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Evaluation of Thermal Conductivity of Gases at Atmospheric Pressure through a Corresponding States Method

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Supporting Information

ABSTRACT: In the present communication, we propose a corresponding states method for calculation/estimation of the vapor thermal conductivity of chemical compounds (mostly organic), applying the gene expression programming (GEP) algorithm. Around 16000 thermal conductivity data of gases at various temperatures from 100 to 1500 K and atmospheric pressure related to about 1600 chemical compounds (mostly organic) are used for development and validation of the method. The quantities used in the corresponding states correlation include temperature, critical pressure, molecular weight, acentric factor, and normal boiling point. More than 14000 thermal conductivity data are randomly selected for developing (training + optimizing) the correlation, and about 1600 data are used for checking its prediction capability. The obtained statistical parameters including average absolute relative deviation of the results from the applied data (about 8%) show acceptable accuracy of the presented method. The most important features of the developed model are its simplicity, its wide range of applicability, and its validity based on the Leverage value test.

1. INTRODUCTION

The ability of a material (or chemical substance) for conducting the heat is generally designated as "thermal conductivity". The Fourier's Law may be the most significant sign of the application of this property that can be expressed in one-dimensional form as follows:[1]

$$q_x = -k \frac{dT}{dx} \quad (1)$$

where q is the heat flow (flux) in the x direction ($W \cdot m^{-2}$), k is the thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$) and T is temperature (K). The thermal conductivity of solids, liquids, or vapors (gases) normally is a slight function of temperature and eventually of spatial location in nonuniform materials.[1] Indeed, the thermal conductivity of gases is also pressure dependent. The effects of pressure at low to moderate pressure regions are negligible; however, they are considerable at high pressures.[1] Physically, heat transfer across materials of high thermal conductivity is greater than that across materials with low thermal conductivity. The speed of heat transfer diffusion depends on the value of thermal diffusivity. In designing processes facilities, there are drastic needs for heat sinks/insulations, which can be achieved applying materials either with high or low thermal conductivities, respectively.[1]

The concept of thermal conductivity is therefore of utmost importance for heat transfer operations/calculations, especially in the petroleum industry. For instance, the effects of non-negligible thermal diffusion because of a geothermal temperature gradient in the oil and gas reservoirs[2] can be modeled reliably provided reliable thermal conductivity values of fluids are available. On the other hand, the Ludwig-Soret effect (thermal diffusion),[3,4] which stands for the mass transfer caused by a temperature gradient is generally defined using thermal conductivity of fluids, density, mass diffusion, etc.[5,6]

The representation and/or prediction of thermal conductivity has been the subject of many studies since the 1950s.[7] Thermal conductivity of monatomic gases can be expressed as a function of Boltzman's constant, molecular weight, characteristic dimensions of molecule, and a collision integral, which finally yields a dimensionless group of parameters called the "Eucken factor".[7,8] However, the aforementioned description may not be valid for polyatomic gases and needs some modifications in order to stand for the translational and internal degrees of freedom (see ref 7 for details).[7,9−16] The final equation of Eucken for evaluation of the thermal conductivity of gases is a function of molecular weight, viscosity, universal gas constant, heat capacity at constant volume, and heat capacity at constant pressure.[9−16] Later, several authors extended the Eucken's correlation for nonpolar gases and also to high temperatures.[17,18]

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In a different approach, Roy and Thodos[19,20] introduced a dimensionless reduced thermal conductivity that can be calculated in two parts. The first part, standing for translational energy, is a function of critical pressure (P_c), critical temperature (T_c), and molecular weight (M_w). The other part that relates to rotational and vibrational interchanges depends on reduced temperature and a specific constant. Roy and Thodos[19,20] reported different functional forms and group contributions for evaluation of this part of reduced thermal conductivity for the chemical families as reported by Poling et al.[7] as "*Saturated hydrocarbons; Olefins; Acetylenes; Naphtalenes and Aromatics; Alcohols; Aldehydes, Ketones, Ethers, and Esters; Amines and Nitriles; Halides; and Cyclic compounds*". Application of low-pressure gas viscosity, heat capacity at constant volume, universal gas constant, molecular weight, acentric factor (ω), and reduced temperature to evaluate the thermal conductivity of gases was studied by Chung et al.[21,22] The effects of pressure have been also taken into account in several efforts introducing the excess thermal conductivity correlations[23−39] or using the transport property prediction method (TRAPP).[40,41]

