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A RELIABLE SIMPLE METHOD FOR PREDICTION OF THE FLASH POINTS OF SATURATED HYDROCARBONS IN ORDER TO IMPROVE THEIR SAFETY

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Abstract. A reliable simple method is presented for predicting the flash point of pure cyclic and acyclic saturated hydrocarbons. The novel model is based on the number of carbon atoms as well as two structural parameters for improvement of the predicted results. The predicted flash points for a data set of 120 linear and branched alkanes as well as 59 cyclic alkanes are in good agreement with the measured values such that the root mean square (rms) error and the average absolute deviation are 4.6 and 5.4 K, respectively. The reliability of the new model for further 15 acyclic alkanes is comparable with several new models, which have been recently developed for acyclic alkanes. For 76 cyclic and acyclic alkanes, where outputs of complex method of neural network-group contribution method were available, the proposed model also provides good predictions. The proposed method can easily be used for different hydrocarbons including cyclic and acyclic compounds with complex molecular structures.

Keywords: flash point, saturated hydrocarbon, correlation, safety

Introduction

The flash point is the lowest temperature at which a liquid produces enough vapor to ignite in the presence of a source of ignition. It characterizes the fire potential of a combustible substance that can be used in categorizing industrial works as constituting the fire hazards and explosion. It has great practical significance in the handling and transporting of such materials in bulk quantities. For liquid propellants, the knowledge of flash points of liquid fuels is important for prevention of accidents. A large variety of liquid fuels including different hydrocarbon chemicals can be used as rocket propellants [1,2]. They may provide relatively good specific impulse with suitable liquid oxidizers [3-5].

Due to the advancement of technology in discovery or synthesis of new compounds, the experimental flash point values are scarce or too expensive to obtain [6]. For some classes of organic compounds that have dangerous properties such as toxicity and explosion of their vapors with air, the experimental determinations of flash point values are more difficult. Thus, the development of reliable estimation methods for different classes of organic compounds is highly desirable. There are many methods for predicting flash points of different classes of organic compounds, which have been extensively reviewed by some authors [7-9]. Flash points can be correlated with some physical properties such as vapor pressure and boiling point for some classes of organic compounds [7-9]. To obtain good predictive results for flash points, the accuracy of the needed physical properties is essential in this approach. However, reliable experimental values of the desired physical property are required to find the flash point.

Different approaches have been recently introduced to give good predictions for acyclic hydrocarbons [10-14]. For cyclic alkanes, group contribution method of Albahri [10] can also be used but Albahri's method [10] cannot be applied for some of cyclic and acyclic alkanes. Albahri [10] and Pan et al. [12] introduced two different correlations for predicting flash points of hydrocarbons. The method of Pan and coworkers [12] relies on a neural network taking bond group occurrences as input, which can be applied only for acyclic alkanes.

Neural networks can be applied in different branches of sciences, e. g. predicting impact sensitivity of energetic compounds [15,16]. They have become an important modeling technique in the field of quantitative structure-activity relationships (QSAR) and/or quantitative structure-property relationships (QSPR). The QSPR method has been used extensively in recent years for the prediction of flash points of organic compounds [17-26]. It is essential in the QSPR analysis to find optimum quantitative relationships between molecular structure and flash point through molecular descriptors. In general, the QSPR method requires special computer programs. Moreover, training set of the QSPR procedure should contain large number of compounds with different molecular structures to obtain suitable results for the compounds with similar molecular structure in test set. Two new neural network-group contribution methods have also been developed to predict flash points of organic compounds [24,25]. These methods require special software to apply with respect to simple methods of Albahri [10] and Pan et al. [12].

The purpose of this work is to introduce a novel simple method for calculating simultaneously both cyclic and acyclic alkanes. The predicted results are compared with experimental data and the estimated values of some predictive methods. It will be shown that the number of carbon atoms is sufficient for predicting flash points of most saturated hydrocarbons. Two correcting terms are also given in the new correlation, which can improve the predicted results on the basis of elemental composition. Some alkanes with complex molecular structures have been tested in the new scheme.

