New Neural Network Group Contribution Model for Estimation of Lower Flammability Limit Temperature of Pure Compounds

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New Neural Network Group Contribution Model for Estimation of Lower Flammability Limit Temperature of Pure Compounds

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In the present study, a group contribution based neural network method is developed to predict the lower flammability limit temperature (LFLT) of pure compounds. The needed parameters of the model are the occurrences of 125 functional groups in every molecule. The average absolute deviation error obtained over 1429 pure compounds used in this study is 2.35%. Therefore, the model is an accurate model and can be used to predict the LFLT of a wide range of pure compounds.

Introduction

The most common accident in chemical and petrochemical plants is fire.[1] To prevent accidents resulting from fire, knowledge about flammability characteristics of materials is necessary.

There are several parameters used to classify compounds according to their degree of flammability. Flash point (FP) is a well accepted and perhaps the most widely used parameter to evaluate the ability of a flammable compound to form an explosive atmosphere. FP is defined as the lowest temperature at which, a liquid produces enough vapor to ignite in air at atmospheric pressure when an ignition source such as an external flame, for instance, is applied under specified test conditions. Research shows that temperatures just below the FP are not safe enough.[2] Therefore, recently, another parameter has been considered by scientists for this purpose. This parameter is the lower flammability limit temperature (LFLT).[2]

The LFLT is defined as the lowest temperature at which the mixtures of vapor or gas with air, if ignited, will just propagate flame. The definition of the LFLT is like the definition of FP, but there is an important difference between definitions of these two properties. The FP is reached when a flame propagates from an ignition source such as an external flame through the vapor−air mixture, but LFLT is essentially independent of the ignition source strength.[2] Therefore, it can be concluded that the LFLT always is lower than FP. This result has been experimentally confirmed.[2] Therefore, attention to this result is very important and it can be found that LFLT is more important than FP in the evaluation of safely operating an industrial process. In other words, operating at temperatures below the FP may not be sufficiently safe, but operating at temperatures below the LFLT gives sufficient safety.[2]

One of the most widely used methods to estimate various physical and chemical properties is quantitative structure−property relationship (QSPR) methodology.[3−17] In QSPR methodology, the property under consideration is correlated using some chemical structure-based parameters. These parameters are calculated by known mathematical algorithms only from the chemical structure of compounds. There are many types of chemical structure-based parameters. Functional groups are one of the simplest classes of these parameters.

The literature surveys by the author of this manuscript showed that there is only one model for prediction of the LFLT of pure compounds.[18] This recently presented model is a classic quantitative structure−property relationship (QSPR). This model has six parameters. These parameters are calculated from the molecular structure of every pure compound. This model respectively shows squared correlation coefficient, average absolute deviation, standard error, and root-mean-square error of 0.9459, 3.98%, 15.554, and 15.613 over 1171 pure compounds. The most important disadvantage of the model is the complexity of procedure to compute the input parameters. Therefore, the main subject of this study is to present a simpler and more accurate method for estimation of LFLT. In the present study, a new collection of functional groups are used to develop an accurate model to predict the LFLT of pure compounds.

Materials and Methods

Data Set. Evaluated databases such as the DIPPR 801 database[19] are useful tools for developing new property prediction models. DIPPR 801 is recommended by AIChE (American Institute of Chemical Engineers) for physical properties of pure compounds. In this study, 1429 pure compounds were found in this database and their LFLTs were used as the main data set. These compounds and their LFLT values are presented in the Supporting Information. It should be noted that most of the LFLT values in the DIPPR 801 database are calculated via intersection of the temperature-dependent vapor pressure and temperature-dependent lower flammability limit (LFL) values.

Development of New Group Contributions. In this step, the chemical structures of all 1429 compounds were analyzed, and to represent the structure of the molecules to predict LFLT, 125 functionally groups were found useful.

The functional groups found and used in this study are extensively presented in Table 1.

These 125 functional groups and their numbers of occurrences in pure compounds are presented in the Supporting Information. These functional groups are used as input parameters for the model.

