Development of a General Model for Determination of Thermal Conductivity of Liquid Chemical Compounds at Atmospheric Pressure

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In this communication, a general model for representation/presentation of the liquid thermal conductivity of chemical compounds (mostly organic) at 1 atm pressure for temperatures below normal boiling point and at saturation pressure for temperatures above the normal boiling point is developed using the Gene Expression Programming algorithm. Approximately 19,000 liquid thermal conductivity data at different temperatures related to 1636 chemical compounds collected from the DIPPR 801 database are used to obtain the model as well as to assess its predictive capability. The parameters of the model comprise temperature, acentric factor, critical pressure, normal boiling temperature, and molecular weight. Nearly 80% of the data set (15,221 data) is randomly assigned to develop the model equation, 10% of the data set (1902 data) is used to validate the model, and the remaining data (1902 data) were implemented to evaluate its predictive power. The average absolute relative deviation of the model results from the DIPPR 801 data is less than 9%. In terms of simplicity and wide range of applicability, this empirical model shows acceptable accuracy. © 2012 American Institute of Chemical Engineers *AIChE J,* 59: 1702–1708, 2013

Keywords: gene expression programming, liquid thermal conductivity, corresponding states, reliable model, prediction

Introduction

Thermal conduction is a mode of energy transfer that occurs within and between bodies of matter as a result of a temperature gradient. It is normally expressed using the law of heat conduction or the well-known Fourier's Law as follows[1]

$$\vec{q} = -k\nabla T \tag{1}$$

where $\vec{q}$, k, and ∇T are the local heat flux (W m^{-2}), thermal conductivity (W m^{-1} K^{-1}), and temperature gradient (K m^{-1}), respectively.

Accurate measurements of thermal conductivity are not straightforward and need special care because of the possible presence of convective currents and heat losses during its experimental determination. Thus, the uncertainty concerning the existing experimental data is almost larger than that of other chemical compounds.[2–6]

Knowledge of reliable and accurate thermal conductivity data is essential for heat transfer operations/calculations, particularly in the petroleum industry. For instance, the effects of non-negligible thermal diffusion as a result of geothermal temperature gradients in oil and gas reservoirs[7] can be

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Additional Supporting Information may be found in the online version of this article.

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described reliably if reliable thermal conductivity data of the fluids are available. Besides, the Ludwig–Soret effect (thermal diffusion)[8,9] which represents the mass transfer which results from a temperature gradient is generally elucidated using thermal conductivity of fluids, density, mass diffusion, and so forth.[9,10]

The estimation of liquid thermal conductivities of chemical compounds has been the subject of many studies. Since 1950, when the first detailed kinetic theories of thermal conductivity of monoatomic liquids were presented,[11] there has not been a correlation adequately developed to be used to accurately estimate the property. It seems almost all the existing techniques are empirical and with limited applicability. In a majority of the methods,[12] thermal conductivity is correlated at a reference temperature. Subsequently, a temperature dependent correlation is developed. For instance, the models proposed by Sato-Riedel,[6,13] and Sastri and Rao[12,14] use the normal boiling temperature as the reference temperature whereas, the models proposed by Missenard[15] and the methods explained in API Technical Data Book[16] implement 293.15 K as the reference temperature.

A detailed review of the methods for the estimation of liquid thermal conductivities has been performed by Poling et al.[17] A summary of the findings are as follows:

(1) The methods proposed by Latini et al. and Baroncini et al.[18–24] and Sastri et al.[25] are reasonably accurate below the normal boiling point of liquids.

(2) The deviation of the model results from experimental data for organic liquids may vary widely, but typically is less than 15%.[17]

(3) There are very few experimental data for $T_r > 0.65$. It can be simply concluded that one of the main drawbacks of the current empirical methods may be inaccurate for $T_r > 0.65$ where T_r represents reduced temperature.

(4) The Latini et al. and Baroncini et al.[18–24] methods have been successfully applied for refrigerants up to $T_r = 0.9$.

