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A QSPR Investigation of Octane Isomers Using Degcity Indices

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Abstract

This study examines the use of degcity indices as molecular descriptors for modelling selected physicochemical properties of octane isomers. Seven indices involving vertex degree and eccentricity are considered. Simple linear regression is first used to investigate the individual correlations between these descriptors and entropy (S), acentric factor (AF), enthalpy of vaporization (ΔH_{vap}), standard enthalpy of vaporization (ΔH^0_{vap}), and heat capacity (CP). Multiple linear regression models are then developed using backward stepwise selection. Their goodness of fit is assessed through the correlation coefficient, coefficient of determination, adjusted coefficient of determination and F-statistic. Predictive performance is further examined by leave-one-out cross-validation (LOOCV). The resulting models give comparatively strong results for S, AF, ΔH_{vap} and ΔH^0_{vap}, whereas the model for CP has limited predictive performance. The findings illustrate the potential, as well as the limitations, of degcity indices for QSPR modelling of the considered octane isomers.

keywords: *Degcity indices, MLR, Octane isomers, QSPR analysis, Topological index*
Mathematics Subject Classification (2020): *05C07, 05C09, 05C10, 05C12.*

1 Introduction

QSPR analysis is concerned with constructing mathematical models that relate the structural representation of a molecule to its physicochemical characteristics. Once an appropriate model has been established, it can be used to estimate a property from molecular descriptors, thereby providing a complementary approach to experimental determination. In chemical graph theory, topological indices are numerical descriptors obtained from the graph representation of a molecule. Their use in structure–property investigations has been discussed in a range of studies; relevant developments and applications are reported in [9, 1, 2, 5, 7, 8, 3, 4, 6].

The IUPAC terminology describes topological indices as numerical quantities associated with molecular constitution and used to relate molecular structure to physical, chemical or biological properties [11]. Different classes of descriptors encode different graph features. For example, degree-based indices reflect vertex connectivity, distance-based indices use shortest-path information, and eccentricity-based indices involve the maximum distances from vertices to the remaining vertices. A descriptor based on only one structural feature may not represent every aspect relevant to a particular molecular property; this motivates the examination of indices that combine more than one graph parameter.

The degcity indices proposed in [10] incorporate vertex degree and eccentricity in their construction. Degree describes the number of edges incident with a vertex and therefore represents a local connectivity feature. Eccentricity, in contrast, is determined by the greatest distance from a given vertex to any other vertex in the graph. Combining these quantities makes it possible to examine descriptors that reflect both local and distance-related structural information. Their usefulness for predicting molecular properties is an issue that can be assessed through an appropriate QSPR analysis.

In this work, the seven degcity indices are considered jointly as candidate explanatory variables in a multiple linear regression framework. This allows the analysis to move beyond the separate, one-descriptor relationships examined through simple linear regression and to investigate whether combinations of indices account for variation in the selected properties. Backward stepwise regression is used to obtain the reported descriptor combinations, and leave-one-out cross-validation is applied as an additional assessment of their predictive performance.

Eighteen octane isomers are selected for the investigation. The study considers five properties: entropy (S), acentric factor (AF), enthalpy of vaporization (ΔH_{vap}), standard enthalpy of vaporization (ΔH^0_{vap}), and heat capacity (CP). The aim is to determine how well the degcity indices describe these properties individually and in combination, and to evaluate the fitted models using the reported statistical measures and cross-validation results.