Generation of Neural Network Based Group Contribution. In this section, there are 125 functional groups and one physical property. We should find a relationship among these functional groups and the property. The simplest way to solve this problem is what is applied in the classical group contributions method. In this method, a multilinear relationship among inputs (125 functional groups in this study) and output (the LFLT in this study) is assumed. Then a computation is attempted of the value

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Table 1. Functional Groups Used to Develop the Model[a]

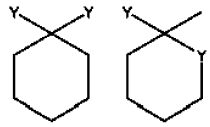
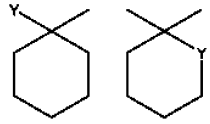
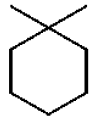
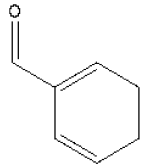
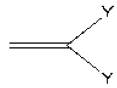
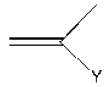
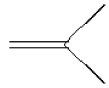
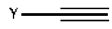
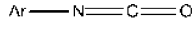
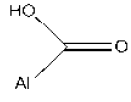
No.	ID	Group	Comments
1	F001	$C\text{-}CY_3$	number of terminal primary C(sp3) Y = any terminal atom or heteroaromatic group (i.e. H, X, OH, NH2, etc.)
2	F002	$C\text{-}CY_2\text{-}C$	number of total tertiary C(sp3) Y = H or any heteroatom
3	F003	$C\text{-}CY_2(C)\text{-}C$	number of total quaternary C(sp3)
4	F004	$C\text{-}C(C)_2\text{-}C$	number of total quaternary C(sp3)
5	F005		number of ring secondary C(sp3) Y = H or any heteroatom
6	F006		number of ring tertiary C(sp3) Y = H or any heteroatom
7	F007		number of ring quaternary C(sp3)
8	F008	Sum of all the carbons belonging to any aromatic and heteroaromatic structure	number of aromatic C(sp2)
9	F009		number of non-aromatic conjugated C(sp2)
10	F010		number of terminal primary C(sp2) Y = any terminal atom or heteroaromatic group (i.e. H, X, OH, NH2, etc.)
11	F011		number of aliphatic secondary C(sp2) Y = H or any heteroatom
12	F012		number of aliphatic tertiary C(sp2)
13	F013		number of allenes groups
14	F014		number of terminal C(sp)
15	F015		number of non-terminal C(sp) Y = C or any non-terminal heteroatom
16	F016		number of isocyanates (aliphatic)
17	F017		number of isocyanates (aromatic)
18	F018		number of carboxylic acids (aliphatic)

Table 1. Continued

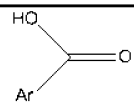
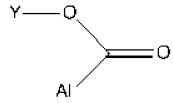
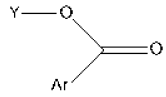
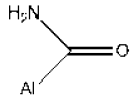
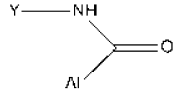
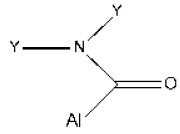
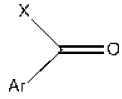
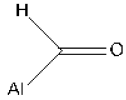
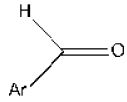
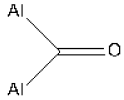
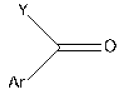
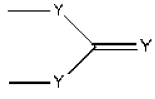
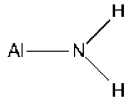
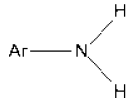
No.	ID	Group	Comments
19	F019		number of carboxylic acids (aromatic)
20	F020		number of esters (aliphatic) Y = Ar or Al (not H) Al = H or aliphatic group linked through C
21	F021		number of esters (aromatic) Y = Al or Ar
22	F022		number of primary amides (aliphatic) Al = H or aliphatic group linked through C
23	F023		number of secondary amides (aliphatic) Y = Ar or Al (not H, not C = O) Al = H or aliphatic group linked through C
24	F024		number of tertiary amides (aliphatic) Y = Ar or Al (not H, not C = O) Al = H or aliphatic group linked through C
25	F025		number of acyl halogenides (aromatic)
26	F026		number of aldehydes (aliphatic)
27	F027		number of aldehydes (aromatic)
28	F028		number of ketones (aliphatic)
29	F029		number of ketones (aromatic) Y = Al or Ar
30	F030		number of carbonate (-thio) derivatives Y = O or S
31	F031		number of primary amines (aliphatic) Al = aliphatic group linked through C (not C = O)
32	F032		number of primary amines (aromatic)

