

Evaluation of the Temperature Dependence of Vaporization Enthalpy and its Correlation with Surface Tension by Machine Learning and Predictive Correlations

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Abstract

Temperature dependence of vaporization enthalpy is one of the most important thermophysical properties of compounds with extensive applications in chemistry and chemical engineering. In the present study, we theoretically developed relationships for evaluation of vaporization enthalpy of pure compounds from diverse chemical families for a wide temperature range from melting point to the critical temperature. Applying the derived relationships for predicting vaporization enthalpy of 767 compounds yielded an accuracy comparable to the most successful empirically derived models. One major outcome of the proposed method is a relationship describing the correlation between the surface tension and vaporization enthalpy which outperforms the extensively applied Kabo method empirically developed for the same purpose. To achieve higher accuracies, we also developed machine learning predictive models which yielded the most accurate evaluation of vaporization enthalpy at various temperatures to date. A C++ code is provided for user-friendly and convenient implementation of the developed machine learning models.

1- Introduction

Temperature dependence of vaporization enthalpy is one of the key properties of chemicals with numerous important applications in chemistry and chemical engineering, including but not limited to estimation of saturation vapor pressure (highly required in major chemical processes such as distillation, evaporation, drying, humidification and dehumidification¹), calculation of Hildebrand solubility parameter (required for evaluation of liquid-liquid equilibria as well as evaluation of the solubility of solids, gases and other liquids²⁻⁴), evaluation of fire hazards⁵, prediction of miscibility of polymer blends as a function of temperature and calculations of liquid-liquid separation processes such as leaching⁶⁻⁷.

Experimental measurement of vaporization enthalpy for a wide temperature range is not always feasible, e.g., due to safety concerns or operational limitations. This has been the motivation of numerous scientific works in the past decades aiming at predicting vaporization enthalpy at various temperatures *in silico*. Although various approaches such as molecular dynamics⁸ or Monte Carlo simulation⁹, group contributions and QSPR based methods¹⁰ have been exploited for this purpose, still the most straightforward and successful models are correlations which predict vaporization

enthalpy as a function of temperature and usually some additional more readily available thermophysical properties.

Some of the most successful previously proposed correlations and a comparison of their performances are reported in table 1.

Despite almost a century of research on this specific topic, almost all of the successful correlations applicable for predicting vaporization enthalpy of diverse compounds at wide temperature ranges have been developed empirically. In a previous study, a correlation was derived for this purpose entirely on a theoretical basis, and it was demonstrated that its accuracy is comparable to that of empirically derived models for a limited temperature range ¹. In the present study we provide an update on our theoretically derived correlation, resulting in a substantial improvement in its accuracy for a much wider temperature range.

In addition to predictive correlations, we also studied predictability of vaporization enthalpy via machine learning models as a widely accepted and powerful tool for finding dependency between model inputs and the target variable. We have recently employed machine learning for remarkably improving predictability of solvation free energy ¹¹ and flash point ¹².

Noteworthy, employing machine learning to predict vaporization enthalpy has been previously proposed in a number of studies before. Nevertheless, the currently available machine learning models are mainly limited to evaluating vaporization enthalpy at a single temperature which is commonly either room temperature ¹³⁻¹⁴ or normal boiling point ¹⁵⁻¹⁶. In the present study we present machine learning models applicable for evaluating vaporization enthalpy at various temperatures.

