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New empirical correlation for estimation of vaporization enthalpy of algerian saharan blend petroleum fractions

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ABSTRACT

A Real-coded Genetic Algorithm has been used to develop a new correlation to estimate the enthalpy of vaporization for pure compounds and petroleum fractions as a function of the normal boiling point and specific gravity. In developing the correlation 80% of the data was used and the remaining are used for validation. The results of the proposed correlations are compared to others in literature. The comparison indicates that the proposed model is simple to use and more accurate than the most common correlations for predicting the enthalpy of vaporization of pure compounds and petroleum fractions.

KEYWORDS

characterization correlation; enthalpy of vaporization; genetic algorithm; petroleum fraction; pure compounds

1. Introduction

Knowledge of the physical, chemical and thermodynamic properties of petroleum mixtures play an important role in the design and operation of almost every part of equipment in the petroleum industry. In chemical processes, we need to know these data to improve the efficiency of equipment and optimize time and energy consumption. That is, to minimize the cost of production (Riazi 2005). Some physical properties of mixtures are easily measurable, such as specific gravity, while other properties such as the critical properties and enthalpy of vaporization cannot be measured easily. (Constantinou, and Gani 1994; Riazi 2005).

The enthalpy of vaporization (ΔH^{vap}) is of great value in various areas of science and engineering applications such as volumetric properties and heat flux calculations. Several correlations have been proposed for predicting the ΔH^{vap} of pure compounds (PC) and petroleum factions (PF). In this study we consider some of the well-recognized analytical models based on the knowledge of some molecular properties or on the properties of the liquid–vapor equilibrium. The most widely used correlations in the industry are available in the literature (Riazi and Daubert 1980; Vetere 1995; Liu 2001; Morgan 2007; Mohammadi and Richon 2007; Cachadina and Mulero 2009; Parhizgar, Dehghani, and Eftekhari 2013; Tatar et al. 2016; Baghban 2016). These methods are categorized into several groups based on a number of several criteria. In the most convenient classification, such methods are categorized into theoretical, semi-theoretical and empirical relations. Many models have been developed based on the principle of the structural groups contributions, however, these group contribution methods cannot be used for mixtures of indefinite compositions such as petroleum fractions (Hosseinifar and Jamshidi 2014).

The main objective of this work is to develop a novel and accurate model for the prediction of the ΔH^{vap} for both pure compounds and petroleum fractions. For this, we proposed a nonlinear function the coefficients of which need to be optimized. Several popular algorithms are available to optimize nonlinear functions such as the least-squares method. However, using this method in the optimization of nonlinear

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functions is sometimes insufficient. The common problem is that it may converge to a local optimum rather than a global optimum (Olinsky et al. 2004). Genetic algorithms have been successfully applied to optimize nonlinear functions and could be more effective against the least-squares method (Olinsky et al. 2004; Jin 2010). For this reason, we used real-coded genetic algorithm (RCGA) to globally optimize the coefficients of the new model.

2. The new generalized empirical correlation

The main objective is to find a function that relates a characteristic property with the input parameters. Riazi and Daubert (2005), constructed a simple equation for predicting the properties of undefined petroleum fractions. The equation is given as

$$\theta = a\theta_1^b\theta_2^c \tag{1}$$

Where, θ is the characteristic property to be predicted. θ_1 and θ_2 are any two input parameters that should represent molecular energy and molecule size, e.g. of properties that may be used as pairs of correlating parameters (θ_1, θ_2) in (Eq. 1) (Normal boiling point, Specific gravity), (Normal boiling point, Refractive index) and (molecular dynamic viscosity, Specific gravity).

The following polynomial function (Eq. 2) was inspired by the above Equation (1) of Riazi and Daubert. The final form is deduced after testing several combinations between the input parameters.

$$\theta = a\theta_1^b + c\theta_2^d + e\theta_1^f\theta_2^g \tag{2}$$

Parameters a-g are constants that have specific values for the ΔH^{vap} correlation. We used a genetic algorithm to obtain the globally optimized values of the constants a-g in Equation (2).

