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# Heat of Vaporization and Refractive Index Estimation for Hydrocarbons and Petroleum Fractions based on Simple Models

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**Abstract:**

The present research reports that simple two parameter and three parameter models integrating normal boiling point, specific gravity and molecular weight of hydrocarbons can effectively be used for estimation of different important properties namely heat of vaporization and refractive index. Multivariate regression analysis was employed for model development based on experimental data of pure hydrocarbons reported in literature. Subsequently, it has been demonstrated that this model can be utilized further for prediction of those properties for different petroleum fractions as well. The developed simple generalized two parameter regression-based models can predict heat of vaporization of pure hydrocarbons (C3 – C30) and petroleum fractions with wide boiling point range from 355.5 to 646.8 K with good accuracy (percentage error less than 10% for pure hydrocarbons and lower than 13% for petroleum fractions) in addition, refractive index of petroleum fractions are estimated with percentage error of less than 4.01%. Moreover, comparison results demonstrated that developed models are more accurate and simpler for practical applications in petroleum industry as compared to earlier published correlations for both pure hydrocarbons and petroleum fractions.

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## 1. INTRODUCTION

Heat of vaporization is an important thermo-physical property of petroleum fractions due to its inherent effect on temperature and to quantify the inherent vapor – liquid phase behavior for effective distillation of multi-component crude oil. Refractive Index is another important physical property of petroleum and their fractions and is measured conventionally using refractometer as a function of temperature. Accurate knowledge of these thermo-physical properties of hydrocarbons and petroleum fractions are important for various engineering applications namely, thermodynamic calculations of multi-component multiphase equilibria process, enthalpy flux calculations of many unit operations, design of separation equipment, oil and gas production processes and petroleum characterization etc. [1-3]. Accurate determination of heat of vaporization of heavy oil components is essential for optimizing the thermal recovery processes in order to enhance the recovery rate of heavy oil with minimum operational cost and energy consumption [4]. Additionally, heat of vaporization is one of the important property for estimation of solubility parameters of hydrocarbons [3, 5]. It is difficult to measure or estimate accurately the thermo-physical properties of petroleum fractions compared to pure hydrocarbons due to inherent complexity of composition petroleum and non-ideal behavior of the mixture. Hence, methods for accurate estimation of heat of vaporization and refractive index is of great practical significance in the petroleum industry [6].

Determination of heat of vaporization and refractive index of petroleum and its fractions through experimentation is a time consuming, costly and labor-intensive affair. Moreover, conventional refractometers are not suitable to handle heavier hydrocarbons due to their high viscous nature and inherent opacity [7]. Hence, development of suitable model to predict these properties utilizing easily measurable properties will be beneficial for both pure hydrocarbons and petroleum fractions as well. Over past decades, researchers have developed various models or methods for estimation of heat of vaporization and refractive index such as group contribution method, empirical correlations and Artificial Neural Network (ANN) approach which are summarized in Table **1** [3, 8-17]. The detailed comparative analysis of existing correlations and methods are also mentioned in Table **1** clearly indicating that empirical correlations are extensively

**Table 1: Summary of Models/Methods of Predictions of Heat of Vaporization and Refractive Index [3, 8-17]**

| Reference | Model/ Method | Petroleum Component | Limitations/Gaps | Significance |
|---|---|---|---|---|
| Joback and Reid [8]<br>Tu and Liu [9]<br>Gharagheizi *et al*. [10] | Group contribution method | Pure components | Requires knowledge of chemical groups in molecule and chemical structure, have limited applicability to complex mixtures | Fast method of estimation with less computational resources requirement |
| Riazi and Daubert [11] | Empirical correlation | Petroleum fractions | Deviation is more for heavier and lighter fractions | Prediction of heat of vaporization for middle fractions quite well and computationally fast |
| Gopinathan and Saraf [12]<br>Fang *et al*. [13] | Empirical correlation | Pure hydrocarbons and crude fractions | Complex correlation for practical applications | Overcomes the shortcomings of previous correlations. |
| Riazi and Roomi [14] | Empirical correlation | Pure hydrocarbons and Petroleum fractions | Limited dataset for training and validation | Proposed empirical correlation with application for petroleum fractions |
| Vetere A. [15] | Empirical correlation | Pure hydrocarbons | Complex equation and wide deviation for heavier hydrocarbons | Demonstrated the applicability of model to great variety molecular structures like pure hydrocarbons, alcohols and esters. |
| Parhizgar *et al*. [16] | Genetic Programming approach | Petroleum fractions as well as pure hydrocarbons | Model is too complex for practical applications, computationally intensive | Highlighted the use of genetic programming for prediction of thermophysical properties |
| Mohammadi and Richon [3]<br>Eghtedaei *et al*. [17] | Artificial Neural Network approach | Pure hydrocarbons and Petroleum fractions | Complex model and highly computation intensive and network parameters | Highlighted the improvement by the use of artificial neural networks as compared to existing methods |

used as they relates heat of vaporization ($\Delta H^{vap}$) and refractive index (*RI*) to easily measurable thermo-physical properties of petroleum and petroleum fractions [17].