2- Methods

2.1- predictive correlation

In the previous study, it was shown that the temperature dependence of vaporization enthalpy follows ¹:

$$\Delta h_{vap} = \Delta \varepsilon_{bs} - \frac{k_B}{2} T \cdot \ln(T) - T \int \frac{\Delta \varepsilon_{bs}}{T^2} dT + CT, \quad (1)$$

where C is a constant and $\Delta \varepsilon_{bs}$ is the energy required for moving one molecule from the bulk of the liquid to the surface. Via the fundamental thermodynamics relationships between energy (ε), Helmholtz free energy (f) and entropy (s), which for our problem imply ¹:

$$\Delta \varepsilon_{bs} = \Delta f_{bs} + T \Delta s_{bs}, \quad (2)$$

$$\Delta s_{bs} = -\frac{d(\Delta f_{bs})}{dT}, \quad (3)$$

and exploiting the thermodynamics relationship among the free energy change for moving one molecule from the bulk of liquid to the surface (Δf_{bs}), surface tension (γ) and contribution of each molecule into the interfacial surface (a_s) which is defined as¹:

$$\Delta f_{bs} = a_s \gamma, \quad (4)$$

we get:

$$\Delta \varepsilon_{bs} = a_s \left(\gamma - T \frac{d\gamma}{dT} \right). \quad (5)$$

By substituting (5) in (1) and using $\frac{d(\frac{\gamma}{T})}{dT} = \frac{T \frac{d\gamma}{dT} - \gamma}{T^2}$ and multiplying both sides by Avogadro's number, the correlation between the surface tension and molar vaporization enthalpy (ΔH_{vap}) is obtained as :

$$\Delta H_{vap} = a \left(2 \gamma - T \frac{d\gamma}{dT} \right) - \frac{R}{2} T \cdot \ln(T) + \beta T, \quad (6)$$

in which a and β are constants.

For a constant temperature, (6) reduces to the Kabo method which describes correlation between vaporization enthalpy and surface tension as:

$$\Delta H_{vap} = \mathcal{A} \left(N_A^{\frac{1}{3}} V^{\frac{2}{3}} \gamma \right) + \mathcal{B}, \quad (7)$$

and has already been extensively applied in numerous works specially in studying ionic liquids¹⁷.

In the previous study, the constant a in eq.(6) was approximated via the liquid molar volume and assuming liquid phase molecules as true spheres, while the constant β was determined using a single item of reference data. Despite all these simplifying approximations, for a limited temperature range (between 50K below the normal boiling point up to 100 K below the critical temperature) the derived correlation yielded accuracies comparable with those of the most successful empirically developed models. Nevertheless, we noticed remarkable inaccuracies for the previously derived correlation when applied for wider temperature ranges, especially close to the critical temperature, which is mainly attributed to the assumption of true spheres for liquid molecules¹.

To overcome the above-mentioned shortcomings, in the present study and in contrast to the previous work, we calculate the constant a using a single reference data while the constant β is determined analytically and using the boundary condition at critical temperature. Accordingly, knowing that at critical temperature both vaporization enthalpy and surface tension approach zero, and due to continuity of the surface tension the $\frac{d\gamma}{dT}$ term also approaches zero, the constant β is found as:

$$\beta = \frac{R}{2} \ln(T_c), \quad (8)$$

which by substitution into eq.(6) results in:

$$\Delta H_{vap} = \alpha \left(2 \gamma - T \frac{d\gamma}{dT} \right) - \frac{R}{2} T \cdot \ln(T) + \frac{R}{2} T \ln(T_c), \quad (9)$$

The constant α in eq.(9) as the only remaining unknown constant can be determined using a single reference data.

To obtain a more straightforward relationship describing temperature dependence of vaporization enthalpy, we also exploit the Guggenheim–Katayama relationship stated as ¹⁸:

$$\gamma = \gamma^\circ \left(1 - \frac{T}{T_c} \right)^{11/9}, \quad (10)$$

which after substitution in eq.(9) results in:

$$\Delta H_{vap} = \alpha \left(2 \left(1 - \frac{T}{T_c} \right)^{11/9} + \frac{11}{9} \frac{T}{T_c} \left(1 - \frac{T}{T_c} \right)^{2/9} \right) - \frac{R}{2} T \cdot \ln(T) + \frac{R}{2} T \ln(T_c). \quad (11)$$

2.1- machine learning

In the present study we employed artificial neural networks to map the dependency between the vaporization enthalpy and potential input variables. We studied 9 potentially relevant thermophysical properties commonly employed in vaporization enthalpy predictive models, namely critical temperature (T_c), critical pressure (P_c), normal boiling point (NBP), liquid molar volume (V), acentric factor (ω), radius of gyration (R_g), van der Waals area (vdW_A) and volume (vdW_V) and dielectric constant (ϵ).