(5) None of the methods can predict the large changes of liquid thermal conductivity near the critical point.

A quick consideration of the models proposed by Latini et al. and Baroncini et al.[18–24] and Sastri et al.[25] reveals some points that should be considered.

The model proposed by Latini et al. and Baroncini et al.[18–24] is presented for several particular chemical families of compounds including saturated hydrocarbons, olefins, cycloparafins, aromatics, alcohols, organic acids, ketones, esters, and refrigerants. These chemical families do not cover a significant number of widely used chemical families such as amines, silanes/siloxanes, inorganic compounds, sulfides/thiophenes, mercaptanes, epoxides, peroxides, nitriles, elements, and aldehydes. This issue significantly affects its applicability domain when using the model. As a result, the model is not general.

Furthermore, the model proposed by Sastri et al.[25] is based on 748 data points for 208 compounds below the normal boiling point, and 186 data points for just 23 pure compounds above the normal boiling point.

The aforementioned remarks encourage us to investigate the possibility of developing a comprehensive model which is able to predict the thermal conductivities of a large number of pure liquids. As a result, in this study, we apply the Gene Expression Programming (GEP)[26,27] algorithm to develop a general model for representation/prediction of the liquid thermal conductivities of more than 1600 liquids (mostly nonelectrolyte organic) at different temperatures but atmospheric pressure for temperatures below the normal boiling point and at saturation pressure for temperatures above the normal boiling point. The details of the GEP technique can be found elsewhere.[28–33]

Providing the Database

To develop a reliable and accurate model, the use of high quality data set is of great importance. For this purpose, the DIPPR 801[34] database was used in the present work to provide nearly 19,000 liquid thermal conductivity data for 1636 pure chemical compounds (mostly organic). The data are used to develop and validate the model.

Developing the Model

The GEP computational steps[26,27] described in the previous works[28–33,35] has been followed here to develop the model. The corresponding states principle parameters which comprise critical temperature (T_c), critical pressure (P_c), critical volume (V_c), acentric factor (ω), normal boiling temperature (T_b), temperature (T), and the molecular weight (M_w) have been introduced as input parameters into the algorithm. It is initially assumed that the liquid thermal conductivity can be formulated as a function of the aforementioned properties as follows

$$k = f(T_c, P_c, V_c, \omega, T_b, T, M_w) \tag{2}$$

As a result of what has been just mentioned, the following computational steps are implemented:

(1) Initialization of the population, that is, randomly generating the chromosomal structures of the individuals by setting various correlations presented as pars trees applying the operators (−, +, *, /, ^) and terminals as functions of the input experimental data and the output desired results (k values);

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

$$\mathrm{OF}(i) = \frac{100}{N}\sum_{i}^{N} \frac{\left| k(i)^{\mathrm{rep/pred}} - k(i)^{\mathrm{exp}} \right|}{k(i)^{\mathrm{exp}}} \tag{3}$$

where N denotes the number of the experimental data points used in the GEP[26,27] algorithm, and superscripts rep/pred and exp are the represented/predicted liquid thermal conductivity values by the final developed correlation and the DIPPR 801[34] dataset values, respectively.

(3) Selection of the individuals to stand for proper parents for replacement, which were evaluated from the fitness values. In this study, the tournament technique has been used to provide an acceptable diversity of the population in each 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).

(b) Mutation operator: It results in efficient adaption of populations of individuals. In this study, the point mutation has been applied, 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 arity taken from the initial (old) set.[26,27] Having defined the mutation rate (p_m), the mutation can happen everywhere in the structural organization of chromosomes; however, with preservation of the original structure. The mutation can be normally performed through changing the heads of genes symbols and terminals of the tails.

(c) Inversion operator: This operator is applied to create new individuals through modification of the heads of randomly selected genes. It has already been argued that all the new individuals created by inversion are considered as correct programs. The performance of this operator can be adapted choosing a value for the inversion rate (p_i).