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2 Definitions and Notation

Throughout this section, let G denote a molecular graph with vertex set $V(G)$ and edge set $E(G)$. For an edge uv, the quantities d_u and d_v represent the degrees of its end vertices, while e_u and e_v denote their eccentricities. The seven degcity descriptors used in this study are defined by combining these parameters over the edges of G [10]:

$$DC_1(G) = \sum_{uv \in E(G)} [e_u + e_v]\,[d_u + d_v] \tag{2.1}$$

$$DC_2(G) = \sum_{uv \in E(G)} \frac{e_u + e_v}{d_u + d_v} \tag{2.2}$$

$$DC_3(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{e_u + e_v} \tag{2.3}$$

$$DC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{e_u + e_v}{d_u + d_v}} \tag{2.4}$$

$$DC_5(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v}{e_u + e_v}} \tag{2.5}$$

$$DC_6(G) = \sum_{uv \in E(G)} \frac{e_u + e_v}{d_u d_v} \tag{2.6}$$

$$DC_7(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{e_u e_v} \tag{2.7}$$

For any undefined graph terminology and notation, the reader may refer to [12].

3 Materials and Methodology

3.1 Dataset

The dataset comprises eighteen octane isomers. For each isomer, the five response variables considered are entropy (S), acentric factor (AF), enthalpy of vaporization (ΔH_{vap}), standard enthalpy of vaporization (ΔH^0_{vap}), and heat capacity (CP). The experimental property values are taken from [8] and are compiled in Table 1. The seven degcity indices calculated for the corresponding molecular graphs are reported in Table 2.

Table 1: Experimental values of physicochemical properties of octane isomers.

No.	Octane Isomers	AF	S	CP	ΔH^0_{vap}	ΔH_{vap}
1	n-Octane	0.398	111.670	24.640	9.915	73.190
2	2-Methyl heptane	0.378	109.840	24.800	9.484	70.300
3	3-Methyl heptane	0.371	111.260	25.600	9.521	71.300
4	4-Methyl heptane	0.372	109.320	25.600	9.483	70.910
5	3-Ethyl hexane	0.362	109.430	25.740	9.476	71.700
6	2,2-Dimethyl hexane	0.339	103.420	25.600	8.915	67.700
7	2,3-Dimethyl hexane	0.348	108.020	26.600	9.272	70.200
8	2,4-Dimethyl hexane	0.344	106.980	25.800	9.029	68.500
9	2,5-Dimethyl hexane	0.357	105.720	25.000	9.051	68.600
10	3,3-Dimethyl hexane	0.323	104.740	27.200	8.973	68.500
11	3,4-Dimethyl hexane	0.340	106.590	27.400	9.316	70.200
12	2-Methyl-3-ethyl pentane	0.332	106.060	27.400	9.209	69.700
13	3-Methyl-3-ethyl pentane	0.307	101.480	28.900	9.081	69.300

Continued on the next page

Table 1 continued from the previous page

No.	Octane Isomers	AF	S	CP	ΔH^0_{vap}	ΔH_{vap}
14	2,2,3-Trimethyl pentane	0.301	101.310	28.200	8.826	67.300
15	2,2,4-Trimethyl pentane	0.305	104.090	25.500	8.402	64.870
16	2,3,3-Trimethyl pentane	0.293	102.060	29.000	8.897	68.100
17	2,3,4-Trimethyl pentane	0.317	102.390	27.600	9.014	68.370
18	2,2,3,3-Tetramethyl butane	0.255	93.060	24.500	8.410	66.200

Table 2: Computed values of the degcity descriptors for the octane isomers.