After trying various models, we noticed that the most successful neural network models are achieved for non-dimensionalized target and input variables. Accordingly, we employed reduced temperature ($\frac{T}{T_c}$) as an additional model input and $\frac{\Delta H_{vap}}{RT_c}$ as the target variable.

Considering that for many compounds not all of the studied model inputs might be readily available, we studied models which take only 2 to 6 of the studied thermophysical quantities. To that end, we exploited the Minimum Redundancy and Maximum Relevance (MRMR) algorithm ¹⁹ as a highly efficient algorithms for selecting most effective sets of variables for developing robust machine-learning-based models ²⁰.

We developed neural network models based on the guidelines proposed in the previous study¹². Accordingly, we used only 60% of the dataset for training the neural network models and assigned 15% and 25% of the dataset for validation and test of the models, respectively. We only studied neural networks with one hidden layer. For each model, maximum numbers of neurons were

determined in a way to yield models for which at least 10 training samples exist per model constant, as proposed in the previous study¹². For each model we studied Levenberg-Marquardt backpropagation and Gradient descent backpropagation training algorithms, and hidden layer transfer functions of the logarithm-sigmoid and tangent-sigmoid types²¹. For each model yielding higher accuracy compared to the best found result for the same neural network configuration, we evaluated its reliability by a 100-fold cross-validation proposed in the previous study. Accordingly, these models were retrained using the found neural network weight and bias constants as the initial guess under 100 different randomly selected training, validation and test sets. The models which in at least 80% of the iterations yielded test and training set error with the same mean and standard deviation as evaluated by the t-test method were selected as reliably trained models.

3.1- dataset

To benchmark the new model, we use thermophysical data of the DIPPR801 database²². Screening the dataset and selecting only the compounds with maximum uncertainty of 5% results in 767 compounds from diverse chemical families. The names of these compounds are provided as supplementary material.

For each compound, the experimentally determined data of vaporization enthalpies for 25 points linearly distributed between the melting point and the critical temperature were evaluated using the provided relationships in the DIPPR database.

Although the performance of vaporization enthalpy predictive correlations is commonly reported as average absolute relative error, in the present study we use Average Absolute Deviation (AAD) defined as

$$AAD = \frac{1}{N} \sum (|y_i^{exp} - y_i^{pred}|). \quad (12)$$

as a more appropriate parameter to evaluate the performance of the models. It is because at temperatures close to the critical point, the vaporization enthalpy approaches zero and as a result, small deviations in predicted data yield a very large relative error, resulting in an inappropriate inference about the performance of the studied models.

3- Result and discussion

3.1- predictive correlation results

In describing the correlation between the vaporization enthalpy and surface tension, the most obvious difference between the proposed relationship in eq.(6) and the widely accepted Kabo method is the existence of the $T \frac{d\gamma}{dT}$ term in our newly derived relationship. To evaluate the significance of this term on improving predictability of the vaporization enthalpy via surface

tension, we calculated the constants of eq.(6) by regression using vaporization enthalpy data of the whole temperature range for two cases: once with and once without the $T \frac{d\gamma}{dT}$ term included.

