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Short Communication

A NEW PARAMETER FOR THE FLAMMABILITY OF COMBUSTIBLE MATERIALS

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Fire hazards are associated with chemicals commonly used in laboratories and industry. The most commonly accepted parameter for comparing the flammability of materials is the Oxygen Index (OI) described first by Wolfhard and co-workers [1,2]. OI can now be determined from commercially available OI test instruments [3]. However, in many places such an instrument is not generally available. In the past, attempts have been made to correlate OI with various physico-chemical properties of materials. Johnson [4] correlated OI with ΔH (heat of combustion in kcal/g) of both polymeric and non-polymeric materials. He observed the following dependence.

$$OI = 1.9/\Delta H \tag{1}$$

This dependence was, however, much better for polymeric materials than for non-polymeric materials. Simmons and Wolfhard [1] found a similar correlation to exist between limiting flame temperature of the non-polymeric materials and the inverse of OI. Redfern [5] has reviewed the implications and interpretations of the OI test and has discussed the usability of OI. Van Krevelen [6] has suggested that there is a distinct correlation between the OI as a measure of the flammability and the elementary composition of a polymer. Recently Ohe and Matsuura [7] related the OI to a parameter called "Mean Heat Energy of Limiting Heat Flux" (MHEF) for various substances. Laskiewiez et al. [8] used a modification of the OI test to study the effect of sample weight and position and the effect of flame retardants. They showed that the OI increased with increasing sample weight and defined an intrinsic OI value, (OI) as follows:

$$(OI) = \lim_{m \to 0} OI \tag{2}$$

The most comprehensive attempt to evaluate the meaning of the test is due to Kaunury [9] who has done a detailed mathematical analysis of the test to understand the dependence of OI on various physical and chemical properties of the system. Abraham [10] proposed a term known as "Acceptability Index" (AI)

TABLE 1

Thermochemical parameters of various substances

	Substances	OI	Flash point T_f (°C)	Ignition temperature, T_i(°C)	Specific heat[a], C_p(cal g^{-1} K^{-1})	Heat of combustion[a] ΔH (kcal g^{-1})	$\frac{C_p T_f}{\Delta H} \times 10^3$	$\frac{C_p T_i}{\Delta H} \times 10^3$
1.	Methane	0.139	gas	537.20	0.528	13.2	—	21.50
2.	Ethane	0.118	gas	515.00	0.386	12.3	—	16.20
3.	Propane	0.127	gas	466.10	—	12.0	—	—
4.	n-Pentane	0.1325	−40	308.90	0.4093	11.6	−1.4	10.90
5.	n-Hexane	0.1335	− 21.7	233.90	0.3646	11.5	−0.7	7.40
6.	n-Octane	0.134	13.3	220.00	0.578	11.4	0.7	11.20
7.	n-Decane	0.1345	46.1	207.8	—	11.3	—	—
8.	Methanol	0.111	11.1	463.9	0.390	5.35	0.8	33;80
9.	Ethanol	0.126	12.8	422.8	0.406	7.1	0.7	24.20
10.	n-Propanol	0.128	25.0	371.1	—	—	—	—
11.	n-Butanol	0.129	28.9	343.3	0.526	8.6	1.768	22.50
12.	n-Pentanol	0.130	32.8	300.0	—	9.0	—	—
13,	Pentanol-2	0.133	42.8	347.2	—	—	—	—
14.	Ethylene	0.105	——	485.0	0.359	11.8	—	14.80
15.	Acetylene	0.085	—	350.0	0.383	12.0	—	11.20
16.	Cyclohexane	0.134	−20.0	—	0.413	11.0	−0.75	—
17.	Benzene	0.133	−11.1	562.2	—	10.0	—	—
18.	Acetone	0.1285	−17.8	537.8	0.528	7.36	−1.3	38.60
19.	Carbon monoxide	0.076	—	590.0	0.2478	2.42	—	60.40
20.	Thiophene	0.166	− 1.1	—	—	7.98	—	—
21.	Toluene	0.166	4.4	536.1	0.42	10.20	0.2	22.10
22.	Ethyl borate	0.166	11.1	—	—	—	—	—
23.	Benzotrifluoride	0.182	12.2	—	—	—	—	—
24.	Pyridine	0.164	20.0	—	0.431	8.32	1.0	—
25.	*m*-Xylene	0.176	25.0	527.8	0.387	10.20	0.949	20.00
26.	Chlorobenzene	0.196	31.0	—	—	—	—	—
27.	*o*-Xylene	0.176	17.2	463.9	0.411	10.20	0.693	18.70
28.	Acetic acid	0.207	42.8	—	—	3.48	—	—
29.	Trimethyl phosphite	0.204	54.4	—	—	—	—	—