No.	$DC_1(G)$	$DC_2(G)$	$DC_3(G)$	$DC_4(G)$	$DC_5(G)$	$DC_6(G)$	$DC_7(G)$
1	270	20.6667	2.5777	11.8942	4.2073	25.0000	1.0595
2	258	16.7167	3.1429	10.7189	4.6522	20.0833	1.4833
3	246	16.7833	3.2756	10.6774	4.7242	20.6667	1.6000
4	236	16.3833	3.4343	10.5190	4.8240	20.1667	1.7667
5	209	14.7500	3.8333	9.9809	5.0912	18.5833	2.1722
6	256	12.8167	4.0952	9.3847	5.3117	15.3750	2.1778
7	227	13.3667	4.0556	9.5534	5.2612	16.3611	2.2722
8	227	13.2500	4.0556	9.5168	5.2698	16.1667	2.2722
9	238	13.3000	3.8730	9.5912	5.1735	15.8333	2.0778
10	230	12.7167	4.5238	9.2335	5.5268	15.8750	2.6333
11	216	13.3000	4.2381	9.4763	5.3569	16.6667	2.4667
12	178	11.0000	5.2000	8.6137	5.9166	13.8889	3.8333
13	178	10.5000	5.8857	8.3212	6.2503	13.6250	4.5833
14	206	9.4976	5.7714	8.0404	6.2678	11.6667	4.1667
15	216	9.5333	5.4857	8.1083	6.1428	11.3750	3.7500
16	192	9.3810	6.1714	7.9313	6.4452	11.7083	4.7500
17	192	9.9167	5.4857	8.2353	6.1090	12.1111	4.0000
18	182	6.5000	8.0000	6.7071	7.4142	7.7500	7.0000

3.2 Model Development

Initially, simple linear regression (SLR) models were developed to examine the relationship between individual degcity indices and physicochemical properties. The general form of the SLR model is:

$$P = C + (DI)M, \tag{3.1}$$

Here, P denotes the property being modelled, DI is the selected degcity descriptor, and C and M are the intercept and slope, respectively. The correlation coefficients obtained from these individual fits are presented in Table 3.

Table 3: Correlation coefficients between the degcity indices and the physicochemical properties.

Degcity Index	AF	S	CP	ΔH^0_{vap}	ΔH_{vap}
$DC_1(G)$	0.7712	0.6687	0.6237	0.5242	0.4198
$DC_2(G)$	0.9622	0.9037	0.4626	0.9015	0.8443
$DC_3(G)$	0.9788	0.9438	0.4107	0.8195	0.7365
$DC_4(G)$	0.9774	0.9228	0.4563	0.8909	0.8268
$DC_5(G)$	0.9854	0.9423	0.4317	0.8480	0.7707
$DC_6(G)$	0.9577	0.9113	0.4101	0.9222	0.8733
$DC_7(G)$	0.9515	0.9269	0.3886	0.7622	0.6735

To improve predictive performance, multiple linear regression (MLR) models were constructed using the backward stepwise regression technique. In this approach, all candidate descriptors are initially included in the model, and the least significant variables are iteratively removed based on statistical criteria (p-value), until an optimal model containing only significant descriptors is obtained. The general form of the MLR model is given by:

$$p = a_0 + a_1t_1 + a_2t_2 + a_3t_3 + ... + a_nt_n + \epsilon \tag{3.2}$$

In this expression, a_0 is the intercept, a_i denotes the regression coefficient associated with descriptor t_i, and ϵ represents the error term. Using (3.2), we have the following MLR models for each property of octane isomers.

$$S = 139.052 - 0.063DC_1 - 4.296DC_3 \tag{3.3}$$

$$\begin{aligned} AF = {} & 3.947 + 0.045DC_2 - 0.251DC_4 \\ & - 0.369DC_5 + 0.062DC_7 \end{aligned} \tag{3.4}$$

$$\Delta H_{vap} = 139.307 - 0.057DC_1 + 7.760DC_3 - 16.848DC_5 \tag{3.5}$$

$$\begin{aligned} \Delta H^0_{vap} = {} & 41.511 - 2.085DC_4 - 3.722DC_5 \\ & + 0.316DC_6 + 0.866DC_7 \end{aligned} \tag{3.6}$$

$$\begin{aligned} CP = {} & -3636.142 - 46.101DC_2 - 143.210DC_3 \\ & + 257.751DC_4 + 455.568DC_5 \end{aligned} \tag{3.7}$$

3.3 Model Evaluation

The developed models were evaluated using statistical parameters including the correlation coefficient (R), coefficient of determination (R^2), adjusted R^2 (R^2_{adj}), and F-statistic. These parameters provide insight into the goodness-of-fit and statistical significance of the models. The corresponding values of these statistical measures for all developed models are presented in Table 4, which summarizes the overall performance and reliability of the regression models.

