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Corresponding States Method for Determination of the Viscosity of Gases at Atmospheric Pressure

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S Supporting Information

ABSTRACT: The accuracy and predictability of empirical/semiempirical correlations for evaluation of the physicochemical properties of chemical compounds are of much interest in chemical industry. In this study, our objective is applying the Gene Expression Programming (GEP) mathematical algorithm to propose a correlation based on the corresponding states method to calculate/estimate the gas viscosity of about 1600 chemical compounds (mostly organic) from 81 chemical families at different temperatures and atmospheric pressure. The parameters of the correlation include the temperature, critical temperature, critical pressure, and molecular weight. Around 13 000 experimental gas viscosity data are randomly selected for developing the correlation, and about 8500 data are treated for checking its prediction capability. The obtained statistical parameters including average absolute relative deviations (AARD %) of the results from the experimental data (about 7%) indicate the accuracy and applicability of the presented correlation along with its simplicity compared with the most widely used corresponding states method (with AARD of about 9%) available in open literature.

1. INTRODUCTION

As discussed in our previous work, accurate values of the thermo-physical, physicochemical, and thermodynamic properties are necessary for the design of various processes in chemical industry.¹ However, producing reliable experimental data is normally time-consuming, costly, and with probable non-negligible uncertainties because of different reasons generally happening in experimental measurements at different experimental conditions.^{1–5} Therefore, numbers of studies including empirical, semiempirical, and molecular theories have been so far developed by the engineers/researchers for correlating/predicting the corresponding properties of chemical compounds.^{1–5} Reliable predictive correlations with parameters defined for representative chemicals pertaining to representative chemical families are of great interest. It is up to the operator to select the best experimental data (through thermodynamic consistency tests, experimental backgrounds, etc.)^{4,5} in order to adjust the most effective model parameters and consequently develop satisfactory ones for data predictions. These models can later be applied to represent the behavior or properties of hazardous chemicals at the conditions where measurements of experimental data are difficult.

To obtain the optimum values of the parameters of the aforementioned methods, suitable mathematical algorithms are required. Selection of a proper mathematical method (optimization algorithm) has always been a challenge for the scientific community.^{6–11} Useful remarks to choose a reliable algorithm for this purpose have already been well-argued.¹

Application of the Genetic Algorithm (GA),¹¹ as a population-based evolutionary optimization technique, has generated considerable attention in engineering fields for several decades.

In later years, an improvement of the original GA¹¹ was developed, in which the solutions are treated as nonlinear structures of parse trees (treated as functions) instead of fixed length binary solutions (the Genetic Programming (GP)).^{12,13} Modification of this new algorithm was continued until its reformulation by Ferreira,¹⁴ who presented the so-called “Gene Expression Programming (GEP)” method.

The GEP strategy¹⁴ totally encodes the ramified structures of different sizes and shapes (parse trees) in the linear solutions of fixed length that contributes to more probability of obtaining the global optimum values of the model parameters.^{9,14} As the GEP¹⁴ has already been proven to have high capabilities in development of accurate correlations in various engineering problems,^{15–19} we are seeking to show its application to propose more accurate corresponding states methods to determine the physicochemical properties of chemical compounds (mostly organic ones). This article deals with calculation/estimation of the viscosity of about 1600 gaseous compounds (mostly organic) at different temperatures and atmospheric pressure.

The general definition of viscosity results from the investigation of the effect of shearing stress to a portion of a fluid, which leads to its movement with a velocity gradient.² In other words, viscosity (internal fluid friction) is a kind of resistance of a fluid against deformation caused through a shear/tensile stress.²⁰ In general, the less viscous the fluid is, the greater fluidity it has.²⁰ This property that is measured at nonequilibrium conditions

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can also be applied to define a state of a material.² The detailed theory of the viscosity of gases has been reported by Millat and co-workers.²¹ The viscosity of species of petroleum fluids is also very significant in study of their flow pattern, especially when they are supposed to contain agglomerated asphaltene particles or precipitated waxy compounds.^{22,23} From the mechanical point of view, the viscosity can be determined by evaluating the ratio of local shear stress per unit area at any point of fluid to the velocity gradient:^{2,20}

$$\tau = \mu \frac{\partial u}{\partial y} \quad (1)$$

where τ is shear stress, μ is the dynamic viscosity, u denotes the velocity gradient in the direction perpendicular to the layer of fluid, and y stands for the direction of the movement of fluid.

