2012; Surowiak, 2013a; b; 2014a; b), wherein it must be noted that they are linked with each other. The evaluation of coal suitability for gasification should be therefore conducted multidimensionally with the use of multidimensional distributions of properties and their statistics (Ahmed & Drzymała, 2005; Brożek & Surowiak, 2005; 2007; 2010; Drzymała, 2007; 2009; Jamróz, 2001; 2009; 2014a; b; c, in print; Jamróz & Niedoba, 2014; 2015; Niedoba & Jamróz, 2013; Niedoba, 2009; 2011; 2013a; b; 2014; Niedoba & Surowiak, 2012; Saramak, 2013; Surowiak & Brożek, 2014a; b; Szostek & Suraj, 2002; Szostek, 2003; Tumidajski, 1997; Tumidajski & Saramak, 2009). It is a natural thing that the analysis of multidimensional properties and statistics begin with the analysis of particle density distribution and particle size distribution of coals and then is extended on the basis of further coal properties, especially the contents of components and reactions to the processes of its processing. While the analysis of coal in terms of distribution of the so-called class-fraction provides the initial information on the coal capability of developing the surface area and concentration of flammable and volatile parts and ash, multidimensional methods of visualisation allow for the combined interpretation of all measured properties in tested terms.

# 2. Data

In order to investigate the mineral beneficiation capability intended for the process of gasification in fluidised bed, i.e. bituminous coals from Janina Mining Plant (coal of 31.2 type) and Wieczorek Coal Mine (coal of 32 type), each of them was subjected to beneficiation process in the laboratory ring jig (10 rings, coal in the class of 0-18 mm). After the completion of the separation process, material was divided into 5 layers (with 2 rings) and each of them was sieved on sieves into 10 grain classes, establishing yields of layers and classes. Subsequently, products obtained in such a way: grain classes, after the separation of analytical samples, were subjected to chemical elemental and technical analysis of coal in order to describe features influencing gasification processes.

In total, from both coal mines, 99 samples (50 from Janina Mining Plant and 49 from Wieczorek Coal Mine; in one of the layers 16-18 mm class was not obtained) were obtained with the following parameters: total sulphur content, hydrogen content, nitrogen content, chlorine content, total carbon content, heat of combustion and ash content. Additionally, the card of technological suitability of coal was used (Sobolewski et al., 2012; 2013), which describes key, relevant and additional parameters affecting the gasification process. The card was used to indentify coal samples, which are subjected to the gasification process in an effective way. The conditions used involved: calorific value [kJ/kg] >18000, ash content <25%, chlorine content <0.1%, total sulphur content <2%, carbon content >60%, 3.5% ≤hydrogen content ≤5.5%, nitrogen content <2%. On the basis of the presented conditions, only 18 out of the analysed 99 samples were identified as suitable for gasification in an effective way. Among the above 18 samples, 17 came from Janina Mining Plant and only one sample from Wieczorek Coal Mine. The whole set of data may be found in (Dzik et al., 2014; Gawenda et al., 2014a; b; Marciniak-Kowalska, 2012-13; Marciniak-Kowalska et al., 2014).

# 3. Multidimensional scaling

## 3.1. Description of the method

Multidimensional scaling (MDS) is the method based on mapping of $n$-dimensional space into $m$-dimensional space. It is based on calculation of a distance between each pair of $n$-dimensional points. On the basis of these distances the considered method determines mutual location of these points images in destined $m$-dimensional space. Let $d_{ij}$ denote distance between $n$-dimensional points of no. $i$ and $j$. Multidimensional scaling is based on such location of points in $m$-dimensional space that distance $D_{ij}$ calculated in this space between mapped points of no. $i$ and $j$ is possibly closest to $d_{ij}$. The operation of algorithm MDS can be based on iterative change of location of randomly (initially) located points in $m$-dimensional space in the way ensuring that the function $S = \sqrt{\sum_{i>j} \left(D_{ij} - d_{ij}\right)^2}$ achieves the smallest possible value. For $m = 2$ this method allows to watch multidimensional data directly on two-dimensional computer screen (Jamróz, 2014b; Kruskal, 1964; Kim et al., 2000).

