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Corresponding States Method for Estimation of Upper Flammability Limit Temperature of Chemical Compounds

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S Supporting Information

ABSTRACT: The accuracy and predictability of predictive methods to determine the flammability characteristics of chemical compounds are of drastic significance in the chemical industry. This work aims at continuing application of the gene expression programming (GEP) mathematical strategy to modify the existing thermophysical properties correlations available in the literature to pursue the following objectives: optimization of the number of independent parameters, amplification of the generality, and improvement of the accuracy and predictability. This work deals with presenting a simple corresponding states model to predict the upper flammability limit temperature of 1462 organic compounds from 76 chemical families. The parameters of the correlation include the critical temperature and the acentric factor of the compounds. The obtained statistical parameters including average absolute relative deviation of the results from DIPPR 801 database values (1.7, 1.8, 1.7% for training, optimization, and prediction sets, respectively) demonstrate improved accuracy of the presented correlations.

1. INTRODUCTION

The knowledge of flammability limits of liquids is essential in the design of different processes, particularly those dealing with combustible materials.^{1–11} Flammability characteristics enable engineers to consider precautionary actions to prevent fire onset and explosion in diverse industrial processes. The term “flammability limits” in the form of concentration or mole fraction is not normally appropriate for application in industry. Instead, the use of some temperature related parameters such as lower flammability limit temperature (LFLT) and upper flammability limit temperature (UFLT) is preferable.

The upper flammability limit temperature (UFLT), or the upper explosion point is defined as the liquid temperature at which the concentration of vapor that is in thermodynamic equilibrium with the liquid equals the upper flammability limit. The experimental details of measuring the UFLT are presented elsewhere.^{12,13}

Because experimentally measuring the UFLT is costly and time-consuming, having an accurate hand-held computational method would be favorable. Our literature survey shows that there is only one method for prediction of the UFLT of pure compounds.⁹ The mentioned tool is an artificial neural-network group contribution method which has been developed by the first author. It demonstrates the average absolute relative deviation (AARD %) of 1.7% for all of the 1294 pure compounds employed for its development. The model has two major drawbacks. First, the number of parameters of the model is quite high, and, second, the implicit nature of the model makes it difficult to apply.

In the majority of problems in chemical engineering, having a theoretical idea may suggest some basic models; however, the majority of these kinds of models seem to be weak to be directly applied in industry because of lack of sufficient

accuracy. As a result, semi/empirical correlations may be taken into account.

Some semi/empirical correlations are normally based on some scientific idea. Perhaps, the most widely used scientific idea that has been so far implemented is the corresponding states theory. Using this theory, the physical properties of compounds may be correlated using their critical properties and acentric factors.

In this study, we apply the gene expression programming (GEP)¹⁴ to develop a corresponding states method for representation and prediction of the UFLT of approximately 1500 pure compounds. The details of the GEP technique can be found elsewhere.^{14–17}

2. DATABASE FOR UPPER FLAMMABILITY LIMIT TEMPERATURE

As the quality and generality of the applied database has a direct influence on the developed model/correlation for determination of the UFLT, the comprehensive DIPPR 801 database¹⁸ has been used in this work. The UFLT temperatures of 1462 pure compounds have been employed for developing and validating an accurate correlation.

3. DEVELOPING THE CORRELATION

A similar calculation procedure described in the previous works^{15,16} has been followed here to develop the corresponding

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state model. The corresponding states principle parameters including critical pressure (P_c), critical temperature (T_c), critical volume (V_c), acentric factor (ω), normal boiling point temperature (T_b), and the molecular weight (M_w) have been introduced as input parameters to the algorithm. It is first assumed that the UFLT value can be formulated as a function of the aforementioned properties as follows:

$$\text{UFLT} = f(T_c, P_c, V_c, \omega, T_b, M_w) \quad (1)$$

Having defined the independent parameters of the correlation, the following computational algorithm has been applied.

(1) Initialization of the population or generating, randomly, the chromosomal structures of the individuals by setting many correlations presented as parse trees using the operators ($-$, $+$, $*$, $/$, \wedge) and terminals as functions of the input data and the output desired results (the UFLT values).