The proposed methods for determination of the viscosity of gases are generally based on the theory of Chapman-Enskog²⁴ or corresponding states principles.² The former one utilizes the integral relations for the transport properties according to the interactions between colliding molecules described by a potential energy function. A numerical solution should be pursued for each choice of intermolecular potential model, for example, the Lennard-Jones (12–6) potential function,^{2,25} to apply this theory. The shortcoming of this method in calculation of the viscosity of different gases can be expressed as

1. Difficulty of evaluation of the required parameters, for example, ε (characteristic energy), σ (the collision diameter), and r (the distance from center of a molecule to the place, where the potential function has a small value)
2. Complex numerical solution for choosing the intermolecular potential model
3. Long time of the viscosity calculation, which is of significance in molecular/process simulators.

The second category of the methods includes the corresponding states equations, which generally relate the viscosity to critical temperature (T_c), critical pressure (P_c), critical volume (V_c), molecular weight (M_w), universal gas constant (R), Avogadro's number (N_A), and/or some other parameters to account for polarity or quantum effects like dipole moment. From 1960s up to now, a remarkable number of efforts have been undertaken to improve the accuracy of these correlations.^{25–33} Meticulous scrutiny of these works shows their probable drawbacks as follows:

1. The numbers of the parameters (up to 9), which makes some of the methods unattractive for engineers
2. Most of these methods have special parameters, which may not be available for particular chemical species, for example, dipole moment. Therefore, these methods may not be concluded to be general or easy-to-use ones.
3. Complex forms of the proposed correlation functions. These formulations may lead to long calculation time and normally enhance the probability of computational errors in calculation of the viscosity.
4. Some of the available correlations do not have a unique function form. For instance, the common method of Lucas^{31–34} uses three forms for different values of a parameter defined as reduced dipole moment for various chemical compounds.
5. Calculations through applying some of these methods^{31–34} demonstrate that they result in complex (not real) or negative values of viscosity for particular gases, which

make them nonapplicable for evaluation of viscosity of these species.

The aforementioned criteria clarify the need of developing accurate, simple, and more applicable method to determine the viscosity of gases, which is the aim of the present work, as already mentioned.

2. DATABASE

The DIPPR 801 database³⁵ has been applied in this work. The gas viscosity values of about 1600 organic compounds at different temperatures and atmospheric pressure have been employed for developing and validating the correlation.

3. DEVELOPING THE CORRESPONDING STATES METHOD

The same GEP computational steps¹⁴ described in our previous work¹ have been followed here to develop the correlation of interest. A concise literature review indicates that the experimental data of viscosity of the pure gaseous compounds can be represented by the corresponding states principle parameters such as critical pressure, critical temperature, reduced temperature (T_r), critical volume, acentric factor (ω), reduced normal boiling point temperature (T_{br}), and the molecular weight. It is preliminarily assumed that the viscosity value can be formulated as the functions of the aforementioned properties as follows:

$$\mu = f(T_c, P_c, V_c, \omega, T_{br}, M_w, T) \quad (2)$$

Having defined the probable input parameters of the method, the following computational steps have been pursued:¹

