Application of Factor Analysis for the Study of Physicochemical Properties in Different Blends of Diesel Fuel with Biodiesel

Tsanaktsidis C.G., Vasiliadis V., Itziou A., Petrakis L.A., Moisiadis S.A.

Abstract*— The present study focused on the investigation of an alternative energy resource, biodiesel. In order to check the appropriateness of biodiesel, its physicochemical properties were analyzed. The main aim of the present study was to investigate the differentiations in the physicochemical properties of several blends of diesel/biodiesel. Thus, the results were integrated through the factorial analysis, and a unit circle was designed in order to study the correlations among the properties (variables) tested. The results of the current study indicated significant correlations among the properties tested. The results of this study can be useful in developing new educational products, with a view to understanding of mathematical concepts through everyday activities such as the use of fuel.

***Index Terms*— factor analysis, diesel, biodiesel, physicochemical properties.**

I. INTRODUCTION

The biggest challenge modern industrial society is facing today is the decline and exhaustion of the fossil energy resources. The primary sources of energy that power our civilization are those fossil fuels [1]. Therefore continued use of petroleum-sourced fuels is now widely recognized as unsustainable because of depleting supplies and increasing demand. In addition, the combustion of the fossil fuels used is considered as the major factor responsible for global warming due to large-scale carbon dioxide emissions. The IPCC Special Report on Emissions Scenarios gives a wide range of future carbon dioxide scenarios, ranging from 541 to 970 ppm by the year 2100. Fossil fuel reserves are sufficient to reach this level and continue emissions past 2100, if coal, tar sands or methane clathrates are extensively used [2]. Fossil fuels are also considered as the main source of local environmental pollution.

Thus, alternative energy sources based on sustainable, renewable and environmentally friendly processes are urgently needed. One of the most prominent alternative energy resources is biodiesel.

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Because of diminishing petroleum reserves and the deleterious environmental consequences of exhaust gases from petroleum diesel, biodiesel has been receiving more attention all over the world due to energy needs and environmental consciousness [3]. It is a renewable and biological origin alternative diesel fuel [4]. Many studies have shown that the properties of biodiesel are very close to diesel fuel [5, 6, 7]. Therefore, biodiesel fuel can be used in diesel engines with little or no modification. Biodiesel has a higher cetane number than diesel fuel, no aromatics, no sulfur, and contains 10-11% oxygen by weight. These characteristics of biodiesel are responsible for a reduction in the emissions of carbon monoxide (CO), hydrocarbon (HC) and particulate matter (PM) in the exhaust gas compared to diesel fuel [8, 9]. However, to be a viable alternative, a biodiesel should provide a net energy gain, be economically competitive, and be producible in large quantities without reducing food supplies [10].

The present study focused on the investigation of the appropriateness of the final product, so that it could be beneficially used as an energy source being at the same time friendly to the environment. The quality testing of liquid alternative fuels principally aims at ascertaining to what extent the fuel is suitable in order to ensure the reduction of environmental pollution, the sound operation of the combustion machine and the highest work output through its use. The qualitative testing is expressed by a series of physicochemical properties, and compared to specific specifications. The proposed methods of analysis are based on the general directions set by ASTM (American Society for Testing Materials) testing process as well as I.P. (Institute of Petroleum) [11].

In the United States, biodiesel is sold as a blend with petroleum diesel, as either B2 (2% biodiesel) or B20 (20%), and is considered oxygenate. Such employment is likely to affect the quantity and the composition of emissions and potential biologic effects of the exhaust [12]. Eventually, research into potential consequences of biodiesel exhaust exposure on human health will have to consider blends. Thus, there is a strong desire and need for alternative fuels. Employment of biodiesel fuel is favorably viewed, and there are suggestions that its exhaust emissions are less likely to present any risk to human health relative to petroleum diesel emissions [13]. However, the speculative nature of a reduction in health effects based on chemical composition of biodiesel exhaust needs to be followed up with investigations using newer biologic approaches gained from years of diesel research. Studies into health effects of exposure to biodiesel exhaust should be initiated [14].

