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Experimental exploration of discrepancies in *F*-number correlation of flammability limits

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Abstract

Flammability limits measurement has been made by ASHRAE method for some 20 kinds of combustible gases and vapors. These compounds have been selected mainly because the literature values of flammability limits are not consistent with the *F*-number calculated ones [J. Hazard. Mater. A 82 (2001) 113]. As a result, it has been found that the newly obtained values of flammable range are classified into three groups. For the first group of compounds, the present values agree well to the literature values. For the second group, the present values do not agree to the literature values but agree with the calculated ones. For the third group ones, the present values neither agree to the literature values nor to the calculated ones. There are 4, 13, and 6 compounds in the respective groups.
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1. Introduction

The flammability limit is the most commonly used index for representing the flammability characteristics of gases and vapors. There is a pretty large volume of flammability limits data, which have been obtained by using various experimental methods [1–3]. From a safety point of view, the data of flammability limits with upward propagation of flame is of particular importance. However, even if the measurements are made using upward propagation of flame, the experimental values of flammability limits can be quite different for different measurement methods. It is quite common that the divergences of flammability

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limits data from different sources are as much as 10% or more. In this connection, we have carried out an extensive study concerning the effect of ignition source on the measurement of flammability limits [4,5].

Another problem concerning the flammability limits is that it is extremely difficult to predict accurately the values for unknown compounds. In a previous paper, we have shown a novel method of predicting flammability limits by using *F*-number, which is defined by the following equation [6,7]:

$$F = 1 - \left(\frac{L}{U}\right)^{0.5} \tag{1}$$

where L is the lower flammability limit and U the upper flammability limit. *F*-number is a sort of normalized flammable range, and it takes values ranging from zero to unity depending on the degree of flammability of substances.

The *F*-number prediction method for L and U utilizes an empirical expression of *F*-number to describe quantitatively the flammability of various organic substances. The parameters appearing in the expression can be determined by the least-squares fit to the observed values of *F*-number for a wide variety of compounds. The value of *F*-number can be predicted for an arbitrary organic compound by using this equation. It has been shown to be an excellent method to predict the flammability characteristics of various organic substances.

Further, the values of *F*-number can be converted to the upper and lower flammability limits, by using the stoichiometric concentration corrected for the effect of selective diffusion. In a previous paper [7], the *F*-number analysis was carried out employing the values of upper and lower flammability limits of 238 compounds [3]. The data seems to have been obtained with various vessels under various conditions [3], but were adopted there simply because the number of data listed is large. As a result, it has been found that there are a certain number of compounds for which discrepancy between the observed and calculated values of flammability limits is unacceptable even if the commonly observed divergences of the values are considered which result from using different methods of measurement.

In the present paper, we have re-measured the values of flammability limits for a number of compounds for which disagreement occurs between the literature values and *F*-number calculated values [7]. The compounds actually measured here are hydrocarbons, oxygen compounds, and nitrogen compounds for which high purity (98% or better) samples can be purchased from chemical companies.

2. Experimental method

The experimental setup in the present study is essentially based on the ASHRAE method [8], which is a revised version of ASTM E-681 [9]. The explosion vessel is a 12 l spherical glass flask and is equipped with a pair of tungsten electrodes for ac electric discharge together with a fan for gas mixing. The electrodes 2 mm in diameter are sharpened at the top and set opposed to each other at 0.25 in. distance. The height of the electrodes is one-third from the bottom to the ceiling of the vessel. The ac electric spark is initiated by a Neon transformer. The temperature of the explosion vessel is 35 °C, and the total pressure of the sample mixture is 760 Torr unless otherwise stated.