According to the results, while for eq.(6) in its original form, estimating the constants by regression results in an AAD of 905.7 Joule/mol, removing the $T \frac{d\gamma}{dT}$ term and recalculating these constants yields an AAD of 2672.2 Joule/mol. This confirms the importance of the $T \frac{d\gamma}{dT}$ term in substantially improving predictability of the vaporization enthalpy. Similarly, calculating the constants without the $\frac{R}{2} T \cdot \ln(T)$ term also results in increasing the AAD by 19.34 Joule/mol. All these findings imply the veracity of the developed method

For eq.(9), estimating α using the enthalpy of vaporization at normal boiling point (ΔH_{nbp}) as the only reference point yielded an AAD of 1077.1 Joule/mol, while for the same compounds and temperature range, finding the two constants of the Kabo method (eq. 7) by regression using all data points of the whole temperature range yielded an AAD of 1714.8 Joule/mol.

These results show that our newly derived relationship between vaporization enthalpy and surface tension (eq. 9) clearly outperforms the Kabo method as it requires only one adjustable parameter, does not require data of liquid molar volume and for the constant determined using only a single reference data yields much higher accuracy at other temperatures compared to the Kabo method even when its constants are determined using reference data at all temperatures.

For direct evaluation of vaporization enthalpy without requiring surface tension data, we examined the performance of the proposed relationship eq. (11). Accordingly, for the constant α calculated via experimentally determined data of vaporization enthalpy at normal boiling point, an AAD of 1150.7 Joule/mol for the whole temperature range was achieved.

Although experimental data at other temperatures can also be used to determine the constant α , using vaporization enthalpy at normal boiling point would be more advantageous due to convenience of its experimental measurement on one hand and existence of several accurate and straightforward to implement correlations for predicting ΔH_{nbp} on the other hand. In the present study we used and compared three such predictive correlations proposed by Chen²³, Vetere²⁴ and LIU²⁵ which provide accurate prediction of ΔH_{nbp} using critical temperature and critical pressure and normal boiling point as the only required data. Accordingly, calculating α in eq.(11) via ΔH_{nbp} predicted via these correlations yielded vaporization enthalpies predicted for the whole temperature range with AADs of 1321.8, 1351.7 and 1470.2 Joule/mol, respectively. These results are compared with those obtained for the same dataset via the most successful empirical models in table 1.

As can be seen in table 1, the theoretically derived relationships proposed in the present study yield accuracies comparable to those of the most successful empirically developed models. Nevertheless, it should be noted that as for the experimentally determined data, inaccuracies up to 5 percent are expected as reported by DIPPR, slight differences in accuracies of different models do not allow a certain judgment about their performances. Specifically, most of the empirically developed models are parameterized to reproduce DIPPR data, which might result in higher

accuracies for those models. For example, the higher accuracy of the model developed by Morgan compared to other empirical models might be due to employing the same relationship as the one provided by the DIPPR database to provide reference data at various temperatures, which was used in the present study to get reference data as well.

The distribution of AAD obtained via eq. (11) over major chemical families is depicted in figure 1 and shows a rather smooth variability for the AAD which is not so dramatically influenced by the chemical families. In our previous study we reported an obvious increasing pattern between the observed average absolute relative errors (AARE%) and molecular weights, especially in 1-alkenes, n-alkanes, methyl alkanes and dimethyl alkanes, which was attributed to a proportional increase in deviation from the true sphere assumption used in calculating the constant α with increasing molecular weight¹. Nevertheless, as depicted in figure 2, the alternative parameterization approach used in the present study to overcome inaccuracies due to the true sphere assumption clearly results in an almost uniform distribution of AARE% over molecular weight for the same groups, as expected.