Development of a new method

For n-alkanes from C_3H_8 to $C_{16}H_{18}$, Mathieu [13] used the experimental data of flash points of these n-alkanes to indicate that their flash points are proportional to the square root variation of n_C (r^2>0.99). The correlation coefficient for linear fitting of flash points of n-alkanes with n_C for mentioned n-alkanes is also relatively good, which is 0.982. In contrast to n-alkanes, isoparaffins have lower flash points with respect to n-paraffins of the same carbon number [10]. For calculation of flash points of acyclic hydrocarbons, Carroll and coworkers [14] have also introduced flash point numbers that are proportional to n_C. For saturated cyclic and acyclic hydrocarbons, the flash point depends upon volatility and the contribution of the various molecular structure parameters. The study of flash points of mentioned hydrocarbons has shown that their flash points are a function of the number of carbon atoms in the molecule. A carful examination of flash points of many hydrocarbons reveals that the predicted flash points on the basis of the number of carbon atoms can be corrected to obtain a reliable predictive model. The presence of the certain length and location of especial type of branching along the hydrocarbon chain or cyclic hydrocarbons may increase or decrease the predicted results on the basis of the number of carbon atoms, which can be described as follows: (a) For cyclic alkanes that have small rings (three and four member rings) with only methyl groups as substituents or without any substituent, the predicted flash points composition can be decreased; (b) Large cyclic compounds with more than seven member rings have opposite effect and their predicted flash points have been increased; (c) The attachment of large linear alkyl groups (n_{alkyl} > 9) to cyclopentane and cyclohexane can improve the predicted flash points; (d) The existence of molecular fragments of isobutyl, i.e. $(CH_3)_3C^-$, in some saturated acyclic hydrocarbons is an important factor in decreasing predicted flash points; (e) Since flash points of small hydrocarbons are very low, some authors have omitted their contributions in selected data sets to obtain good results for the other saturated hydrocarbons, e.g. the method of Pan et al. [12].

For most hydrocarbons, the number of carbon atoms is sufficient to obtain a reliable prediction of flash points. A suitable correlation on the basis of the number of carbon (n_C) atoms as well as increasing (*ISP*) and decreasing (*DSP*) structural parameters can be given as follows:

$$FP(K) = A + 16.15.n_C + 16.68\ ISP - 24.71\ DSN \qquad (1)$$

where *A* is a constant that is equal to 146.6 and 154.9 for acyclic and cyclic alkanes, respectively. A multiple linear regression method and experimental data given in Table 1 were used to derive Eq. (1). The change of the value of constant *A* in Eq. (1) can be validated only in transition from alkanes (i.e. n-paraffins and iso-paraffins) to cycloalkanes. The new correlation can be easily applied for a wide range of saturated hydrocarbons including n-alkanes, iso-alkanes and cycloalkanes. Moreover, as indicated in Table 1, the new correlation can be applied to different types of hydrocarbons over a wide range of molecular weights, e.g. methane and cyclohexyltetradecane.

Correcting terms *ISP* and *DSP* of the new correlation can revise deviations of the predicted results of flash points of saturated hydrocarbons on the basis of n_C. They have been specified for some saturated cyclic and acyclic hydrocarbons according to the following situations: ***ISP***- This parameter can be used only for large cycloalkanes that have more than seven-membered rings. However, it is equal to 1.0 for these cyclic compounds; ***DSP***- The specification of this parameter for cyclic and acyclic compounds depends on the presence of particular molecular fragments, which can be classified as: (i) *Cycloalkanes with three- or four-membered rings:* For these compounds without any substituent or with the attachment of only methyl groups, the value of *DSP* is 1.0; (ii) *Cycloalkanes with five- or six-membered rings*: For the attachment of large n-alkyl with more than nine carbon atoms ($n_{C>9}$), *DSP* is equal to $(n_{C>9} - 9) \times 0.3$; (iii) *Acyclic hydrocarbons with isobutyl molecular fragment (i.e. $(CH_3)_3C$-R)*: If alkyl group has less than four carbons ($n_{C<4}$), the contribution of this structural parameter should be considered. The value of *DSP* can be calculated for this case as $DSP = 0.3\ n_{C<4}$; (iv) *Small acyclic hydrocarbons*: If $n_C \leq 4$, then $DSP = 4.25 - n_{C\leq 4}$.

The parameters *ISP* and *DSP* are equal to zero if the conditions for giving them various values are not met. The coefficient of determination or the r^2- value of Eq. (1) is relatively good, which is equal to 0.986 [27].

Results and discussion

The calculated flash points of various cyclic and acyclic saturated hydrocarbons compounds are given in Table 1 and compared with corresponding experimental data. Experimental data from different authors as well as organizations can differ by as much as 30 K [12]. The measured data of cyclic and acyclic alkanes were also taken from Ref. 28 in which all flash points are from the chemical database of the department of chemistry at the University of Akron (USA). As seen in Table 1, the root mean square (rms) error and the average absolute deviation in the new method are 4.6 and 5.4 K, respectively. Furthermore, maximum deviation of predicted results from experimental values in Table 1 is less than 16 K, which is acceptable with respect to uncertainty of experimental data

from different sources. A total of 179 some acyclic and cyclic aliphatic given in Table 1 were considered in the new method, and 94.4% of the estimated flash points were within ±10 K of the measured flash points. A visual comparison of the predicted results of the new correlation with the experimental data is also shown in Fig. 1. The predicted results show that this simple method can be easily applied to both cyclic and acyclic alkanes with complex molecular structures.