Table 1. Continued

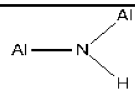
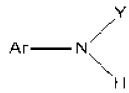
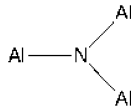
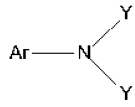
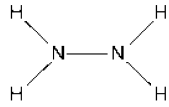
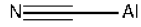
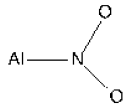
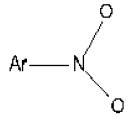
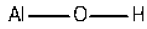
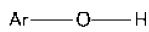
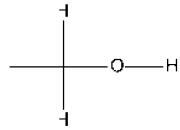
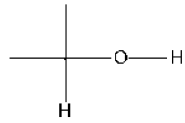
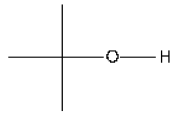
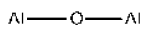
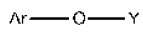
No.	ID	Group	Comments
33	F033		number of secondary amines (aliphatic) Al = aliphatic group linked through C (not C = O)
34	F034		number of secondary amines (aromatic) Y = Ar or Al (not C = O)
35	F035		number of tertiary amines (aliphatic) Al = aliphatic group linked through C (not C = O)
36	F036		number of tertiary amines (aromatic) Y = Ar or Al (not C = O)
37	F037		number of N hydrazines Y = C or H
38	F038		number of nitriles (aliphatic)
39	F039		number of nitriles (aromatic)
40	F040		number of nitro groups (aliphatic) Al = H or aliphatic group linked through carbon
41	F041		number of nitro groups (aromatic) Al = aromatic group linked through carbon
42	F042		number of hydroxyl groups Al = aliphatic group linked through any atom
43	F043		number of aromatic hydroxyls Ar = aromatic group linked through any atom
44	F044		number of primary alcohols
45	F045		number of secondary alcohols
46	F046		number of tertiary alcohols
47	F047		number of ethers (aliphatic) Al = aliphatic group linked through C (not C = O, not C # N)
48	F048		number of ethers (aromatic) Y = Ar or Al (not C = O, not C # N)

Table 1. Continued

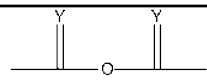
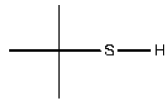
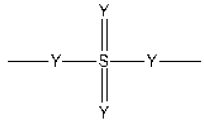
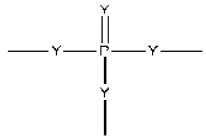
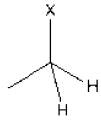
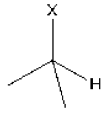
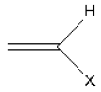
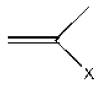
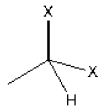
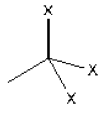
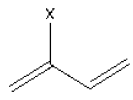
No.	ID	Group	Comments
49	F049		number of anhydrides (thio-) Y = O or S
50	F050		number of thiols
51	F051		number of sulfides
52	F052		number of sulfates (thio- / dithio-) Y = O or S
53	F053		number of phosphates / thiophosphates Y = O or S
54	F054		number of CH2RX
55	F055		number of CHR2X
56	F056		number of R=CHX
57	F057		number of R=CRX
58	F058		number of CHRX2
59	F059		number of R=CX2
60	F060		number of CRX3
61	F061		number of X on aromatic ring
62	F062		number of X on exo-conjugated C
63	F063		number of Aziridines