The results of this study can be useful in developing new educational products, in the development of teaching methodologies, with a view to understanding of mathematical concepts through everyday activities such as the use of fuel. Moreover, the proposed results can be included in textbooks for educational institutions. Finally, they could be used in industrial research in the design of new products, through exported software which would foresee the physicochemical properties of the fuel by applying a simple equation. This would lead to cost reduction analysis as well as to more immediate deliverables.

The main aim of the present study was to investigate the differentiations in the physicochemical properties of several blends of diesel/biodiesel. Thus, the results were integrated through the factorial analysis, and a unit circle was designed in order to study the correlations among the properties (variables) tested.

II. MATERIALS AND METHODS

A. Production of biodiesel

Biodiesel is produced through transesterification [15] and it involves reacting vegetable oils or animal fats with a short-chain aliphatic alcohol (typically methanol or ethanol), with the presence of a catalyst, usually a strong base such as sodium or potassium hydroxide, or, preferably and more commonly, alkoxides (Fig. 1). The resulting product may contain not only the desired alkyl ester as a product, but non-reacting material, residual alcohol, and residual catalyst as well. Glycerol is formed as a by-product and is separated from biodiesel during the production process. Nevertheless, traces of glycerol may be detected in the final biodiesel product.

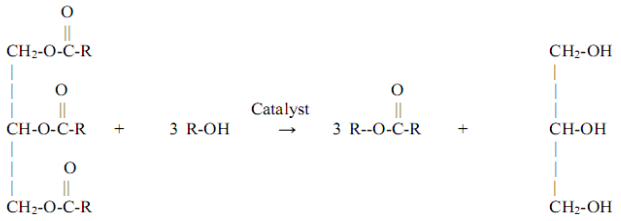

Fig 1. Transesterification reaction.

B. Analysis of physicochemical properties of biodiesel and diesel

After the production of biodiesel, it was considered necessary to check the appropriateness of the final product, by studying its physicochemical properties and by measuring their values. These values were then checked for meeting certain specifications, referred to as biodiesel standards. The European Biodiesel Standards EN 14214 for Vehicle Use are referred in Table 1. It is worth mentioning that some specifications in biodiesel standards are similar to diesel standards, nevertheless, not all test methods applied for diesel analysis are suitable for biodiesel analysis as well.

Diesel oil constitutes a mixture of many hydrocarbons, while each one of them is characterized by different properties. Diesel of internal combustion should have attributes that ensure the auto ignition of the fuel, as well as a secure and smooth combustion without problems in the booth combustion conditions. The properties of the fuel depend on the type and the concentration of the hydrocarbons that it contains. The Greek specifications of fuel Diesel have as objective the satisfaction of certain properties, described by [11]. In the present study, the analysis of the physicochemical properties of both diesel and biodiesel was performed with ASTM.

C. Blends of diesel and biodiesel

Pure diesel and biodiesel by vegetables (vegetable oil fuel) were used. These samples met the specifications of diesel fuel and biodiesel standards described above. Eleven different blends were used. The total volume of each blend was 100 mL and in each blend the volume fraction of diesel/biodiesel was different (100% diesel, 90% diesel-10% biodiesel, 80% diesel-20% biodiesel, 70% diesel-30% biodiesel, 60% diesel-40% biodiesel, 50% diesel-50% biodiesel, 40% diesel-60% biodiesel, 30% diesel-70% biodiesel, 200% diesel-80% biodiesel, 10% diesel-90% biodiesel, and 100% biodiesel).

III. RESULTS AND DISCUSSION

A. Analysis of physicochemical properties of pure biodiesel and diesel

The analysis of the physicochemical properties both of biodiesel and diesel as well are presented in Table 1. The results indicate that both fuels fulfill the necessary requirements that render them as highly qualitative fuels.

Table 1. Laboratory values of pure diesel and Greek specifications (harmonized with the European Community) of diesel fuel (FEK 332/B/11-2-2004, EN 590:1999), as well as laboratory values of vegetable biodiesel and biodiesel standards (European Biodiesel Standards EN 14214 for Vehicle Use).