A detailed investigation of the proposed literature models[7] shows the following: (1) Most of the models require special quantity values as inputs, which are supposed to be estimated, where experimental values are not available, for example, gas viscosity and heat capacity. Furthermore, when the experimental values are available, they contain, generally, high uncertainties, leading to excess errors through the corresponding models. (2) Calculation procedures of some of the recommended methods are not normally easy to follow, especially those utilizing group contributions. This may make them not very interesting for the industry, where straightforward and easy-to-use correlations are preferred. (3) Applications of the available models have been checked for calculation or estimation of limited chemical compounds or families such as polar or nonpolar ones, hydrocarbons, alcohols, etc. To the best of our knowledge, none of the aforementioned methods have been validated using a database as large as the one concerning the current manuscript. (4) The absolute relative deviations of the results obtained applying these methods are very high (more than 30%) for some of the commonly used organic compounds, which may lessen their reliability.

In this study, we apply the gene expression programming (GEP)[42−47] to develop a corresponding states method for representation and prediction of the thermal conductivity of around 1600 gases (mostly nonelectrolyte organic) at different temperatures but atmospheric pressure. The details of the GEP technique[46,47] can be found elsewhere.[42−47]

2. DATABASE

The thermal conductivity values of about 1600 chemical compounds (mostly organic ones) including around 16000 data at different temperatures from 100 to 1500 K and atmospheric pressure available in the DIPPR 801 database[48] have been used for developing and validating the method.

3. DEVELOPING THE CORRESPONDING STATES MODEL

A similar calculation procedure described in previous works[42−45] has been followed here to develop the corresponding states model. The introduced corresponding states principle parameters including critical temperature, critical pressure, reduced temperature (T_r), critical volume (V_c), acentric factor, normal boiling point temperature (T_b), and the molecular weight along with temperature are input quantities to the algorithm (decision variables of the optimization procedure). It is first assumed that the thermal conductivity is a function of the aforementioned properties as follows:

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

Having defined the probably most relevant input quantities of the method, the following computational steps have been pursued:[42−45]

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 ($-$, $+$, $*$, $/$, $\wedge$) and terminals as functions of the input data and the output desired results (B values).
2. Calculation of the fitness value for every individual of the generated population by the following objective function (OF):

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

where N stands for the number of the employed data points used in the GEP[46,47] algorithm, n denotes the number of the correlation parameters, and superscripts rep/pred and expt are the represented/predicted thermal conductivity values by the final developed correlation and the applied data, respectively.

3. Selection of the individuals to stand for proper parents for replacement, which were evaluated from the fitness values. In this work, the tournament technique[46,47] 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).[46,47]
   (b) Mutation operator. It results in efficient adaptation of populations of individuals.[46,47] In this article, 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.[46,47] 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.[46,47] The mutation can be normally performed through changing the heads of genes symbols and terminals of the tails.[46,47]
   (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.[46,47] The performance of this operator can be adapted choosing a value for inversion rate (p_i).[46,47]

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5. Transposition and insertion sequence elements. The transposable elements of gene expression programming 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:[46,47] "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,[46,47] randomly chooses two chromosomes to exchange specific material with each other, leading to appearance of two new chromosomes.[46,47] Consequently, a 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.[46,47]

4. RESULTS AND DISCUSSION

A corresponding states model has been developed undertaking the described computational algorithm. The main database[48] has been divided into three subdata sets including the "Training" set (12742 data points, about 80% of the whole data set), the "Validation (Optimization)" set (1592 data points, about 10% of the whole data set), and the "Test (Prediction)" set (1592 data points, about 10% of the whole data set) to develop and test the method. The process of division of database into three subdata sets is performed randomly. In this division procedure, we generally undertake many distributions to prevent the local accumulations of the data in the feasible region of the problem. Hence, the acceptable distribution is the one with homogeneous distributions of the data on the whole domain of the three subdata sets. The GEP[46,47] technique determines the required parameters, which yield the most accurate model from the introduced inputs (T, T_c, T_r, P_c, V_c, ω, T_b, M_w).[42−45] Therefore, one can introduce several independent types of inputs for a particular problem and obtain the ones that have the most positive effects on the desired output results. The final correlation is

$$k = 7.9505 \times 10^{-4} + 3.989 \times 10^{-5} T - 5.419 \times 10^{-5} M_w + 3.989 \times 10^{-5} A \quad (4)$$

where

$$A = \frac{\left(2\omega + T - \frac{(2\omega + 3.2825)T}{T_b} + 3.2825\right)}{0.1 M w P_c T} \times (3.9752\omega + 0.1P_c + 1.9876B + 6.5243)^2 \quad (5)$$

and

$$B = T + \frac{2\omega + 2T - \frac{2T(2\omega + 3.2825)}{T_b} + 3.2825}{2\omega + T - \frac{T(2\omega + 3.2825)}{T_b} + 3.2825} - \frac{T(2\omega + 3.2825)}{T_b} \quad (6)$$