## 2.2. Algorithm

The initial data set consists of parts described by n features. It can be treated then as a set of $n$-dimensional vectors. Let $i^{th}$ denote initial data vector $x_i = (x_{i,1}, x_{i,2}, \dots x_{i,n})$. The algorithm used for the visualization by means of multidimensional scaling consists of several steps:

1. Scaling of initial data. Individual features represented by individual data dimensions must be scaled in a way ensuring their suitability in the same desired range. It was decided to scale individual coordinates (features) of data set vectors to range (0, 1).
2. Randomization of initial location of points images in 2-dimensional space. Let us assume that image of $i^{th}$ point $x_i$, so the point related to it in 2-dimensional space will be marked as $p_i=(u_i, v_i)$. Because in the previous point each coordinate of data vectors was scaled to range (0, 1) the data set fits $n$-dimensional box of side length equal to 1. It occurs that the greatest distance between two points of this set can be the same as the length of $n$-dimensional box diagonal, so it is equal to $\sqrt{n}$. Therefore, the initial coordinates $u_i$ and $v_i$ are being randomized from range $\left(0, \sqrt{n}\right)$ by means of uniform probability distribution.

   Next points 3-5 are realized for each possible pair $i, j$ of initial data vectors ITER Times (where ITER means parameter accepted in a certain moment):
3. For the next pair of points $x_i$, $x_j$ their distance is calculated by means of Euclidean metric:

$$d_{ij} = \sqrt{\sum_{k=1}^{n} \left(x_{i,k} - x_{j,k}\right)^2} \tag{1}$$

4. For the next pair of points images $p_i = (u_i, v_i)$, $p_j = (u_j, v_j)$ their distance is calculated by means of Euclidean metric:

$$D_{ij} = \sqrt{\left(u_i - u_j\right)^2 + \left(v_i - v_j\right)^2} \tag{2}$$

5. The location of image $p_j$ is changed in the way ensuring distance $D_{ij}$ to be possibly closest to $d_{ij}$:

$$\tilde{u}_j = u_j + 0.01\frac{\left(u_j - u_i\right)\left(d_{ij} - D_{ij}\right)}{D_{ij}} \tag{3}$$

$$\tilde{v}_j = v_j + 0.01\frac{\left(v_j - v_i\right)\left(d_{ij} - D_{ij}\right)}{D_{ij}} \tag{4}$$

where $\tilde{u}$ and $\tilde{v}$ are values after change. Equations (3) and (4) cause that point $p_j$ is closer to the point $p_i$ when $D_{ij} > d_{ij}$ and farther from $p_i$ when $D_{ij} < d_{ij}$. The allocation of point $p_j$ occurs on straight line passing through points $p_i$ and $p_j$. The constant 0.01 means the speed of points allocation in proper directions.

The application of the abovementioned procedure made it possible to obtain multidimensional initial data points in two-dimensional space. It is sufficient now to present image of each vector on computer screen. It is realized by drawing a symbol representing a fraction to which related data vector $x_i$ belongs in location of coordinates $(u_i, v_i)$. This is how the image of multidimensional points is created on computer screen for which the mutual distances are possibly preserved.

## 4. Experimental results

A computer program was developed based on the assumptions presented in the previous chapter for the purpose of visualization of 7-dimensional data describing coal samples. It was written in programming language C++ by means of Microsoft Visual Studio software. The efficiency of this program was verified multiple times. It was successfully applied in many previous works (Jamróz, 2014; in print; Jamróz & Niedoba, 2015). The obtained results were presented in Figs. 1-5. These views show the way 7-dimensional data is transformed into two dimensions by means of multidimensional scaling method. It should be noticed that these Figures show the best obtained results which in Multidimensional Scaling method depend significantly on a choice of initial random values. By selecting other random values these results were less readable or even did not allow to make any conclusions. The algorithm of multidimensional scaling works in the way ensuring to maintain mutual distances between any two points despite a significant reduction of dimensions number. In this way it is possible to see important features of 7-dimensional data on 2-dimensional computer screen.