Several empirical correlations have been reported for estimation of heat of vaporization and refractive index of pure hydrocarbons and petroleum fractions as a function of specific gravity, normal boiling point and molecular weight [3, 11-15] and those are listed in Table **2**. Mohammadi and Richon [3] have developed an empirical correlation of heat of vaporization in terms of specific gravity and normal boiling point using Artificial Neural Network approach whereas Gopinathan and Saraf [12] have reported an empirical model as a function of specific gravity, normal boiling point and molecular weight based on pure hydrocarbons and petroleum fractions. Riazi and Roomi [14] have developed different correlation of refractive index for light and heavy petroleum fractions as a function of specific gravity, normal boiling point, kinematic viscosity and molecular weight. Vetere [15] has presented heat of vaporization model in terms of normal boiling point and molecular weight. Buckley and Wang [18] have utilized linear regression for development of refractive index relationship with API gravity based on seven types of crude oil data. Later, Genetic Programming model for prediction of heat of vaporization of petroleum fractions as well as pure hydrocarbons presented by Parhizgar *et al*. [16]. Surprisingly, they have developed model based on training data set of petroleum fractions and tested against pure hydrocarbons. In recent years, Huang and Yang [4] have fitted new thermodynamic correlation by incorporating modified alpha function into Peng-Robbinson equation of state for prediction of vaporization enthalpies of pure hydrocarbons mainly normal (straight chain) alkanes and alkenes for wide range of temperatures and pressures. They proposed modified alpha parameter as a function of reduced temperature and acentric factor of components. They have validated the developed model with light naphtha and Alaska naphtha fractions at different temperatures and pressures. It is important to note that their model requires critical properties, compressibility factor as input parameters along with physical properties. Similar form of empirical correlation was also utilized by some researchers for prediction of flash point; for instance, Satyanarayana and Rao [19] have developed and tested the non-linear exponential type correlation for flash point estimation of petroleum fractions as a function of their normal boiling point due to obvious brevity. Estimation of refractive index of hydrocarbons are always challenging and very few studies are available.

Santos *et al*. [20] have reviewed the empirical correlations for flash point estimation of pure hydrocarbons, petroleum fractions, biodiesel, vegetable oil, hydrocarbon blends and diesel-biodiesel blends for their practical their applicability. As instantaneous flash point values are required for online blending in refineries, empirical equations are frequently utilized for obvious simplicity in their usage [19, 20].

Literature analysis revealed that all these models reported in [3, 12, 13, 16] differ greatly in accuracy of predictions such as percentage relative deviation was up to 20% for Gopinathan and Saraf model [12] and less than 10 % for model proposed by Mohammadi and Richon [3], Fang *et al*. [13], and Parhizgar *et al*. [16]. It is worth mentioning that even though percentage

**Table 2: Some Empirical Models Available for Heat of Vaporization and Refractive Index of Petroleum Fractions**

| Model Ref. | Equation |
|---|---|
| Mohammadi and Richon [3] | $\Delta H^{vap} = 10.6988 + 0.000511 s^{0.1520} T_b^{0.8008} (\ln T_b + T_b)$ |
| Gopinathan and Saraf [12] | $\Delta H^{vap} = 1081 + (s^{-0.01418} \times T_b)[31.98 \log_{10} T_b + (22.12 T_b^{-1.573}/M)]$ |
| Fang *et al*. [13] | $\Delta H^{vap} = T_b[9.549 + 14.811 \ln T_b + 12.34(T_b/M) - 0.06662\,(T_b^2/M) + 7.833\times10^{-5}(T_b^3/M) + 19.334 \ln S]$ |
| Riazi and Roomi [14] | $RI_{20} = 0.336 M^{-0.006} S^{0.894}$, for $M \le 300$<br>$RI_{20} = 0.328\, v^{-0.003} S^{0.915}$, for $M > 300$<br>$RI_{20} = 0.01102 \exp(-8.61126\times10^{-4}\, M + 3.22861\, S + 8.61126\times10^{-5} S + 9.07171\times10^{-4} MS)\, M^{0.02426} S^{-2.25051}$, for $M > 300$ |
| Vetere [15] | $\Delta H^{vap} = 4.1868 T_b[9.08 + 4.36 \ln T_b + 0.0068\,(T_b/M) + 0.0009\,(T_b^2/M)]$ |
| Parhizgar *et al*. [16] | $\Delta H^{vap} = A_1 + A_2$<br>$A_1 = 15.1845 - 0.922 \ln\lvert\ln\rvert -61.311 + S^{-0.0376841 T_b + 1}\rVert$<br>$A_2 = 0.000203975\, T_b^{\left(\frac{-21.212111}{-10.969 + 41.0027905 \times S^{56.27}}\right)} - 0.33135 \ln\lvert 75.2754 - S^{-0.03959 T_b}\rvert$ |