The ASHRAE method is a practical method which is expected to give pretty reliable result. Firstly, the vessel size is 12 l which is never too small. Secondly, this method uses ac spark ignition of 0.4 s duration time from a Neon transformer which gives enough energy to ignite ordinary combustible gases. Thirdly, if the ignition energy is more than enough for some of the fuel gases, the evil effect due to excess energy can be avoided by the facility of the vessel that even a small overpressure may lift the top cover of the vessel so that the hot gas heated up by the excess energy may be driven out from the vessel.

Gas mixtures were prepared in the explosion vessel by the partial pressure method. MKS baratron was used for the pressure measurement. The gas mixture was stirred with a fan in the vessel for 10 min and was left quiet for one minute before ignition. Determination of the flammability limit has been made according to the ASHRAE criteria. Namely, the mixture is considered flammable if the flame moves upward and outward from the point of ignition to reach an arc of the vessel wall which subtends an angle larger than 90° as measured from the ignition point. In the present study, the flammability decision was made by watching the flame propagation in the dark. Since the movement of the flame in the flammability limit region inside a spherical vessel of this size is quite slow, there is no difficulty in determining the position up to where the flame-front has reached.

The samples have been purchased from Tokyo Kasei Co. or Wako Chemicals Co. Most of the samples are in the liquid phase at room temperature. The purity of the samples are at least 98% or better unless otherwise stated. They have been used without further purification.

3. Results

In the following, the result of the measurement is described for each compound. Here, comparison of the present values with [3] is of particular importance because the *F*-number analysis in [7] has essentially been made based on the data reported in the literature [3]. The obtained values of flammable range are classified into three groups. For the first group of compounds, the observed values agree well to the literature values. For the second group, the observed values do not agree to the literature values but agree with the calculated ones. For the third group, the observed values neither agree to the literature values nor to the calculated ones. The numbers in parenthesis attached to each compound are from [7].

3.1. Group 1—measured values agree with literature

(1) Dimethyl ether (#41)

The flammable range of dimethyl ether has been found to be 3.3–26.2%. In general, the flame color of hydrocarbon is a whitish blue at fuel lean concentrations and an orange red at fuel rich concentrations. On the other hand, the flame color at the upper limit region of this compound has been found to be a pale blue. This fact indicates the existence of the effect of cool flame upon the upper flammability limit. The present value of flammable range is well justified and accord with the literature value 3.4–27.0% [3]. The calculated value in [7] is 2.6–18.3%, which is very different from the observed one. In this connection, it is of interest to note that the flammability limits with upward propagation in a cylinder 5 cm in diameter and 150 cm in length open at

the firing end is reported to be 3.45–18.1% [1]. In this case, since the vessel diameter is relatively small and the length is large, it is possible that the upper limit is not much affected by the cool flame and the measured value comes close to the calculated one.

(2) Ethyl formate (#45)

The flammable range of ethyl formate has been found to be 2.76–15.7%, which agrees well to the literature value 2.8–16.0% [3]. This is also close to the value 2.75–16.40% obtained with upward propagation in a closed tube 4 in. in diameter and 38 in. in length [1]. At the same time, the calculated value 3.0–15.1% [7] is in reasonable agreement with the observed values. The flame color at the upper limit region is a pale blue instead of orange, which could indicate a possibility of existence of cool flame at the upper limit region of this compound.

(3) Allyl amine (#70)

The flammable range of allyl amine has been found to be 2.03–24.3%. The literature value 2.2–22.0% [3] was reportedly obtained by igniting at 450–500 Torr in a tube 5 cm in diameter and 150 cm in length [1], but is in fair agreement with the present value obtained at 760 Torr. On the other hand, the calculated value is 1.9–11.8% [7]: the upper limit is quite different from the observed values. This indicates that the analytical form of *F*-number or the mean of the flammable range should be revised in some way. The flame color at the lower flammability limit region is a whitish orange, which is similar to that in other nitrogen compounds. The flame color at the upper limit region is a dark red.