It was decided to examine whether the multi-parameter visualization method allows to divide space of samples into areas of various suitability for fluidal gasification process. Figs. 1-5 show the views of points representing 7-dimensional data vectors describing coal samples obtained from Janina Mining Plant or Wieczorek Coal Mine. From Figs. 1-3 it can be seen how grouping of the points representing discussed data grows according to division into coal samples less or

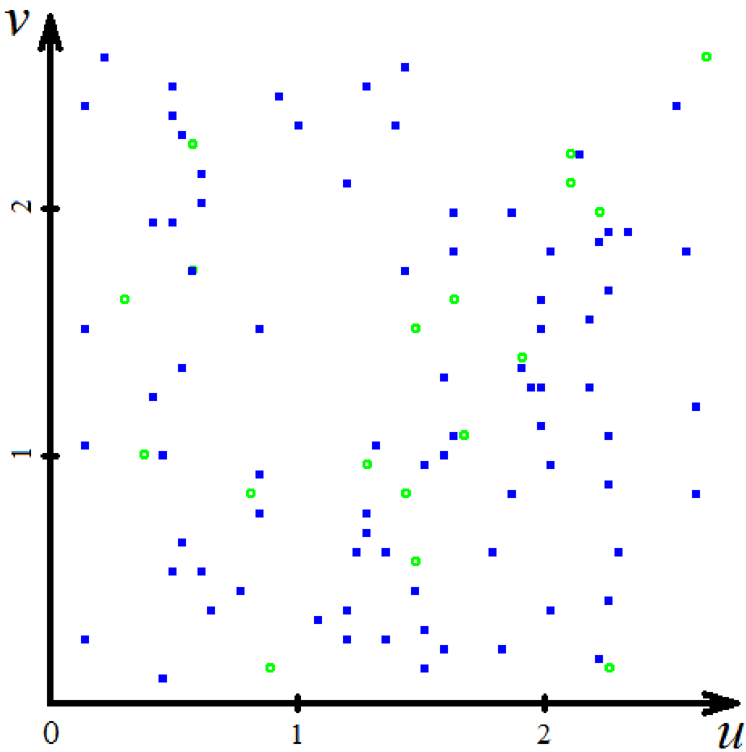


Fig. 1. Initial setting in which each point image representing 7-dimensional coal samples is random. The images of points representing coal samples less suitable for fluidal gasification process were marked as (■), images of points representing coal samples more suitable for fluidal gasification process were marked as (○)

more suitable for gasification along with the growth of value of the parameter ITER. It can be noticed that point images of data representing the same coal fractions start to locate in separated sub-areas and start to group. The clearness of the space division grows with the growth of the value of parameter ITER, which means that the distance of points images $D_{ij}$ in 2-dimensional space and original distances $d_{ij}$ between points in $n$-dimensional space are more and more fitted. Figure 1 presents the initial setting in which each image of point is randomly located on the screen. Figure 2 shows that even by a small value of the parameter ITER = 5 the images of points representing the same fractions start to group.

Fig. 3 reveals the clearest result of division of coal more and less reliable for gasification which was achieved for the discussed data. It occurred by value of the parameter ITER = 340. It can be seen from this Figure that images of points representing coal samples more or less reliable for gasification are located in the separated sub-areas. In the whole area of the picture, these sub-areas can be easily separated. Based on this figure it is further possible to state that multidimensional scaling allows to divide samples space into areas of various applicability to fluidal gasification process. Thanks to it, following analyses of unknown samples will make it possible to qualify them to a group more or less reliable to gasification. It is particularly important because samples of coal more reliable to gasification in the analyzed situation are inside the 7-dimensional cuboid,