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

$$OF(i) = \frac{100}{N - n} \sum_i \frac{|\mu(i)^{rep/pred} - \mu(i)^{exp}|}{\mu(i)^{exp}} \quad (3)$$

where N stands for the number of the data points used in the GEP¹⁴ algorithm, n denotes the number of the correlation parameters, and the superscripts rep/pred and exp are the determined viscosity values by the final developed correlation and 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^{36,37} 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 steps.
 - a. Replication operator: It copies exactly the chromosomes of the individuals chosen in the selection step (step 3).⁹
 - b. Mutation operator: It results in efficient adaption of populations of individuals.⁹ 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.⁹ 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.⁹ The mutation can be normally performed through changing the heads of genes symbols and terminals of the tails.^{9,14}

- 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.⁹ The performance of this operator can be adapted choosing a value for inversion rate (p_i).⁹
5. Transposition and insertion sequence elements: The transposable elements of gene expression programming are a part of the genome that can be activated and jump to another place in the chromosome, which include three types as implemented by Ferreira:⁹ "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,⁹ randomly chooses two chromosomes to exchange specific material with each other, leading to the appearance of two new chromosomes.⁹ Consequently, a new generation is created. The preceding procedure is repeated until the defined stopping criteria (can be either user-defined convergence criteria or maximum number of generations) is satisfied. The details of this procedure along with comprehensive examples have been provided by Ferreira.⁹

4. RESULTS AND DISCUSSION

An easy-to-use corresponding states correlation has been obtained following the explained algorithm. In this work, the main data set³⁵ has been (randomly) divided into the "Training" set (4257 data points, about 20% of the whole data set), the "Validation (Optimization)" set (8514 data points, about 40% of the whole data set), and the "Test (Prediction)" set (8514 data points, about 40% of the whole data set) to develop and test the method. The division of the database into three subdata sets is performed randomly. It is worth pointing out that the GEP¹⁴ technique determines the required parameters, which yield the most accurate correlation from the introduced parameters (T , T_c , P_c , V_c , ω , T_{bw} , M_w). Therefore, one can introduce several independent parameters for a particular problem and obtain the ones that have the most positive effects on the desired output results. The final correlation can be reported as follows:

$$\mu = 10^{-7} \left[10^5 P_c T_r + \left(0.091 - \frac{0.477}{M_w} \right) T + M_w \left(10^5 P_c - \frac{8M_w^2}{T^2} \right) \left(\frac{10.7639}{T_c} - \frac{4.1929}{T} \right) \right] \quad (4)$$

In eq 4, the viscosity is calculated in (Pa·s) and P_c , T and T_c are in (Pa) and (K), respectively. The number of the digits of the coefficients in this correlation has been evaluated through

performing sensitivity analysis of the calculated/estimated results to these values. The statistical parameters of the obtained results (Table 1) indicate that the absolute average

Table 1. Statistical Parameters of the Developed Corresponding States Method (eq 4)

statistical parameter	value
Training Set	
R^{2a}	0.959
average absolute relative deviation, ^b %	7.8
standard deviation error	1.7×10^{-6}
root mean square error (RMSE)	1.7×10^{-6}
N^c	4257
Optimization Set	
R^{2a}	0.954
average absolute relative deviation, %	7.8
standard deviation error	1.8×10^{-6}
root mean square error	1.8×10^{-6}
N	8514
Prediction Set	
R^{2a}	0.952
average absolute relative deviation, %	7.7
standard deviation error	1.9×10^{-6}
root mean square error	1.9×10^{-6}
N	8514
Training + Optimization + Prediction Set	
R^{2a}	0.954
average absolute relative deviation, %	7.2
standard deviation error	1.8×10^{-6}
root mean square error	1.8×10^{-6}
N	21285

^a R^2 : Squared correlation coefficient. ^b%AARD = $[100/(N - n)] \sum_i^N [(\text{rep}(i)/\text{pred}(i) - \text{exp}(i))/\text{exp}(i)]$, where n is the number of the model parameters. ^cNumber of data points.

relative deviation (AARD) of the calculated/estimated viscosity values from all of the data³⁵ is 7.2%. This issue shows an acceptable accuracy of the correlation for determination of the viscosity of many of chemical compounds in the gas state at different temperatures and atmospheric pressure. Figures 1 and 2 show comparisons between the represented/predicted viscosity values/percent relative deviations and the applied data.³⁵ Four tables containing all of the detailed results along with the values of the input parameters to the correlation are reported as Supporting Information. The effective parameters of the applied GEP¹⁴ technique are reported in Table 2, including the numbers of treated chromosomes, genes, the mutation and inversion coefficients, and the applied operators.