(4) Propylene oxide (#85)

The flammable range of propylene oxide obtained in the present study is 2.2–35.5%, which is in accord with the literature value 2.3–36.0% [3]. For this compound, Coward and Jones report that the flammable range with upward propagation of flame in a tube 6 cm in diameter open at the firing end is about 2.1–21.5% [1]. The upper limit is much lower than the present one. On the other hand, the calculated value is 1.9–16.7% [7], which is different from any of the observed values. At any rate, the *F*-number parameters related to this compound may have to be revised in some way.

3.2. Group 2—measured values agree with predictions

(5) Methyl formate (#13)

The flammable range of methyl formate has been obtained as 5.2–23.0%. The lower limit is a little higher than the value 4.5% of [3], but agrees well to the calculated value 5.1% [7]. On the other hand, the upper limit agrees well to both the literature value and the calculated one [3,7]. Jones et al. [11] have reported that the flammable range obtained in a closed tube 4 in. in diameter and 38 in. in length, with upward propagation of flame, is 5.05–22.7%, which agrees well with the present result. It is noted that the flame color in the upper flammability limit region is a pale blue, which suggests that the upper limit is affected to some extent by the existence of cool flame.

(6) Methyl acetate (#44)

The flammable range of methyl acetate has been obtained as 3.13–14.0%. The lower limit is in accord with the literature value 3.1%, while the upper limit is a little lower

than the literature value 16.0% [3]. Jones et al. have also reported that the flammable range measured in a closed tube 4 in. in diameter and 38 in. in length with upward propagation of flame is 3.15–15.6% [1], which rather agrees to that of [3]. It is noted that the flame color in the upper flammability limit region is pale blue, which may indicate a possibility of cool flame in the upper flammable region of this compound as well.

(7) Methacrylonitrile (#71)

The lower flammability limit of this compound has been determined to be 1.89%. Because of the low vapor pressure of the compound the upper limit 11.0% has only been determined at a reduced pressure of about 580 Torr. The obtained range does not agree well to the literature values 2.0–6.8% [7], but it agrees well to the calculated values 1.9–10.6% [3]. It seems that the literature value of upper limit is a little too low. The flame color at the lower limit region is a whitish orange which is characteristic of nitrogen compounds.

(8) Methyl acrylate (#83)

The flammable range 2.18–14.4% obtained in the present study for this compound is quite different from the literature value 2.8–25.0% [3]. It is remarkable, however, that the present value is in good accord with the calculated one 2.1–14.6% [7], suggesting that the literature values are in error.

(9) *n*-Butyl alcohol (#93)

Because of the low vapor pressure of *n*-butyl alcohol, only the lower flammability limit has been determined as 1.63% at a reduced pressure of 350 Torr. This is a little larger than the literature value 1.4% [3], but is in accord with the calculated one 1.6% [7]. On the other hand, Coward and Jones report that the flammable range in a closed vessel 4 in. in diameter and 38 inches in length with upward propagation of flame at a temperature sufficient to vaporize the sample (100 °C) is 1.45–11.25% [1]. It could be that the value of lower limit is consistent with the present one if the difference of measurement temperature is taken into account.

(10) *tert*-Butyl alcohol (#96)

The vapor pressure of *tert*-butyl alcohol is not high enough to reach the upper flammability limit at room temperature. The value of lower flammability limit has been obtained as 1.84%, which is to be compared with the literature value 2.4% [3]. The calculated value 1.6% is closer to the present value rather than the literature. On the other hand, another reference reports that the lower limit measured in a 0.5 l flask is 1.68% [12]. The size of the vessel of the latter experiment seems to be too small.

(11) Vinyl ethyl alcohol (#108)

Due to the low vapor pressure of the compound, only the lower flammability limit has been obtained to be 1.75% at a reduced pressure of 475 Torr. The present value is completely different from the literature value 4.7% [3] but is close to the calculated one 1.6% [7]. The present value is close to both the values of lower flammability limit of *n*-butyl alcohol 1.63% and *tert*-butyl alcohol 1.84%, which are also four carbon alcohols except without one double bond. There is no question that the value of lower flammability limit in [3] is in error. The upper limit of this compound is reported to be 34.0% [3], which is also extremely different from the calculated one 12.3% [7].