(2) Calculation of the fitness value for every individual of the generated population by the following objective function (OF):

$$\text{OF}(i) = \frac{100}{N} \sum_i \frac{|\text{UFLT}(i)^{\text{pred}} - \text{UFLT}(i)^{\text{expt}}|}{\text{UFLT}(i)^{\text{expt}}} \quad (2)$$

where N is the number of the data points used in the GEP¹⁹ algorithm, and subscripts *pred* and *expt* denote the determined the UFLT values by the final developed correlation and experimental data, respectively.

(3) Selection of the individuals to stand for appropriate parents for replacement, which were evaluated from the fitness values. In this work, the tournament technique^{19,20} has been applied to provide an acceptable diversity of the population in every generation.

(4) Use of the genetic operators including replication, mutation, and inversion for gene reproduction with modification computational steps.

(a) Replication operator: It copies exactly the chromosomes of the individuals chosen in the selection step (step 3).¹⁹

(b) Mutation operator: It contributes to efficient adaption of populations of individuals.¹⁹ In this study, the point mutation has been used, in which a random node (in the structures of the chromosomes) is selected and the stored information is replaced with a different random primitive of the same parity taken from the initial (old) set. Having defined the mutation rate (*pm*), the mutation can occur everywhere in the structural organization of chromosomes though with preservation of the original structure.¹⁹ Generally, the mutation can be performed through changing the heads of genes symbols and terminals of the tails.^{14,19}

(c) Inversion operator: This operator is applied to create new individuals through modification of the heads of randomly selected genes. It has already proven that all the new individuals created by inversion are correct programs. The performance of this operator can be set choosing a value for inversion rate (*pi*).¹⁹

(5) Transposition and insertion sequence elements: The transposable elements of gene expression programming are the portion of the genome that can be activated and jump to another place in the chromosome, which include three types as implemented by Ferreira:¹⁹ "Short fragments with either a function or terminal in the first position transpose to the head of genes, short fragments with a function in the first position that transpose to the root of genes (root IS elements or RIS

elements), and entire genes that transpose to the beginning of chromosomes."

(6) Recombination: This step, which is conducted in three manners including one-point recombination, two-point recombination, and gene recombination, randomly chooses two chromosomes to exchange specific material with each other, leading to appearance of two new chromosomes.¹⁹ Consequently, new generation is created. The preceding procedure is repeated until the defined stopping criteria (can be user-defined convergence criteria or maximum number of generations) is satisfied. The details of this procedure along with comprehensive examples are provided by Ferreira.¹⁹

During the calculation steps, the database is randomly divided into the "Training" set (1170 data points, about 80% of the whole data set), the "Optimization" set (146 data points, about 10% of the whole data set), and the "Prediction" set (146 data points, about 10% of the whole data set).²¹ The training set is used to develop the model. Then the model is calibrated using the optimization set. To ensure the predictive power, the third data set, namely, the prediction set, is implemented.

4. RESULTS AND DISCUSSION

The explained procedure has been followed to obtain an accurate and simple correlation. As a matter of fact, the GEP¹⁹ algorithm computational steps define the required parameters, which yield the most accurate correlation from the introduced parameters (T_c , P_c , V_c , ω , T_b , M_w). Therefore, one can consider several independent parameters for a particular problem and obtain the ones, which have the most effects on the desired output results. The final correlation can be expressed as follows:

$$\text{UFLT} = 2\omega + 11.799 + T_c(0.1401\omega - 0.1401(0.4943\omega - 0.3851)^2 + 0.4943) \quad (3)$$

In the above equation, the unit of both UFLT and T_c is Kelvin. The number of the digits of the coefficient in eq 3 has been determined by performing sensitivity analysis of the estimated results to the corresponding value. The statistical parameters of the obtained results indicate that the average absolute relative deviations of the three subdata sets results are about 1.7% from the corresponding experimental values.¹⁸ This issue shows acceptable accuracy of the correlation for determination of the UFLT of the investigated compounds. A comparison between the predicted UFLT values and the experimental ones are interpreted in Figures 1 and 2.

The significant parameters/factors in the GEP¹⁹ calculation steps are reported in Table 1. As can be seen, the numbers of treated chromosomes, genes, the mutation and inversion coefficients, and the applied operators are among the effective parameters of the algorithm required for obtaining an acceptable correlation of interest. We would rather point out that the time of the calculations using the GEP algorithm is of drastic importance in this work. In this study, we have defined a stopping criterion for the algorithm. It may be possible to obtain a slightly more accurate correlation if one continues the calculation steps following more generations from the subsequent populations.