In eq 4, k is calculated in $W \cdot m^{-1} \cdot K^{-1}$, T is in K, P_c and T_b are in MPa and K, respectively. The numbers of the digits of the coefficients in this correlation have been determined through simultaneous performing sensitivity analysis of the calculated and estimated results to these values during the optimization processes of GEP[46,47] algorithm.

Table 1 reports the applied parameters of the applied GEP[46,47] technique including the numbers of treated chromosomes, genes, the mutation and inversion coefficients, and the applied operators. The statistical parameters of the obtained results (Table 2) indicate that the absolute average relative deviation of the determined thermal conductivity values from the ones of the database[48] is about 9%. Therefore, it is figured out that the developed corresponding states model brings about acceptable accuracy for calculation and estimation of the thermal conductivity of the investigated chemical compounds in the gaseous state at different temperatures and atmospheric pressure. Comparisons between the results of the proposed model and the corresponding thermal conductivity values from the database[48] accompanied with the percent relative deviations are convincingly 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. In addition, the capability of the proposed

Table 1. The Parameters of the GEP[46,47] Algorithm Applied in the Computational Steps

GEP[46,47] algorithm parameters	value
number of chromosomes	20
head size	6
number of genes	6
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	+, −, ∗, /, √, exp, $\log_e$, power

[a]Calculated as

$$\%AARD = \frac{100}{N - n} \sum_{i}^{N} \frac{|rep(i)/pred(i) - expt(i)|}{expt(i)}$$

where N is the number of data and n is the number of parameters.

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Table 2. The Statistical Parameters of the Developed Corresponding States Model (eq 4)

statistical parameter	value
Training Set	
R^{2a}	0.938
average absolute relative deviation,[b] %	8.5
standard deviation error	0.005
root mean square error	0.005
N^c	12742
Optimization Set	
R^2	0.935
average absolute relative deviation, %	8.6
standard deviation error	0.005
root mean square error	0.005
N	1592
Prediction Set	
R^2	0.939
average absolute relative deviation, %	8.6
standard deviation error	0.005
root mean square error	0.005
N	1592
Training + Optimization + Prediction Set	
R^2	0.937
average absolute relative deviation, %	8.2
standard deviation error	0.005
root mean square error	0.005
N	15926

[a] R^2: Squared correlation coefficient. [b] Calculated as

$$\%\text{AARD} = \frac{100}{N-n}\sum_{i}^{N}\frac{|\text{rep}(i)/\text{pred}(i) - \text{expt}(i)|}{\text{expt}(i)}$$

where n is the number of the model parameters. [c] Number of data points.

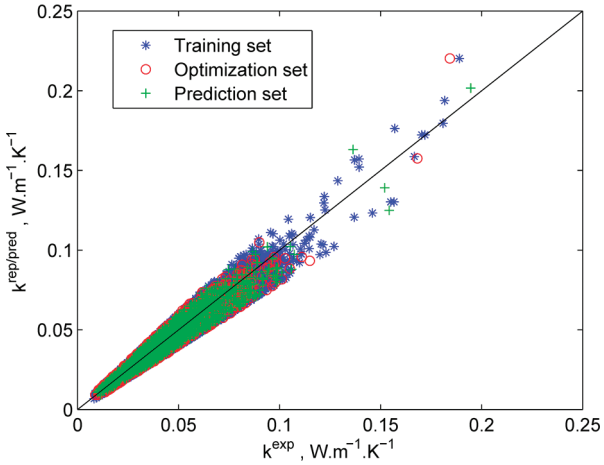

Figure 1. Comparison between the represented/predicted results of the developed correlation (eq 4) and the applied data[48] of thermal conductivity of investigated gases at different temperatures and atmospheric pressure.

method for determination of the gas thermal conductivity values for different chemicals/chemical families is shown in the Supporting Information files. Acceptable deviations from the applied data are observed. This issue argues about the acceptable applicability of the proposed correlation for many of the chemical families (mostly organic and nonelectrolyte).