	Substances	OI	Flash point, T_f (°C)	Ignition temperature, T_i (°C)	Specific heat[a], C_p(cal g^{-1} K^{-1})	Heat of combustion[a], ΔH (kcal g^{-1})	$\frac{C_p T_f}{\Delta H} \times 10^3$	$\frac{C_p T_i}{\Delta H} \times 10^3$
30.	*o*-Chlorophenol	0.211	63.9	—	—	—	—	—
31.	Borneol	0.155	65.6	—	—	10.60	—	—
32.	*p*-Dichlorobenzene	0.225	70.0	—	—	—	—	—
33.	Aniline	0.163	—	530.00	0.52	8.7	—	31.70
34.	*o*-Dichlorobenzene	0.231	75.0	—	—	4.6	—	—
35.	*o*-Bromotoluene	0.345	79.0	—	—	—	—	—
36.	*p*-Bromotoluene	0.236	85.0	—	—	—	—	—
37.	Acetophenone	0.165	96.0	—	0.474	8.2	5.55	—
38.	Hexadecane	0.155	100.0	—	0.495	11.3	4.40	—
39.	Diphenyl ether	0.165	115.0	—	—	—	—	—
40.	Anthracene	0.171	121.1	—	—	9.54	—	—
41.	1,4-Butanediol	0.165	121.1	—	—	—	—	—
42.	Anthraquinone	0.195	185.0	—	—	—	—	—
43.	Aniline—HCl	0.192	193.3	—	—	—	—	—
44.	Diphenylmethane	0.153	130.0	—	—	9.85	—	—
45.	Triphenyl phosphite	0.210	218.3	—	—	—	—	—
46.	Diethyl ether	0.165	—	180.00	0.547	8.80	—	11.20
47.	Ethylene glycol	0.148	111.1	412.80	0.571	—	—	—
48.	Lauric acid	0.156	—	—	0.510	8.87	—	—
49.	Acetophenone	0.165	—	—	0.474	8.25	—	—
50.	Phenol	0.17	—	—	0.561	7.80	—	—
51.	Nicotine	0.171	—	—	—	8.80	—	—
52.	Benzamide	0.174	—	—	—	7.00	—	—
53.	Phtalimide	0.174	—	—	—	5.77	—	—
54.	Phenylalanine	0.174	—	—	—	6.72	—	—
55.	*o*-Naphthoic acid	0.162	—	—	—	7.14	—	—
56.	*m*-Toluic acid	0.181	—	—	—	6.72	—	—
57.	Ethyliodine	0.240	—	—	0.17	2.28	—	—
58.	Malonic acid	0.240	—	—	0.275	1.99	—	—
59.	Methyl iodide	0.296	—	—	—	1.37	—	—
60.	Acetaldehyde	0.120	−37.8	185.0	—	—	—	—
61.	Carbon	0.372	—	600.0	0.165	8.08	—	—

[a]At 25°C.

for evaluating combustibility of materials. AI was defined as follows:

$$AI = (OI)^2 T_i / \Delta H \quad (3)$$

where T_i is the ignition temperature of the material.

