Autoignition Temperature Data for Methanol, Ethanol, Propanol, 2-Butanol, 1-Butanol, and 2-Methyl-2,4-pentanediol

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Although autoignition temperature (AIT) is indispensable information to safely handle and operate flammable substances, the AITs reported in different data compilations are, however, very diverse. In this work, the AITs of six frequently used alcohols are measured in compliance with the ASTM E659 method. The measured AITs are (433.1 ± 8.7) °C, (368.8 ± 7.4) °C, (380.0 ± 7.6) °C, (397.1 ± 8.0) °C, (314.0 ± 6.3) °C, and (409.8 ± 8.2) °C for methanol, ethanol, propanol, 2-butanol, 1-butanol, and 2-methyl-2,4-pentanediol, respectively. It is found that the AIT reported in DIPPR 2009 is beyond the reproducibility in cases of ethanol, 1-butanol, and 2-methyl-2,4-pentanediol, and the difference is up to 104 °C in the case of 2-methyl-2,4-pentanediol. The International Programme on Chemical Safety's (IPCS) INCHEM service reports the AIT beyond the reproducibility in methanol, 1-butanol, and 2-methyl-2,4-pentanediol with differences of 33 °C, 31 °C, and 104 °C, respectively. The Sax's dangerous properties of industrial materials only report the AIT of 2-butanol within the reproducibility. The Chemical Database reports the AIT of all investigated chemicals within the reproducibility except for the propanol with the difference of 32 °C which is only a little bit beyond the reproducibility.

Introduction

Autoignition temperature (AIT), which is also known as spontaneous ignition temperature (SIT), is defined as the lowest temperature at which a substance will produce hot-flame ignition in air at atmospheric pressure without the aid of an external energy source such as a spark or flame. On the basis of the classical thermal theory of ignition, AIT was regarded as that temperature to which a combustible mixture must be raised so that the rate of heat evolved by the exothermic oxidation reactions of the system will just overcome the rate at which heat is lost to the surroundings.[1] Obviously, the ability of a substance to spontaneously ignite is an important index of fire hazards for people who handle, transport, and store the flammable materials.

The principal application of AIT is to define the maximum acceptable surface temperature in a particular area, usually for electrical classification purposes to prevent fire and explosion hazards. For example, article 500.8 of NFPA 70 (also known as the National Electric Code) provides that "Class I equipment shall not have any exposed surface that operates at a temperature in excess of the ignition temperature of the specific gas or vapors".[2] AIT is also frequently used to determine the possible consequence associated with leakage of flammable chemicals in hazard risk assessment methods. For example, API Publication 581, which is also known as Risk-based inspection base resource document, requires the AITs of flammable chemicals to determine if the consequence of a leakage is an explosion or a fire while a leakage of flammable chemicals is occurring.[3]

Although AITs are indispensable information to safely handle and operate flammable liquids, the AITs reported in different data compilations are very diverse. The difference between different data compilations might be up to more than 300 °C for many flammable liquids. Such diversity is attributed to many experimental factors and has been discussed in Chen and Hsieh's study.[4] One of the factors that contributes to this diversity is that the method to determine the AIT of liquid chemicals is not unified yet. Most methods for measuring the AIT of liquid chemicals introduce the sample into the apparatus container which is preheated to a specific temperature, and autoignition is evidenced by the sudden appearance of a flame inside the container and by a sharp rise in the temperature of the gas mixture. However, the container shape and container size are different in each test method.[5,6] When the AITs reported in different data compilations are inconsistent, it is generally hard for the users to determine which value is more feasible for their problems at hand because most of the data compilations do not report the test method of their AIT data.