(5) Transposition and insertion sequence elements: The transposable elements of GEP are a part of the genome that can be activated and jumped to another place in the chromosome, which include three types as implemented by Ferreira[26,27]: "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. 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.[26,27]

Results and Discussion

An explicit model has been developed undertaking the described computational algorithm. The database[34] has been divided into three sub-datasets including the "training" set, the "optimization" set, and the "prediction" set. The process of division of database into three subdatasets is performed randomly. The "Training" set has 15,221 data points, about 80% of the whole dataset, the "Optimization" set has 1902 data points, about 10% of the whole dataset, and the "Prediction" set has 1902 data points. The GEP[26,27] technique allows determining the convenient parameters for the most accurate model from the following parameters: T_c, P_c, V_c, ω, T_b, T, M_w. In general for a particular problem, one can introduce several independent parameters and define the ones, which have the most positive effects on the desired output results. The final correlation can be reported as follows

$$k = 1\times10^{-4}\left(10\omega + 2P_c - 2T + 4 + 1.908\left(T_b + \frac{1.009B^2}{M_w^2}\right) + \frac{3.9287M_w^4}{B^4} + \frac{A}{B^8}\right) \qquad (4)$$

where

$$A = 3.8588M_w^8(1.0045B + 6.5152M_w - 8.9756) \qquad (5)$$

and

$$B = 16.0407M_w + 2T_b - 27.9074 \qquad (6)$$

Table 1. The Parameters of the GEP Algorithm[26,27] Applied in the Computational Steps

GEP[26,27] Algorithm Parameters	Value
Number of chromosomes	20
Head size	6
Number of genes	6
Linking function	+
Generations without change	2000
Fitness function	AARD%*
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	+, −, *, /, $\sqrt{}$, exp, log$_e$, power

*$\text{AARD\%} = \frac{100}{N}\sum_i^N \frac{|\text{Calc.}(i)/\text{Est.}(i) - \text{Exp.}(i)|}{\text{Exp.}(i)}$, where N is the number experimental data.

Table 2. The Statistical Parameters of the Developed Model (Eq. 4)

Statistical Parameters	
Training set	
R^2	0.8835
Average absolute relative deviation*	8.96
Standard deviation error†	0.0146
Root mean square error‡	0.0148
N§	15221
Optimization set	
R^2	0.8715
Average absolute relative deviation	8.95
Standard deviation error	0.0150
Root mean square error	0.0152
N	1902
Prediction set	
R^2	0.9105
Average absolute relative deviation	8.96
Standard deviation error	0.0144
Root-mean-square error	0.0147
N	1902
Total set	
R^2	0.8856
Average absolute relative deviation	8.68
Standard deviation error	0.0146
Root mean square error	0.0149
N	19025

$$R^2 = 1 - \frac{\sum_i^N (\text{Calc.}(i)/\text{Est.}(i) - \text{Exp.}(i))^2}{\sum_i^N (\text{Calc.}(i)/\text{Est.}(i) - \text{average}(\text{Exp.}(i)))^2}$$

$$^{*}\text{AARD\%} = \frac{100}{N}\sum_i^N \frac{|\text{Calc.}(i)/\text{Est.}(i) - \text{Exp.}(i)|}{\text{Exp.}(i)}$$

$$^{\dagger}\text{Std} = \frac{1}{N}\sum_i^N \sqrt{(\text{Calc.}(i)/\text{Est.}(i) - \text{average}(\text{Calc.}(i)/\text{Est.}(i)))^2}$$

$$^{\ddagger}\text{RMSE} = \left(\frac{\sum_{i=1}^N (\text{Calc}(i)/\text{Est.}(i) - \text{Exp}(i))^2}{N}\right)^{1/2}$$

§Number of data points.