2.1. Sources of data

There are several sources that provide experimental data. In this work a number of 243 enthalpy of vaporization data for pure compounds and 127 data points for petroleum fractions were collected from previous studies; Parhizgar, Dehghani, and Eftekhari (2013) databank contains 62 data points for pure hydrocarbon and 58 data points for petroleum fractions, DIPPR's data banks (DIPPR Data files 2003) developed by the Institute of Chemical Engineering at the University of Pennsylvania, and the data banks of the Thermodynamical Research Center (TRC) (Tables, T.T. 1994). For petroleum fractions, the experimental data in the literature is scarce. For example, the data of Gray et al. (1985) is limited to only 8 narrow boiling coal liquid fractions. We therefore used experimental data of three Algerian crude oils (called Sahara Blend) with 61 petroleum fractions.

3. Genetic Algorithms

Genetic Algorithms (GA) are powerful tools for problem solving developed by John Holland (Sivanandam and Deepa 2007). They are widely applicable stochastic research and optimization methods based on the mechanics of natural selection and natural evolution (Golberg 1989). Genetic Algorithms work on a population of individuals. These individual consist of strings of genes called chromosomes. Each individual represents candidate solutions to the optimization problem at hand and each individual is evaluated to give some measure of its fitness. Some individuals undergo stochastic transformations by means of genetic operations to form new individuals (Sivanandam and Deepa 2007).

3.1. Definitions of GA operators

The main operators used by GA are the selection, crossover and mutation. The "initial population" corresponds to the starting set of individuals (Figure 1 shows an example of an individual) which are to be evolved by the GA. These individuals are formed by randomly selecting a group of probable solutions for the problem under study. "Fitness" is the representative of the objective function in the genetic

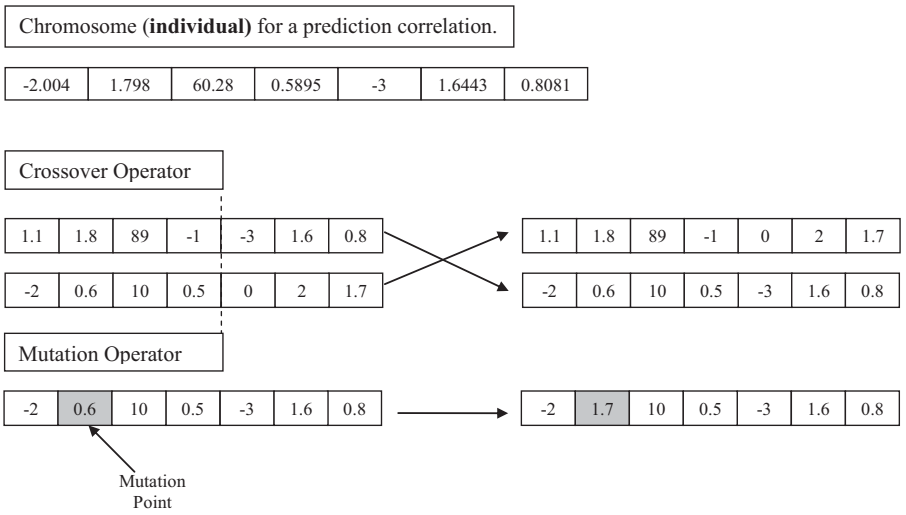

Figure 1. Main operators used by Genetic Algorithm.

algorithm. It is a measure of the quality of the candidate solution represented by the chromosomes following their ability to achieve the objective function criteria. "Selection" randomly chooses the reproduction candidate, parent. However, the best individuals, according to their fitness, will have a higher probability of contributing one or more times in the next generation. Out of the many available selection methods we used the roulette wheel selection in this study.

"Crossover" mixes information of parents; selecting a point where the chains interchange information. Figure 1 shows an example of some commonly used crossover operators for GA. "Mutation" occasionally changes the value of a string of genes, which creates new individuals by making changes in a single individual. Mutation operator helps to augment population diversity by introducing new genetic material. As shown in Figure 1. A small mutation rate ranging between (0.001) and (0.01) have always been adopted (Chambers 1998; Chieng and Wahid 2014). We set this mutation probability for our implementation at 0.0033.

When new individuals are evaluated, a new population is formed by selecting the more fit individuals from the parent population and new individuals. After several generations, genetic algorithm converges to the best individual, which represents an optimal solution to the problem. The general structure of the Genetic algorithms is shown in Figure 2.