Moreover, it was believed that in the literature most AITs of liquid chemicals were measured by a now-discontinued procedure of the ASTM D2155 method, which used a 200 mL flask as the ignition container.[2,7] The now-existing ASTM method of ASTM E659 uses a spherical 500 mL flask instead of a 200 mL one.[5] The ASTM E659 method is proposed to replace the ASTM D2155 method because of a higher ratio of heat generation to heat removal in the larger flask and the reduction of catalytic wall effects.[2] In Europe, the existing method to measure the AIT of liquid chemicals is the DIN 51794 method, determining the ignition temperature of petroleum products,

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Table 1. Auotoignition Temperatures (θ_{AIT}) of Selected Compounds in Different Data Compilations

	θ_{AIT}/°C				
compound name	DIPPR 1996[8]	DIPPR 2009[9]	The Chemical Database[20]	Sax's Dangerous Properties of Industrial Materials[21]	IPCS INCHEM[22]
hexadecanoic acid	377	215	377	NA	NA
piperazidine	455	455	320	NA	320
1,3-diisopropylbenzene	77	449	449	NA	449
benzoyl chloride	85	85	600	NA	197
methylhexanone	191	191	455	NA	191
2-methylnitrobenzene	305	305	420	NA	420
2,4-dihydroxy-2-methylpentane	306	306	425	NA	306
1-methyl-2-pyrrolidinone	346	248	245	NA	270
2-heptanone	393	393	532	533	393
crotonic acid	396	396	460	NA	396
1,4-benzenedicarboxylic acid	496	496	678	NA	496
1,3-benzenedicarboxylic acid	496	496	700	NA	NA
phenol	715	715	595	NA	715
acetaldehyde	185	130	140	238	185

which adopts a narrow-neck conical flask having a capacity of 200 mL to be the ignition container.[6] Results of these two existing methods are reported to be not comparable, and it is deemed that the ASTM E659 method will give a lower AIT because of the larger volume of ignition container employed in the ASTM E659 method.

To satisfy industry needs for better data to meet new and more stringent requirements, such as environmental and safety regulations, the DIPPR project sponsored by the American Institute of Chemical Engineering (AIChE) has critically reviewed many data to ensure their consistency and soundness; however, AIT values reported in the DIPPR database are still flagged as currently unevaluated.[8,9] This situation might be attributed to the following two reasons. First, there are two now-existing standard methods to measure the AIT of flammable liquids, i.e., ASTM E659 and DIN 51794 methods, but it is very common that results obtained from these two methods are different. Second, measuring AIT is a very laborious experiment, and it requires a lot of patience. Usually the test time required to measure the AIT of an unknown compound will last (48 to 60) h, and in most instances the operator must be present. Consequently, experimental research of reporting AITs has been very rare in recent years,[10−13] although research on predicting the AIT of flammable liquids has been very active in recent years.[7,14−19]

To highlight the diversity of AITs reported in different data compilations, Table 1 summarizes the reported AITs for selected compounds in different data compilations. Table 1 includes the following data compilations: (1) the DIPPR project supported by the American Institute of Chemical Engineers; (2) The Chemical Database compiled by the department of chemistry at the University of Akron;[20] (3) Sax's Dangerous Properties of Industrial Materials edited by Lewis;[21] and (4) the INCHEM service supported by the International Programme on Chemical Safety (IPCS).[22] The following facts could be observed from this table: (1) the difference of reported AIT for the same compound between the DIPPR 1996 and DIPPR 2009 might be up to more than 350 °C, for example, 1,3-diisopropylbenzene, and there are many chemicals for which this difference is more than 100 °C; (2) although the new DIPPR value conforms to other compilations in most cases, there are some cases that the difference is more than 500 °C, for example, benzoyl chloride; (3) there is no trend which data compilation will always report a higher or lower AIT. Thus, as shown in Table 1, it is generally hard for users to decide which one is feasible for their problems at hand. So, although experimentally determining the AIT of flammable liquids is tedious work, there is an emergent need to reevaluate such data by experiments.

To the researcher, the first problem encountered is to make a choice from the two now-existing test methods for measuring AIT: ASTM E659 and DIN 51794. Because the principal application of AIT is to define the maximum acceptable surface temperature for electrical classification purposes and NFPA 70, 497, and 921 codes require the AIT of flammable liquids to be measured by the ASTM E659 method, we decide to adopt the ASTM E659 method in the present study. The other reason for such a decision is that the AIT measured by ASTM E659 is usually lower than the one obtained by DIN 51794, so results of hazard assessments will produce safer protection strategies if the AIT obtained by ASTM E659 is employed.