Physicochemical Property	Diesel Laboratory Values	Diesel Standards	Vegetable Biodiesel Laboratory Values	Biodiesel Standards	Methods of Determination ASTM
Density 15°C, g/mL	0.8259	0.820-0.845	0.8807	0.860-0.900	D1298 - 99(2005) [3]
Conductivity, pS/m	172	50-600	>2000	0-2000	D2624
Humidity, mg/kg	15	<200.0	179.7	<500	D 1744-92(2000) [5]
Kinematic Viscosity, (40°C) mm^2/s (cSt)	2.72	2.00-4.50	4.98	1.9–6.0	D 445 – 06 [4]
Calorific value, kJ/gr	46.428	>43000	40.036	>35000	D4809
Flash point, °C	64	>55	167		D93

B. Analysis of physicochemical properties of blends of diesel and biodiesel

Eight different properties were analyzed in eleven different blends of diesel and biodiesel. The results are presented below (Table 2).

Table 2. Measurement of physicochemical properties in eleven different blends of diesel/biodiesel, where D=diesel, B=biodiesel, V1=density, V2=api, V3=conductivity, V4=humidity, V5=kinematic viscocity, V6=dynamic viscocity, V7=calorific value, V8=flash point.

Diesel/Biodiesel Blends	Physicochemical properties							
	V_1	V_2	V_3	V_4	V_5	V_6	V_7	V_8
100% D	0.8259	39.3	172	15	2.72	2.25	46.428	64
90%D 10%B	0.8299	38.5	206	27.6	2.82	2.34	45.668	67
80%D 20%B	0.8324	38.0	388	52.2	2.95	2.46	44.908	73
70%D 30%B	0.8405	36.3	412	54.6	3.14	2.64	44.152	81
60%D 40%B	0.8473	35.0	450	56.3	3.40	2.88	43.488	90
50%D 50%B	0.8531	33.9	553	65.6	3.74	3.19	42.955	100
40%D 60%B	0.8584	32.9	767	83.2	3.94	3.38	42.399	112
30%D 70%B	0.8714	30.4	1135	95.6	4.14	3.61	41.819	125
20%D 80%B	0.8734	30.0	1240	106.8	4.38	3.83	41.219	138
10%D 90%B	0.8757	29.6	1655	149.8	4.61	4.04	40.619	152
100% B	0.8807	28.7	>2000	179.7	4.98	4.39	40.036	167

Since the previous variables had different values and were expressed in different units of measurement, Table 3 was normalized. Therefore, the following formula was applied to every variable of every column:

$$\frac{v_{ij} - \bar{v}_j}{sj\sqrt{n-1}}$$

where $\bar{v}_j$ is the mean and s_j is the standard deviation of the j column and n is the number of rows of the above matrix. Thus, the following normalized Table 3 resulted:

Table 3. Normalized matrix including the values of the physicochemical properties tested.

-0.43973	0.44599	-0.33372	-0.41529	-0.40859	-0.40639	0.51072	-0.37737
-0.37604	0.38025	-0.31610	-0.33550	-0.36736	-0.35855	0.39537	-0.35059
-0.33624	0.33916	-0.22182	-0.17972	-0.31375	-0.31507	0.28003	-0.29702
-0.20727	0.19946	-0.20938	-0.16452	-0.23541	-0.23679	0.16530	-0.22561
-0.09900	0.09263	-0.18970	-0.15376	-0.12820	-0.13243	0.06452	-0.14526
-0.00665	0.00224	-0.13634	-0.09487	0.01199	0.00237	-0.0163	-0.05599
0.07772	-0.07993	-0.02547	0.01657	0.09446	0.08499	-0.1007	0.05112
0.28471	-0.28537	0.16516	0.09510	0.17693	0.18501	-0.1887	0.16718
0.31655	-0.31824	0.21956	0.16602	0.27589	0.28067	-0.2798	0.28323
0.35317	-0.35111	0.43455	0.43831	0.37073	0.37199	-0.3708	0.40821
0.43278	-0.42507	0.61328	0.62765	0.52330	0.52419	-0.4593	0.54211

The values of Table 3 were characterized by the following properties:

- They were net numbers (they do not have units of measurement)
- Their values were between -1 and 1
- They were of equal magnitude
- The sum of every column was equal to 0 (the sum of all squares was equal to 1)
- The vectors defined by each column had length equal to1

Then, an inertia table (Table 4) was calculated by multiplying the normalized Table 3 with the inversion Table3.