Since OI is a dimensionless quantity we tried to develop a dimensionless

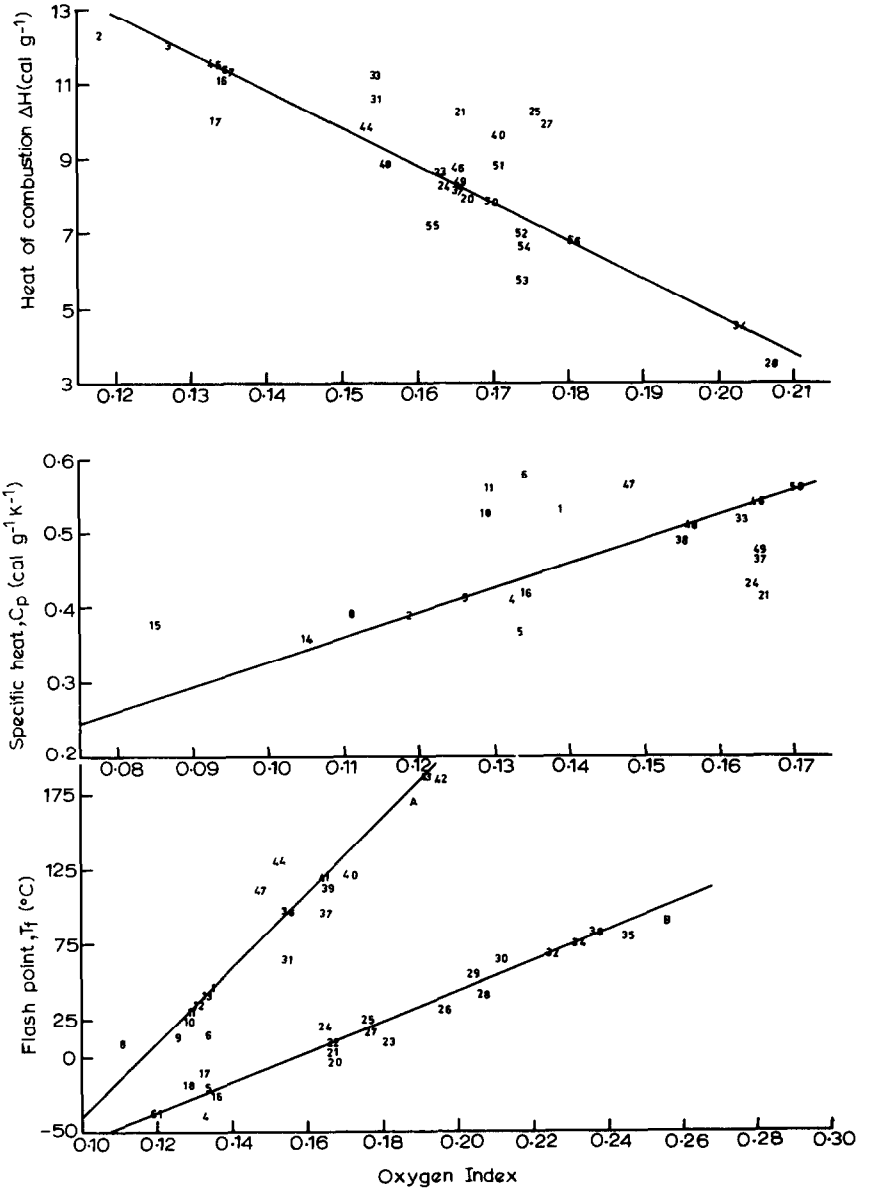

Fig. 1. Dependence of Oxygen Index on heat of combustion, specific heat and flashpoint.