We believe that the upper limit of [3] is also in error. It could be that polymerization or something occurred during the time when the liquid was warmed for the sampling procedure.

(12) Ethyl acrylate (#125)

The lower limit has been determined as 1.60%, which is closer to the calculated one 1.7% [7] rather than the literature value 1.4% [3]. Because of the low vapor pressure, the upper limit has only been obtained as 11% under a very low pressure of 275 Torr. The calculated value 11.4% [7] is closer to this value rather than the literature value 14.0% as well.

(13) Morpholine (#132)

The low vapor pressure of the compound made it impossible to determine the upper limit at an ambient pressure and the experimental temperature. The lower limit has been determined to be 1.67% under a pressure of 640 Torr. This is a little higher than the literature value 1.4% [3], but is close to the calculated one 1.6% [7].

(14) Amyl amine (#149)

Due to the low vapor pressure of this compound, the upper flammability limit has not been obtained in the present study. The lower limit has been determined as 1.32%. This value is quite different from the literature value 2.2% [3], but is in good accord with the calculated one 1.3% [7]. The literature value of this compound is of the same number as that of allyl amine in the same literature [3], so there is a possibility of mixing-up of the data from allyl amine.

(15) Isobutyl acetate (#158)

Because of the low vapor pressure, only the lower flammability limit has been determined at the ambient pressure. The obtained value is 1.42% which is fairly close to both the literature value 1.3% [3] and the calculated value 1.5% [7]. The upper flammability limit has been measured to be 8.0% at a reduced pressure as low as 205 Torr. The obtained value is close to the calculated one 8.3% [7] and lower than the literature 10.5% [3].

(16) 1,4-Hexadiene (#174)

The flammable range of 1,4-hexadiene has been determined to be 1.18–7.9%. The lower limit is different from the literature value 2.0% [3], but is close to the calculated one 1.1% [7]. The upper limit is also close to the calculated one 8.2% [7] rather than the literature value of 6.1% [3].

(17) 2,4,4-Trimethyl-1-pentene (#211)

The flammable range of this compound has been determined to be 0.88–6.0%. This does not agree to the UFL in literature value 0.8–4.8% [3], but agrees well to the calculated UFL in range 0.9–6.0% [7]. Since the prediction of flammability limits is easiest for this kind of compounds (moderate sized hydrocarbons), we suspect that the literature value must be in error.

3.3. Group 3—measured values disagree with literature and predictions

(18) Acetaldehyde (#12)

In the present study, the flammable range of acetaldehyde was observed as 4.0–57%. The lower limit is in accord with the literature value, but the upper limit is much

higher than the literature value of 36.0% [3]. The sample used in the present study contains about 10% water, but since the vapor pressure of water at room temperature of about 20° at which the sample container was kept is very small compared to that of acetaldehyde, the effect on the resulting value of flammable range is small. On the other hand, the flammable range with upward propagation of flame in a 2 in. diameter tube open at the lower end is 4.12–55.0% [1], which is very close to the present result. This is further rationalized by the literature support with the upper flammability limit 57% [10]. The flame color in the upper limit region of acetaldehyde has been found to be an extremely pale blue, which is due to the cool flame. This is indeed the main reason why the observed values of upper flammability limit is much higher than the *F*-number calculated value 20.3% [7].

(19) Ethyl amine (#18)

The flammable range of ethyl amine has been found to be 2.80–14.9%. Both lower and upper values showed match either with reported values or with calculated values. The lower limit is close to the calculated value 2.5% [7] rather than the literature value 3.5% [3], while the upper limit is a little higher but close to the literature value 14.0% [3]. On the other hand [1] reports that the flammable range measured in a closed cylinder of 2 in. in diameter at 450 Torr is 3.55–13.95% [1], which is practically the same as that of [3]. The flame color in the lower flammability limit region is a whitish orange, which is quite different from that of hydrocarbons. The flame color in the upper flammability limit region is a reddish blue.