Table 4. The inertia matrix is a rectangular m×m table, where m is the count of variables, that is m=8. The total inertia of the table is equal to m, which is equal to 8. The table is symmetrical to its main diagonal.

1.	-0.99987	0.93673	0.92653	0.98720	0.98803	-0.98792	0.9792
-0.99987	1.	-0.93216	-0.92303	-0.98561	-0.98630	0.98848	-0.97665
0.93673	-0.93216	1.	0.98820	0.96349	0.96638	-0.93510	0.98343
0.92653	-0.92303	0.98820	1.	0.96179	0.96246	-0.94761	0.97545
0.98720	-0.98561	0.96349	0.96179	1.	0.99981	-0.98718	0.99483
0.98803	-0.98630	0.96638	0.96246	0.99981	1.	-0.98607	0.99598
-0.98792	0.98848	-0.93510	-0.94761	-0.98718	-0.98607	1.	-0.97667
0.9792	-0.97665	0.98343	0.97545	0.99483	0.99598	-0.97667	1.

After the calculation of the inertia table as well as its total inertia, it was necessary to calculate the eigenvalues of Table 4. The eigenvalues appear in the following Table 5, called Jordan Table, while Table 6 shows the eigenvalues of the matrix of inertia with the corresponding unitary eigenvectors.

Table 5. Jordan of the matrix of inertia.

7.80625	0	0	0	0	0	0	0
0	0.15105	0	0	0	0	0	0
0	0	0.02760	0	0	0	0	0
0	0	0	0.01354	0	0	0	0
0	0	0	0	0.00138	0	0	0
0	0	0	0	0	0.00010	0	0
0	0	0	0	0	0	0.00003	0
0	0	0	0	0	0	0	9.23323×10^{-6}

Table 6. Eigenvalues of the matrix of inertia with the corresponding unitary eigenvectors.

λ	v
$\lambda_1 = 7.8062$	v_1 = (0.3535,0.3529,0.3489,0.3480,0.3569,0.3571,-0.3537,0.3570)
$\lambda_2 = 0.1510$	v_2 = (0.3756,-0.4062,-0.5342,-0.5610,0.0789,0.0672,-0.2647,-0.1130)
$\lambda_3 = 0.0276$	v_3 = (-0.2121,0.1614,-0.4181,0.4894,-0.0165,-0.0966,-0.6666,-0.2458)
$\lambda_4 = 0.0135$	v_4 = (-0.3312,0.3599,-0.3320,-0.1352,0.5746,0.4866,0.1373,0.2151)
$\lambda_5 = 0.0013$	v_5 = (-0.2024,0.1307,-0.0080,-0.2814,-0.2714,-0.2430,,-0.3507,0.7789)
$\lambda_6 = 0.0001$	v_6 = (0.0797,-0.3148,-0.5209,0.4573,0.0179,-0.2552,0.4616,0.3679)
$\lambda_7 = 0.0000$	v_7 = (0.1350,0.0963,-0.1722,0.1238,-0.6734,0.6809,0.0709,0.0715)
$\lambda_8 = 9.23 \times 10^{-6}$	v_8 = (-0.7166,0.6551,0.0811,-0.0510,-0.0914,0.1837,-0.0155,-0.0754)

The above eigenvectors consist an orthonormal base of vector space R^8. The percentage of data that each axis gave was calculated and the axes with the two highest percentages formed a level, where the projections of all vectors were defined and studied. Each axis was correlated with an eigenvalue, and thus the percentage of each axis was calculated by the following formula:

$$\frac{l_i}{\sum_{t=1}^{m} l_i} * 100$$

Each axis had the same direction and sense of the eigenvector with which it was correlated. The denominator was the inertia which was equal to 8. That gave the following results (Table 7):

Table 7. Percetages of data given by each factorial axis.

Factorial axis	% of the total information
1st	97.5782
2nd	1.8882
3rd	0.3451
4th	0.1692
5th	0.0173
6th	0.0013
7th	0.0004
8th	0.0001

In order to study the previous results, a transport to another reference system was considered necessary, the coordinate system defined by the m eigenvectors. This was fulfilled with the use of a transformed table (Table 8), where the values in columns are the eigenvectors of the inertia table, as it is indicated below:

Table 8. The transformation matrix from the matural base to the above "eigenvectors" orthonormal base.