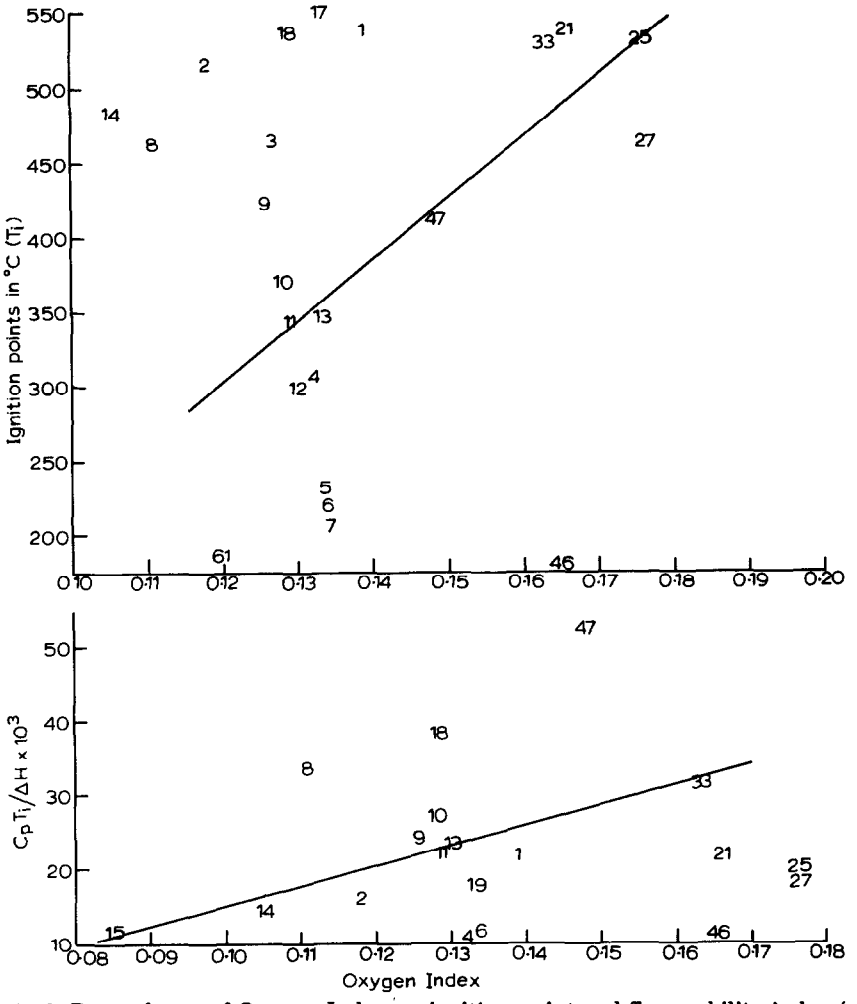

Fig. 2. Dependence of Oxygen Index on ignition point and flammability index (using ignition point data).

parameter which could be evaluated from available thermochemical quantities. It may be noted that the parameters proposed earlier which correlate with OI are not dimensionless. We venture to define this new dimensionless quantity as "Flammability Index" (FI). Flammability Index can be represented mathematically as

$$\mathrm{FI} = C_p\, T/\Delta H \qquad (4)$$

where C_p (cal g^{-1} K^{-1}) is the specific heat and T can be either the Flash temperature (T_f) or T_i of the material.

The data on T_i, T_f, ΔH and C_p were collected from several sources [1,4, 11—14] and are presented in Table 1. Justification for the definition of FI can

be had from Fig. 1 where OI has been plotted against ΔH, C_p and T_f. Whereas C_p and T_f show a direct dependence, ΔH shows an inverse dependence on OI. A plot of OI versus T_i was also made in a similar manner (Fig. 2) which shows a lot of scattering, showing that T_i is not a better quantity compared to T_f for FI. Dependence of $C_pT_i/\Delta H$ and $C_pT_f/\Delta H$ on OI is shown in Figs. 2 and 3, respectively. It can be seen that $C_pT_f/\Delta H$ shows a better dependence on OI compared to $C_pT_i/\Delta H$. This may be due to the fact that dependence of T_f on OI is much better than that of T_i.