The statistic parameters of the model for training, optimization, and prediction sets are presented in Table 2.

As depicted in eq 3, the model is very simple and has just two input parameters. The results demonstrate that the model is much more accurate than the previously proposed model by the first author. It should be noted that the data set previously

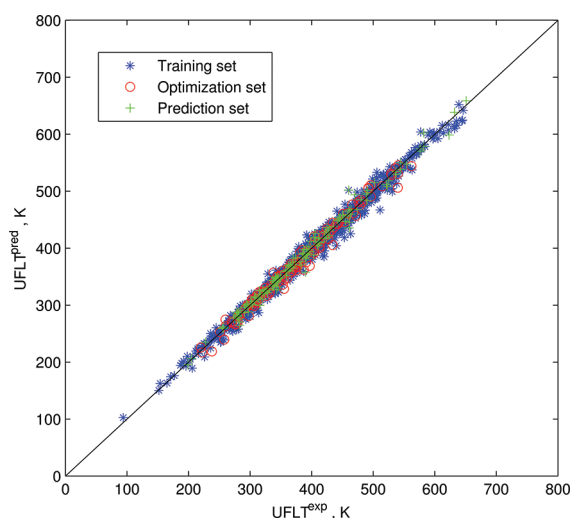


Figure 1. Comparison between the results of the developed correlation (eq 3) and the database¹⁸ values for the UFLT of investigated chemical compounds. Superscripts pred and expt represent the UFLT values predicted/represented by eq 3 and the UFLT values reported in DIPPR 801¹⁸ data set, respectively.

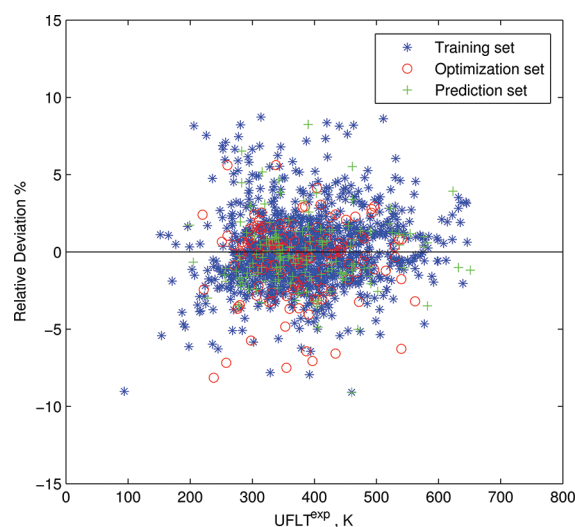


Figure 2. Relative deviations of the UFLT values of the investigated chemical compounds obtained by eq 3 from database¹⁸ values. Superscripts pred and expt represent the UFLT values predicted/represented by eq 3 and the UFLT values reported in DIPPR 801¹⁸ data set, respectively.

studied has 1294 UFLT data, whereas the data set employed in this work has 1462 UFLT data. The evaluation of the current model for the 1294 compounds of previous study shows an AARD % of 1.2. This latter reveals the superiority of the current model over the previously proposed model. Additionally, it is much simpler than the previous one.

As can be found, the obtained correlation in this work is simple and leads to reasonable deviations of the determined the UFLT values from the database values. Table 3 reports the deviations of the results of the aforementioned correlation for the chemical families categorized in 76 chemical families.

One significant point should be emphasized in our discussion. As mentioned earlier, the proposed correlation is very simple to apply and does not require any computer program for computations. The obtained results denote

Table 1. The Parameters of the GEP¹⁹ Algorithm Applied in the Computational Route

GEP algorithm parameters	value
number of chromosomes	30
head size	8
number of genes	7
linking function	+
generations without change	2000
fitness function	AARD% ^a
mutation	0.044
inversion	0.1
IS transposition	0.1
RIS transposition	0.1
one-point recombination	0.3
two-point recombination	0.3
gene recombination	0.1
gene transposition	0.1
constant per gene	2
operators used	+, −, *, /, √, expt, log _ω power

^a%AARD = $(100/N) \sum_i^N (|lpred(i) - expt(i)| / expt(i))$, where N is the number of data points used in the GEP¹⁹ algorithm.