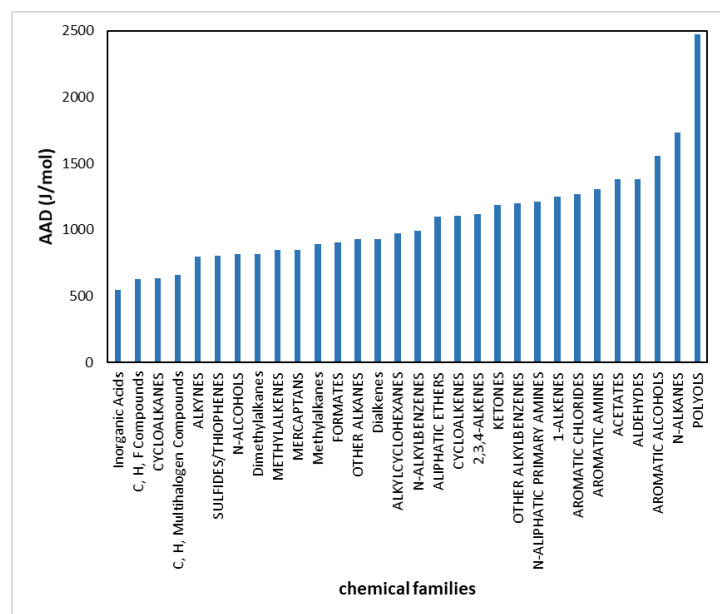


Figure 1- distribution of AAD among various chemical families

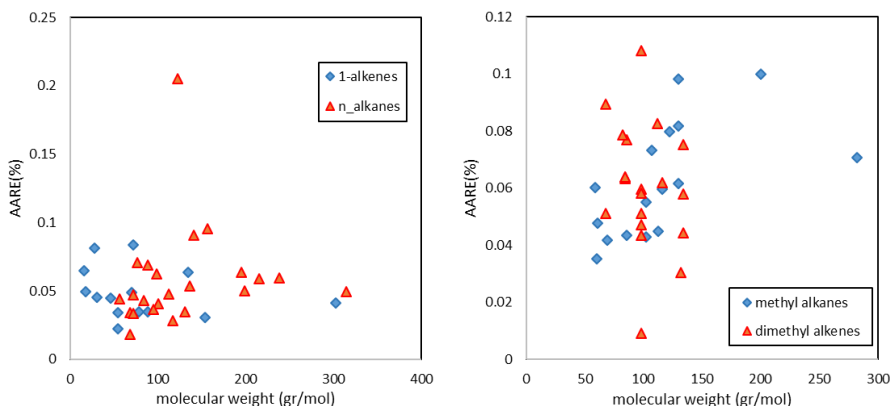


Figure 2- distribution of AARE(%) over molecular weights

Table 1- comparison of the results predicted via various models		
	Model inputs	AAD (Joule/mol)
Machine learning	<i>See table 2 for details</i>	865.383- 1066.57
New relationship (eq. 11)	$T_{nbp}, T_c, \Delta H_{nbp}$	1158.99
(α determined via experimentally determined data)		
New relationship (eq. 11)	T_{nbp}, T_c, P_c	1321.8
(α determined via the Chen model ²³)		
New relationship (eq. 11)	T_{nbp}, T_c, P_c	1351.7
(α determined via the Vetere model ²⁴)		
New relationship (eq. 11)	T_{nbp}, T_c, P_c	1470.2
(α determined via the Liu model ²⁵)		
Fish-Lielmezs ²⁶	$T_{nbp}, T_c, \Delta H_{nbp}$	1085.4
Morgan ²⁷	T_c, ω	1021
Morgan-Kobayashi ²⁸	T_c, ω	1217.3
Sivaraman et. al. ²⁹	T_c, ω	1218.6
Carruth-Kobayashi ³⁰	T_c, ω	1350.1
Meyra et al. ³¹	$T_{nbp}, T_c, \Delta H_{nbp}$	1959.3