Table 1. Continued

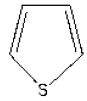
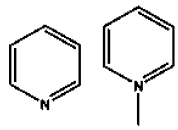
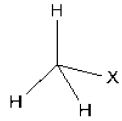
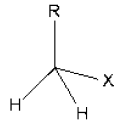
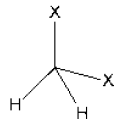
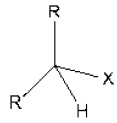
No.	ID	Group	Comments
64	F064		number of Oxiranes
65	F065		number of Pyrrolidines
66	F066		number of Oxolanes
67	F067		number of tetrahydro-Thiophenes
68	F068		number of Furanes
69	F069		number of Thiophenes
70	F070		number of Pyridines
71	F071	Sum of the hydrogens linked to all of the Os and Ns in the molecule	number of donor atoms for H-bonds (N and O)
72	F072	Total number of Ns, Os and Fs in the molecule, excluding N with a formal positive charge, higher oxidation states and pyrrolyl form of N	number of acceptor atoms for H-bonds (N, O, F)
73	F073		X represents any electronegative atom (O, N, S, P, Se, halogens)
74	F074		X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon
75	F075		X represents any electronegative atom (O, N, S, P, Se, halogens)
76	F076		X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon

Table 1. Continued

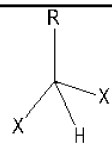
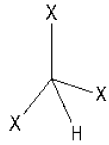
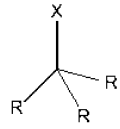
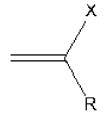
No.	ID	Group	Comments
77	F077		X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon
78	F078		X represents any electronegative atom (O, N, S, P, Se, halogens)
79	F079		X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon
80	F080		X represents any electronegative atom (O, N, S, P, Se, halogens)
81	F081		X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon
82	F082	R--CR--R	R represents any group linked through carbon -- represents an aromatic bond as in benzene or delocalized bonds such as the N-O bond in a nitro group
83	F083	R--CX--R	R represents any group linked through carbon -- represents an aromatic bond as in benzene or delocalized bonds such as the N-O bond in a nitro group
84	F084	R--CH--X	X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon -- represents an aromatic bond as in benzene or delocalized bonds such as the N-O bond in a nitro group
85	F085	R--CR--X	X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon -- represents an aromatic bond as in benzene or delocalized bonds such as the N-O bond in a nitro group
86	F086	R--CH..X	X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon -- represents an aromatic bond as in benzene or delocalized bonds such as the N-O bond in a nitro group .. represents aromatic single bonds as the C-N bond in pyrrole
87	F087	R--CR..X	X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon -- represents an aromatic bond as in benzene or delocalized bonds such as the N-O bond in a nitro group .. represents aromatic single bonds as the C-N bond in pyrrole
88	F088	R-C(=X)-X or R-C#X or X=C=X	X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon = represents a double bond; # represents a triple bond
89	F089	X-C(=X)-X	X represents any electronegative atom (O, N, S, P, Se, halogens) = represents a double bond
90	F090	H^a attached to C^0(sp3) no X attached to next C	X represents any electronegative atom (O, N, S, P, Se, halogens)
91	F091	H attached to C^0(sp3) no X attached to next C	X represents any electronegative atom (O, N, S, P, Se, halogens)
92	F092	H attached to C^1(sp3) / C^0(sp2)	