Table 2. Statistic Parameters of the Obtained Model Using GEP¹⁹ Strategy

statistical parameter	value
Training Set	
R^2 ^a	0.990
average absolute relative deviation ^b	1.7
standard deviation error ^c	8.7
root mean square error ^d	8.7
N ^e	1170
Optimization Set	
R^2	0.985
average absolute relative deviation	1.8
standard deviation error	8.9
root mean square error	9.1
N	146
Prediction Set	
R^2	0.990
average absolute relative deviation	1.7
standard deviation error	9.0
root mean square error	9.0
N	146
Total Set	
R^2	0.989
average absolute relative deviation	1.7
standard deviation error	8.8
root mean square error	8.8
N	1462

^a R^2 = square correlation coefficient:

$$R^2 = 1 - \frac{\sum_i^N (\text{calc}(i)/\text{est}(i) - \text{expt}(i))^2}{\sum_i^N (\text{calc}(i)/\text{est}(i) - \text{av}(\text{expt}(i)))^2}$$

^b%AARD = $(100/N) \sum_i^N (|lcalc(i)/est(i) - expt(i)| / expt(i))$. ^cstd = $(1/N) \sum_i^N (((\text{calc}(i)/\text{est}(i) - \text{av}(\text{calc}(i)/\text{est}(i))))^2)^{1/2}$. ^dRMSE = $\sum_{i=1}^N (((\text{calc}(i)/\text{est}(i) - \text{exp}(i))^2)/n)^{1/2}$. ^eNumber of experimental data.

obviously that the applied algorithm is very promising for evaluation of other physical properties.

Apart from that, the applied UFLT data set values contain definite uncertainties,¹⁸ which generally affect, indeed, the

Table 3. Average Percent Errors of the Model Predictions over Each One of Chemical Families of Compounds Used in This Study