(20) Methylal (#80)

The flammable range of this compound has been determined to be 2.54–18.5%. The literature value is 2.2–13.8% [3]. The calculated value of lower limit 2.2% [7] agrees well to the literature value, while that of upper limit 16.4% [7] is rather close to the present observation. The flame color at the upper limit region is a pale blue, indicating an existence of cool flame as observed on many other oxidized compounds.

(21) Diethyl ether (#112)

The flammable range of diethyl ether has been obtained to be 1.7–46%. The lower limit is close to both the literature value 1.9% [3] and the calculated one 1.6% [7]. On the other hand, the upper limit is very different either from the literature value 36% [3] or from the calculated value 10.1% [7]. For this compound, a variety of results have been obtained from different measurements, and some of them have reported 47 and 48% as the upper limit [1]. It is clear that the upper limit of diethyl ether has been extremely expanded by the effect of cool flame.

(22) Vinyl ethyl ether (#126)

The flammable range of vinyl ethyl ether has been determined as 1.67–19.0%. The lower limit is close to both the literature value 1.7% [3] and the calculated one 1.6% [7]. However, the upper limit neither agrees with the literature value 28.0% [3] nor with the calculated one 12.2% [7]. On the other hand, the flammable range with upward propagation of flame in a tube 6.3 cm in diameter and 150 cm in length open at the firing end is reported to be 2.04–16.6% [13]. Because of the effect of cool flame, the value of upper flammability limit seems to strongly depend on how the measurement is done for this compound.

(23) Furan (#136)

The flammable range of furan has been determined to be 2.0–23.0%. This is quite different from the literature value 2.3–14.3% [3]. It is also different from the calculated value 1.4–19.2% [7]. The flame color at the upper flammability region of this compound is orange and it does not seem to be suffering from the effect of cool flame. It may be necessary to revise in some way the *F*-number parameters related to this compound as well.

4. Discussion

The values of flammability limits obtained in the present study are classified into three groups (Table 1). For the first group of compounds, the present values of flammability limits agree well to the literature values, which means in turn that the calculated values of these compounds are not good [7]. Four compounds out of 23 measured in this study belong to this group, i.e. methyl ether (#41), ethyl formate (#45), allyl amine (#70), and propylene oxide (#85). For the second group of compounds, the observed values of flammable range are different from the literature values, and are rather close to the calculated ones. This group contains such compounds as methacrylonitrile (#71), methyl acrylate (#83), 1,4-hexadiene (#174), and 2,4,4-trimethyl-1-pentene (#211). Although the lower limit only has been measured, *n*-butyl alcohol (#93), *tert*-butyl alcohol (#96), vinyl ethyl alcohol (#108), morpholine (#132), and amyl amine (#149) also belong to this group. Thirteen compounds out of 23 belong to this group. For the third group, the observed values neither coincide with the literature values nor with the calculated ones. This group contains six compounds: ethyl ether (#112), vinyl ethyl ether (#126), furan (#136) and so on.

In summary, for 19 compounds out of 23, the present values are different from that in [3]. We believe that the literature values of these compounds should be replaced by the present ones.

Among others, we assert for the flammable range of vinyl ethyl alcohol (#108) that the literature value of flammable range is definitely in error. In this connection, the flammable range of crotyl alcohol (#107) is of interest [3], though the value has not been measured in the present study. Crotyl alcohol has the same chemical formula and a similar molecular structure as vinyl ethyl alcohol (#108). In addition, the literature value of flammable range 4.2–35.3% is very close to that of vinyl ethyl alcohol 4.7–34.0% [3]. On the other hand, the calculated value of flammable range for this compound is the same as that of vinyl ethyl alcohol 1.6–12.3% [7]. Measurements may find that the literature for the flammable range of this compound is largely in error.