Table 4: Statistical performance measures of the developed MLR models.

Property	**R**	**R^2**	**R^2_{adj}**	**F**
S	**0.968**	**0.938**	**0.929**	112.785
AF	**0.999**	**0.997**	**0.996**	1199.593
ΔH_{vap}	**0.967**	**0.935**	**0.921**	67.354
ΔH^0_{vap}	**0.975**	**0.950**	**0.935**	62.048
CP	0.882	0.778	0.709	11.358

4 Results and Discussion

The correlation coefficients obtained from simple linear regression (Table 3) indicate that most degcity indices exhibit strong relationships with entropy (S) and acentric factor (AF), while their correlations with enthalpy of vaporization (ΔH_{vap}), standard enthalpy of vaporization (ΔH^0_{vap}), and heat capacity (CP) are comparatively weaker.

To improve predictive performance, multiple linear regression (MLR) models were developed using a backward stepwise regression approach. The resulting models (3.3) to (3.7) incorporate two to four degcity indices as descriptors. The statistical parameters of these models are summarized in Table 4.

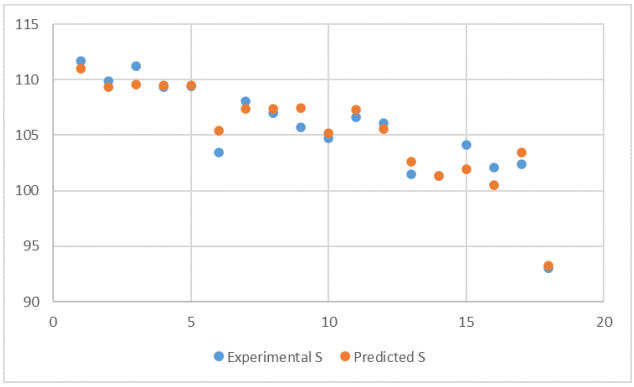
The high values of the correlation coefficient ($R > 0.96$) for S, AF, ΔH_{vap}, and ΔH^0_{vap} indicate strong linear relationships between the selected degcity indices and the corresponding physicochemical properties. The adjusted coefficient of determination (R^2_{adj}) values ($0.921-0.996$) further confirm that a substantial proportion of the variance in these properties is explained by the proposed models. Additionally, the F-statistic and corresponding significance values ($Sign.F < 0.05$) demonstrate that all models are statistically significant.

Among the developed models, the MLR model for acentric factor (AF) shows particularly high predictive accuracy ($R^2_{adj} = 0.996$), indicating an excellent fit. Similarly, the models for entropy (S), ΔH_{vap}, and ΔH^0_{vap} exhibit strong predictive capability, with R^2_{adj} values exceeding 0.92. However, the model for heat capacity (CP) shows comparatively lower performance ($R^2_{adj} = 0.709$), suggesting that CP may depend on additional molecular factors not fully captured by the considered topological descriptors.

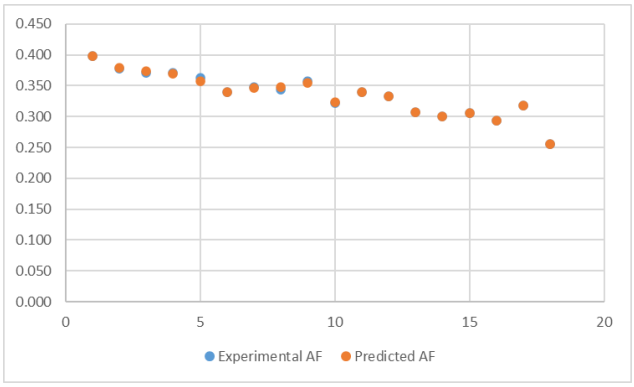
It is important to note that degcity indices exhibit a certain degree of inter-correlation, which may introduce multicollinearity in multi-descriptor regression models. While the stepwise regression procedure helps in selecting statistically significant variables, the presence of multicollinearity may influence the stability and interpretability of regression coefficients.