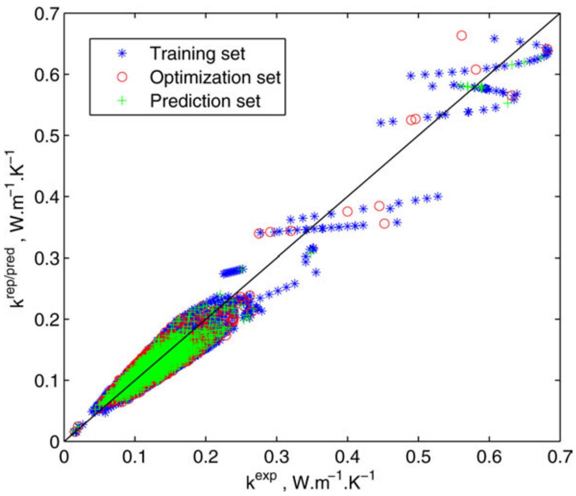

Figure 1. Comparison between the represented/predicted results of the developed model (Eq. 4) and DIPPR 801 data[34] at different temperatures at atmospheric pressure.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

In Eq. 4, units for k, P_c, and M_w are W m^{-1} K^{-1}, bar, g mol^{-1}, respectively. T, T_b, and T_c are in K.

The parameters used for the GEP technique[26,27] including the numbers of treated chromosomes, genes, the mutation and inversion coefficients, and the applied operators are presented in Table 1.

The statistical parameters of the obtained results (Table 2) indicate that the average absolute relative deviation of the determined liquid thermal conductivity values from the experimental ones[34] is about 8.7%. Therefore, it is figured out that the developed model results in acceptable accuracy for representation/prediction of the thermal conductivity of the investigated chemical compounds in liquid state at different temperatures and atmospheric pressure. Comparisons between the results of the proposed model and the corresponding thermal conductivity values of the DIPPR 801[34] dataset accompanied with the percent relative deviations are illustrated in Figures 1 and 2. The detailed results using the developed model for all of the studied compounds along with the values of the input parameters of the model are presented as Supporting Information files.

Furthermore, the capability of the proposed method for determination of the liquid thermal conductivity values for different chemicals/chemical families are, respectively, presented in Supporting Information table and Table 3.

It should be noted that the model could not predict the temperature dependence of liquid thermal conductivity of water, and deuterium oxide well. The model gives an almost correct average value for the liquids over a wide range of temperature, however, it cannot appropriately predict the property as a function of temperature.

Reasonable deviations from the DIPPR 801[34] dataset values can be observed. This issue asserts the acceptable applicability of the proposed model for many of the chemical families. This point is confirmed when taking a look at the uncertainty of the DIPPR 801 data.[34] The average uncertainty of DIPPR 801 data[34] for each chemical family is reported in Table 3. According to the results, it can be concluded that the deviation of the model results are mostly within or very close to the average uncertainty of DIPPR 801 data.[34] This latter demonstrates the capability of the model.

Regarding those points for which the model does not produce very accurate thermal conductivity values [generally in the 17–19 AARD (average absolute relative deviations) % range], some possible explanation is stated further. There are four chemical families for which the model results show AARD% more than 17%; Inorganic Halides (18.9%), Inorganic Acids (18.1%), N-Aliphatic Primary Amines (17.7%) and Inorganic Gases (17.1%).

As stated earlier, experimental measurement of accurate liquid thermal conductivity data is very difficult. Thus, the first possibility which may prevent the model in providing good representation/prediction for the data points may be due to the high experimental uncertainties. A quick consideration of Supporting Information table demonstrates that the uncertainties of the data generally lie between 1 and 50% (see Supporting Information). According to Table 3, the average uncertainties of the chemical families for which the model produces AARD% more than 17% are <23% (Inorganic Halides), <16% (Inorganic Acids), <9% (N-Aliphatic Primary Amines), and <14% (Inorganic Gases), respectively. Therefore, the high uncertainty of the data may directly affect the quality of the model as can be observed for the four chemical families that have higher deviations than 17% as well as other chemical families.