0.35357	0.37569	-0.21218	-0.33121	-0.20248	0.07971	0.13502	-0.71660
-0.35296	-0.40623	0.16148	0.35998	0.13075	-0.31485	0.09634	-0.65514
0.34894	-0.53429	-0.41814	-0.33202	-0.00802	-0.52090	-0.17229	0.08119
0.34801	-0.56102	0.48941	-0.13525	-0.28144	0.45734	0.12380	-0.05108
0.35692	0.07891	-0.01656	0.57460	-0.27145	0.01790	-0.67347	-0.09140
0.35715	0.06729	-0.09664	0.48667	-0.24302	-0.25525	0.68098	0.18375
-0.35371	-0.26471	-0.66667	0.13739	-0.35079	0.46167	0.07092	-0.01557
0.35700	-0.11307	-0.24588	0.21512	0.77898	0.36795	0.07158	-0.07545

Table 9. Application of transformation matrix to normalized matrix.

-1.18024	-0.08720	-0.10003	0.02960	0.00347	0.00177	-0.00267	0.00024
-1.01844	-0.05676	-0.02747	0.00508	-0.00210	-2.3465×10^{-6}	0.00497	-0.00017
-0.80816	-0.13126	0.05289	-0.02762	-0.00307	-0.00544	-0.00140	-0.00124
-0.58162	-0.00748	0.05527	-0.04410	0.00375	0.00402	-0.00019	0.00171
-0.35515	0.09310	0.04765	-0.01057	0.00814	-0.00071	-0.00045	0.00005
-0.09281	0.13442	0.03660	0.05486	-0.01227	-0.00215	-0.00056	0.00089
0.17053	0.10004	0.03418	0.04449	-0.00178	0.00451	0.00001	-0.00155
0.54781	0.13877	-0.06508	-0.06300	-0.01960	0.00031	-0.00032	-0.00036
0.75746	0.12046	-0.04389	0.00284	0.02148	-0.00468	0.00055	0.00033
1.09609	-0.09645	0.00597	-0.01601	0.01277	0.00346	-0.00019	-0.00072
1.46552	-0.20765	0.00389	0.02442	-0.01079	-0.00110	0.00028	0.00081

The coordinates of our initial variables, in relation of the "eigenvectors" orthonormal base, are the columns of this table. If we restrict in the first factor level we have the 97.5+82+1,8882% of the total information. In the next figure we can show the projection of the cases (rows) on the first factor level. The next step was to take the level defined by the first two factorial axes mentioned previously, and on this level all values were presented, as it is shown in Fig. 2.

Factor Level 1

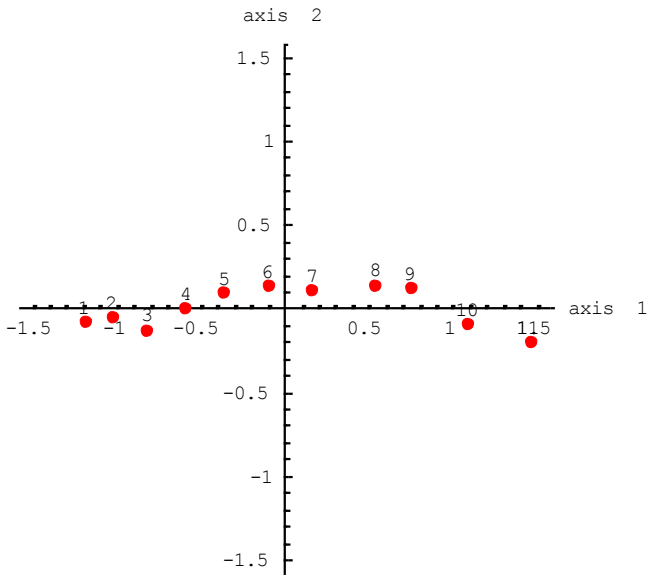

Fig. 2. Projection of the cases on the first factor level.

The next step is to project the variables (columns) on the first factor level. These projections should be on a unit circle. Therefore, the first two coordinates were picked and by dividing each coordinate by the norm of the variable-vector we obtain unit vectors.