Figure 1 compares the experimental and model-predicted values for entropy, acentric factor, enthalpy of vaporization

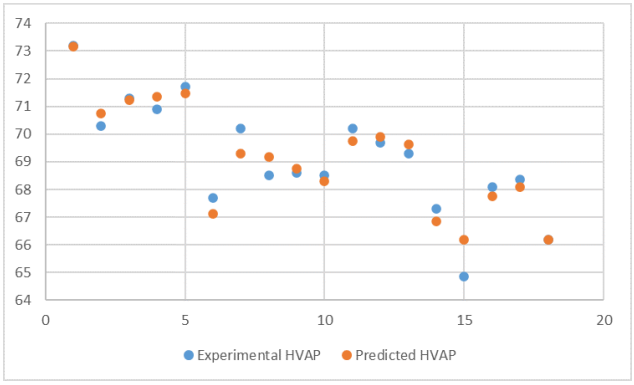
and standard enthalpy of vaporization. The plotted comparisons provide a visual assessment of how closely the fitted values follow the corresponding experimental observations. The heat-capacity model is not included in this figure.



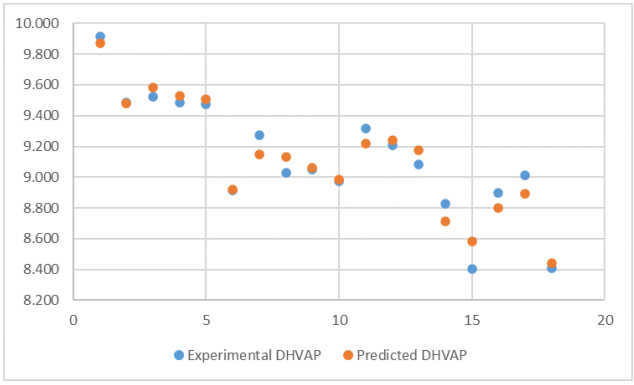
(a) S



(b) AF



(c) ΔH_{vap}



(d) ΔH^0_{vap}

Figure 1: Experimental vs Predicted values of S, AF, ΔH_{vap} and ΔH^0_{vap}

4.1 Validation of QSPR Model

The predictive performance of the developed models was evaluated using the leave-one-out cross-validation (LOOCV) technique. The cross-validated coefficient of determination, Q^2, is calculated as follows:

$$R^2_{CV} \equiv Q^2 = 1 - \frac{PRESS}{TSS}, \tag{4.1}$$

where PRESS is the Predictive Error Sum of Squares and TSS is the Total Sum of Squares.

A model is generally considered reliable if $Q^2 > 0.5$, while values greater than 0.9 indicate excellent predictive ability. The computed Q^2 values for the models are presented in Table 5.

The results show that the models for S, AF, ΔH_{vap} and ΔH^0_{vap}, yield high Q^2 values $(0.901 - 0.996)$, confirming their strong predictive capability and robustness. In contrast, the Q^2 value for CP is negative, indicating poor predictive performance and suggesting that the corresponding model is not suitable for reliable prediction.

Table 5: Leave-one-out cross-validation results for the proposed QSPR models.

Model No.	Property	Q^2
(3.3)	S	**0.913**
(3.4)	AF	**0.996**
(3.5)	ΔH_{vap}	**0.901**
(3.6)	ΔH^0_{vap}	**0.913**
(3.7)	CP	-0.122

4.2 The residuals

Residual analysis was carried out to assess the adequacy of the developed models. The residuals, defined as the differences between experimental and predicted values, are presented in Tables 6 and 7. The corresponding residual plots (Figure 2) indicate that the residuals are randomly distributed around zero without any systematic pattern.
This behavior suggests that the assumptions of linear regression are satisfied and that the proposed models are appropriate for describing the relationship between degcity indices and the selected physicochemical properties.