Of particular interest is the fact that the capability of the proposed correlation for determination of the gas viscosity of the investigated compounds is compared to the results obtained by the common corresponding states method reported in the literature, which is that of Lucas.^{31–34} To deal with this issue, the following points should be taken into account:

1. The correlation of Lucas^{31–34} contains nine parameters (almost twice those of our proposed correlation), including T , T_c , P_c , M_w , dipole moment, R , N_A , Z_c (critical compressibility factor), and another parameter that accounts for polar or quantum effects.
2. The special form of the correlation of Lucas^{31–34} leads to obtaining negative or even complex values for gas viscosity of some of the chemical compounds. The names of these

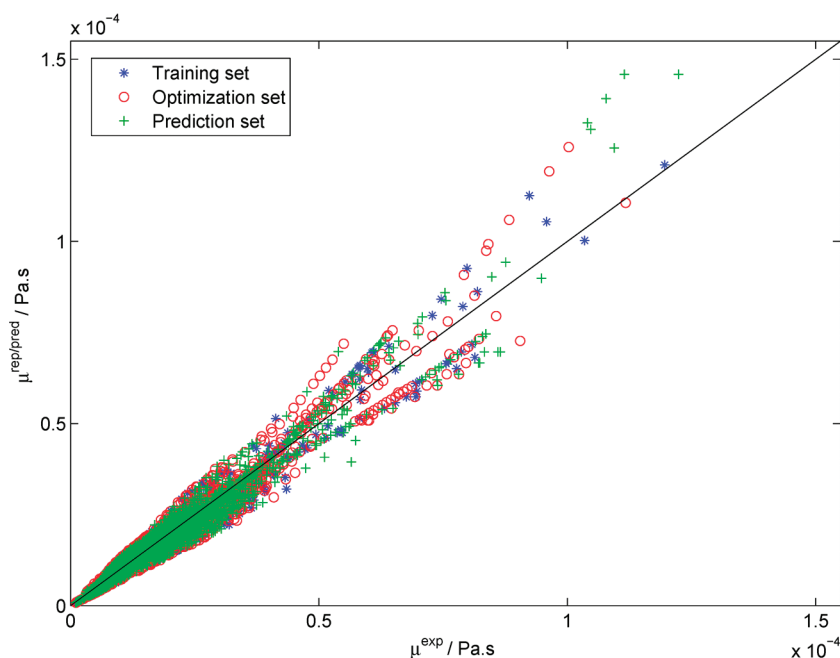


Figure 1. Comparison between the represented/predicted results of the developed correlation (eq 4) and the applied data³⁵ of gas viscosity of investigated compounds at different temperatures and atmospheric pressure.