To compare the predicted results of new method with some new correlations, fifteen further compounds were also given in Table 2. These alkanes are compared with the methods of Pan et al. [12], infrared spectra [11], Albahri [10] and Carroll et al. [14]. The measured values of flash points were also taken from Ref. 28 except 2,7-dimethyloctane [29]. Based on the average flash point 282 K in Table 2, the average absolute deviations are 4.4, 6.3, 5.6, 3.6 and 4.4 K for the methods of new, Pan et al. [12], infrared spectra [11], Albahri [10] and Carroll et al. [14], respectively. According to the rms values from the new model and the other works [10-12,14], the reliability of this novel simple method for acyclic alkanes is comparable with mentioned methods. Pan et al. [12] showed that the absence of the predicted result for 2,7-dimethyloctane is a shortcoming of Albahri method [10]. A visual comparison of the predictions of the methods of new, Pan et al. [12], infrared spectra [11], Albahri [10] and Carroll et al. [14] with experiment is also given in Fig. 2. Although some of available correlations may also provide better results for a number of acyclic alkanes, e.g. Refs. [13,14], Eq. (1) provides good predictions not only for acyclic alkanes, but also for cyclic hydrocarbons.

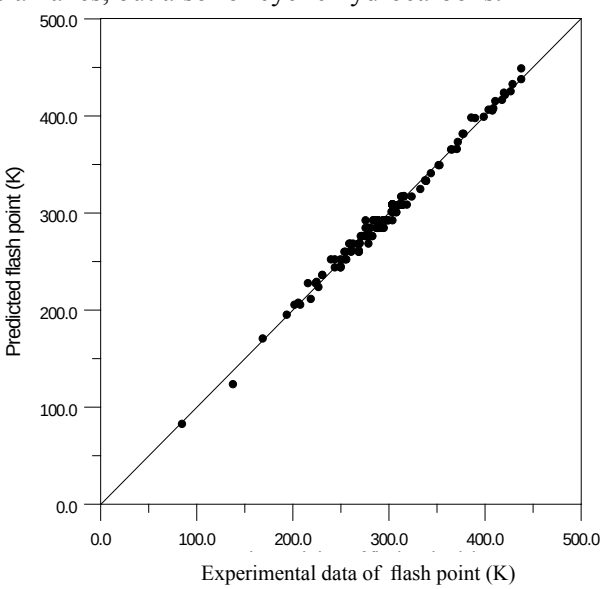

Fig. 1. Calculated flash points versus experimental data for different 179 cyclic and acyclic saturated hydrocarbons given in Table 1. The solid lines represent exact agreement between predictions and experiment. Filled circles denote the calculated results of the new method

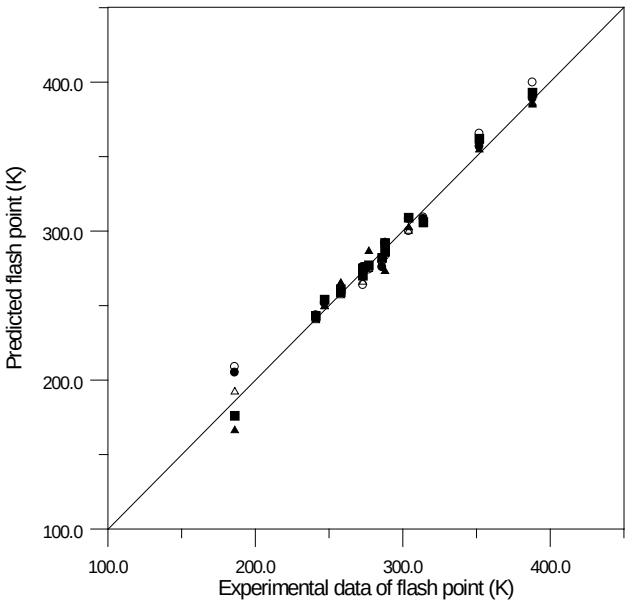

Fig. 2. Calculated flash points versus experimental data for different 15 acyclic alkanes given in Table 2. The solid lines represent exact agreement between predictions and experiment. Filled circles, hollow circles, filled triangles, hollow triangles and filled squares denote calculated results of the new, Pan et al. [12], infrared spectra [11], Albahri [10] and Carroll et al. [14] methods, respectively