3.2- results obtained via machine learning

After training the neural network models and selecting the reliable ones based on the guidelines discussed in section 2-1 and screening out the models which for the same or additional input variables yielded lower accuracy, we obtained 26 models reported in table 2. Based on the number and type of input variables, the developed machine learning models yield different AAD ranging from 865.383 to 1066.57 Joule/mol. As implied from these results, one main advantage of

employing machine learning is achieving higher accuracies as well as flexibility in treating different input variables. Furthermore, for the same input variables the results obtained via the machine learning models still show higher accuracy compared to the most successful predictive correlations which are the outcome of several decades of developing such correlations. For example, for predicting the vaporization enthalpy via critical temperature and acentric factor as the only model inputs, the neural network model specified with ID 23 in table 2 can be used which results in an AAD of 992.158 Joule/mol. This result shows a higher accuracy compared to the predictive correlations reported in table 1 which require the same model inputs. Among the developed machine learning models, the most interesting results are those obtained via a model specified in table 2 with ID 26 which requires only experimental data at the critical point and yields an AAD of 1066.57 Joule/mol. In comparison to all predictive correlations reported in table 1, this model shows an obvious advantage because all those correlations in addition to experimentally determined data at the critical point also require at least one additional reference data item of vaporization enthalpy either at $0.7 T_c$ (required for calculating the acentric factor) or at normal boiling point, nevertheless resulting in lower accuracy compared to the machine learning model. Despite the remarkable advantage of machine learning models compared to empirical correlations, one drawback of those models is the requirement of having technical knowledge for their application. With that in mind, we provide a C++ code with detailed used instructions for a user-friendly and straightforward application of the developed machine learning models.

4- Conclusion

In the present study we proposed theoretically derived relationships and machine learning models for prediction of vaporization enthalpy of pure chemical compounds at wide temperature ranges. We have demonstrated the success of the theoretically derived relationship in predicting vaporization enthalpy with an accuracy comparable to the most successful correlations as well as in describing the correlation between the vaporization enthalpy and surface tension. We have also developed and provided neural network models which, unlike other machine learning models proposed elsewhere, are not limited to a single temperature and can be used to evaluate vaporization enthalpy at various temperatures. We emphasize significant advantages of machine learning models compared to the predictive correlations: They possess higher flexibility in input variables, which for some models are more readily available, and can yield a higher accuracy.

Table 2- Performance of the developed machine learning models

Model ID	AAD(Joule/mol)	Model inputs:					
1	865.383	T/T_c	T_c	ω	vdW_A	ε	$\Delta H_{nbp}/RT_c$
2	867.641	T/T_c	ω	vdW_A	ε	$\Delta H_{nbp}/RT_c$	
3	868.492	T/T_c	NBP	V	ω	ε	$\Delta H_{nbp}/RT_c$
4	869.496	T/T_c	NBP	ω	ε	$\Delta H_{nbp}/RT_c$	
5	877.668	T/T_c	T_c	Pc	ω	ε	$\Delta H_{nbp}/RT_c$
6	890.629	T/T_c	ω	ε	$\Delta H_{nbp}/RT_c$		
7	897.208	T/T_c	NBP	ω	$\Delta H_{nbp}/RT_c$		
8	912.854	T/T_c	P_c	NBP	ε	$\Delta H_{nbp}/RT_c$	
9	913.738	T/T_c	ω	$\Delta H_{nbp}/RT_c$			
10	945.2	T/T_c	T_c	NBP	ω	vdW_A	ε
11	946.728	T/T_c	NBP	V	ω	vdW_V	ε
12	952.052	T/T_c	T_c	NBP	ω	ε	
13	952.575	T/T_c	ω	vdW_A	ε		
14	957.393	T/T_c	Pc	NBP	ω	ε	
15	958.143	T/T_c	T_c	P_c	ω	ε	
16	961.256	T/T_c	NBP	ω	ε		
17	961.524	T/T_c	Pc	ω	ε		
18	970.587	T/T_c	ω	ε			
19	977.585	T/T_c	Pc	ω			
20	980.281	T/T_c	NBP	V	ω		
21	981.209	T/T_c	T_c	NBP	ω		
22	984.434	T/T_c	NBP	ω			
23	992.158	T/T_c	ω				
24	997.771	T/T_c	T_c	P_c	NBP	vdW_A	ε
25	1019.28	T/T_c	P_c	NBP	ε		
26	1066.57	T/T_c	P_c	NBP			

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