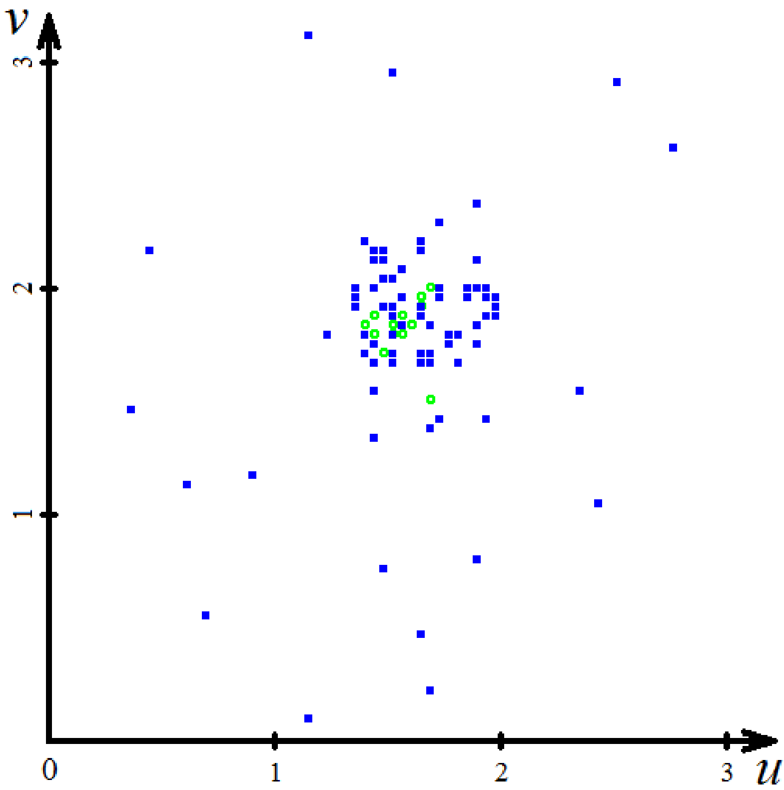


Fig. 2. View of 7-dimensional data representing coal samples of various suitability for fluidal gasification process by value of the parameter ITER = 5. The start of grouping is visible. The images of points representing coal samples less suitable for fluidal gasification process were marked as (■), images of points representing coal samples more suitable for fluidal gasification process were marked as (○)

which is a considerable simplification. It occurs directly from the fact that accepted conditions determining membership to this group are simple inequalities by which means is easy to verify such membership (Technological applicability card for coals). However, in reality it can occur that an area of membership can have much more complicated shape. Then, on the basis of the higher amount of samples whose membership to a group more or less reliable to gasification was empirically proved, it will be possible to try to divide the space into areas representing coal samples more or less reliable to gasification by means of multidimensional scaling. It can occur that obtained mapping will express the reality more adequately. That is why the previous statement referring to the fact that multidimensional scaling allows to divide space of samples into areas of various reliability to fluidal gasification process becomes essential.

Additionally, as it occurs, the same division of space contains much more information. This is shown in Fig. 4, which presents the discussed data according to division into coal samples more or less reliable to gasification without the condition concerning chlorine contents (by the same value of the parameter ITER = 340). It is also the place where, despite avoiding the condition concerning chlorine contents, images of points representing coal samples more or less reliable

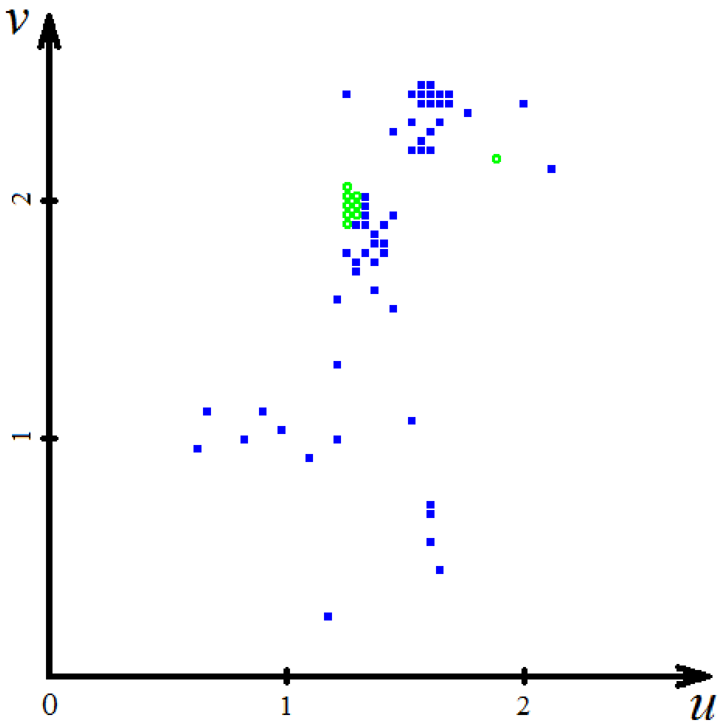


Fig. 3. The clearest view obtained for 7-dimensional data representing coal samples of various suitability for fluidal gasification process by value of the parameter ITER = 340. The images of points representing coal samples less suitable for fluidal gasification process were marked as (■), images of points representing coal samples more suitable for fluidal gasification process were marked as (○)

