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Correlation Between Self-Ignition Temperature And Physicochemical Characteristics Of Hydroalcoholics Gels

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Abstract
The aim of the work presented in this paper was to study the correlation between self-ignition temperature and physicochemical characteristics (pH, density and alcoholic degree)characterizing the hydroalcoholic gel.Data of self-ignition temperatures were obtained using the isothermal oven procedure described in standard DIN 51794.The results obtained throw light on that any correlation were observedbetween the alcoholic degree and the self-ignition point (r = -0.022)and between density and alcoholic degree (r = -0.232) the variables evolve in anopposite direction. Also, negative correlation,but not significant,were observedbetween the alcoholic degree and the pH(r = -0.527) andno correlation were observed between self-ignition temperature and the pH (r = 0.054). These results mean that alcoholic degree and the pH therefore evolve in an opposite direction.

Key-words: *Hydroalcoholic gel, physicochemical characteristics, self-ignition, DIN 51794, correlation*

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I. Introduction

Knowledge of the tendency of materials to self-ignite and explode is essential to plants and populations that handle, store or process flammable materials.Self-ignition not only involves fires but also explosions, which can occur when the dust or vapors originated in the handling of materials results in the formation of an explosive atmosphere [1–2]. The assessment of the minimum temperatures that can lead to self-ignitionis therefore essential if accidents are to be prevented. The potential sources of self-ignition must therefore be clearly established when it results from improper storage in an environment where the heat could be very excessive due to exposure to direct sunlight for exemple.

Following long and laborious experimental work by researchers worldwide, a standardized method was proposed for characterizing materials with respect to their spontaneous combustion; this is enshrined in European standard DIN 51794 [3]. The method involves the isothermal oven test to obtain the relationships between volumes, temperatures and storage times [1, 4]. The results obtained can be analyzed using simple scaling procedures or methods based on the thermal explosion theory (which differ in their mathematical background) [5–7] to provide the correlation between physicochemical characteristics of material and its self-ignition temperature. Therefore, other simplified methods also exist to determine the susceptibility of materials to self-ignite [8], but their use is limited to defining the safety characteristics of the packaging that should be used when transporting them [1].

The year 2020 was marked by the pandemia of the COVID-19 which upset and affected stability of many countries throughthe world [9].To prevent and limit the contamination, most countries, including Cote d'Ivoire, have mobilized material and financial resources to support populations against this pandemic.Among these resources, the production of hydroalcoholic gels on a large scale has been set up in order to participate in the fight against COVID-19[10].Indeed, hydroalcoholic gels consist of three types of constituents: The active ingredient (alcohol or isopropanol), water and emollients (glycerin or glycerol) [11].However, the use ofhydroalcoholic gels presents some drawbacks, among which flammability is those which requires some precautions during their use and storage [12].

Several facts reported in the literature report misuse or improper storage of hydroalcoholic gels resulting in bodily injury and / or fires. Majority of these cases arise from an application of a heat energy source such as a pilot flame, however rare, unproven cases report the possibility of self-ignition of the hydroalcoholic gels due to excessive heat source. The risk of self-ignition in the handling and storage of gels is therefore one of the primary causes of fire and personal injury [13]. Indeed, the self-ignition of a compound is considered to be the ignition of this compound in air in general, resulting from the release of heat produced by an exothermic oxidation reaction in the absence of a source external incandescence such as a spark or flame [14-15].

Therefore, it is important to find the relationship between the self-ignition temperature observed and the physicochemical characteristics characterizing the hydroalcoholic gelsto estimate the risk of fire and injuries incidents in the areas where gels is stored. The study of the correlation between the minimumself-ignition temperature observed and physicochemical characteristics characterizing the hydroalcoholic gelswas the subject of the work presented in this paper.