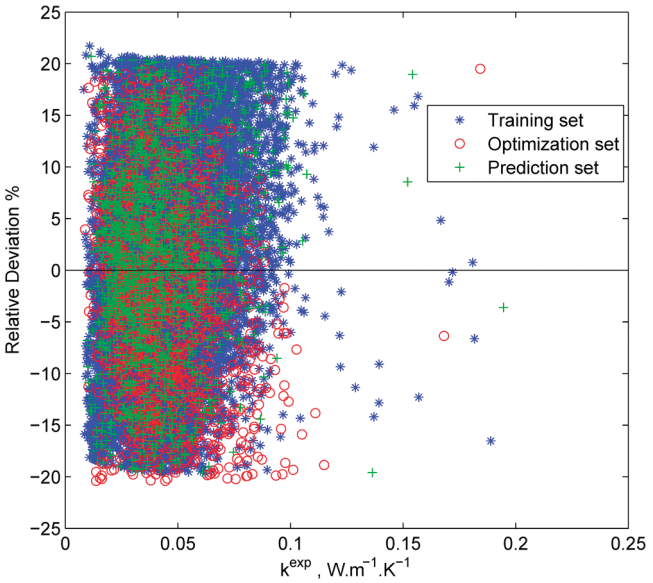

Figure 2. Relative deviations of the represented/predicted thermal conductivity values of the studied compounds by eq 4 from the corresponding data.[48]

It seems to be very fruitful here to point out some discussions on the aforementioned data, for which the correlation does not result in very accurate thermal conductivity values (generally in the 17−19 AARD % range). We may be able to connect these results to the data mainly from the chemical families including multiring cycloalkanes, some alkanes, alkylcyclopentanes, and cycloaliphatic alcohols. First, it is worth knowing that the computational steps in each generation of the GEP[46,47] strategy needs parallel computing and consequently high amounts of time. For development of the method, we have defined a stopping 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 (we have herein used 0.1 AARD%/hr i.e. 0.1 % deviation in each hour of calculations). Consequently, it is possible to develop a more accurate model through continuation of the calculation steps producing more generations from the subsequent populations. However, careful investigation using more powerful computers should be made to verify this concept.

In the second place, the applied data[48] contain definite uncertainties (see the Supporting Information). These uncertainties affect, indeed, the prediction capability of the obtained correlation. It is possible to detect the doubtful data using a mathematically exact statistical approach. In this article, we have applied the method of Leverage Value Statistics[49,50] for this purpose. The subsequent results show that there are no evident outliers for the proposed model (the results of applying the leverage value statistics method[49,50] are freely available upon request to the authors). Therefore, we can reach into this conclusion that the developed corresponding states model is a valid one from the statistical point of view, and we may have no doubt about the applied data using the characteristics of the model.

5. CONCLUSION

In this work, the gene expression programming[46,47] mathematical strategy was utilized to develop a straightforward

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corresponding states model for determination of the thermal conductivity of about 1600 gases at various temperatures (100 to 1500 K) and atmospheric pressure. Temperature, critical pressure, molecular weight, acentric factor, and normal boiling point are the input parameters of the method. More than 14000 data points of thermal conductivity (about 90% of the whole data set) and about 1600 ones (around 10% of the whole data set) were applied for developing and predictability testing the proposed corresponding states model, respectively. The statistical parameters of the obtained correlation show about 9% absolute average relative deviation of the results from the corresponding database values.[48] Investigation of the capability of the proposed method for evaluation of the thermal conductivity of various gases at different temperatures and atmospheric pressure demonstrates its wide range of applicability compared with the available methods in the literature. Additionally, the Leverage Value Statistics[49,50] test indicates that there are no evident outliers regarding the proposed corresponding states model. Indeed, more calculation time of the GEP[46,47] algorithm for converging to more probable global optimum of the objective function of the problem may lead to developing more predictive tools for the same purpose.[42−45]

■ ASSOCIATED CONTENT

Supporting Information

All of the evaluated thermal conductivity values of the investigated compounds along with their absolute relative deviations from the applied data[48] and the capability of the proposed method for determination of the gas thermal conductivity values for different chemicals/chemical families. 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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