no.	family	AARD%	UFLT ^{expt} range (K)	UFLT ^{pred} range (K)	N	no.	family	AARD%	UFLT ^{expt} range (K)	UFLT ^{pred} range (K)	N
1	1-alkenes	1.1	152–574.49	150.3–574.72	20	41	N-aliphatic acids	1.1	340–553	324.9–542.13	20
2	2,3,4-alkenes	0.8	225–468	232.5–471.27	24	42	N-aliphatic primary amines	1.3	237–454	238.2–457.32	13
3	acetates	0.7	286–446	282.9–444.12	25	43	N-alkanes	1.5	94–622	102.5–617.03	32
4	aldehydes	1.5	277–438	257.9–443.65	35	44	N-alkylbenzenes	1.3	288–543	300.4–536.16	19
5	aliphatic ethers	2.0	222–491	216.6–479.68	35	45	naphthalenes	1.9	383–530	397.3–514.33	17
6	alkylcyclohexanes	1.1	300–459	308.2–453.86	18	46	nitriles	2.2	277–541	262.4–526.4	29
7	alkylcyclopentanes	2.1	281–345	287.1–348.33	11	47	nitroamines	1.1	477–635	482.2–622.92	6
8	alkynes	4.7	238–370	218.6–362.75	17	48	organic salts	2.9	320–481	310.1–457.9	6
9	anhydrides	2.2	349–568	348.6–576.59	9	49	other aliphatic acids	1.6	344–530	344.3–528.57	21
10	aromatic alcohols	2.2	385–632	396.3–614.12	36	50	other aliphatic alcohols	1.3	304–476	306.4–471.69	37
11	aromatic amines	1.6	329–632	333.2–638.4	33	51	other aliphatic amines	1.2	230–505	234–505.45	22
12	aromatic carboxylic acids	1.3	445–651	446.8–658.67	9	52	other alkanes	1.6	281–544	288.3–550.33	24
13	aromatic chlorides	1.9	329–428	340.9–438.46	14	53	other alkylbenzenes	1.2	334–459	340.4–460.77	47
14	aromatic esters	1.2	386–614	393–603.87	32	54	other amines, imines	1.8	280–574	281.5–568.85	33
15	C, H, Br compounds	3.5	236–497	250.1–511.87	18	55	other condensed rings	1.2	442–582	448.1–578.59	8
16	C, H, F compounds	1.5	165–309	163.2–308.27	11	56	other ethers/diethers	2.3	274–551	265.2–546.21	27
17	C, H, I compounds	3.1	268–367	281.6–376.2	5	57	other hydrocarbon rings	2.5	309–488	319.9–494.48	13
18	C, H multihalogen compounds	3.4	226–373	209–368.67	4	58	other monoaromatics	1.1	337–423	347.4–421.21	19
19	C, H, NO ₂ compounds	1.2	330–505	328.2–512.94	16	59	other polyfunctional C, H, O	2.1	332–623	329.2–601.5	60
20	C1/C2 aliphatic chlorides	1.7	215–340	221.2–335.74	12	60	other polyfunctional organics	0.7	537–576	542.9–574.12	2
21	C3 and higher aliphatic chlorides	2.0	253–420	252.1–384.91	24	61	other saturated aliphatic esters	1.8	338–563	333.3–544.02	22
22	cycloaliphatic alcohols	2.0	361–645	363.8–624.69	12	62	peroxides	1.5	316–561	311.2–563.19	10
23	cycloalkanes	3.4	198–341	210.1–348.95	6	63	polyfunctional acids	1.4	385–612	386.2–615.37	19
24	cycloalkenes	1.4	266–348	270.8–353.17	10	64	polyfunctional amides/ amines	1.4	314–530	313.6–528.18	29
25	dialkenes	2.2	205–394	206.4–419.32	28	65	polyfunctional C, H, N, halide, (O)	1.7	397–531	391.4–498.89	11
26	dicarboxylic acids	1.1	523–577	513.9–580.35	12	66	polyfunctional C, H, O, halide	3.3	192–474	201.3–477.9	33
27	dimethylalkanes	1.0	259–349	265–350.32	20	67	polyfunctional C, H, O, N	1.4	307–636	298.3–615.67	25
28	diphenyl/polyaromatics	1.6	428–622	434.6–607.14	20	68	polyfunctional C, H, O, S	5.0	380–421	369–395.16	3
29	epoxides	2.9	260–453	262.7–461.86	13	69	polyfunctional esters	2.3	360–646	346.7–641.91	26
30	ethyl and higher alkenes	0.5	257–318	259.9–318.83	12	70	polyfunctional nitriles	2.5	382–428	366.9–432.62	6
31	formates	0.8	268–412	266–412.31	15	71	polyols	2.3	402–560.69	408.4–545.01	37
32	inorganic bases	3.7	215–215	223.3–223.32	1	72	propionates and butyrates	0.6	301–356	297.1–356.94	13
33	inorganic gases	4.7	199–387	189.2–359.21	4	73	silanes/siloxanes	4.6	301–511	291.9–493.59	16
34	isocyanates/diisocyanates	1.4	280–508	270.4–501.2	9	74	sulfides/thiophenes	1.4	271–545	268.6–538.95	40
35	ketones	1.1	279–470	281.6–479.26	40	75	terpenes	1.0	337–375	343.6–373.69	8
36	mercaptans	0.5	246–439	248.6–438.28	13	76	unsaturated aliphatic esters	1.7	314–538	299.6–513.14	24
37	methylalkanes	1.2	212–393	219.3–386.12	17						
38	methylalkenes	0.8	217–356	225.3–355.64	23						
39	multiring cycloalkanes	3.2	363–370	375.4–381.63	2						
40	N-alcohols	1.3	314–530	306.1–517.07	20						

prediction capability of the obtained correlation. The uncertainties of the UFLT data can be normally reduced by careful calibration of the measuring devices such as temperature probes, using the chemicals with high purity, and pursuing accurate and reliable experimental procedure for measuring the corresponding values.

5. CONCLUSION

In this communication, the gene expression programming¹⁹ algorithm was successfully applied for determination of the UFLT temperatures of 1462 chemical compounds. A total of 1170 experimental UFLT data was applied for developing (about 80% of the whole data set), and about 146 (around 10% of the whole data set) were utilized for optimizing the correlation and evaluating its predictive power. The remaining

146 (around 10% of the whole data set) were implemented for testing the correlation. The statistical parameters of the obtained correlation show 1.7% average absolute relative deviation of the results from data set values.¹⁸ Comparison of the estimated results of the proposed correlation and the only previously proposed one demonstrates high capability of the proposed correlation to determine the UFLT of the chemical compounds from 76 chemical families.

■ ASSOCIATED CONTENT

Supporting Information

Table that includes the model parameters, results, and absolute relative deviation from DIPPR 801 data.¹⁸ This material is available free of charge via the Internet at <http://pubs.acs.org>.

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Notes

The authors declare no competing financial interest.

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