To show the reliability of the new model with complex neural networks that were used for organic compounds, the predicted results of Eq. (1) are compared with complex neural network-group contribution method of Gharagheizi et al. [25] that are given in Table 3. Several points should be considered: (1) Different database DIPPR 801 [30] was used by Gharagheizi et al. [25] in which some of experimental data are different from the chemical database of the department of chemistry at the University of Akron (USA) [28], e.g. 2,2,5,5-tetramethylhexane; (2) Of 194 different compounds in Tables 1 and 2, only 76 saturated hydrocarbons were considered by Gharagheizi et al. [25] in their training and test sets; (3) some cyclic compounds such as cyclopropane and cyclobutane as well as their derivatives cannot be calculated by method of Gharagheizi et al. [25]; (4) many of compounds given in Table 1, which have ISP or DSP, were not included in the database of Gharagheizi et al. [25]. As seen in Table 3, although different database of DIPPR 801 [30] and only 39.2% of compounds in Tables 1 and 2 were used by Gharagheizi et al. [25], the rms values and the average absolute deviations of new model are also less than method of Gharagheizi et al. [25]. Thus, the predicted results of new simple model are comparable with output of complex neural networks. A visual comparison of the predictions of the new and Gharagheizi et al. [25] methods with database of DIPPR 801 [30] is also given in Fig. 3.

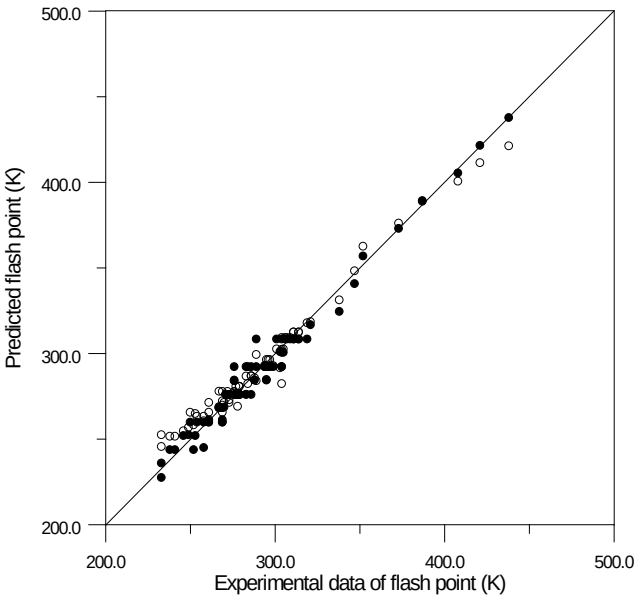

Fig. 3. Calculated flash points versus experimental data for different 76 cyclic and acyclic alkanes given in Table 3. The solid lines represent exact agreement between predictions and experiment. Filled and hollow circles denote calculated results of the new and Gharagheizi et al. [25] methods, respectively

Table 1. Comparison of the predicted flash points for 120 acyclic alkanes and 59 cycloalkanes with experimental data

No.	Compound	Experimental flash point (K)	Predicted flash point (K)	Deviation (K)
1	Methane	85	82.4	2.7
2	Ethane	138	123.3	14.9
3	Propane	169	170.4	-1.2
4	Butane	202	205.1	-2.9
5	Pentane	224	227.4	-3.3
6	2,2-Dimethylpropane	208	205.2	3.0
7	2-Methylbutane	216	227.4	-11.3
8	Hexane	250	243.6	6.6
9	2,2-Dimethylbutane	225	228.7	-3.6
10	2,3-Dimethylbutane	244	243.6	0.6

Table 1 (continued)

No.	Compound	Experimental flash point (K)	Predicted flash point (K)	Deviation (K)
11	2-Methylpentane	250	243.6	6.6
12	Heptane	269	259.7	9.4
13	3,3-Dimethylpentane	254	259.7	-5.6
14	2,4-Dimethylpentane	261	259.7	1.4
15	3-Ethylpentane	255	259.7	-4.6
16	2,2-Dimethylpentane	250	244.9	5.2
17	2-Methylhexane-	269	259.7	9.4
18	2,2,4-Trimethylpentane	261	261.1	0.1
19	2,2,3-Trimethylpentane	270	268.5	1.7
20	3-Methyl-3-ethylpentane	276	275.9	0.2
21	3-Ethylhexane	278	275.9	2.2
22	3-Methylheptane	279	275.9	3.2
23	3,3-Dimethylhexane	272	275.9	-3.8
24	2,3-Dimethylhexane	283	275.9	7.2
25	2,4-Dimethylhexane	283	275.9	7.2
26	2,5-Dimethylhexane	271	275.9	-4.8
27	2,3,3-Trimethylpentane	273	275.9	-2.8
28	2-Methylheptane	278	275.9	1.6
29	2,2-Dimethylhexane	269	261.1	8.1
30	4-Methylheptane	278	275.9	2.2
31	3-Ethyl-2-methylpentane	276	275.9	0.2
32	Nonane	304	292.1	12.1
33	2,5-Dimethylheptane	288	292.1	-3.9
34	3,3-Dimethylheptane	300	292.1	8.1
35	3,4-Dimethylheptane	288	292.1	-3.9
36	2,3-Dimethylheptane	288	292.1	-3.9
37	2,6-Dimethylheptane	299	292.1	7.1
38	2,3-Dimethyl-3-ethylpentane	288	292.1	-3.9
39	2,2,5-Trimethylhexane	286	292.1	-5.9
40	4-Methyloctane	295	292.1	3.1
41	2-Methyloctane	297	292.1	5.1
42	3-Methyloctane	297	292.1	5.1
43	2,2,3,4-Tetramethylpentane	284	292.1	-7.9