Table 6: Comparison of observed and model-estimated entropy and acentric factor values with corresponding residuals.

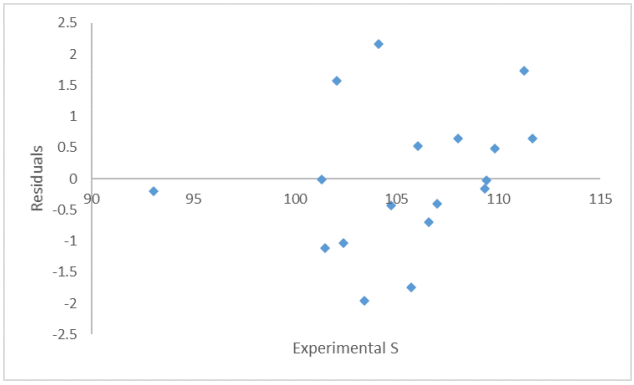
Octane Isomers No.	Experimental S	Predicted S	Residual	Experimental AF	Predicted AF	Residual
1	111.670	111.024	0.646	0.398	0.398	-0.001
2	109.840	109.350	0.490	0.378	0.379	-0.002
3	111.260	109.533	1.727	0.371	0.374	-0.003
4	109.320	109.479	-0.159	0.372	0.369	0.003
5	109.430	109.460	-0.030	0.362	0.358	0.005
6	103.420	105.384	-1.964	0.339	0.340	-0.001
7	108.020	107.375	0.645	0.348	0.347	0.001
8	106.980	107.375	-0.395	0.344	0.348	-0.004
9	105.720	107.469	-1.749	0.357	0.355	0.002
10	104.740	105.175	-0.435	0.323	0.323	0.000
11	106.590	107.282	-0.692	0.340	0.340	0.000
12	106.060	105.535	0.525	0.332	0.333	0.000
13	101.480	102.589	-1.109	0.307	0.307	0.000
14	101.310	101.322	-0.012	0.301	0.301	0.000
15	104.090	101.922	2.168	0.305	0.305	0.000
16	102.060	100.483	1.577	0.293	0.294	0.000
17	102.390	103.429	-1.039	0.317	0.319	-0.001
18	93.060	93.255	-0.195	0.255	0.255	0.000

Table 7: Comparison of observed and model-estimated enthalpy of vaporization and standard enthalpy of vaporization values with corresponding residuals.

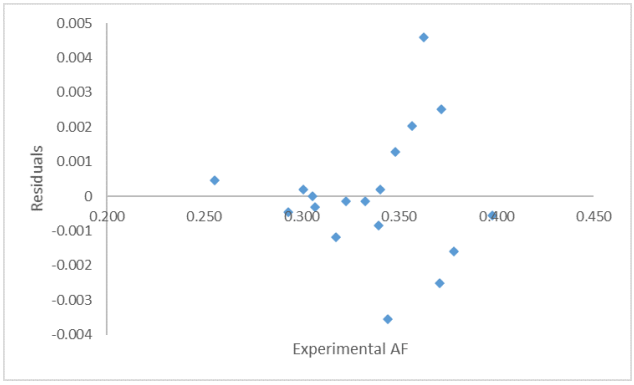
Octane Isomers No.	Experimental ΔH_{vap}	Predicted ΔH_{vap}	Residual	Experimental ΔH^0_{vap}	Predicted ΔH^0_{vap}	Residual
1	73.190	73.169	0.021	9.915	9.871	0.044
2	70.300	70.737	-0.437	9.484	9.478	0.006
3	71.300	71.230	0.070	9.521	9.582	-0.061
4	70.910	71.346	-0.436	9.483	9.527	-0.044
5	71.700	71.467	0.233	9.476	9.506	-0.030
6	67.700	67.128	0.572	8.915	8.919	-0.004
7	70.200	69.309	0.891	9.272	9.148	0.124
8	68.500	69.165	-0.665	9.029	9.131	-0.102
9	68.600	68.749	-0.149	9.051	9.061	-0.010
10	68.500	68.299	0.201	8.973	8.986	-0.013
11	70.200	69.736	0.464	9.316	9.218	0.098
12	69.700	69.916	-0.216	9.209	9.239	-0.030
13	69.300	69.615	-0.315	9.081	9.173	-0.092
14	67.300	66.852	0.448	8.826	8.714	0.112
15	64.870	66.176	-1.306	8.402	8.584	-0.182
16	68.100	67.758	0.342	8.897	8.799	0.098
17	68.370	68.100	0.270	9.014	8.894	0.120
18	66.200	66.186	0.014	8.410	8.443	-0.033