relative error in above mentioned correlations [3, 13, 16] is less, they are too complex for practical applications as it requires complex computations. Most of these models utilizes molecular weight as an important variable for estimation of heat of vaporization and refractive index, however, determination of molecular weight for crude oils and petroleum fractions are not easy task. In addition, correlation suggested by Riazi and Daubert (1980) reported in Gopinathan and Saraf [12] as a function of specific gravity and normal boiling point is simpler than previous models [3, 12, 13, 15, 16] but their results indicated higher deviation for lighter and heavier petroleum fractions. Hence it is necessary to develop more accurate and simpler correlation to estimate the heat of vaporization and refractive index of petroleum fractions over wide range of boiling points. Main objective of this study is to develop a simple and generalized model for the estimation of heat of vaporization and refractive index for both pure hydrocarbon compounds and petroleum fractions based on their easily measurable properties. Excel based multivariate regression analysis was employed to develop simple non-linear three and two parameter models and to estimate the optimal coefficients for the developed models. The novelty of the present work is development of models based on only two easily measurable input properties of hydrocarbons namely specific gravity (*S*) and normal boiling point ($T_b$) and hence, have more practical applicability. The comprehensive experimental data of published literature for petroleum fractions and pure hydrocarbons were utilized for model development and validation purposes.

## 2. MODEL DEVELOPMENT FOR PREDICTION OF HEAT OF VAPORIZATION OF PETROLEUM FRACTIONS

Simple regression-based models relating heat of vaporization and refractive index as a functions of normal boiling point ($T_b$), specific gravity (*S*) and molecular weight (*M*) of hydrocarbons were targeted. Experimental data points of pure hydrocarbons reported by Parhizgar *et al*. [16] from previous literature [12, 15, 21] were utilized for model development. This database covers 64 pure hydrocarbon compounds with a boiling point range of 231.1 K to 722.8 K and specific gravities of 0.508 to 0.885. In order to develop the efficient model, 45 data points out of total data set of 64 pure hydrocarbons were selected for training set and 19 data points were used as validation set. Thorough analysis of the available data helped to segregate data points into training and validation set such a way that complete characteristics of both light and heavy hydrocarbons are picked up. The details of pure hydrocarbons data are provided in supplementary information Table **S1**.

In addition, 58 data points of petroleum fractions from published literature of Fang *et al*. [13] were used for further validation of developed model. This petroleum fractions data set comprises of four different crude oils (one from Russia, one from Iran and two from China).

The following simple, generalized three parameter model is proposed:

$$\Delta H^{vap} or\ RI = a \times T_b^b \times S^c \times M^d \quad (1)$$

where, $\Delta H^{vap}$ represents heat of vaporization (kJ/g-mol), RI denotes Refractive index (at 70° C), $T_b$ is normal Boiling point temperature (K), *S* is specific gravity (-), *M* indicates molecular weight (g/g-mol) and *a*, *b*, *c*, *d* are the coefficients of model equations to be determined.

Subsequently, it was attempted to develop a model with two easily measurable parameters namely normal boiling point ($T_b$) and specific gravity (*S*) based on the available literature data. The molecular weight factor of three parameter model (Eqn. 1) is excluded in modified model, as the measurement of molecular weight of petroleum fractions is a difficult task. The new two parameter model for heat of vaporization and refractive index was proposed as:

$$\Delta H^{vap} or\ RI = l \times T_b^m \times S^n \quad (2)$$

The optimal parameters *a*, *b*, *c*, *d*, *l*, *m*, and *n* of the proposed models (Eqns. 1 and 2) were estimated using multivariate regression analysis tool in Excel.