The result of the present study suggests that the *F*-number analysis has an excellent potential ability of predicting flammability of combustible gases and vapors. However, it has also been found that there are a number of compounds for which the flammability limits predicted by the *F*-number analysis do not agree well to the observed values, so there is still room to improve the *F*-number analysis.

In this connection, the disagreement between the observed and calculated values of flammability limits is found for compounds containing particular chemical groups, for example ethers and oxides. According to [7], *F*-number is expressed by the following

Table 1
Samples used for the measurements and the values of flammability limits

No.	Compound	Formula	No. in [7]	Molecular weight	Boiling point (°C)	Purity (%)	L_{ref} (%)	U_{ref} (%)	F_{ref}	L_{calc} (%)	U_{calc} (%)	F_{calc}	L_{exp}[a] (%)	U_{exp}[a] (%)	Flame color		Pressure[b] (Torr)	Group[c]
															LFL	UFL		
	Methane	CH_4	1	16.04	−164	Gas	5.0	15.0	0.42	4.7	16.5	0.47	4.9 (0.1)	15.8 (0.1)	Whitish blue	Orange		
1	Dimethyl ether	C_2H_6O	41	46.07	−24.8	99	3.4	27.0	0.65	2.6	18.3	0.62	3.3 (0.1)	26.2 (0.5)	Whitish blue	Blue		1
2	Ethyl formate	$C_3H_6O_2$	45	74.08	54.5	99	2.8	16.0	0.58	3.0	15.1	0.55	2.76 (0.03)	15.7 (0.4)	Whitish blue	Pale blue		1
3	Allylamine	$C_3H_5NH_2$	70	57.10	55–58	99	2.2	22.0	0.68	1.9	11.8	0.60	2.03 (0.03)	24.3 (0.3)	White–orange	Dark red		1
4	Propylene oxide	C_3H_6O	85	58.08	34.23	99	2.3	36.0	0.75	1.9	16.7	0.66	2.2 (0.1)	35.5 (0.5)	Whitish blue	Reddish blue		1
5	Methyl formate	$HCOOCH_3$	13	60.05	31.8	98	4.5	23.0	0.56	5.1	22.6	0.52	5.2 (0.2)	23.0 (0.5)	Whitish blue	Pale blue		2
6	Methyl acetate	$C_3H_6O_2$	44	74.08	56.9	98	3.1	16.0	0.56	3.0	15.1	0.55	3.13 (0.05)	14.0 (0.5)	Whitish blue	Blue		2
7	Methacrylonitrile	C_3H_5CN	71	67.09	90.3	99	2.0	6.8	0.46	1.9	10.6	0.58	1.89 (0.02)	11.0 (0.5)*	White–orange	Orange	*580	2
8	Methyl acrylate	$C_4H_6O_2$	83	86.09	80	99	2.8	25.0	0.67	2.1	14.6	0.62	2.18 (0.04)	14.4 (0.2)	Whitish blue	Reddish blue		2
9	*n*-Butyl alcohol	$C_4H_{10}O$	93	74.12	117.7	99	1.4	11.2	0.65	1.6	10.1	0.60	1.63 (0.04)*	–	Whitish blue	–	*346	2
10	*tert*-Butyl alcohol	$C_4H_{10}O$	96	74.12	82.4	99	2.4	8.0	0.45	1.6	10.1	0.60	1.84 (0.03)	–	Whitish blue	–		2
11	Vinyl ethyl alcohol	C_4H_8O	108	72.11	114	98	4.7	34.0	0.63	1.6	12.3	0.64	1.75 (0.06)*	–	Whitish blue	–	*475	2
12	Ethyl acrylate	$C_5H_8O_2$	125	100.12	99.4	99	1.4	14.0	0.68	1.7	11.4	0.61	1.60 (0.02)	11*	Whitish blue	Reddish blue	*276	2