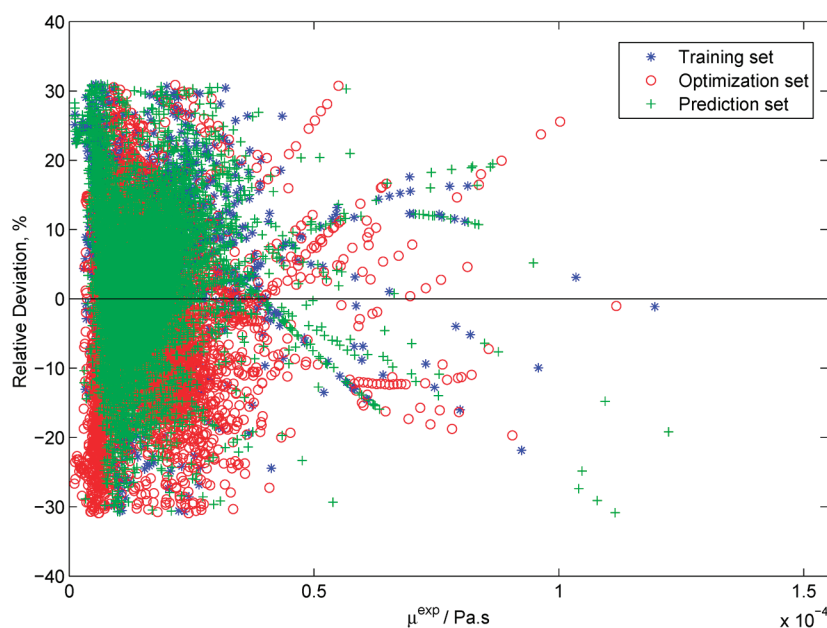


Figure 2. Relative deviations of the represented/predicted gas viscosity values of the studied compounds by eq 4 from the corresponding data.³⁵

compounds for which the complex viscosity values are obtained are listed in a table in Supporting Information. In the case of $T_r < 12$, the calculated gas viscosity values for hydrogen and helium are negative.

3. The required parameters for application of the mentioned correlation,^{31–34} including the dipole moment, are sometimes not available (for particular species from the main data set³⁵).

According to the preceding criteria, we have to eliminate some of the compounds and the related data points from the main data set³⁵ to undertake the comparison study. The treated compounds have been categorized in 81 chemical families, and

the deviations of the results using the two correlations have been reported in Supporting Information. The detailed results of this comparison are presented as Supporting Information, which show the average absolute relative deviations of about 8% and 9% with respect to our correlation and the correlation proposed by Lucas.^{31–34} However, the AARD % of the developed correlation results from the whole data set³⁵ (without eliminating those points, for which the method of Lucas^{31–34} is not applicable) in this work is evaluated to be around 7%.

As can be seen in Figures 1 and 2, the proposed correlation does not bring about accurate representation/predictions for some of the investigated viscosity values. We may not be able to

Table 2. Parameters of the GEP¹⁴ Algorithm Applied in the Computational Route

GEP ¹⁴ algorithm parameters	value
number of chromosomes	30
head size	8
number of genes	3
linking function	+
generations without change	3000
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

^aAARD = $[100/(N - n)] \sum_i^N [(|rep.(i)/pred.(i) - exp.(i)|)/exp.(i)]$, where n is the number of the model parameters.

correspond these points to the data for chemical compounds grouped in definite chemical families. However, it can be stated that it is probably due to development of this correlation based on the limited number of compounds from particular chemical families or some inaccurate data. On the other hand, the time of the calculations using the GEP¹⁴ algorithm plays also an important role. The computational steps in each generation of the GEP¹⁴ 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. Consequently, it may be possible to develop a more accurate correlation through continuation of the calculation steps producing more generations from the subsequent populations along with a different stopping criterion and application of more viscosity data from wider ranges of chemical families as a training set. However, careful investigation using powerful computers should be made to verify this concept.

Furthermore, some of the predictions show almost the same trends (i.e., probable systematic deviations from the related gas viscosity values³⁵) in Figure 1 (refer to the Supporting Information for better observing these points). We may first conclude that these data correspond to the chemical compounds, which are highly polar, and consequently their viscosity could be better represented considering the dipole moment parameter in our correlation (according to application of dipole moment for prediction of viscosity in some available methods). However, careful investigation of these data indicates that they pertain to nonpolar compounds including helium, argon, neon, and sulfur hexafluoride (with the zero values for dipole moments). The detailed results of the representations/predictions of the proposed correlation for viscosity values of

the aforementioned compounds are presented in Supporting Information. In addition, we tried developing the correlation this time considering the dipole moment as the input parameter. However, the GEP algorithm has not selected this parameter as a very efficient one in the corresponding state method; that is, we may conclude that any of the obtained parameters have had more positive effects on the final viscosity values of the studied chemicals.