In this study, AITs of six frequently used alcohols are measured in compliance with the ASTM E659 method. These six alcohols are methanol, ethanol, propanol, 2-butanol, 1-butanol, and 2-methyl-2,4-pentanediol. These alcohols are selected in the present study because of their wide applications in the process industry. The largest use of methanol is in making other chemicals, for example, formaldehyde. The largest single use of ethanol is as a motor fuel and fuel additive. Propanol is used as a solvent in the pharmaceutical industry and for resins and cellulose esters. 2-Butanol is mainly converted to butanone which is an important industrial solvent and found in many cleaning agents and paint removers. 1-Butanol is mainly used as a solvent for paints, coatings, and natural resins. The dominating uses of 2-methyl-2,4-pentanediol are as solvents in paints, lacquers, and varnishes and as a solvent plasticizer in surface coatings. Table 2 summarizes the reported AITs in different data compilations for these investigated alcohols. As it is shown in Table 2, the reported values are very diverse. For example, the difference between the DIPPR 2009 compilation and The Chemical Database is about 120 °C in the case of 2-methyl-2,4-pentanediol. The main purpose of this article is to provide the AIT data of aforementioned alcohols in compliance with the ASTM E659 method. Moreover, the ignition delay time and the sample quantity associating the AIT are also reported in this work because these two values are important factors in the hazard assessment phase. This article is organized as follows. First, the experimental apparatus, materials, and procedures are briefly discussed in section 2. Section 3 gives the experimental results and discussions. Finally, this work is concluded in section 4.

Experimental Section

Experimental Apparatus and Procedure. Autoignition temperature measurements were made on the K47000 autoignition apparatus manufactured by the Koehler instrument company.

Table 2. Auotoignition Temperatures (θ_{AIT}) for Explored Alcohols in Different Data Compilations

		θ_{AIT}/°C				
chemical name	CAS no.	DIPPR 1996[8]	DIPPR 2009[9]	The Chemical Database[20]	Sax's Dangerous Properties of Industrial Materials[21]	IPCS INCHEM[22]
methanol	67-56-1	464	464	455	470	464
ethanol	64-17-5	423	423	363	423	363
propanol	71-23-8	371	371	412	440	371
2-butanol	78-92-2	406	390	390	406	406
1-butanol	71-36-3	343	343	340	416	345
2-methyl-2,4-pentanediol	107-41-5	306	306	425	NA	306

Table 3. Chemical Information for Substances Used in This Investigation

chemical name	formula	CAS no.	mass fraction purity 100 w	manufacturer
methanol	CH_4O	67-56-1	99.9	TEDIA
ethanol	C_2H_5OH	64-17-5	99.9	Merck
propanol	C_3H_8O	71-23-8	99.98	TEDIA
2-butanol	$C_4H_{10}O$	78-92-2	99.8	Fisher Chemical
1-butanol	$C_4H_{10}O$	71-36-3	99.9	Echo Chemical
2-methyl-2,4-pentanediol	$C_6H_{14}O_2$	107-41-5	99.0	ACROS ORGANICS

The K47000 instrument is designed to meet the test requirements described by the test method of ASTM E659-78 (2005).[5] This apparatus consists of an ignition chamber of a commercial 500 mL borosilicate round-bottom, short-necked boiling flask wrapped with aluminum foil and an electrical heated furnace with a cylindrical interior shape to maintain uniform temperature. Furnace temperatures were monitored at the bottom, side, and neck of the flask with three external thermocouples. A fine Chromel-Alumel thermocouple was used for measuring the gas temperature inside the flask. A furnace provides rapid response and ± 1 °C stability throughout the operating range of (200 to 1200) °C. A 500 μL hypodermic syringe with a 15 cm stainless needle was used to inject the sample into the flask. A mirror was mounted above the flask at a 45 degree angle to see into the flask without having to be directly over it.

The sample, approximately (50 to 250) μL, was injected into the uniformly heated flask containing air at a predetermined temperature. After insertion of the sample, the contents of the flask were observed in a dark room for 10 min or until autoignition occurred. Autoignition was evidenced by the sudden appearance of a flame inside the flask and by a sharp rise in the temperature of the gas mixture. When the mixture exhibited flames at the preset temperature, the next sample was tested at a lower temperature. These procedures were repeated until the lowest temperature at which the mixture exhibited flame was obtained. The quantity of added sample was then systematically varied to determine the lowest temperature at which the hot-flame ignition occurs, and the lowest internal flask temperature at which hot-flame ignition occurred was taken to be the autoignition temperature (AIT) of the chemical in air at atmospheric pressure. Hot-gun air was used to purge the product gases after a test was completed and before the next test. To avoid interference from the ambient temperature, 10 min elapsed time is considered to allow time for ambient temperature of thermal equilibrium between trials. During the experiment, the ambient temperature is controlled to be about 20 °C.