4. Results and discussion

In this work, a new empirical method was developed to predict the enthalpy of vaporization at NBP for both pure compounds and petroleum fractions. The optimized values for the coefficients of Eq. (2) are shown in Eq. (3). After developing this generalized correlation, we compared it against some of the well-recommended correlations by Riazi and Daubert (1980), Vetere (1995), Morgan (2007) and Parhizgar, Dehghani, and Eftekhari (2013).

$$\Delta H^{vap} = 0.2065 T_b{}^{0.9265} + 0.6545 SG^{-0.9197} - 0.5590 T_b^{0.5806} SG^{-0.3265} \quad (3)$$

Using all the experimental data compiled in this study, the Average Absolute Error (AAE%) and the correlation coefficient (R^2) for all methods were calculated for pure compounds per chemical families and for petroleum fraction, as shown in Figure 3. As shown in Figure 3 our new correlation is more accurate than all other empirical models and has the potential for calculating the enthalpy of vaporization of both pure compounds and petroleum fractions. Therefore, the superiority of the new correlation over the other empirical methods has been verified for the experimental data available. The proposed correlation in this work is more convenient to use as it requires only the specific gravity and

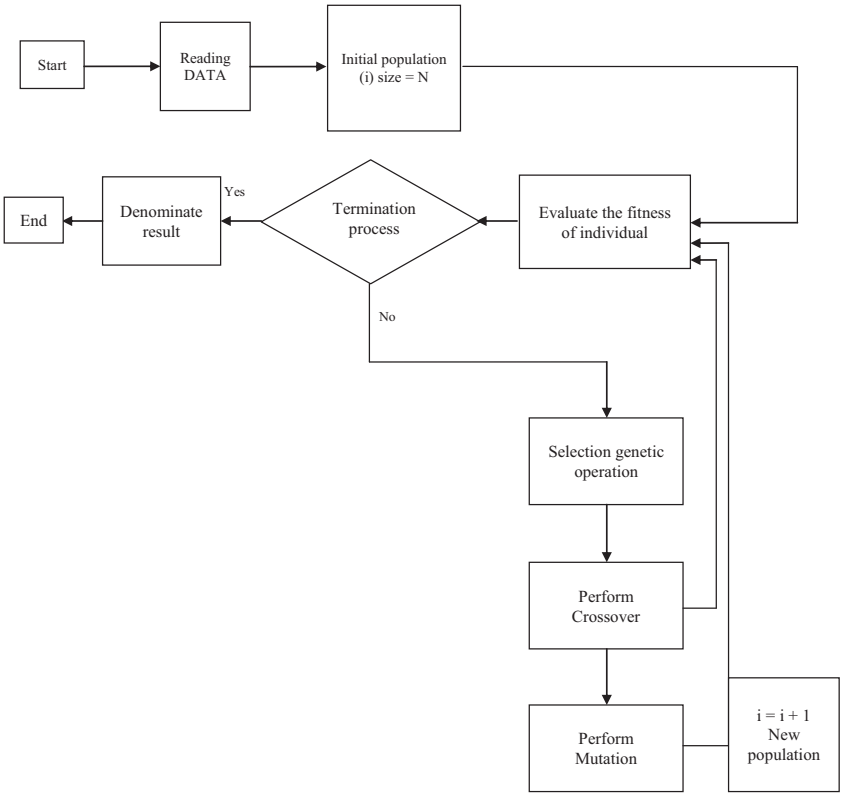

Figure 2. Flow chart showing the various steps in our genetic algorithm program.

boiling point as input parameters and can further be applied for both pure compounds and petroleum fractions.

To estimate the ability of the developed correlation to predict the enthalpy of vaporization of pure compounds we tested this correlation to predict the enthalpy of an independent set of data (about 20% of the experimental data compiled in this study) which are not used in the data base of GA during the development of the proposed correlation. The ΔH^{vap} predicted from our model versus the corresponding experimental data is shown in Figure 4 for petroleum fractions and Figure 5 for pure compounds. A tight