5 Conclusion

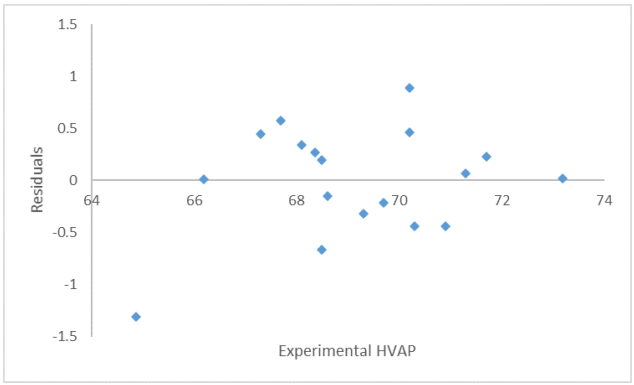
In this study, quantitative structure–property relationship (QSPR) models were developed to predict selected physicochemical properties of octane isomers using degcity indices. The results demonstrate that multiple linear regression (MLR)



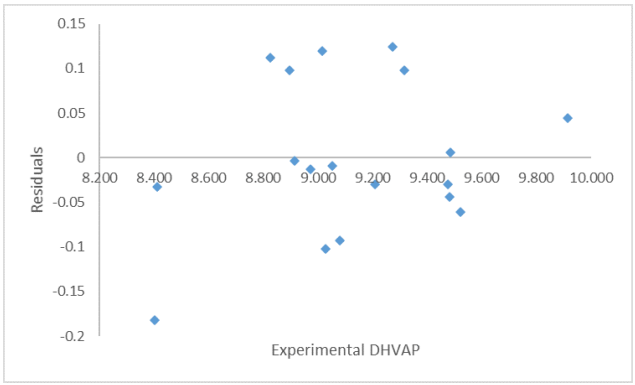
(a) Residual plot of S



(b) Residual plot of AF



(c) Residual plot of ΔH_{vap}



(d) Residual plot of ΔH^0_{vap}

Figure 2: Residual plots of S, AF, ΔH_{vap} and ΔH^0_{vap}

models constructed through backward stepwise regression provide strong predictive performance for entropy (S), acentric factor (AF), enthalpy of vaporization (ΔH_{vap}), and standard enthalpy of vaporization (ΔH^0_{vap}), as evidenced by high statistical parameters and cross-validated (Q^2) values. These findings indicate that degcity indices, which incorporate both degree and eccentricity information, effectively capture essential structural features of molecular graphs.

However, the model for heat capacity (CP) shows comparatively weaker performance, suggesting that this property may depend on additional molecular characteristics not fully described by the considered descriptors. The study also highlights that multicollinearity among degcity indices may influence coefficient stability in multi-descriptor models.

Overall, the results confirm that degcity indices are reliable and informative descriptors for QSPR modeling of octane isomers, particularly for entropy and enthalpy-related properties. Future work may focus on incorporating additional descriptors or advanced modeling techniques to further improve prediction accuracy, especially for properties such as heat capacity.

6 Disclosure Statement

There is no conflict of interest regarding the publication of this article.

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