The plots of $C_pT_f/\Delta H$ and T_f versus OI show two distinct straight lines. A careful look at Fig. 3 reveals that line A applies to materials like alcohols, ketones and acids, whereas line B represents mainly hydrocarbons. Why alcohols, ketones and acids fall on the same line can be explained by the fact that oxidation of alcohols yields ketones and acids. That the combustion of alcohols involves oxidation processes has already been demonstrated earlier [15]. Similarly, the combustion behaviour of all hydrocarbons should be similar and hence they give a dependence corresponding to line B. An exactly similar dependence of T_f is reflected in Fig. 3 for the plot of $C_pT_f/\Delta H$ versus OI. The same explanation holds good here also. This further shows that FI is a quantity which strongly depends on T_f.

Figure 3 has been used to calculate theoretical values of OI of different substances by using the following empirical equations.

$$(OI) = 0.014\,(FI) + 0.100 \quad (5)$$

(for alcohols, ketones, acids, etc.)

$$(OI) = 0.019\,(FI) + 0.148 \quad (6)$$

(for hydrocarbons etc.)

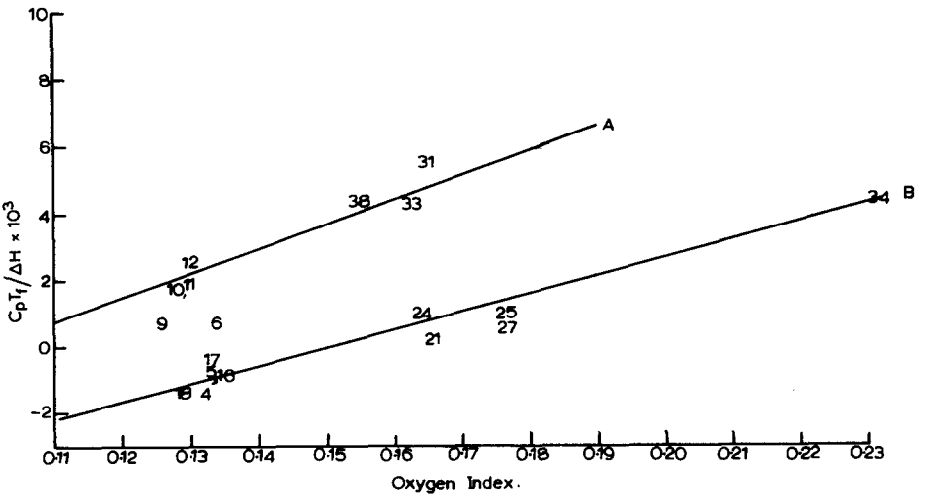

Fig. 3. Dependence of Oxygen Index on flammability index (using flashpoint data).

The theoretical values have been compared with the experimental values in Table 2. It may be seen from Table 2 that theoretically derived values agree well with the experimental values. Thus eqns. 5 and 6 can be used to get information about the flammability of those materials whose experimental OI's are not known.

TABLE 2

Comparison between theoretical and experimental values of Oxygen Index OI

Substances	Calculated OI	Observed OI
Methanol	0.111	0.111
Ethanol	0.110	0.126
n-Butanol	0.125	0.129
n-Propanol	0.125	0.128
n-Pentanol	0.136	0.130
Aniline	0.159	0.165
Acetophenone	0.178	0.165
Hexadecane	0.162	0.155
Anthraquinone	0.190	0.195
n-Pentane	0.121	0.1325
n-Hexane	0.135	0.1335
Cyclohexane	0.134	0.134
Benzene	0.141	0.133
Acetone	0.123	0.128
Toluene	0.152	0.166
Pyridine	0.167	0.164
m-xylene	0.166	0.176
o-xylene	0.161	0.176
o-Dichlorobenzene	0.232	0.231

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