Table 1. Continued

No.	ID	Group	Comments
93	F093	H attached to C^3(sp3) or C^2(sp2) or C^3(sp2) or C^3(sp)	
94	F094	H attached to alpha-C	An alpha-C may be defined as a C attached through a single bond with -C=X, -C#X, -C--X = represents a double bond; # represents a triple bond
95	F095	H attached to C^0(sp3) with 1X attached to next C	X represents any electronegative atom (O, N, S, P, Se, halogens)
96	F096	H attached to C^0(sp3) with 2X attached to next C	X represents any electronegative atom (O, N, S, P, Se, halogens)
97	F097	H attached to C^0(sp3) with 3X attached to next C	X represents any electronegative atom (O, N, S, P, Se, halogens)
98	F098	alcohol	
99	F099	phenol or enol or carboxyl OH	
100	F100		
101	F101	Al-O-Al	Al represents aliphatic group
102	F102	Al-O-Ar or Ar-O-Ar or R..O..R or R-O-C=X	Al and Ar represent aliphatic and aromatic groups = represents a double bond .. represents aromatic single bonds as the C-N bond in pyrrole
103	F103	R-O-O-R	R represents any group linked through carbon
104	F104	Ar-NH-Al	Al represents aliphatic group
105	F105	Ar-NAl2	Al represents aliphatic group
106	F106	RCO-N< or >N-X=X	X represents any electronegative atom (O, N, S, P, Se, halogens) R represents any group linked through carbon = represents a double bond; # represents a triple bond
107	F107	Ar2NH or Ar3N or Ar2N-Al or R..N..R†	Al and Ar represent aliphatic and aromatic groups R represents any group linked through carbon .. represents an aromatic bond as in benzene or delocalized bonds † Pyrrole-type structure
108	F108	R#N or R=N-	.. represents an aromatic bond as in benzene or delocalized bonds = represents a double bond; # represents a triple bond
109	F109	R--N--R§ or R--N--X	R represents any group linked through carbon X represents any electronegative atom (O, N, S, P, Se, halogens) -- represents an aromatic bond as in benzene or delocalized bonds § Pyridine-type structure
110	F110	F attached to C^1(sp3)	
111	F111	F attached to C^2(sp3)	
112	F112	F attached to C^3(sp3)	
113	F113	F attached to C^1(sp2)	
114	F114	F attached to C^2(sp2)-C^4(sp2) or C^1(sp) or C^4(sp3) or X	X represents any electronegative atom (O, N, S, P, Se, halogens)
115	F115	Cl attached to C^1(sp3)	
116	F116	Cl attached to C^2(sp3)	
117	F117	Cl attached to C^3(sp3)	
118	F118	Cl attached to C^1(sp2)	
119	F119	Cl attached to C^2(sp2)-C^4(sp2) or C^1(sp) or C^4(sp3) or X	X represents any electronegative atom (O, N, S, P, Se, halogens)

Table 1. Continued

No.	ID	Group	Comments
120	F120	Br attached to C^1(sp3)	
121	F121	Br attached to C^1(sp2)	
122	F122	R2S or RS-SR	R represents any group linked through carbon
123	F123	R=S	R represents any group linked through carbon
124	F124	R-SO-R	R represents any group linked through carbon
125	F125	R-SO2-R	R represents any group linked through carbon

[a] The superscript represents the formal oxidation number. The formal oxidation number of a carbon atom equals the sum of the conventional bond orders with electronegative atoms; the C−N bond order in pyridine may be considered as 2 when we have one such bond and 1.5 when we have two such bonds; the C···X bond order in pyrrole or furan may be considered as 1.

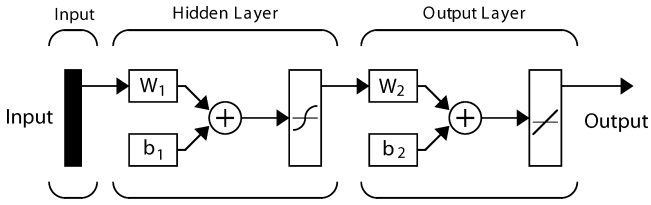


Figure 1. Schematic structure of the three layer feed forward neural network (FFNN) used in this study.

of every functional group contribution using the least-squares method. We used this method, but the results are very poor compared to what can be used as an accurate estimation model (the squared correlation coefficient of the linear group contribution model obtained using these 125 functional groups is 0.7618). Therefore, we should find a nonlinear relationship among inputs and output in this study.

Neural networks are extensively used in various scientific and engineering areas such as estimations of physical and chemical properties.[20] These powerful tools are usually applied to study of complicated systems such as the problem defined here. Theoretical explanations of neural networks can be found in many references such as ref 21.

This solution is found useful, and therefore, using the Neural Network toolbox of the MATLAB software (Mathworks, Inc.), three layer feed forward neural networks were evaluated for the problem. The schematic of the typical structure of three layer feed forward neural networks is presented in Figure 1.