The resulting vectors are as follows and are depicted on the unit circle:

Var[1]=(0.685346,0.728218),Var[2]=(-0.655888,-0.754858)

Var[3]=(0.546814,-0.837254),Var[4]=(0.527138,-0.84978), Var[5]=(0.976422,0.215872), Var[6]=(0.982709,0.185158), Var[7]=(-0.80062,-0.599172),Var[8]=(0.953324,-0.301949)

Variables which are close to each other on the circle are positively correlated, while variables which are at different quarters and perpendicular to each other show no correlation. Finally, variables which are at opposite quarters are negatively correlated (Fig. 3).

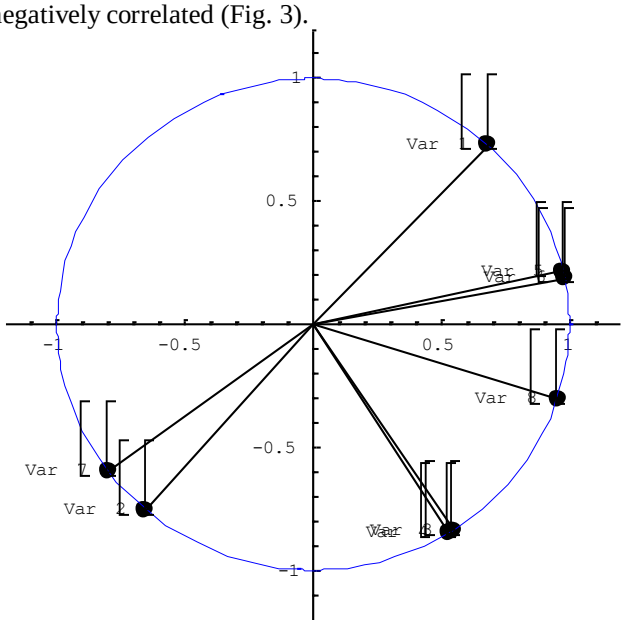

Fig. 3. Graph of "variables" and "cases" on unitary circle.

Variables v_5 and v_6 are very close positioned, so they can be considered to form a cluster. The same thing holds for the pairs of variables v_3 and v_4, and also for the variables v_2 and v_7. In a second hierarchical level we can consider that v_1, v_5 and v_6 also consist a cluster of variables (v_1, v_5, v_6). The cluster (v_3, v_4) is almost perpendicular to the clusters (v_2, v_7) and (v_1, v_5, v_6). The clusters (v_2, v_7) and (v_1, v_5, v_6) are diametrically opposed to each other. Variables which belong to the same cluster are positively correlated. Variables which belong to diametrically opposed clusters are negatively correlated. Variables which belong to perpendicular to each other clusters are not correlated.

Points that belong on a cluster or that are close to a cluster are characterized from the properties of variables of the cluster. So the cases 7, 8 and 9 are characterized by the properties v_1, v_5 and v_6. The cases 1, 2, 3, 4 and 5 are characterized by the properties v_2 and v_7, but not in a very significant way.

As it was previously discussed, all vectors have been depicted on a level defined by the first two factorial axes. A table of square cosines (Table 10) was calculated, including the points of the first factorial level (which results from the first two axes of Table 7). This means that when the values (only of the first column of Table 10) are close to 1, then they are close to the first factorial level, while when they are close to 0, then they are away from the first factorial level [16].

Table 10.Square cosines table.

	$\cos^2[\varphi_1]$	$\cos^2[\varphi_2]$
1	0.98688	0.00538
2	0.99612	0.00309
3	0.96908	0.02556
4	0.98517	0.00016
5	0.91898	0.06316
6	0.27616	0.57935
7	0.68808	0.23681
8	0.91508	0.05872
9	0.97133	0.02456
10	0.99191	0.00769
11	0.97999	0.01967

The first column of Table 10, represents the square cosines of angle φ_1, that each variable forms with the first factorial axis. The second column of Table 10, represents the square cosines of angle φ_2, that each variable forms with the second factorial axis.

In order to have a clearer view on the exact relative position of these points regarding the axes, the square of cosines of the angle formed by each vector with each axis were calculated, and the following table (Table 11) occurred.

Table 11. Table indicating the square cosines of the angle formed by each vector with each axis.