The experimental precision of the ASTM E659 is defined in its document which includes: (1) repeatability—duplicate results by the same operator should be considered suspect if their difference $\delta\theta_{AIT}$ is more than $\delta\theta_{AIT}/\theta_{AIT} = 0.02$ where the temperature θ_{AIT} is in degrees Celsius; (2) reproducibility—the results submitted by each of two laboratories should be considered suspect if the two results as $\delta\theta_{AIT}$ differ by more than $\delta\theta_{AIT}/\theta_{AIT} = 0.05$ where the temperature θ_{AIT} is in degree Celsius. In this work, the reproducibility will be taken as the admissible error to compare experimental results with those reported in other data compilations.

Materials. All investigated chemicals are purchased from commercial companies with guaranteed mass fraction purity. The details of chemical information for the compounds used in this investigation are summarized in Table 3, which includes: (1) the Chemical Abstract registry number, (2) the supplier, and (3) the mass fraction purity. The guaranteed mass fraction purities of all chemicals used in the present study are more than 99.8 % except for 2-methyl-2,4-pentanediol of which guaranteed purity is 99.0 %.

Results and Discussions

Figures 1 to 6 show the combustion plots of experiments for methanol, ethanol, propanol, 2-butanol, 1-butanol, and 2-methyl-2,4-pentanediol, respectively. In these figures, the x-axis is the amount of sample added into the combustion container, and the y-axis is the preheated temperature of the combustion container. If the sample introduced generates a hot flame in ten minutes, this case is taken as a flammable one and denoted as a circle. If the sample introduced can not be ignited or it generates a

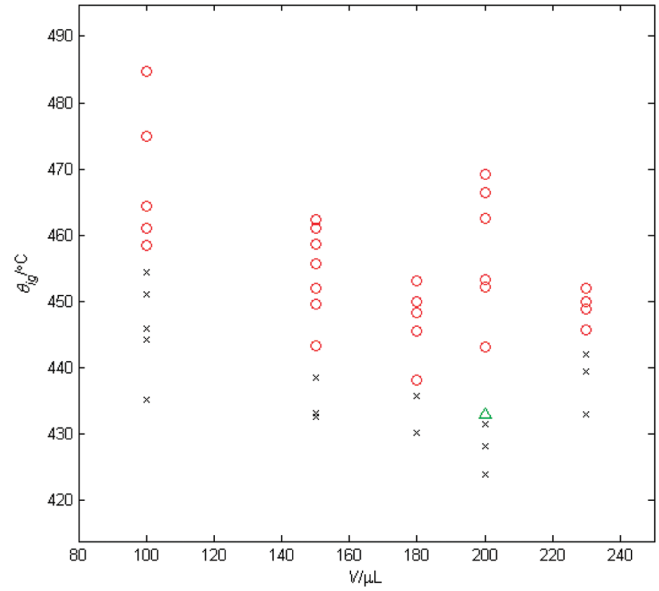

Figure 1. Ignition temperature (θ_{ig}) at different sample volumes (V) for methanol: circle, flammable case; cross, nonflammable case; triangle, the lowest flammable temperature.