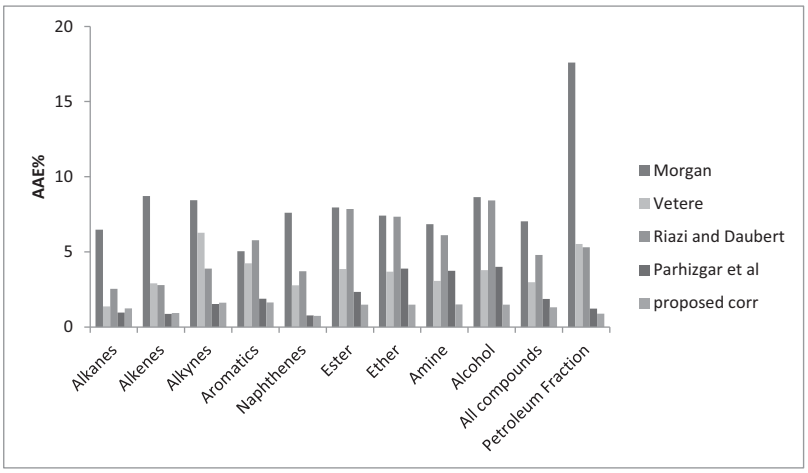

Figure 3. A comparison of all methods in prediction of enthalpy of vaporization for various types of compounds and petroleum fractions.

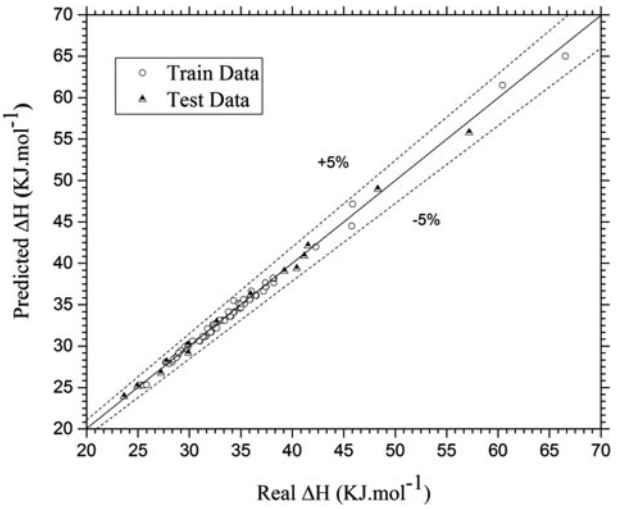

Figure 4. Predicted enthalpies of vaporization of algerian saharan blend petroleum fractions from the new model versus the experimental enthalpies of vaporization values.

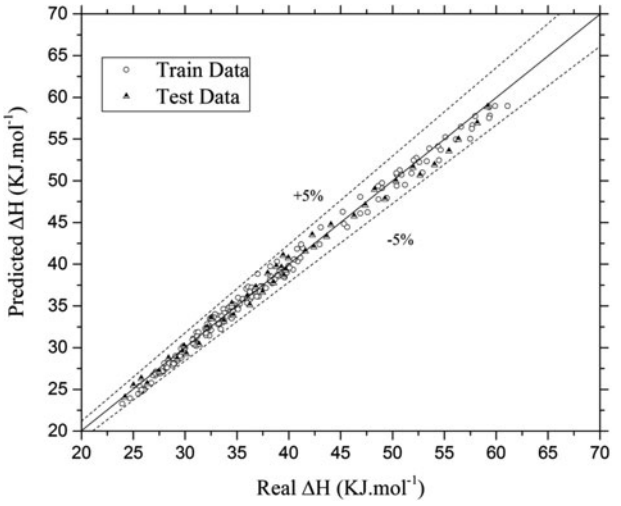

Figure 5. Predicted enthalpies of vaporization of pure compounds from the new model versus the experimental enthalpies of vaporization values.

alliance of points around the 45° line for the data illustrates a good correlation and the ability of the new model to predict of ΔH^{vap}. We notice that the predicted values of ΔH^{vap} for the new set of data as shown in Figures 4–5 are comparable to those of the training data which demonstrates the predictive ability of the proposed correlation for new data. The new correlation has successfully predicted more than 49% of the experimental data with AAE% less 1% and 84% less 2.5% and 100% of the data with AAE% less than 5% and $R^2 = 0.99$. It can be concluded that there is admirable accord between the literature experimental data and calculated values by the new model.

5. Conclusion

In this paper we proposed a general equation model to predict the enthalpy of vaporization at the NBP for both pure compounds and petroleum fractions. We used genetic algorithms to determine the coefficients of the proposed equation. The model gave very good results, thus fulfilling the main objective of this work

which is to provide a simple correlation model that predicates the ΔH^{vap} of pure compounds as well as petroleum fractions using two input parameters; the boiling point and specific gravity. The comparison with the literature shows that our model is more accurate compared to other conventional methods and gave comparable results to those obtained experimentally.

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