II. Material and methods

a. Material

All investigated hydroalcoholic gels are purchased from Nouvelle PSP-CI (Abidjan, Côte d'Ivoire) with guaranteed quality and purity. Theprecision balance used is manufactured by SHIMADZU model UW4200H (Philippines), while the muffle oven apparatus used for self-ignition temperature measurements, with temperature range between 30 and 3000°C, is manufactured by Nabertherm GmbH (Bremen, Germany). The pHmeteris manufactured by Lovibondmodel SensoDirect 150 (Dortmund, Germany).In this study, the analysis were carry out by the using of aluminium tanks,with volume of 100, 150 and 200 cm^3 as well as graduated test-tubes of volume 100, 250 and 500 ml.

b. Experimental Apparatus and Test Procedure

The density of a material is the ratio of its specific mass to that of the pure water measured under the same conditions. The density of the hydroalcoholic gels is measured using a glass pycnometer as indicated by Rodier et al. [16]. The pH is measured, using a pHmeter with glass electrode manufactured by Lovibond model SensoDirect 150 (Dortmund, Germany), according to the method described by Rodier et al. [16].The alcoholic degree of our hydroalcoholic gelsamples is evaluated by infra-red spectrometry according to the method described per Mtoe Y. et al.[17].

The self-ignition temperatures of of hydroalcoholic gelsampleswere determined using methods based on DIN 51794 [3]. The analysis is based on different heating volumes of test material at a constant temperature in an isothermal oven. The aim is to determine the self-ignition temperatures of these different volumes, so that the extrapolation of the results can identify the minimum volumes to obtain self-ignition. The Nabertherm brand muffle oven used has an internal volume of 18.15 L (37.5cmx22cmx22cm) and can reach a temperature of 3000°C. The self-ignition temperature was measured by introducing, in the oven at temperatures ranging from 30 to 550 °C, different volumes of hydroalcoholic gels in different sizes of aluminum tanks to determine the optimal volume of gel topour according to the size of the aluminum tanks [13]. The choice of aluminum tanks is justified by the high melting temperature of aluminum, which is around 657 °C [18]. The hydroalcoholic gel samples were poured into aluminum tanks of different sizes (volume of 100, 150 and 200 cm^3), open at the top and closed at the bottom.A sufficient number of tests was carried out with each volume of hydroalcoholic gel on each size of aluminium tanks until to the self-ignition. These different volumes were measured to remain in conformity with the conditions presented by standard DIN 51794 [3].

c. Statistical analysis

The statistical tests used for data processing: means, minimum, maximum, standard deviations and correlations were performed using XLSTAT software (version 7.5) and Microsoft Excel 2013. Barlett testwas used to test the existence of correlation between at least two parameters.

III. Results

a. Physicochemical characteristics of hydroalcoholic gels

Results of physicochemical characteristics (pH, density and alcoholic degree) of52 hydroalcoholic gels analysed are shown in table 1 below. pH of the hydroalcoholic gels analysed range between 5.10 and 7.41 with an average of 5.72 ± 0.54. Values of density obtained range between 0.80 and 1.12 with an average of 0.87 ± 0.08, while average of alcoholic degree is74.43 ± 6.09°with range between 61.30 and 83.02°.

Table 1: Physicochemical characteristics of hydroalcoholics gels

Sample numbers	pH	Density	Alcoholic degree
1	6.06	0.83	62.56°
2	6.11	0.88	70.45°
3	6.20	0.84	66.30°
4	6.21	0.88	61.33°
5	6.27	0.81	75.07°
6	6.22	0.84	62.02°
7	7.24	0.83	72.74°
8	7.41	0.84	74.71°
9	6.3	0.83	65.68°
10	6.44	0.83	75.36°
11	5.87	0.80	64.61°
12	5.50	0.87	69.50°
13	6.4	0.83	61.30°
14	6.33	0.85	70.01°
15	5.54	0.83	68.56°
16	6.54	1.10	73.93°
17	6.23	1.12	64.08°
18	6.21	1.11	71.05°
19	6.40	1.07	65.42°
20	6.00	1.06	65.41°
21	5.94	1.04	78.65°
22	5.16	0.89	64.08°
23	5.17	0.85	80.80°
24	5.39	0.87	76.18°
25	5.81	0.90	81.66°
26	5.23	0.84	78.67°
27	5.34	0.85	84.95°
28	5.79	0.85	67.69°
29	5.24	0.84	76.87°
30	5.27	0.85	77.16°
31	5.40	0.87	77.01°
32	5.55	0.88	83.27°
33	5.35	0.88	79.58°
34	5.40	0.88	83.02°
35	5.49	0.84	78.40°
36	5.55	0.85	80.01°
37	5.20	0.84	75.46°
38	5.22	0.84	79.23°
39	5.40	0.84	77.38°
40	5.10	0.83	75.49°
41	5.40	0.83	75.01°
42	5.27	0.84	80.02°
43	5.45	0.83	83.01°
44	5.39	0.83	80.06°
45	5.23	0.85	76.23°
46	5.44	0.83	79.56°
47	5.27	0.81	80.46°
48	5.41	0.82	80.26°
49	5.48	0.84	81.10°
50	5.12	0.83	80.09°
51	5.11	0.83	78.80°
52	5.28	0.90	80.02°
AVERAGE	**5.72 ± 0.54**	**0.87 ± 0.08**	**74.43 6.09°**