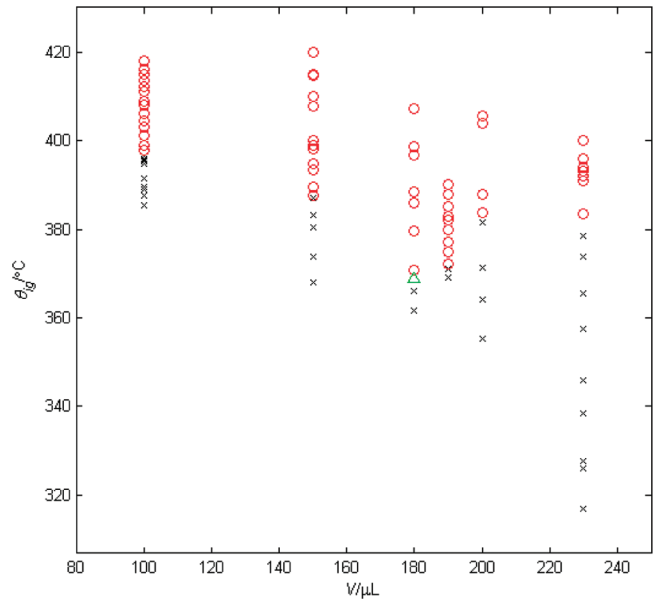

Figure 2. Ignition temperature (θ_{ig}) at different sample volumes (V) for ethanol: circle, flammable case; cross, nonflammable case; triangle, the lowest flammable temperature.

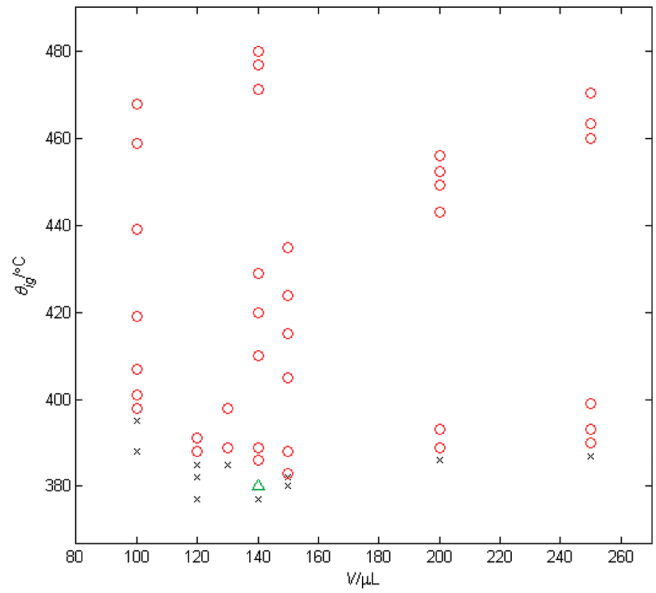

Figure 3. Ignition temperature (θ_{ig}) at different sample volumes (V) for propanol: circle, flammable case; cross, nonflammable case; triangle, the lowest flammable temperature.

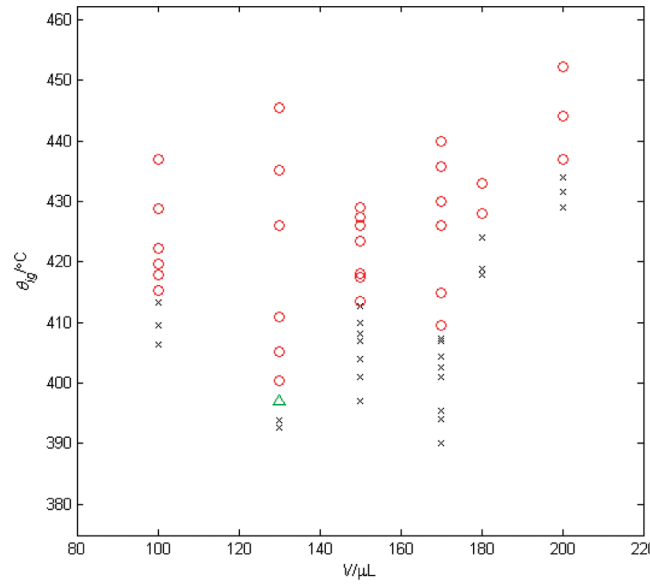

Figure 4. Ignition temperature (θ_{ig}) at different sample volumes (V) for 2-butanol: circle, flammable case; cross, nonflammable case; triangle, the lowest flammable temperature.