It seems to be very fruitful here to point out some discussions on the aforementioned data, for which the correlation does not result in acceptable ARD (absolute relative deviation) % values (data of viscosity of helium, argon, neon, and sulfur hexafluoride). The applied viscosity data³⁵ contain definite uncertainties, which generally lie between 3 and 25% (see the Supporting Information). These uncertainties affect, indeed, the prediction capability of the obtained correlation.¹ We are well aware that there are several methods to detect the outlier data for the model as follows:

1. It is possible to eliminate these data from the training set and develop a new correlation. Later, these omitted data can be predicted using the new correlation. If these predictions are again within the unacceptable deviations from the data (i.e., with almost the same ARD % obtained from application of the previous correlation), we may conclude the high probability of considering these viscosity data as outliers. On the contrary, if the new correlation acceptably predicts these data, we may not be able to report them as the outliers of the model, and consequently the new correlation would not be more accurate than the current one.
2. The numerical methods such as neural networks³⁸ or support vector machine^{39–41} could be used on the whole database in the training step only to try identifying the outliers of the correlation (the GEP algorithm can also be used in this method; however, it may not be possible at this time because of the high computational time as already stated). Later, a new data set can be constructed, eliminating the outliers. This time, the new data set would be used for training, optimizing, and predictability test steps.
3. There are other statistical methods for definition of the outliers that are independent of the new divisions (data allocations) of the data in the three subdata sets like the method of Leverage Value Statistics.^{42,43}

Each of the preceding solutions can be pursued to determine the outliers of the developed method. However, our objective, in this work, has been to study the ability of the investigated corresponding states method for representation/prediction of all of the gas viscosity values from one of the most comprehensive data sets in the literature.³⁵ These phenomena reveal some broad recommendations to improve the correlation's predictive capability in future works. It should be noted that the uncertainties of the data³⁵ could be normally reduced by designing more appropriate equipment and careful calibration of the measuring devices.¹

5. CONCLUSION

In this article, the Gene Expression Programming¹⁴ mathematical algorithm was used to develop an easy-to-use corresponding states method for determination of the gas viscosity values of about 1600 chemical compounds (mostly organic) at different temperatures and atmospheric pressure. The parameters

of the correlation include the temperature, critical temperature, critical pressure, and molecular weight of the compounds. Around 13 000 data points of gas viscosity (about 60% of the whole data set) and about 8500 ones (around 40% of the whole data set) were applied for developing and testing the proposed correlation, respectively. The statistical parameters of the obtained correlation show about 7% absolute average relative deviation of the results from the corresponding data.³⁵ Comparison of the calculated/estimated results of the proposed method and those through application of the well-known correlation of Lucas^{31–34} (with AARD % of about 9%) demonstrates high capability of the proposed correlation for determination of the gas viscosity of many of chemical compounds (mostly organic) from 81 chemical families at different temperatures and atmospheric pressure. In addition, the proposed correlation is much simpler than that of Lucas^{31–34} and requires the values of only four input parameters instead of nine parameters proposed in the work of Lucas.^{31–34} Moreover, the correlation of Lucas^{31–34} cannot be used to determine the gas viscosity values for particular compounds because of its special functional terms. Indeed, using more accurate viscosity data (in the case of availability) and considering more calculation time for the GEP¹⁴ algorithm to converge to more probable global minimum of the objective function of the problem shall contribute to developing more predictive tools for the same purpose.

■ ASSOCIATED CONTENT

■ Supporting Information

All of the evaluated gas viscosity values of the investigated compounds accompanied with their absolute relative deviations from the applied data,³⁵ the chemical compounds for which the correlation of Lucas^{31–34} leads to complex gas viscosity values, and the average absolute relative deviations of the investigated correlation results from the corresponding data³⁵ for each chemical families. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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