13	Morpholine	C_4H_9NO	132	87.12	128.9	99	1.4	11.2	0.65	1.6	12.4	0.64	1.67 (0.03)*	–	White–orange	–	*640	2
14	Amylamine	$C_5H_{11}NH_2$	149	87.17	105.3	98	2.2	22.0	0.68	1.4	7.2	0.56	1.32 (0.02)	–	White–orange	–		2
15	Isobutyl acetate	$C_6H_{12}O_2$	158	116.16	117.3	99	1.3	10.5	0.65	1.5	8.3	0.57	1.42 (0.03)	8.0*	Whitish blue	Pale blue	*207	2
16	1,4-Hexadiene	C_6H_{10}	174	82.15	72	99	2.0	6.1	0.43	1.1	8.2	0.63	1.18 (0.03)	7.9 (0.2)	Whitish blue	Orange		2
17	2,4,4-Trimethyl-1-pentene	C_8H_{16}	211	112.22	100	99	0.8	4.8	0.59	0.9	6.0	0.61	0.88 (0.03)	6.0 (0.1)	Whitish blue	Orange		2
18	Acetaldehyde	CH_3CHO	12	44.05	20.8	90	4.0	36.0	0.67	3.3	20.3	0.60	4.0 (0.2)	57 (3)	Whitish blue	Thin blue		3
19	Ethyl amine	$C_2H_5NH_2$	18	45.08	16.6	99	3.5	14.0	0.50	2.5	12.4	0.55	2.80 (0.03)	14.9 (0.2)	White–orange	Reddish blue		3
20	Methylal	$C_3H_8O_2$	80	76.10	41.5	98	2.2	13.8	0.60	2.2	16.4	0.63	2.54 (0.04)	18.5 (0.5)	Whitish blue	Pale blue		3
21	Diethyl ether	$C_4H_{10}O$	112	74.12	34.6	99	1.9	36.0	0.77	1.6	10.1	0.60	1.7 (0.1)	46 (1)	Whitish blue	Thin blue		3
22	Vinyl ethyl ether	C_4H_8O	126	72.11	35.8	98	1.7	28.0	0.75	1.6	12.2	0.64	1.67 (0.03)	19.0 (0.5)	Whitish blue	Reddish blue		3
23	Furan	C_4H_4O	136	68.08	32	99	2.3	14.3	0.60	1.4	19.2	0.73	2.0 (0.1)	23.0 (0.5)	Whitish blue	Orange		3

[a] Numbers in parenthesis are the estimated errors.
[b] Total pressure is 760 Torr unless otherwise stated.
[c] See text for details.

equation:

$$F = p_1(1 + p_2C_1 + p_3R_{OE} + p_4R_{CO} + p_5R_{COO} + p_6R_{NH} + p_7R_{RNG} + p_8R_{ARM} + p_9R_{US})(1 + p_{10}R_F + p_{11}R_{Cl} + p_{12}R_{Br} + p_{13}R_{OH} + p_{14}R_{NO_2} + p_{15}R_{NH_2} + p_{16}R_{CN} + p_{17}R_{COOH}) \quad (2)$$

Then, the values of flammability limits are calculated from F-number together with the geometric mean of upper and lower flammability limits through the following equations [7]:

$$L = (UL)^{0.5}(1 - F) \quad (3)$$

and

$$U = \frac{(UL)^{0.5}}{(1 - F)} \quad (4)$$

where the value of $(UL)^{0.5}$ is derived from the stoichiometric concentration corrected for the effect of selective diffusion.

Considering a certain level of success of the present scheme of F-number analysis in predicting the flammability limits, the degree of predictability of flammability limits is essentially dependent upon what kind of chemical groups the compound contains, and on how well we know the coefficient for that group.

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