Table 1 (continued)

No.	Compound	Experimental flash point (K)	Predicted flash point (K)	Deviation (K)
44	2,3,3,4-Tetramethylpentane	284	292.1	-7.9
45	2,2,3,3- Tetramethylpentane	289	292.1	-2.9
46	2,2,4,4-Tetramethylpentane	276	292.1	-15.9
47	3-Ethylheptane	295	292.1	3.1
48	4-Ethylheptane	288	292.1	-3.9
49	2,2-Dimethylheptane	297	292.1	5.1
50	2,4-Dimethylheptane	288	292.1	-3.9
51	2,3,4-Trimethylhexane	288	292.1	-3.9
52	3,3,4-Trimethylhexane	288	292.1	-3.9
53	2,3,5-Trimethylhexane	288	292.1	-3.9
54	2,2,3-Trimethylhexane	288	292.1	-3.9
55	3,5-Dimethylheptane	288	292.1	-3.9
56	3,3-Diethylpentane	294	292.1	2.1
57	Tetraethylmethane	294	292.1	2.1
58	3-Ethyl-2,2-dimethylpentane	286	292.1	-5.9
59	4,4-Dimethylheptane	288	292.1	-3.9
60	3ethyl-2-methylhexane	288	292.1	-3.9
61	3-Ethyl-3-methylhexane	288	292.1	-3.9
62	4-Ethyl-2-methylhexane	288	292.1	-3.9
63	2,4-Dimethyl-3-ethylpentane	288	292.1	-3.9
64	2,2,4-Trimethylhexane	288	292.1	-3.9
65	2,3,3-Trimethylhexane	288	292.1	-3.9
66	Decane	319	308.3	10.9
67	3-Ethyloctane	314	308.3	5.9
68	4-Ethyloctane	314	308.3	5.9
69	2,2,4-Trimethylheptane	304	308.3	-4.1
70	3,4,4-Trimethylheptane	304	308.3	-4.1
71	3,3,4-Trimethylheptane	304	308.3	-4.1
72	2,4,4-Trimethylheptane	304	308.3	-4.1
73	2,3,6-Trimethylheptane	304	308.3	-4.1
74	2,3,5-Trimethylheptane	304	308.3	-4.1

Table 1 (continued)

No.	Compound	Experimental flash point (K)	Predicted flash point (K)	Deviation (K)
75	2,3,3-Trimethylheptane	304	308.3	-4.1
76	2,2,5-Trimethylheptane	304	308.3	-4.1
77	2,2,6-Trimethylheptane	304	308.3	-4.1
78	2,4,5-Trimethylheptane	304	308.3	-4.1
79	2,5-Dimethyloctane	314	308.3	5.9
80	2,4-Dimethyloctane	314	308.3	5.9
81	4,4-Dimethyloctane	314	308.3	5.9
82	4,5-Dimethyloctane	314	308.3	5.9
83	3,4-Dimethyloctane	314	308.3	5.9
84	3,6-Dimethyloctane	314	308.3	5.9
85	2,3-Dimethyloctane	314	308.3	5.9
86	3,3-Diethylhexane	311	308.3	2.9
87	3,3-Dimethyloctane	314	308.3	5.9
88	3,5-Dimethyloctane	314	308.3	5.9
89	2,6-Dimethyloctane	314	308.3	5.9
90	3-Ethyl-2,2-dimethylhexane	311	308.3	2.9
91	3,3,4,4-Tetramethylhexane	304	308.3	-4.1
92	2,2,5,5-Tetramethylhexane	304	308.3	-4.1
93	2,2,3,5-Tetramethylhexane	304	308.3	-4.1
94	2,3,3,5-Tetramethylhexane	304	308.3	-4.1
95	2,2,4,5-Tetramethylhexane	304	308.3	-4.1
96	2,3,4,5-Tetramethylhexane	304	308.3	-4.1
97	2,2,4,4-Tetramethylhexane	304	308.3	-4.1
98	3,3,5-Trimethylheptane	304	308.3	-4.1
99	2,3,5-Trimethylheptane	304	308.3	-4.1
100	3-Ethyl-3-Methylheptan	314	308.3	5.9
101	5-Ethyl-2-Methylheptan	314	308.3	5.9
102	3-Ethyl-4-Methylheptan	304	308.3	-4.1
103	4-Ethyl-3-Methylheptan	314	308.3	5.9
104	4-Methylnonane	311	308.3	2.9
105	3-Methylnonane	314	308.3	5.9