### 2.1. Description of Multivariate Regression Approach

Multivariate regression is a standard statistical method to estimate relationship between the dependent variable (also known as response variable, i.e., the targeted output) and multiple independent variables (called predictor variables).

The multivariate regression model can be written in the general form as

$$Y = \beta_0 + \beta_1 X_1 \pm \ldots + \beta_i X_k + \varepsilon \quad (3)$$

where, *Y* represents the experimental outputs ($\Delta H^{vap}$ or *RI* here), $X_i$ represents the experimental inputs ($T_b$, *S*

and *M*), $\beta_i$'s are the coefficients of the proposed model (*i* = 1, 2, …, *n*) and ε stands for the residuals (errors) between model predictions and corresponding experimental values.

In multivariate analysis, the optimal parameters for the model that best fit the data points are estimated using least square method that minimizes the square of residuals (SSR).

$$SSR = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{k} \beta_j X_{ij}\right)^2 \quad (4)$$

In this study, the present non-linear models (Eqns. 1 and 2) were converted to linear form using logarithms and then model parameters were found using multivariate regression tool in Excel.

### 2.2. Statistical Error Analysis

The efficiency and accuracy of the developed regression-based models were evaluated by utilizing statistical methods namely coefficient of determination ($R^2$), percentage error (% Error), and Absolute Average Relative Deviation (AARD).

$$R^2 = 1 - \frac{\sum_{i=1}^{N}\left[\Delta H_{pred.}^{vap} - \Delta H_{expt.}^{vap}\right]^2}{\sum_{i=1}^{N}\left[\Delta H_{expt.}^{vap} - \overline{\Delta H}_{expt.}^{vap}\right]^2} \quad (5)$$

$$\%\ \text{Error} = \left(\frac{\Delta H_{pred.}^{vap} - \Delta H_{expt.}^{vap}}{\Delta H_{expt.}^{vap}}\right) \times 100 \quad (6)$$

$$\text{AARD}\ \% = \frac{1}{N}\sum \left(\frac{\left|\Delta H_{pred.}^{vap} - \Delta H_{expt.}^{vap}\right|}{\Delta H_{expt.}^{vap}}\right) \times 100 \quad (7)$$

where, *N* is number of experimental data points.

## 3. RESULTS AND DISCUSSION

Two generalized models encompassing two and three parameters to predict heat of vaporization of pure hydrocarbon compounds were developed based on multivariate regression analysis. The optimal values of coefficients of these models (three parameter model as depicted in Eqn. 1 and two parameter models of Eqn. 2) were determined by minimizing sum of square errors and are represented by following expressions (Eqns. 8 and 9):

$$\Delta H^{vap} = 0.00373 \times T_b^{1.605} \times S^{-0.248} \times M^{-0.115} \quad (8)$$

$$\Delta H^{vap} = 0.01035 \times T_b^{1.348} \times S^{-0.150} \quad (9)$$

Similarly, models for estimation of refractive index with optimized coefficients are expressed as (Eqns. 10 and 11)

$$RI = 0.842 \times T_b^{0.1515} \times S^{0.196} \times M^{-0.069} \quad (10)$$

$$RI = 1.557 \times T_b^{-0.0033} \times S^{0.255} \quad (11)$$

As evident from Figure **1**, both the two parameter and three-parameter models can able to predict both heat of vaporization ($\Delta H^{vap}$) and refractive index (*RI*) quite accurately ($R^2$> 0.98) and ($R^2$> 0.89) respectively. The data points used for training and test set are represented with different symbols for easy comparison purposes. Also, percentage error (% Error), Absolute Average Relative Deviation (AARD %) (using Eqns. 6 and 7) were calculated for all the predictions and the obtained values are provided in Table **3** and supporting information (Table **S1** for heat of vaporization and Table **S2** for refractive index).

Furthermore, it is observed from Table **S1** that the maximum % Error of prediction of heat of vaporization for training data set of 45 pure hydrocarbons is 7.88 % for Eqn. (8), whereas for Eqn. (9) maximum % Error is 7.45 %. The average absolute relative deviation for Eqns. 8 and 9 is 2.75 % and 2.79 % respectively. Similarly, result in Table **S2** indicates that prediction of refractive index for training data set of 45 pure hydrocarbons using Eqn. 10 exhibited maximum % Error of (– 3.59 %), whereas (– 4.01 %) for Eqn. 11 and AARD is of 0.72 and 0.71 % respectively.