b. *Self-ignition temperatures of hydroalcoholic gels*

The self-ignition temperatures of the hydroalcoholic gels are given by direct reading on the display of the oven by the operator according to the method describe by Gnonsoro *et al.* [13]. Indeed, self-ignition temperatures were determined at atmospheric pressure and at ambient temperature located around 30°C. Thus, the optimal self-ignition conditions obtained by Gnonsoro *et al.* [13] were applied to the 52hydroalcoholics gels samples purchased from Nouvelle PSP-CI (Abidjan, Cote d'Ivoire). The self-ignition temperatures of the gels obtained at the end of these tests are presented in Figure 1 below. The self-ignition temperatures obtained varied from 380 to 425°C with an average of 406.94 ± 12.09 °C.

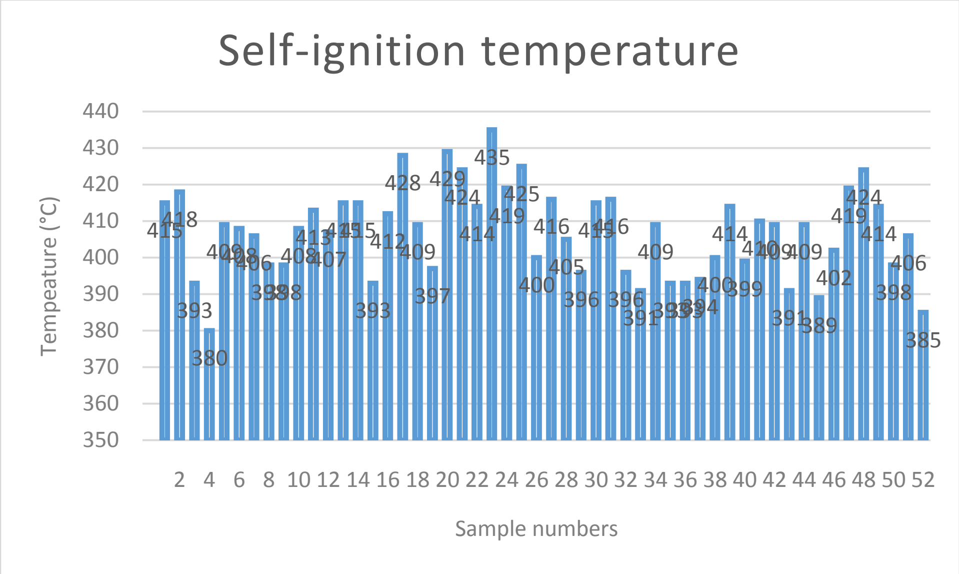

Figure 1: Self-ignition temperatures of hydroalcoholic gels

c. Correlations among physicochemical characteristics of hydroalcoholic gels

Results of correlationtests among physicochemical characteristics of hydroalcoholic gels are shown in Table 2. Significant negative correlation was observed between alcoholic degree and pH (r = -0.527, P<0.05). These variables therefore evolve in oppositedirections.For the others parameters, correlations between them were not significant (Table 2).

Table 2 : Correlations among physicochemical characteristics of hydroalcoholic gels

	pH	Density	Alcoholic Degree
pH	**1.000**	0.295	-0.527
Density	0.295	**1.000**	-0.232
Alcoholic Degree	-0.527	-0.232	**1.000**

d. Correlation between self-ignition temperatures andphysicochemical characteristics

Results of correlations between self-ignition temperatures and physicochemical characteristics of hydroalcoholic gelsare shown in Table 3 below. Both pH and density showed no correlation with self-ignition temperature (r = 0.054 ; 0.252, P<0,05 respectively). In addition, alcoholic degree showed any correlation withself-ignitiontemperature of hydroalcoholic gels(r = -0.022, P<0,05). All values obtained through this study showed no correlation between alcoholic degree, pH and density with self-ignitiontemperature.