Table 1 (continued)

No.	Compound	Experimental flash point (K)	Predicted flash point (K)	Deviation (K)
106	2-Methylnonane	314	308.3	5.9
107	2,4,6-Trimethylheptane	304	308.3	-4.1
108	3-Ethyl-2,3,4-Trimethylpentane	304	308.3	-4.1
109	2,3,4,4-Tetramethylhexane	304	308.3	-4.1
110	3,4,5-Trimethylheptane	304	308.3	-4.1
111	3-Ethyl-5-methylheptane	304	308.3	-4.1
112	5-Methylnonane	312	308.3	3.9
113	2,2,3,4-Tetramethylhexane	304	308.3	-4.1
114	4-Propylheptane	314	308.3	5.9
115	Undecane	333	324.4	8.7
116	Dodecane	344	340.6	3.6
117	Tetradecane	372	372.9	-0.8
118	Hexadecane	408	405.3	2.9
119	Heptadecane	421	421.4	-0.3
120	Octadecane	438	437.6	0.5
121	Methylcyclopropane	194	194.9	-0.7
122	Cyclobutane	206	207.2	-1.1
123	Cyclopentane	231	235.8	-4.6
124	trans1,2-Dimethylcyclopropane	219	211.1	8.1
125	Methylcyclobutane	227	223.4	3.7
126	Ethylcyclopropane	231	235.8	-4.6
127	Cyclohexane	255	251.9	3.2
128	Methylcyclopentane	256	251.9	4.2
129	Ethylcyclobutane	250	251.9	-1.8
130	cis-1-Ethyl-2-methylcyclopropane	244	251.9	-7.8
131	1-Ethyl-1-methylcyclopropane	240	251.9	-11.8
132	Cycloheptane	279	268.1	11.0
133	Methylcyclohexane	269	268.1	1.0

Table 1 (continued)

No.	Compound	Experimental flash point (K)	Predicted flash point (K)	Deviation (K)
134	Ethylcyclopentane	269	268.1	1.0
135	trans-1,2-Dimethylcyclopentane	263	268.1	-5.0
136	Cis-1,2-Dimethylcyclopentane	269	268.1	1.0
137	Cis-1,3-Dimethylcyclopentane	259	268.1	-9.0
138	trans-1,3-Dimethylcyclopentane	260	268.1	-8.0
139	Cyclooctane	303	301.0	2.2
140	Ethylcyclohexane	292	284.3	7.9
141	Isopropylcyclopentane	287	284.3	2.9
142	n-Propylcyclopentane	289	284.3	4.9
143	1,1-Dmethylcyclohexane	276	284.3	-8.1
144	1-Ethyl-1-methylcyclopentane	279	284.3	-5.1
145	1,2-Dmethylcyclohexane	288	284.3	3.9
146	Cis-1,2-Dmethylcyclohexane	295	284.3	10.9
147	trans-1,2-Dmethylcyclohexane	290	284.3	5.9
148	1,3-Dmethylcyclohexane	279	284.3	-5.1
149	Cis-1,3-Dmethylcyclohexane	279	284.3	-5.5
150	Trans-1,3-Dmethylcyclohexane	281	284.3	-3.1
151	Cyclononane	316	317.1	-1.0
152	Isopropylcyclohexane	308	300.5	7.7
153	Butylcyclopentane	308	300.5	7.7
154	Propylcyclohexane	304	300.5	3.7
155	Cyclodecane	338	333.3	4.9
156	n-Butylcyclohexane	314	316.6	-2.5
157	1,1,4,-Trimethylcycloheptane	316	316.6	-0.5

Table 1 (continued)

No.	Compound	Experimental flash point (K)	Predicted flash point (K)	Deviation (K)
158	Pentylcyclopentane	324	316.6	7.5
159	tert-Butylcyclohexane	313	316.6	-3.5
160	Hexylcyclopentane	339	332.8	6.4
161	Pentylcyclohexane	339	332.8	6.4
162	Cyclododecane	371	365.6	5.5
163	1-Cyclohexylhexane	353	349.0	4.2
164	Heptylcyclopentane	352	349.0	3.2
165	1-Cyclohexylheptane	366	365.1	1.0
166	Octylcyclopentane	365	365.1	0.0
167	Nonylcyclopentane	377	381.3	-4.2
168	Cyclotetradecane	386	398.0	-11.8
169	Cyclohexyloctane	378	381.3	-3.2
170	Cyclohexylnonane	390	397.5	-7.3
171	Cyclopentylundecane	399	398.8	0.3
172	Cyclohexyldecane	404	406.2	-2.1
173	Undecylcyclohexane	411	415.0	-3.8
174	Cyclopentyldodecane	409	407.6	1.6
175	Cyclohexyldodecane	420	423.7	-3.6
176	Cyclopentyltridecane	418	416.3	1.8
177	Cyclohexyltridecane	429	432.5	-3.3
178	Cyclopentyltetradecane	427	425.1	2.1
179	Cyclohexyltetradecane	438	448.7	-10.5
The average absolute deviation				4.6
The rms deviation				5.4