Developed two and three parameter models of heat of vaporization (Eqns. 8 and 9) and refractive index (Eqns. 10 and 11) were later validated with 19 validation data sets of pure hydrocarbons and detailed results are also provided in Table **3** and Supporting information in Table **S1** and **S2**. It is clearly evident that the maximum % Error of prediction of heat of vaporization is 8.11 % for Eqn. (8), whereas for Eqn. (9) maximum % Error is 7.58 % with corresponding AARD of 3.08 % and 3.03 % respectively. In a similar way, maximum % Error of prediction of refractive index is (– 1.55) % for Eqn. (10), whereas for Eqn. (11) maximum % Error is (–1.64 %) with corresponding AARD of 0.53 % and 0.45 % respectively.

It is important to note that molecular weight cannot be easily measured for petroleum fractions, so, for practical applications Eqns. 9 and 11 are to be considered as simple and effective models to predict heat of vaporization and refractive index as a function of only two easily measured input parameters namely normal boiling point and specific gravity. Moreover, the capability of developed models was evaluated based on comparative study of model predicted values of heat

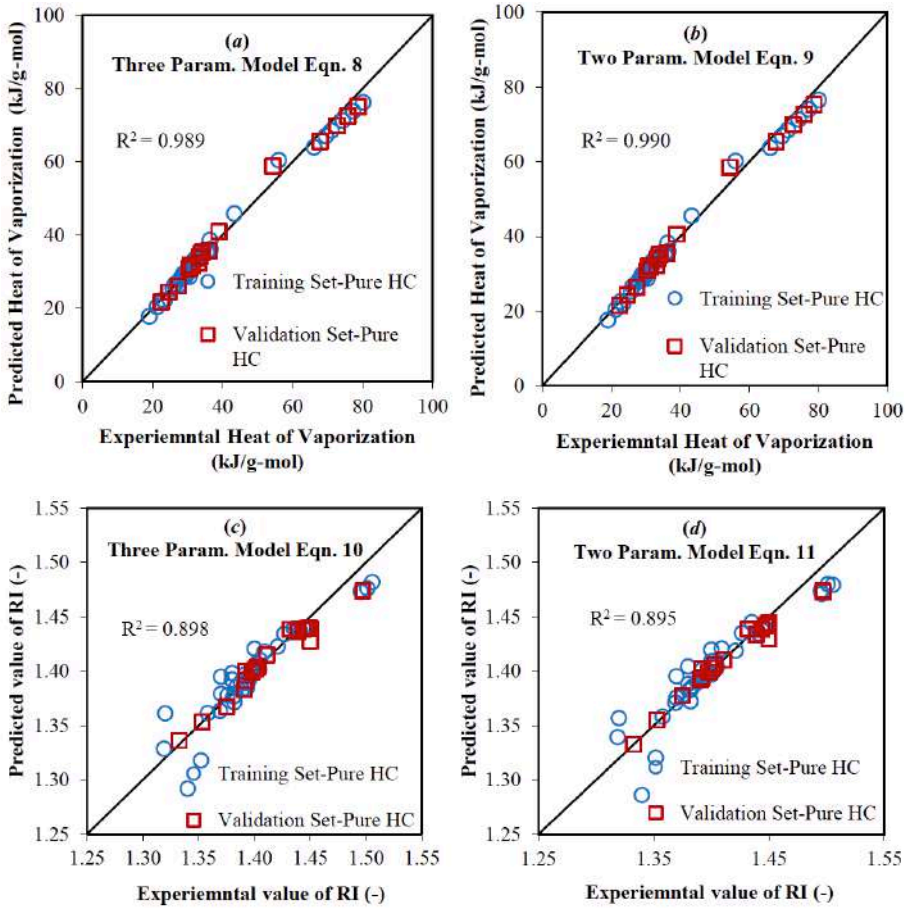


**Figure 1:** Predicted heat of vaporization and refractive index of pure hydrocarbons (training and validation data set) versus experimental heat of vaporization (data available in Ref. [16]) and Refractive Index using (***a***) Three parameter model Eqn. 8, (***b***) Two parameter model Eqn. 9, (***c***) Three parameter model Eqn. 10, (***d***) Two parameter model Eqn. 11.