to gasification gather in different sub-areas. It is visible that in the whole area of the Figure these sub-areas can be easily separated. So, it can be stated that multidimensional scaling allows to divide space of samples into areas of various reliability to fluidal gasification process even by change of conditions determining this reliability. In this case, it has a significant meaning because chlorine contents have the influence only on the pollution level created as a result of gasification, not on the efficiency of the process itself. However, the assignment of the samples changes. For example, in Fig. 3 only 18 samples were marked as these which can be gasified efficiently. Out of these 18 samples, 17 originated from Janina Mining Plant and only one originated from Wieczorek Coal Mine. In contrast, after omitting the condition concerning chlorine contents (Fig. 4), out of the analyzed 99 coal samples as many as 78 samples were marked as these which can be gasified efficiently. In this case,, 37 out of 78 samples originated from Janina Mining Plant and 41 from Wieczorek Coal Mine. It can be stated that if pollution with chlorine contents can be omitted, the gasification of coal originating from Wieczorek Mining Plant will be more efficient as opposed to the case with Janina Coal Mine.

Fig. 5 presents view of the discussed data according to a completely new division: the division into coal samples from Janina Mining Plant and Wieczorek Coal Mine. It can be seen from this figure that images of points representing coal samples from various mines gather in

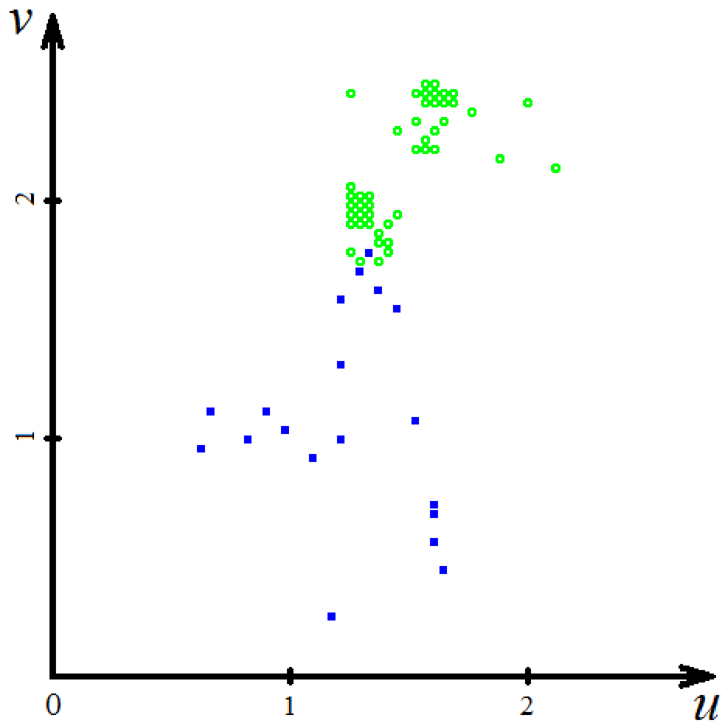


Fig. 4. View of 7-dimensional data with division regarding various suitability for fluidal gasification process without chlorine contents condition by value of the parameter ITER = 340. The images of points representing coal samples less suitable for fluidal gasification process were marked as (■), images of points representing coal samples more suitable for fluidal gasification process were marked as (○)

separated sub-areas. It is visible even more clearly that these gatherings can be easily separated in the whole area of the figure. On this basis it can be stated that multidimensional scaling allows to divide samples space into areas representing various mines. Thanks to that, it is possible to qualify samples originating from Janina Mining Plant or Wieczorek Coal Mine by their visualization during analysis of other unknown samples.

It is worthpaying attention to the fact that the algorithm of multidimensional scaling does not benefit from information about membership of points representing data to certain fractions. In this situation the grouping of images of points representing certain fraction depends only on some data properties noticed by the algorithm. That is why Figures 3, 4 and 5 differ only in terms of membership of individual points to various fractions. It occurs from the fact that these three Figures were created as the result of multidimensional scaling algorithm work on precisely the same 7-dimensional data and by the same value of the parameter ITER = 340 with omitting the information about membership of the points to individual fractions. That is why the location of points in Figures 3, 4 and 5 is identical. Only allocation of individual points to appropriate fractions is different.