Conclusions

A new method has been developed for simple and reliable predictions of flash points of both cyclic and acyclic aliphatic compounds. The present method is based on the number of carbon atoms as well as the contribution of two *ISP* and *DSP* structural parameters. The reliability of the methodology presented here is relatively good compared to the best available methods. The present model is especially useful for simple and reliable calculation of flash points of pure component of saturated hydrocarbons for which no data exist.

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Table 2. Comparison of the predicted flash points of new model with group contribution method of Pan et al. [12] and infrared spectra method [11]

No.	Compound	Experimental flash point (K)	Predicted flash point (K)	Deviation (K)	Pan et al.	Deviation (K)	Infrared spectra method	Deviation (K)
1	2-Methylpropane	186	205.1	-13.9	208.9	-22.9	166.1	19.9
2	3-Methylpentane	241	243.6	-2.6	242.4	-1.4	240.8	0.2
3	2,3-Dimethylpentane	258	259.7	-1.7	261.6	-3.6	265	-7.0
4	3-Methylhexane	258	259.7	-1.6	259.6	-1.5	264.5	-6.4
5	2,2,3-Trimethylbutane	247	252.3	-5.2	251.5	-4.4	249.5	-2.4
6	Octane	286	275.9	10.2	279.6	6.5	282.4	3.8
7	2,2,3,3-Tetramethylbutane	273	275.9	-2.8	263.9	9.3	273.3	-0.2
8	2,3,4-Trimethylpentane	273	275.9	-2.8	272.7	0.4	274.2	-1.1
9	3,4-Dimethylhexane	277	275.9	1.2	274.3	2.8	286.4	-9.3
10	3-Ethyl-4-Methylhexane	288	292.1	-3.9	291.1	-3.0	273	15.2
11	2,4,4-Trimethylhexane	288	292.1	-3.9	283.3	4.8	287.2	0.9
12	2,7-Dimethyloctane	314	308.3	5.8	309.3	4.7	304.3	9.7
13	2,3,3,4-Tetramethylhexane	304	308.3	-4.1	300.1	4.0	302.4	1.8

14	Tridecane	352	356.8	-4.6	365.5	-13.4	354.6	-2.5
15	Pentadecane	388	389.1	-1.1	399.9	-11.9	384.8	3.2
The average absolute deviation				4.4		6.3		5.6
The rms deviation				5.5		8.5		7.9

Table 3. Comparison of the predicted flash points of new model with method of Gharagheizi et al. [25]

No.	Compound	DIPPR 801 (K)	Predicted flash point (K)	Deviation (K)	Gharagheizi et al.	Deviation (K)
1	Pentane	233	227.4	5.8	245.46	-12.3
2	Hexane	252	243.6	7.9	258.1	-6.6
3	2-Methylpentane	238	243.6	-5.6	251.47	-13.5
4	3-Methylpentane	241	243.6	-2.6	251.47	-10.5
5	Heptane	269	259.7	9.4	272.1	-3.0
6	3,3-Dimethylpentane	254	259.7	-5.6	263.1	-9.0
7	2,4-Dimethylpentane	261	259.7	1.4	260.5	0.6
8	3-Ethylpentane	261	259.7	1.3	265.5	-4.5
9	2,2-Dimethylpentane	258	244.9	13.2	263.1	-5.0
10	2,3-Dimethylpentane	258	259.7	-1.7	260.5	-2.5
11	2-Methylhexane-	250	259.7	-9.7	265.5	-15.5
12	3-Methylhexane*	269	259.7	9.3	265.5	3.5
13	2,2,3-Trimethylbutane	249	252.3	-3.3	256.6	-7.6
14	Octane	286	275.9	10.2	286.9	-0.8
15	2,2,3,3-Tetramethylbutane	278	275.9	2.1	269	9.0
16	2,3,4-Trimethylpentane	273	275.9	-2.8	272.8	0.3
17	3,4-Dimethylhexane	277	275.9	1.1	276	1.0
18	2,2,4-Trimethylpentane	261	261.1	0.1	271.2	-10.1
19	2,2,3-Trimethylpentane	270	268.5	1.7	271.2	-1.1
20	3-Methyl-3-ethylpentane	276	275.9	0.2	277.6	-1.5
21	3-Ethylhexane	279	275.9	3.1	280.6	-1.6
22	3-Methylheptane	279	275.9	3.2	280.6	-1.5
23	3,3-Dimethylhexane	272	275.9	-3.8	277.6	-5.5
24	2,3-Dimethylhexane	279	275.9	2.6	276	2.5
25	2,4-Dimethylhexane	283	275.9	7.2	276	7.1