**Table 3: Obtained Values of Coefficient of Determination, Percentage Relative Error and Coefficient of Determination of Three and Two Parameter Models for Heat of Vaporization and Refractive Index for Training and Validation Dataset of Pure Hydrocarbons**

| Model and dataset | Coefficient of determination [$R^2$] | | Relative percentage error [ % $E_i$] | | Absolute Average Relative Deviation (AARD %) | |
|---|---|---|---|---|---|---|
| | $\Delta H^{vap}$ | *RI* | $\Delta H^{vap}$ | *RI* | $\Delta H^{vap}$ | *RI* |
| 3 parameter Training | 0.989 | 0.898 | 7.88 | – 3.59 | 2.75 | 0.72 |
| 3 parameter Validation | | | 8.11 | – 1.55 | 3.08 | 0.53 |
| 2 parameter Training | 0.990 | 0.895 | 7.45 | – 4.01 | 2.79 | 0.71 |
| 2 parameter Validation | | | 7.58 | – 1.64 | 3.03 | 0.45 |

of vaporization along with earlier published correlations by Gopinathan and Saraf [12] and Genetic Programming model by Parhizgar *et al*. [16] and results are reported in supporting information Table **S3**. The obtained values of % Error of developed models for heat of vaporization utilizing training and validation data set of pure hydrocarbons along with earlier published correlations are also illustrated in Figure **2*a*** and ***b***. It is clearly seen from Figure **2** and Table **S3** that developed simple generalized two parameter model (Eqn. 9) for prediction of heat of vaporization exhibits higher accuracy (% maximum Error of 7.58 %) as compared to previously developed complex Genetic Programming model by Parhizgar *et al*. [16] with (–7.97 %) and Gopinathan and Saraf model [12] with (–15.92 %) based on training and validation data set of pure

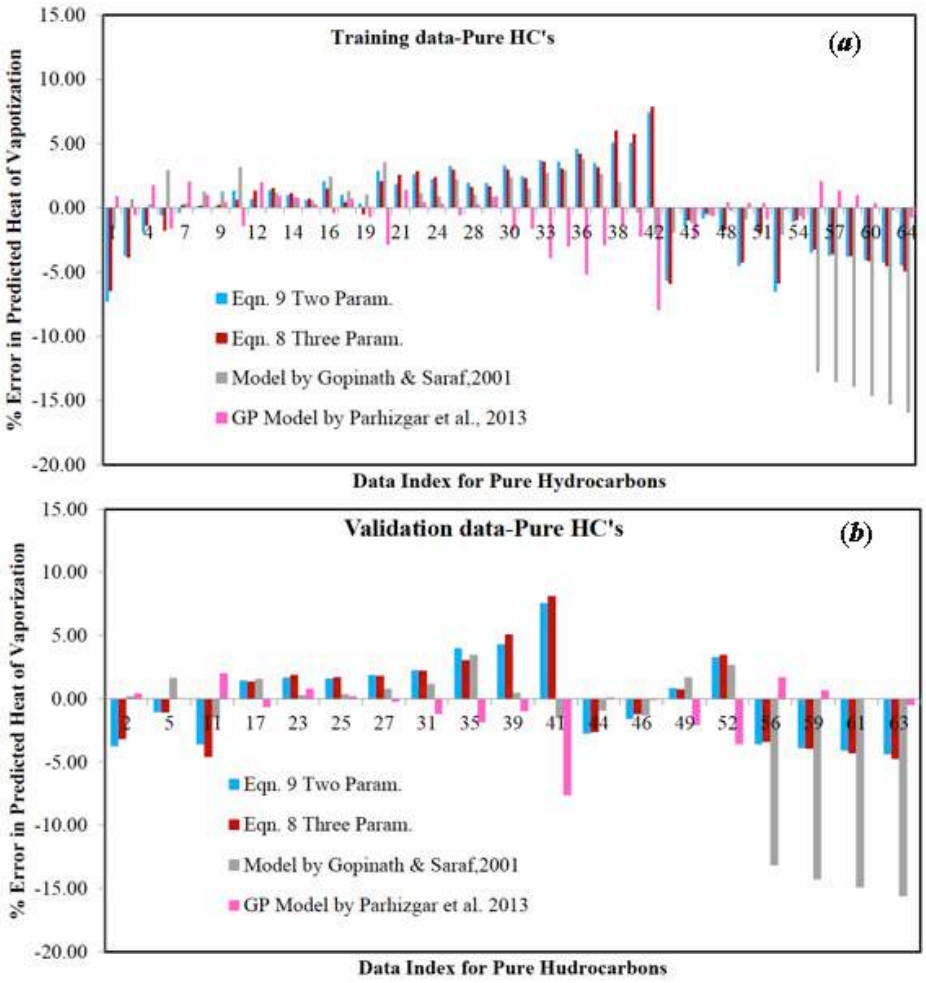


**Figure 2:** Comparison of % Error for Predicted heat of vaporization of (***a***) training data of pure hydrocarbons (***b***) validation data of pure hydrocarbons using developed two and three parameter models (Eqns. 8 and 9) in this study against earlier published models [12, 16].