Apart from that, it is worth to know that the computational steps in each generation of the GEP[26,27] strategy needs parallel computing and consequently high amounts of CPU time. For development of the method, we have defined a convergence criterion for the algorithm, which is the difference between the accuracy of the obtained results from the current generation and the previous one in each step. Consequently, it is possible to develop a more accurate model through continuation of the calculation steps producing more generations from the subsequent populations. However,

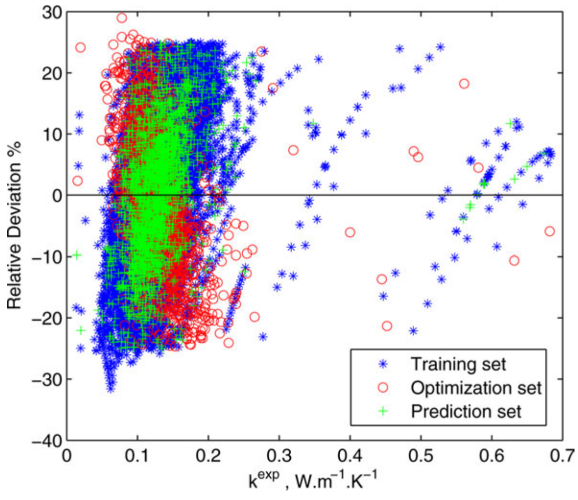

Figure 2. Relative deviations of the represented/predicted liquid thermal conductivity values of the studied compounds by Eq. 4 from the corresponding DIPPR 801 data.[34]

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 3. The Average Absolute Relative Deviations of the Proposed Model Results from the Corresponding DIPPR 801 Data[34] for Each Chemical Family of the Studied Compounds