This type of neural network has been used by the author in his previous works; therefore, detail explanations of the three layer feed forward used in this study can be found elsewhere.[5,9,12−15,17]

All 125 functional groups and the LFLT should be normalized between −1 and +1 to decrease computational errors. This work can be performed using maximum and minimum values of every 125 functional groups for inputs and using maximum and minimum values of the LFLT for output. After this step, the main data set should be divided into two new data sets. These two data sets include: the training and test sets. The training set is used to generate and optimized neural networks, and the test set is used only to check the validity of the obtained model. The process of division of the main data set into two new data sets is usually randomly performed. For this purpose, 80% of the main data set is randomly selected for the training set and the other 20% is used for the test set. Regarding the percent of the test set from the main data set, it should be noted that researchers have used various percents of the main data set for the test set. For example, Albahri and George[22] used 5% of the main data set for the test set (20 compounds from 490 compounds). In another work, Albahri[23] used 5% of the main data set for the test set (9 compounds from 200 compounds). Besides these works, Gharagheizi et al.[5] used 10% of the main data set for the test set (137 compounds from 1378 compounds). The effect of the percent of the test set from the main data set on the accuracy of the neural networks has been studied.[7] The results of this study show that the percent of the test set from the main data set should be between 5−35%. If this percent is lower than 5%, the accuracy of the model over the training set is greater than the test set. Also, if the percent is greater than 40%, the obtained model cannot predict the test set as well as the training set. On the other hand, the experiences of the author shows that the optimum percent of the test set is dependent on the nature of the problem. While solving a problem, different percents of the main data set should be used for the test set. The optimum percent is the percent at which the accuracy of the model over the test set approaches the training set.

We come back to the problem. Various percents of the main data set were used for the test set. Of them, for several times, application of 20% of the main data set for the test showed the least difference among accuracies of the model over the test set and the training set. As a result, 20% of the main data set was used for the test set and the rest of the data was used in the training set (285 compounds for the test set and 1144 compounds for the training set). These compounds were selected randomly.

Using the training set and the test set, the three layer feed forward neural networks were applied to generate a model to predict LFLT.

Generating a neural network means determination of the weight matrices and bias vectors. As shown in the Figure 1, there are two weight matrices and two bias vectors in a three layer feed forward neural network; $\mathbf{W}_1$ and $\mathbf{W}_2$, b_1 and b_2. These parameters should be obtained by minimization of an objective function. The objective function used in this study is sum of squares of error among the outputs of the neural network (estimated LFLT) and the target values (real LFLT of those compounds). This minimization was performed with

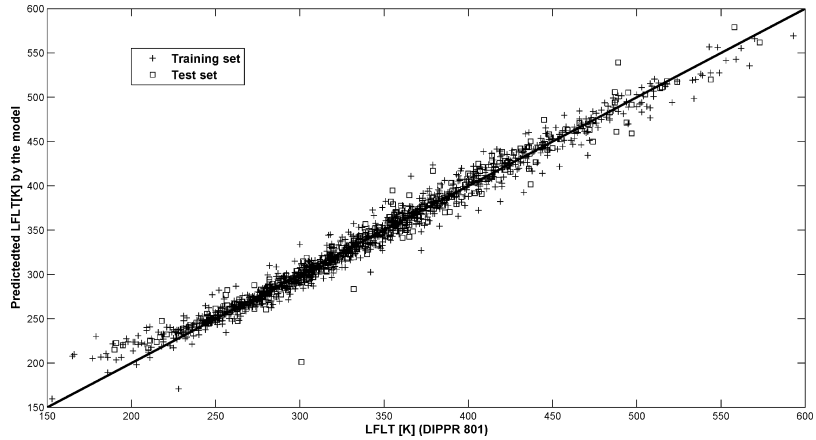


Figure 2. Comparison between LFLT predicted by the model and the DIPPR 801 data.

a Levenberg−Marquardt algorithm. This algorithm is rapid and accurate in the process of training neural networks.[20]