hydrocarbons. There exists higher deviation of prediction of heat of vaporization of heavier hydrocarbons (refer to Supplementary Data Table **S3** for n-heneicosane $C_{21}H_{44}$ to n-triacontane $C_{30}H_{62}$) for Gopinathan and Saraf model [12]. It may be due to the fact, the model was developed based on obtained values of heat of vaporization of petroleum fractions using commercial simulator (as measured heat of vaporization data for crude fractions were not available) and the model were later tested to pure hydrocarbons [12].

In contrast, the developed model (Eqn. 9) in this study has better accuracy for heat of vaporization prediction not only for light hydrocarbons, but also for heavier hydrocarbons. This is because of classification and subsequent inclusion of light and heavy hydrocarbons data for training and validation set during model development. Later, the developed two and three parameter regression-based models are validated utilizing comprehensive experimental data set of petroleum fractions.

### 3.1. Validation of Model Based on Data of Petroleum Fractions

In order to verify the validity of the developed models of heat of vaporization and refractive index, 58 experimental data points for petroleum fractions of Fang *et al*. [13] were utilized. Their reported data of petroleum fractions are from four different crude oils (one from Russia, one from Iran, and two from China). The developed three and two parameter model (Eqns. 8, 9, 10 and 11) were utilized to predict the heat of vaporization and refractive index of these 58 samples of petroleum fractions. Model predicted results of enthalpy of vaporization using developed models in this study (Eqns. 8 and 9) are tabulated in Supplementary Information Table **S4**, whereas comparison results with previous correlation of Gopinathan and Saraf [12] and

**Table 4: Obtained Values of Coefficient of Determination, Percentage Relative Error and Coefficient of Determination of Three and Two Parameter Models for Heat of Vaporization and Refractive Index of Petroleum Fractions Dataset**

| Model and dataset | Coefficient of determination [$R^2$] | | Relative percentage error [ % $E_i$] | | Absolute Average Relative Deviation (AARD %) | |
|---|---|---|---|---|---|---|
| | $\Delta H^{vap}$ | *RI* | $\Delta H^{vap}$ | *RI* | $\Delta H^{vap}$ | *RI* |
| 3 parameter Validation | 0.9798 | 0.8452 | – 12.14 | 3.81 | 3.18 | 0.89 |
| 2 parameter Validation | 0.9827 | 0.9067 | – 11.06 | 4.01 | 3.07 | 0.96 |