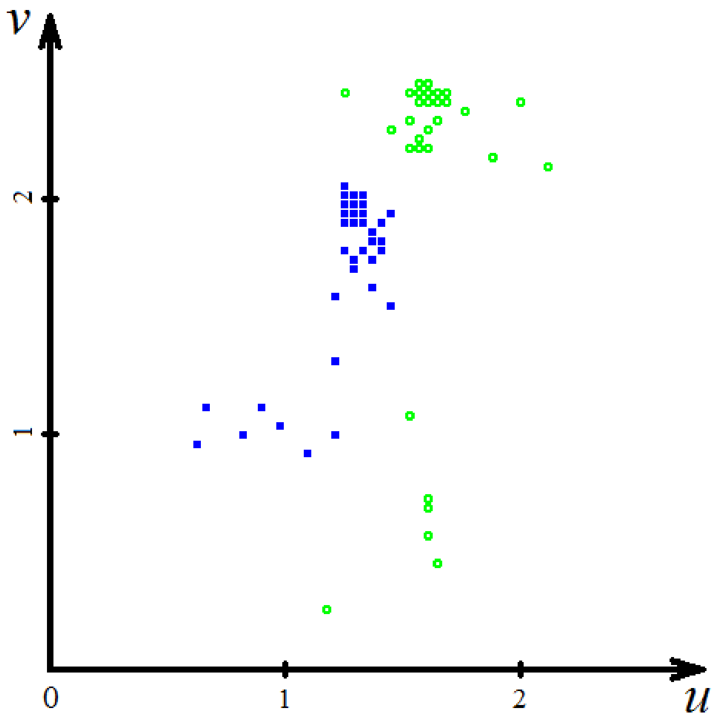


Fig. 5. View of 7-dimensional data with division regarding the location of sampling by value of the parameter ITER = 340. The images of points representing coal samples obtained in "Janina" mine were marked as (■), images of points representing coal samples obtained in "Wieczorek" mine were marked as (○)

## 5. Conclusions

The conducted experiments based on visualization of 7-dimensional data by means of multidimensional scaling allowed to arrive at the following conclusions:

1. Multi-parameter visualization by means of multidimensional scaling allows to state that images of points representing coal samples more or less reliable to gasification are located in separated sub-areas of the space. Thus, multidimensional scaling allows to divide view of samples space into areas of various reliability to fluidal gasification process. Thanks to it, the analysis of other unknown samples by their visualization makes it possible to qualify them to a group more or less reliable to gasification.
2. As a result of visualization drawing upon multidimensional scaling it is possible to state that images of points representing coal samples from Janina Mining Plant and Wieczorek Coal Mine are located in separated sub-areas which can be easily separated. Thanks to it, the space of samples can be divided into areas representing various mines, thus allowing other unknown samples to be qualified through visualization according to their origin to group originated from Janina Mining Plant or Wieczorek Coal Mine.
3. Algorithm of visualization by multidimensional scaling does not benefit from information about membership of points representing data to specified fractions. In this situation

the grouping of images of points representing certain fraction depends only on some properties of thedata noticed by the algorithm, regardless of their affiliation to individual fractions.

4. The same division of samples space conducted by means of multidimensional scaling groups at the same time points representing analyzed data according to both location of their extraction (Janina Mining Plant and Wieczorek Coal Mine) and their reliability on fluidal gasification process.
5. On the basis of "Technological applicability card for coals", only 18 out of the 99 analyzed coal samples were marked as these which can be gasified efficiently. 17 out ofthese 18 samples originated from Janina Mining Plant and only one from Wieczorek Coal Mine.
6. Situation changes completely by omitting a condition concerning chlorine contents. In such case, on the basis of the same "Technological applicability card for coals" 78 out of 99 samples, were marked as these which can be gasified efficiently, 37 of which originated from Janina Mining Plant and 41 from Wieczorek Coal Mine.
7. The transparency of the results grows with more precise fitting of distances $D_{ij}$ of points images in 2-dimensional space to original distances $d_{ij}$ between points in n-dimensional space (with the growth of the value of parameter ITER).
8. The transparency of obtained results depends significantly on accepted parameters.
9. One problem occurring from such visualization is the necessity of selecting parameters for the purpose of obtaining a view which clearly presents the information pursued by the researcher. It is worth mentioning that during the conducted experiments the views were obtained by the value of parameter ITER rangingfrom 1 to 10000. The experiments were conducted many times by renewed generation of random initial values. On some occasions, it led to clearer results. Also, various speeds of learning were accepted before obtaining the one presented in equations (3) and (4). The paper presents the clearest of all obtained results.

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