26	2,5-Dimethylhexane	271	275.9	-4.8	276	-4.9
27	2,3,3-Trimethylpentane	273	275.9	-2.8	271.2	1.9
28	2-Methylheptane	277	275.9	1.2	280.6	-3.5
29	2,2-Dimethylhexane	269	261.1	8.1	277.6	-8.5
30	4-Methylheptane	279	275.9	3.2	280.6	-1.5
31	Nonane	304	292.1	12.1	302.2	1.9
32	2,6-Dimethylheptane	299	292.1	7.1	292.7	6.4
33	2,2,5-Trimethylhexane	286	292.1	-5.9	286.6	-0.5
34	4-Methyloctane	295	292.1	3.1	296.3	-1.2
35	2-Methyloctane	296	292.1	3.9	296.2	-0.2
36	3-Methyloctane	297	292.1	5.1	296.3	0.8
37	2,2,3,4-Tetramethylpentane	284	292.1	-7.9	282.2	1.9
38	2,3,3,4-Tetramethylpentane	304	292.1	11.9	282.2	21.8
39	2,2,3,3-Tetramethylpentane	289	292.1	-2.9	283.9	5.3
40	2,2,4,4-Tetramethylpentane	276	292.1	-15.9	283.9	-7.8
41	2,2-Dimethylheptane	297	292.1	5.1	292.7	4.4
42	3,3-Diethylpentane	294	292.1	2.1	292.7	1.4
43	Tetraethylmethane	294	292.1	2.1	292.7	1.4
44	2,4,4-Trimethylhexane	283	292.1	-9.1	286.6	-3.6
45	Decane	319	308.3	10.9	317.8	1.3
46	2,5-Dimethyloctane	306	308.3	-2.2	309.1	-3.1
47	2,4-Dimethyloctane	304	308.3	-4.2	309.1	-5.1
48	2,3-Dimethyloctane	309	308.3	0.8	309.1	-0.1
49	2,6-Dimethyloctane	307	308.3	-1.2	309.1	-2.1
50	2,2,5,5-Tetramethylhexane	289	308.3	-19.2	299.2	-10.2
51	3,3,5-Trimethylheptane	301	308.3	-7.2	302.5	-1.5
52	4-Methylnonane	311	308.3	2.9	312.4	-1.3
53	3-Methylnonane	314	308.3	5.9	312.4	1.8
54	2-Methylnonane	314	308.3	5.9	312.4	1.8
55	5-Methylnonane	311	308.3	2.8	312.4	-1.4
56	Undecane	338	324.4	13.7	331.1	7.0
57	Dodecane	347	340.6	6.4	348.1	-1.1
58	Tridecane	352	356.8	-4.6	362.5	-10.4

59	Tetradecane	373	372.9	0.2	376	-2.9
60	Pentadecane	387	389.1	-2.1	388.7	-1.7
61	Hexadecane	408	405.3	2.9	400.5	7.6
62	Heptadecane	421	421.4	-0.3	411.3	9.8
63	Octadecane	438	437.6	0.5	421.1	17.1
64	Cyclopentane	233	235.8	-2.8	252.4	-19.4
65	Cyclohexane	253	251.9	1.2	264.7	-11.6
66	Methylcyclopentane	246	251.9	-5.9	254.6	-8.6
67	Cycloheptane	267	268.1	-1.0	277.8	-10.7
68	Methylcyclohexane	267	268.1	-1.0	268.7	-1.6
69	Ethylcyclopentane	269	268.1	1.0	269.6	-0.5
70	Cyclooctane	303	301.0	2.2	291.5	11.7
71	Ethylcyclohexane	295	284.3	10.9	284.6	10.6
72	n-Propylcyclopentane	288	284.3	3.7	285.6	2.4
73	1,1-Dmethylcyclohexane	276	284.3	-8.1	276.8	-0.7
74	Butylcyclopentane	305	300.5	4.6	302.5	2.5
75	Propylcyclohexane	304	300.5	3.7	301.3	2.8
76	n-Butylcyclohexane	321	316.6	4.4	318.4	2.6
The average absolute deviation			4.9		5.1	
The rms deviation			6.3		7.0	

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