Table 3 : Correlationsbetween self-ignition temperatures and physicochemical characteristics

	pH	Density	Alcoholic Degree	Self-ignition temperature
Self-ignition temperature	0.054	0.252	-0.022	**1.000**

IV. Discussion

The pH of the hydroalcoholic gels obtained is in the range of 5.10 - 7.41 with an average of 5.72 ± 0.54 (Table 1). The pH values thus obtained agree for some gels with the values given by the formulation guide for alcohol-based products recommended by the WHO, whose standards are between 6.0 and 7.0 [19]. The density values obtained for the hydroalcoholic gels analyzed which varied from 0.81 to 1.12 with an average of 0.87 ± 0.08 (Table 1). These density values are within the range of values set by the WHO recommended formulation guide for alcohol-based products, whose standards are between 0.8 and 1.0 [19]. As for the alcohol content (alcoholic degree) of the hydroalcoholic gels analyzed, the values varied between 61.30° and 84.95° with an average of 74.43 ± 6.09°. The average alcohol content of hydroalcoholic gels obtained is in agreement with the World Health Organization (WHO) [20] which recommends a concentration of 60-80° of alcohol in hydroalcoholic solutions. Thus some gels whose alcohol levels is greater than 80° do not comply with the recommendations of the WHO, but it is within the range of the recommendations of the Food and Drug Administration (FDA) of the United States which recommends a concentration of 60-95° [21]. So, the hydroalcoholic gels analyzed are generally of satisfactory quality with regard to their physicochemical characteristics (pH, density and alcoholic degree) with the standards established by the WHO [19-20] and FDA [21].

In addition, self-ignition temperatures of the hydroalcoholic gels analyzed, varied from380 to 425 °C with an average of 406.94 ± 12.09 °C, are in agreement with the range of variation of self-ignition temperatures of hydroalcoholic gels indicated in the literatureand set between 400 and 425 °C [22-24].Also, the fact that no significant correlation was found between the physicochemical parameters considered in pairs shows that none of the physicochemical parameters analyzed (pH, density and alcohol content) depends on the others. The lack of correlation between the physicochemical parameters of the gels analyzed is in opposition to the results of No et al. [25] who observed a correlation between physicochemical characteristics and binding capacities of chitosan products. Indeed, No et al. noted a significant correlations between molecular weight and viscosity and between nitrogen and degree of deacetylation ofchitosan products and between fat binding capacity and viscosity. The lack of correlation between the self-ignition temperature and the physicochemical characteristics of the hydroalcoholic gels analyzed is also in opposition to the results obtained on the correlation between self-ignition of a dust layer on a hot surface and baskets volums in an ovenby Janes et al. [26]. Janes et al have demonstrated an acceptable correlation to deduce self-ignition temperature of a dust layer, based on results of self-ignition of the dust in heating ovens. Asimilar resultto Janes et al was obtained by Adam Smoliński [27] who determined a relationship between the experimentally determined value of the maximum temperature observed during the coal mine waste fire and physicochemical parameters characterizing the coal mine waste.

V. Conclusion

This study has clearly demonstrated that there is nosignificantcorrelation between physicochemical characteristics of hydroalcoholic gels (pH, density and alcoholic degree)in one hand and between physicochemical characteristics and self-ignition temperatures in other hand. In fact, in physicochemical characteristics, only alcoholic degree were correlated negatively, but not significantly with pH. Any correlations were observed between alcoholic degree and self-ignitiontemperature of hydroalcoholic gels. In hydroalcoholic gels, any parameter studied may be used to predictthe value of self-ignition temperatures. Thus, to effectively utilize hydroalcoholic gelsfor human applications and to predict value of self-ignition temperatures, relationships between self-ignition temperatureand other physicochemical characteristicsmust be considered.

Conflict of interests

The authors declare that no competing interests exist.

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