Results and Discussion

By the presented procedure in the previous section, an optimized feed forward neural network was obtained for prediction of LFLT. For determination of the number of neurons of the hidden layer of the neural network, the numbers 1−50 were checked and the number 12 showed the best results. Therefore, the best three layer feed forward neural network has the structure: 125−12−1. This result confirms the empirical rule among the number of input parameters, the number of output parameters, and the number of neurons of the hidden layer:

$$N = \sqrt{I \times O} \tag{1}$$

where in this equation, N, I, and O are respectively the number of neurons in the hidden layer, number of input parameters, and number of output parameters in a three layer feed forward neural network. It should be noted that in this study, I and O are respectively equal to 125 and 1. Therefore, N should be between 11 and 12. In these cases, N should be rounded to next integer number.

The mat file (MATLAB file format) of the obtained neural network containing all parameters of the obtained model can be requested by email from the author of this manuscript. The predicted LFLTs using this model in comparison with the real values are shown in Figure 2. Also, these values are reported in the Supporting Information.

The upper and lower LFLT used in the training set and the test set are respectively 153, 593, 190, and 573 K. The results obtained by model are presented in Table 2. These results show that the squared correlation coefficient, average absolute deviation, standard deviation error, and root-mean-square error of the model over the training, test, and main data sets are respectively 0.981, 0.97, 0.9786, 2.30%, 2.55%, 2.35%, 10.45, 12.95, 11, 10.43, 13, and 11. The average absolute deviation error obtained by the model over all 1429 compounds is shown in Figure 3. As can be found, the obtained model is an accurate model to predict the LFLT of pure components.

In comparison with the previously presented method,[18] this model is more accurate and validated using a larger data set. Also, computation of parameters of this model is simpler than that model.

Conclusion

In the presented study, a molecular-based model was presented for prediction of LFLT of pure compounds. The model is the result of a combination of group contributions and neural networks. The needed parameters of the model are the number of occurrences of 125 functional groups in every molecule. It should be noted that many of these 125 functional groups are not simultaneously available in a molecule; therefore, computation of these parameters from chemical structure of every molecule is simple. For developing the model, 1429 pure compounds were used; therefore, this model can be used to predict LFLT of every regular compound with some limitations. These 1429 pure compounds cover many families of compounds; therefore, the model has a wide range of applicability,

Table 2. Statistical Parameters of the Obtained Model

statistical parameter	value
training set	
R^2	0.981
average absolute deviation	2.30%
standard deviation error	10.45
root mean square error	10.43
n	1144
test set	
R^2	0.97
average absolute deviation	2.55%
standard deviation error	12.95
root mean square error	13
n	285
training set + test set	
R^2	0.9786
average absolute deviation	2.35%
standard deviation error	11
root mean square error	11
n	1429

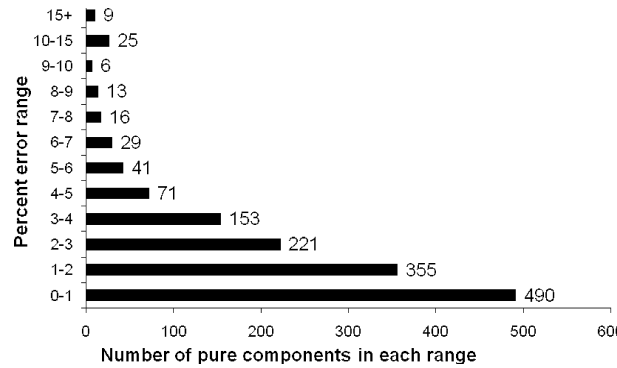


Figure 3. Percent errors obtained using the presented model and number of pure compounds in each range.

but application of the model is restricted to those compounds similar to the compounds used to develop this model. Application of the model to those compounds which are completely different from compounds used to develop the model is not recommended. Finally, it should be noted that the average absolute deviation reached with this method cannot replace the safety margins which are necessary in practice.

Supporting Information Available: Table showing 125 functional groups computed for 1429 pure compounds used in this study. This material is available free of charge via the Internet at http://pubs.acs.org.

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