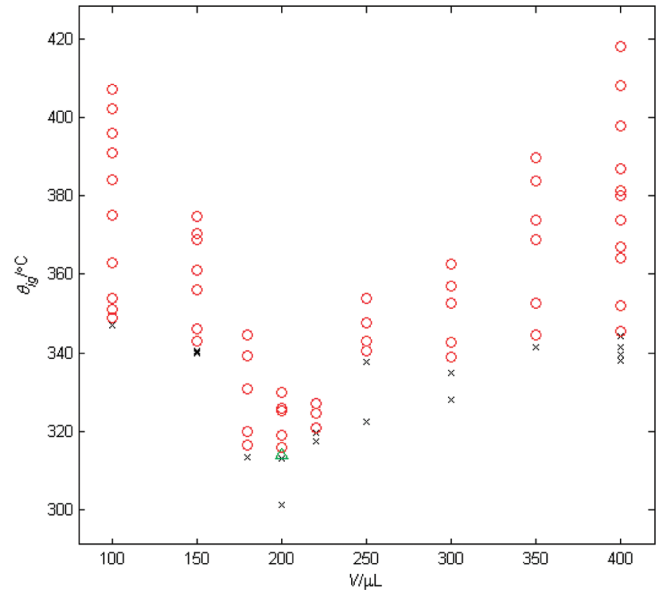

Figure 5. Ignition temperature (θ_{ig}) at different sample volumes (V) for 1-butanol: circle, flammable case; cross, nonflammable case; triangle, the lowest flammable temperature.

cold flame, this case is taken as a nonflammable one and denoted as a cross. While varying the sample quantity, the case of the lowest preheated temperature of the ignition container to ignite the sample with a hot flame is denoted by a triangle. This lowest temperature is, by definition, the AIT of the explored compound.

Table 4 summarizes all the measured AITs with the estimated uncertainties for all chemicals investigated in this work. As mentioned earlier, there is a specific amount of sample quantity at which this minimum ignition temperature of a chemical occurs. If the quantity added is higher or less than this specific amount, it needs higher temperature to ignite the chemical. Such phenomena could be clearly observed in Figures 1 to 6. This specific sample amount that results in the autoignition temperature is listed in the third column in Table 4 for all investigated chemicals. The ignition delay time is defined to be the time lapse between application of heat to a material and its ignition. Obviously it is an important characteristic of flammable liquids for assessing fire safety hazards. Table 4 also lists the ignition delay time at the experimental condition that AIT occurs for all investigated chemicals. The ignition delay times are found to be of 53.3 s, 56.0 s, 56.7 s, 36.5 s, 91.4 s, and 25.8 s for methanol, ethanol, propanol, 2-butanol, 1-butanol, and 2-methyl-2,4-pentanediol, respectively. As shown in the table, the ignition delay time is shorter than one minute for all explored compounds except for 1-butanol.

The equivalence ratio, which is defined as the ratio of fuel−air ratio to stoichiometric fuel−air ratio, is also listed in Table 4. The equivalence ratio is a frequently used index to quantitatively indicate whether a fuel−oxidant mixture is rich, lean, or stoichiometric. It is found in the present study that autoignition occurs in a rich fuel−oxidant condition with the equivalence ratio of about 3 for all explored alcohols. While measuring AIT of a flammable chemical, an estimate of the sample quantity

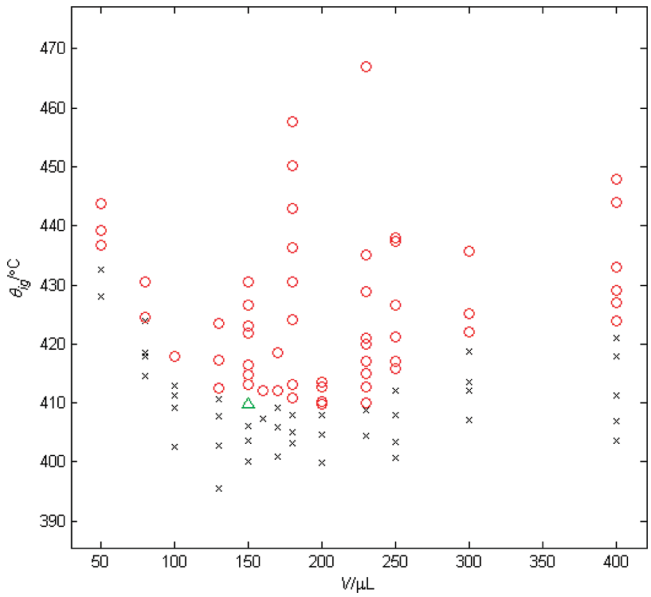

Figure 6. Ignition temperature (θ_{ig}) at different sample volumes (V) for 2-methyl-2,4-pentanediol: circle, flammable case; cross, nonflammable case; triangle, the lowest flammable temperature.