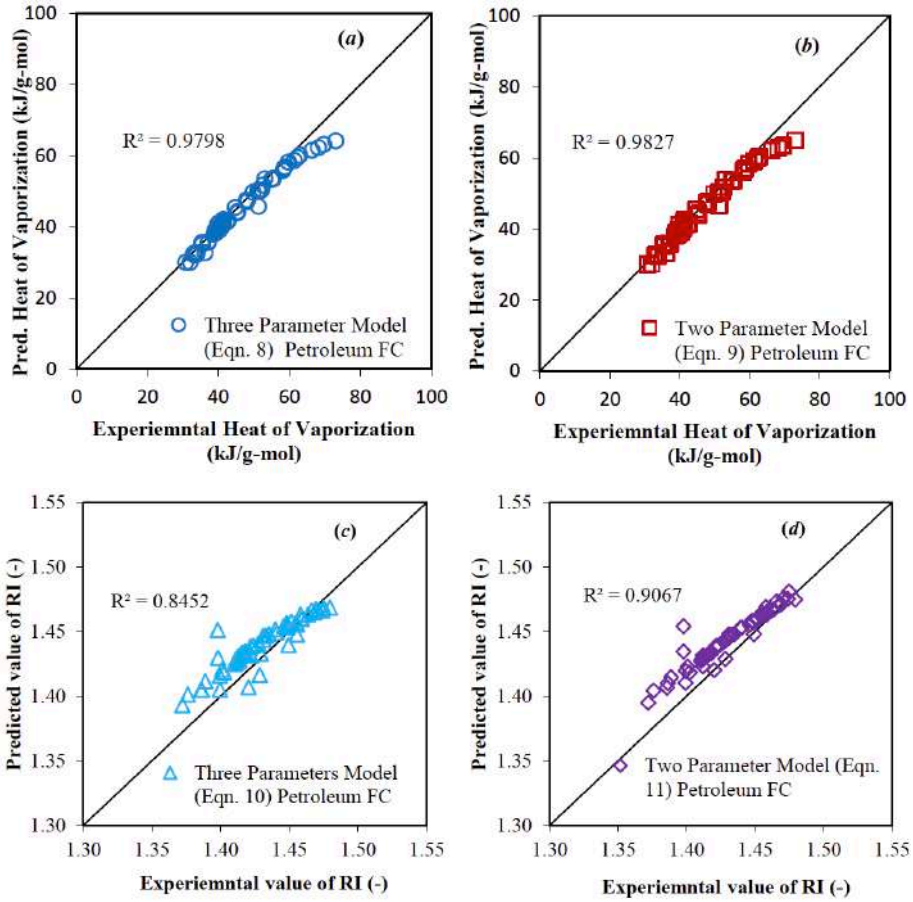


**Figure 3:** Predicted heat of vaporization and refractive index values of petroleum fractions versus the experimental heat of vaporization and refractive index [data obtained from Ref. 13] values using (***a***) Three parameter model Eqn. 8 (***b***) Two parameter model Eqn. 9 (***c***) Three parameter model Eqn. 10 and (***d***) Two parameter model Eqn. 11.

GP model by Parhizgar *et al*. [16] are provided in Supplementary Information Table **S5**. The corresponding % Error and AARD values are displayed in Table **4**. Similarly, model predicted (using Eqns. 10 and 11) refractive index for petroleum fractions along with experimental data are provided in Appendix Table **S6** and % Error and AARD values are exhibited in Table **4**. As clearly seen from results that maximum % Error and AARD values of heat of vaporization for 58 petroleum fractions using Eqns. 8 and 9 are (– 12.14 %, 3.18 %) and (– 11.06 % and 3.07 %) respectively which are comparable with GP model by Parhizgar *et al*. [16] (8.50 %, 1.44 %) and demonstrated better accuracy than Gopinathan and Saraf model [12] (– 18.78 %, 6.53 %). Similarly, maximum % Error of prediction of refractive index of 58 data points of petroleum fraction using developed models (Eqns. 10 and 11) are quite low (3.81 % and 4.01 %) along with AARD value smaller than 0.99 %.

Figure **3*a***, ***b***, ***c*** and ***d*** depicts predicted values of heat of vaporization utilizing Eqns. 8 and 9 and refractive index using Eqns. 10 and 11 against experimental data

of petroleum fractions. As depicted in the figures, the prediction of developed models are in good agreement with the experimental data with coefficient of determination ($R^2$ > 0.97) for heat of vaporization and with $R^2$ value higher than 0.90 for refractive index with two parameter model. It is clearly evident that the developed simple generalized model can reasonably predict heat of vaporization and refractive index of petroleum fractions based on easily measurable two input parameters namely normal boiling point and specific gravity.

## 4. CONCLUSION

The two generalized, simple models were developed using multivariate regression analysis tool in Excel for the estimation of the heat of vaporization and refractive index of hydrocarbons as a function of two easily measurable input parameters namely normal boiling point and specific gravity. The models were developed based on experimental data of pure hydrocarbon available in literature. Later, the efficacy of the model was validated with a comprehensive experimental data of petroleum fractions from published literature. The developed regression-based model is simple to use and able to predict heat of vaporization of pure hydrocarbon and petroleum fractions with percentage error of less than 10 % and 13 % respectively. Similarly, refractive index model prediction demonstrated better accuracy of 96 % for petroleum fractions and for pure hydrocarbons as well. Prediction analysis of three and two input parameter models indicates that if the experimental values of two easily measured parameters namely normal boiling point and specific gravity are known, developed two parameter model demonstrated better performance than the developed three parameter model presented in this study or previously published two or three parameter models as well. Therefore, proposed simple generalized two parameter model based on multivariate regression analysis provide an efficient tool which can be used to predict heat of vaporization and refractive index of petroleum fractions with reasonably good accuracy. The novelty of the study is that all the models are developed based on data of pure hydrocarbons and they are predicting properties of petroleum fractions from diversified reservoirs (one from Russia, one from Iran, and two from China) quite accurately.

## SUPPLEMENTARY TABLES

The supplementary tables can be downloaded from the journal website along with the article.

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