1	2	3	4	5	6	7	8	9	10	11
0.99227	0.99922	0.99465	0.98594	0.98214	0.85552	0.92489	0.97380	0.99590	0.99961	0.99966

The second row of Table 11, represents the square cosines of angle φ, that each variable forms with the first factorial level.

The elements of the second row of Table 12 are the distances of the points-variables from the origin of the axes in the n-th dimensional space (where n is the number of cases-rows).

Table 12. Table of distances of each point from the axes origin.

1	2	3	4	5	6	7	8	9	10	11
1.18805	1.02042	0.82095	0.58598	0.37047	0.17661	0.20558	0.57266	0.76856	1.09955	1.48041

We have to check if two points that their projections are neighboring points in the first factorial level, are also neighboring points in the n-th dimensional space. If the square cosines are close to 1, this means that the projected points are very close to the first factorial level. Therefore, the points-cases 1, 2, 3, 9, 10 and 11 are very close to the first factorial level. In addition, the points-cases 4, 5 and 8 are relatively close to the first factorial level. Finally the points-cases 6 and 7 are the most distant from the above level (Fig. 4).

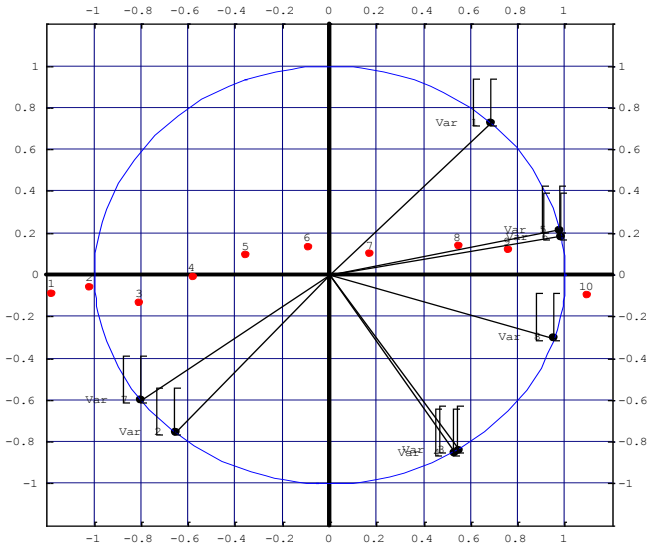

Fig. 4. Graph indicating the distances between points and variables.

IV. CONCLUSIONS AND FUTURE WORK

The results of the factorial analysis indicated significant and innovative data, but they also confirmed in a mathematical way familiar data on the studied properties. The study of information percentage that each factorial axis provides, showed that the first factorial axis, which referred to density, gave 97.57% of the total information, together with the second factorial axis (which referred to api and gave 1,88% of the total information), gave 99.45% of the total information (Table 7).

We have seen that the variables v_5 and v_6 are very close positioned, so they can be considered to form a cluster. The same thing holds for the pairs of variables v_3 and v_4, and also for the variables v_2 and v_7. In a second hierarchical level we can consider that v_1, v_5 and v_6 also consist a cluster of variables (v_1, v_5, v_6). The cluster (v_3, v_4) is almost perpendicular to the clusters (v_2, v_7) and (v_1, v_5, v_6). The clusters (v_2, v_7) and (v_1, v_5, v_6) are diametrically opposed to each other. Variables which belong to the same cluster are positively correlated. Variables which belong to diametrically opposed clusters are negatively correlated. Variables which belong to perpendicular to each other clusters are not correlated.

Dynamic and cinematic viscosity (presented here by variables 5 and 6) were known to be related properties, a fact that was reinforced by the results of the present study, which indicated a positive correlation between their values. The same results were given for conductivity and humidity (variables 3 and 4 respectively). However, an innovative result occurred regarding variables 7 and 2 (referring to calorific value and api), which seem to belong to the same group with several similar characteristics. Finally conductivity and humidity (presented by variables 3 and 4) are not correlated to the density, api, cinematic viscosity, dynamic viscosity and calorific value (presented by properties 1, 2, 5, 6 and 7). In conclusion, the results of the current investigation could be regarded as an applied example of integrating mathematics in everyday activities such as the use of fuel and can be included in textbooks for educational institutions, or used in industrial research in the design of new software products.

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