No.	Family	AARD%	Temperature Range (K)	$k^{\mathrm{rep/pred.}}$ Range ($\mathrm{W\ m^{-1}\ K}$)	N	Average Uncertainty (%)
1	1-Alkenes	7.0	87.8–721.2	0.069–0.163	173	<8
2	2,3,4-Alkenes	7.1	121.8–592.0	0.077–0.159	246	<10
3	Acetates	11.3	167.7–561.2	0.078–0.151	341	<9
4	Aldehydes	6.2	175.6–633.2	0.074–0.219	571	<14
5	Aliphatic ethers	8.6	138.9–523.2	0.075–0.152	429	<9%
6	Alkylcyclohexanes	8.8	161.8–449.8	0.097–0.155	190	<10
7	Alkylcyclopentanes	5.6	133.2–429.8	0.101–0.157	120	<10
8	Alkynes	5.3	141.3–447.1	0.097–0.174	186	<10
9	Anhydrides	9.9	199.9–658.2	0.094–0.181	96	<26
10	Aromatic alcohols	5.3	252.0–771.0	0.073–0.161	346	<12
11	Aromatic amines	7.8	209.6–679.0	0.090–0.182	424	<18
12	Aromatic carboxylic acids	9.6	225.3–802.1	0.092–0.177	73	<15
13	Aromatic chlorides	7.1	211.5–673.2	0.056–0.152	163	<8
14	Aromatic esters	7.0	209.4–815.0	0.066–0.171	342	<19
15	C, H, BR compounds	7.0	141.9–673.2	0.047–0.150	216	<11
16	C, H, F compounds	10.6	128.4–423.1	0.052–0.152	351	<9
17	C, H, I compounds	12.9	170.1–453.1	0.078–0.131	79	<11
18	C, H, multihalogen compounds	9.2	113.2–513.8	0.048–0.131	553	<7
19	C, H, NO_2 compounds	7.5	169.2–663.7	0.080–0.179	239	<19
20	C1/C2 aliphatic chlorides	7.7	129.6–549.4	0.060–0.145	224	<6
21	C3 and higher aliphatic chlorides	6.8	143.1–534.4	0.077–0.151	287	<11
22	Cycloaliphatic alcohols	4.9	274.8–778.0	0.071–0.157	110	<12
23	Cycloalkanes	4.4	145.6–398.1	0.114–0.167	64	<9
24	Cycloalkenes	4.1	131.5–431.6	0.103–0.163	114	<9
25	Dialkenes	6.0	124.9–514.7	0.096–0.170	322	<10
26	Dicarboxylic acids	4.7	242.7–665.7	0.095–0.189	110	<12
27	Dimethylalkanes	11.9	138.7–437.5	0.093–0.149	234	<9
28	Diphenyl/polyaromatics	6.2	255.2–756.2	0.063–0.151	230	<8
29	Elements	12.6	1.6–785.0	0.016–0.108	144	<12
30	Epoxides	9.9	156.3–661.3	0.080–0.191	142	<21
31	Ethyl and higher alkenes	9.5	125.0–393.0	0.101–0.152	132	<10
32	Formates	14.7	156.0–603.2	0.067–0.150	333	<9
33	Inorganic acids	18.1	171.9–423.1	0.082–0.400	41	<16
34	Inorganic bases	11.7	300.0–390.0	0.340–0.358	24	<9
35	Inorganic gases	17.1	100.0–623.2	0.083–0.277	36	<14
36	Inorganic halides	18.9	151.1–493.4	0.085–0.142	102	<23
37	Isocyanates/diisocyanates	7.3	180.0–601.2	0.085–0.161	100	<24
38	Ketones	9.1	171.9–593.2	0.073–0.174	492	<10
39	Mercaptans	4.5	125.3–545.2	0.085–0.179	250	<25
40	Methylalkanes	5.2	113.5–524.0	0.082–0.151	202	<9
41	Methylalkenes	9.4	112.6–443.6	0.096–0.155	266	<9
42	Multiring cycloalkanes	11.1	276.8–506.8	0.096–0.142	48	<5
43	N-Alcohols	10.6	190.8–645.5	0.077–0.224	250	<10
44	N-Aliphatic acids	10.8	253.1–663.2	0.072–0.220	277	<7
45	N-Aliphatic primary amines	17.7	180.1–473.1	0.098–0.232	207	<9
46	N-Alkanes	6.4	85.5–714.0	0.070–0.165	436	<5
47	N-Alkylbenzenes	5.8	180.0–673.2	0.075–0.157	296	<13
48	Naphthalenes	8.2	200.0–648.2	0.079–0.162	186	<9
49	Nitriles	9.8	161.3–623.0	0.121–0.282	290	<24
50	Nitroamines	8.0	344.6–743.0	0.079–0.159	54	<25
51	Organic salts	10.1	212.5–560.0	0.097–0.198	140	<25
52	Organic/inorganic compounds	10.1	139.4–473.1	0.069–0.175	62	<25
53	Other aliphatic acids	7.8	192.9–659.6	0.075–0.187	330	<12
54	Other aliphatic alcohols	5.8	163.5–563.1	0.086–0.219	466	<10
55	Other aliphatic amines	8.6	130.0–639.2	0.071–0.177	276	<16
56	Other alkanes	11.6	150.8–519.5	0.080–0.149	265	<10
57	Other alkylbenzenes	7.4	177.6–613.2	0.074–0.157	553	<9
58	Other amines, imines	10.7	183.1–660.0	0.080–0.219	376	<22
59	Other condensed rings	8.5	362.6–716.2	0.094–0.151	98	<8
60	Other ethers/diethers	12.4	159.9–708.0	0.074–0.156	263	<13
61	Other hydrocarbon rings	4.7	193.0–600.2	0.080–0.156	170	<11
62	Other inorganics	7.7	272.4–787.2	0.113–0.663	80	<5
63	Other monoaromatics	7.5	172.1–623.2	0.075–0.164	218	<13
64	Other polyfunctional C, H, O	13.5	173.0–751.0	0.079–0.181	657	<22
65	Other polyfunctional organics	10.4	302.0–644.4	0.084–0.154	48	<25
66	Other saturated aliphatic esters	12.2	183.1–678.0	0.067–0.198	275	<13
67	Peroxides	8.3	213.0–661.2	0.085–0.167	109	<25
68	Polyfunctional acids	10.4	281.0–659.2	0.088–0.185	235	<24
69	Polyfunctional amides/amines	12.8	214.1–723.2	0.081–0.316	346	<19
70	Polyfunctional C, H, N, halide, (O)	4.8	262.8–588.0	0.090–0.161	125	<25