Table 4. Autoignition Temperature (θ_{AIT}), Sample Volume (V), Ignition Delay Time (t_{delay}), and Equivalence Ratio (ϕ) for Explored Alcohols

chemical name	θ_{AIT} / °C	V / μL	t_{delay} / s	ϕ/−
methanol	433.1 ± 8.7	200	53.3	3.8522
ethanol	368.8 ± 7.4	180	56.0	3.2787
propanol	380.0 ± 7.6	140	56.7	2.8403
2-butanol	397.1 ± 8.0	130	36.5	3.0846
1-butanol	314.0 ± 6.3	200	91.4	3.6362
2-methyl-2,4-pentanediol	409.8 ± 8.2	150	25.8	3.4177

for the first trial is critical to the whole experimental time needed, so the aforementioned ratio gives a good initial estimate of the sample quantity needed to begin the first trial.

In this work, the measured AIT of methanol is 433.1 °C which is lower than all values reported by the data compilations listed in Table 2. However, as the reproducibility of the ASTM E659 method is announced to be of 5 % of the reported value in degrees Celsius, this measured AIT value should be taken to be the same as the one reported in The Chemical Database. The measured AIT of ethanol is 368.8 °C in this work, and this value conforms to the one reported in The Chemical Database and IPCS INCHEM; however, the AITs of ethanol reported by the DIPPR 2009 and Sax's dangerous properties of industrial materials are about 60 °C higher than the measured value. The AIT of propanol is measured to be of 380.0 °C in this work, and this value conforms to the 371 °C reported in DIPPR 2009 and IPCS INCHEM while considering the announced reproducibility. The AITs of propanol reported by The Chemical Database and Sax's dangerous properties of industrial materials are (412 and 440) °C which are about (40 and 70) °C higher than the measured value, respectively. The measured AIT of 2-butanol is 397.1 °C which is the same as the reported value in all data compilations while considering the reproducibility. The measured AIT of 1-butanol is 314.0 °C which is lower than the reported value in all data compilations. The AIT of 1-butanol reported by Sax's dangerous properties of industrial materials is 416 °C, which is higher than the measured value by 100 °C. Although the AIT of 1-butanol reported in other data compilations is closer to the measured value, the differences are still a little bit beyond the reproducibility for all compilations. The measured AIT of 2-methyl-2,4-pentanediol is found to be 409.8 °C. The DIPPR 2009 and IPCS INCHEM, however, report its AIT to be 306 °C, and this value is lower than the measured value by 100 °C, which is of course beyond the reproducibility; however, The Chemical Databases reports the AIT of 2-methyl-2,4-pentanediol to be 425 °C, which conforms to the measured value of 409.8 °C while considering the reproducibility.

Conclusions

In this work, the AITs of six frequently used alcohols are measured in compliance with the ASTM E659 test method. The measured AITs are (433.1 ± 8.76) °C, (368.8 ± 7.4) °C, (380.0 ± 7.6) °C, (397.1 ± 8.0) °C, (314.0 ± 6.3) °C, and (409.8 ± 8.2) °C for methanol, ethanol, propanol, 2-butanol, 1-butanol, and 2-methyl-2,4-pentanediol, respectively. It is found that the differences in measured AIT and the one reported in DIPPR 2009 are beyond the reproducibility in ethanol, 1-butanol, and 2-methyl-2,4-pentanediol. The differences are 54 °C, 30 °C, and 104 °C for ethanol, 1-butanol, and 2-methyl-2,4-pentanediol, respectively. As compared with the experimental results, IPCS INCHEM service reports the AIT beyond the reproducibility in methanol, 1-butanol, and 2-methyl-2,4-pentanediol with difference of 33 °C, 31 °C, and 104 °C, respectively. The Sax's dangerous properties of industrial materials only report the AIT of 2-butanol within the reproducibility. The Chemical Database reports the AIT of all investigated alcohols within the reproducibility except for propanol, and in the case of propanol the difference is 32 °C which is merely a little bit beyond the reproducibility. It should also be noted that in the case of 2-methyl-2,4-pentanediol all data compilations except The Chemical Database report its AIT to be 306 °C. However, in the present study, the experimental value is 409.8 °C which is closer to the 425 °C provided by The Chemical Database.

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