(*Continued*)

Table 3. (Continued)

No.	Family	AARD%	Temperature Range (K)	$k^{\text{rep/pred.}}$ Range (W m^{-1} K)	N	Average Uncertainty (%)
71	Polyfunctional C, H, O, halide	10.8	107.1–627.6	0.066–0.175	334	<22
72	Polyfunctional C, H, O, N	9.7	193.0–686.4	0.076–0.205	259	<29
73	Polyfunctional C, H, O, S	8.3	173.1–558.0	0.097–0.193	134	<25
74	Polyfunctional esters	10.8	192.9–715.0	0.074–0.162	270	<22
75	Polyfunctional nitriles	7.2	201.0–503.1	0.121–0.258	73	<21
76	Polyols	10.2	196.2–690.4	0.079–0.236	352	<12
77	Propionates and butyrates	11.1	165.9–493.1	0.081–0.147	198	<8
78	Silanes/siloxanes	15.4	103.1–550.0	0.063–0.146	303	<18
79	Sulfides/thiophenes	5.9	155.0–660.3	0.084–0.179	560	<23
80	Terpenes	6.3	199.0–450.0	0.097–0.152	87	<10
81	Unsaturated aliphatic esters	8.5	176.1–561.8	0.081–0.152	222	<11

careful investigation using more powerful computers should be made to verify this concept.

In comparison with the models proposed by Latini et al. and Baroncini et al.[18–24] and Sastri et al.,[25] the presented model here is simpler and has smaller number of parameters. The previous models have a major drawback. As, both the models have several chemical family dependent parameters; many compounds may be fitted into more than one chemical family of compounds. As a result some difficulties may happen when predicting of the liquid thermal conductivity of multifunctional compounds.

Another important drawback of the model proposed by Latini et al. and Baroncini et al.[18–24] is that it cannot be used for any pure compounds. The parameters of the model are presented just for several chemical families of compounds comprised of saturated hydrocarbons, olefins, cycloparafins, aromatics, alcohols, organic acids, ketones, esters, and refrigerants. These chemical families do not cover a significant number of widely used chemical families such as amines, silanes/siloxanes, inorganic compounds, sulfides/thiophenes, mercaptanes, epoxides, peroxides, nitriles, elements, and aldehydes. This point reveals that the model is not a general model.

Furthermore, the major advantage of the presented model over previous models is that it has been evaluated using nearly 19,000 experimental data for nearly 1600 compounds.

Therefore, we can conclude that the developed model is a valid one from a statistical point of view and we may not be able to doubt about the applied data using the characteristics of the model.

Conclusion

In this study, the GEP[26,27] mathematical strategy was implemented to develop an explicit model for determination of the thermal conductivity of 1636 liquids (mostly non-electrolyte organic) at different temperatures but atmospheric pressure. Temperature, critical pressure, molecular weight, acentric factor, and normal boiling temperature are the compound input parameters of the method. Almost 15,000 thermal conductivity data and about 1900 ones (around 10% of the whole dataset) were utilized for developing the model. Additionally, the remaining 10% of the data were used to evaluate its predictive power. The statistical parameters of the obtained correlation show about 9% absolute average relative deviation of the results from the corresponding DIPPR 801 data.[34] Investigation of the capability of the proposed method for evaluation of the thermal conductivity of various liquids at different temperatures and atmospheric pressure demonstrates its wide range of applicability compared with the available methods in the literature. Indeed, more calculation time of the GEP[26,27] algorithm for converging to a more probable global optimum of the OF of the problem may lead to developing more predictive tools for the same purpose.

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