QSPR analysis of certain degree based topological invariants using MLR model

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Abstract
QSPR models are vital role for molecular design of new compounds. In this paper, we calculate the degree based topological invariants of alkanes and also to find the correlation coefficient, linear regression and multiple linear regression models (MLR) for the prediction of boiling point of alkenes.

Keywords
Multiple correlation coefficient, MLR models, Topological invariants and boiling point.

AMS Subject Classification
05C05, 05C07, 05C12.

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1. Introduction and Preliminaries

Chemical graph theory is a study of graph theory together with chemistry. It is very useful in physic-chemical and biological properties of organic compounds. Topological invariants are a numerical value which can be used for Quantitative Structure Property Relationship (QSPR) and Quantitative Structure Activity Relationship (QSAR) studies [1-4]. Alkane contains carbon and hydrogen atoms and also carbon-carbon single bonds. It is very useful in chemical engineering and chemical reactions of molecules. Alkanes are important raw materials of the chemical industry and the principal constituent of gasoline and lubricating oils. In this article, we study correlation between the topological indices and the boiling points of corresponding alkanes. [5] Also we study the linear regression equation of boiling points also MLR model for boiling points. Besides we compare the experimental boiling points and the calculated boiling points of alkanes using topological invariants. The main goal of this article is to find the Multiple Linear Regression model (MLR) for the prediction of boiling points of alkenes in terms of its topological invariants.

In this study, we consider multiplicative topological invariants like Second Multiplicative Zagreb index, New Multiplicative version of first Zagreb index, Multiplicative Sum Connectivity index, Multiplicative Product Connectivity index, Multiplicative Atom Bond Connectivity index and Multiplicative Geometric Arithmetic index also we consider additive indices like Randic, Geometric-Arithmetic, Sum connectivity, Harmonic, First Zagreb, Second Zagreb, Second Modified Zagreb, Inverse sum, Alberston, Atom-Bond connectivity, Symmetric Division, Augmented Zagreb indices respectively. [6-11]

Correlation: Correlation analysis is to determine the degree of relationship between variables. Also this is the co variation between two or more variables. If the ratio of change between two variables is uniform then it is called the linear correlation. Positive or negative correlation depends upon the direction of change of the variables in the same direction or opposite direction.

Coefficient of determination ($r^2$): The coefficient of...
determination is the ratio of the expected variance to the total variance.

\[ r^2 = \frac{\text{Expected Variance}}{\text{Total Variance}} \]

**Regression:** Regression is the study of the average relationship between two or more variables. Regression analysis predicts the value of dependent variables from the values of independent variables. Regression equation of X on Y is

\[ \overline{Y} = \beta_0 + \beta_1 \overline{X} \]

Regression equation of Y on X is

\[ \overline{X} = \frac{\beta_0}{\beta_1} \overline{Y} - \frac{\beta_0}{\beta_1} \overline{X} \]

where, \( \overline{X} \) = Mean of X series, \( \overline{Y} \) = Mean of Y series

We have used here Eight Multiplicative degree based topological invariants and twelve Additive degree based topological invariants which are listed in Table 1 and Table 2. Also the experimental boiling points of alkanes are in Table 3. Besides the calculated values of these indices are listed in table 4, 5, 6, 7. Also table 8 and 9 indicated that the correlation coefficient between boiling points and its corresponding indices. Linear Regression equations of boiling points in terms of its indices are noted in table 10 and table 11 respectively. In table 12 and table 13 indicated the MLR model for prediction of boiling points. Table 14 has contained predicted boiling points and its residuals.

### 1.1 Multiple Linear Regression model

Multiple Linear Regression is a statistical method which uses several variables to find the outcome of a dependent variable. The objective of MLR is to calculate the linear relationship between the independent variables and dependent variable. The formula for MLR is

\[ Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \cdots \]

Where, \( Y \) = dependent variable, \( X \) = independent variable and \( \beta_0, \beta_1, \beta_2, \ldots, \beta_p \) = Regression coefficients.

### 2. MLR Model and Correlation analysis

#### Table 1. Formulae for degree based Multiplicative invariants

| Topological Invariants | Formulae |
|------------------------|----------|
| Second Multiplicative Zagreb index \((MT_1)\) | \( I_1(G) = \prod_{uv \in E(G)} d_G(u)d_G(v) \) |
| New multiplicative version of first Zagreb index \((MT_2)\) | \( I_2'(G) = \prod_{uv \in E(G)} [d_G(u) + d_G(v)] \) |
| First multiplicative hyper-Zagreb index \((MT_3)\) | \( H1_1(G) = \prod_{uv \in E(G)} [d_G(u) + d_G(v)]^2 \) |
| Second multiplicative hyper-Zagreb index \((MT_4)\) | \( H1_2(G) = \prod_{uv \in E(G)} [d_G(u)d_G(v)]^2 \) |

#### Table 2. Formulae for degree based Additive Topological invariants

| Topological Invariants | Formulae |
|------------------------|----------|
| Randic index \((AT_1)\) | \( \chi(G) = \sum_{e \in E(G)} \frac{1}{\sqrt{d_G(e)}} \) |
| Geometric-Arithmetic index \((AT_2)\) | \( GA(G) = \sum_{e \in E(G)} \frac{d_G(e)}{\sqrt{d_G(e)}} \) |
| Sum Connectivity index \((AT_3)\) | \( SC(G) = \sum_{e \in E(G)} \frac{1}{\sqrt{d_G(e)}} \) |
| Harmonic index \((AT_4)\) | \( HI(G) = \sum_{e \in E(G)} \frac{1}{d_G(e)} \) |
| First Zagreb index \((AT_5)\) | \( M_1(G) = \sum_{e \in E(G)} i + j \) |
| Second Zagreb index \((AT_6)\) | \( M_2(G) = \sum_{e \in E(G)} ij \) |
| Second Modified Zagreb index \((AT_7)\) | \( M_2'(G) = \sum_{e \in E(G)} \frac{1}{i} \) |
| Inverse Sum index \((AT_8)\) | \( IS(G) = \sum_{e \in E(G)} \frac{i}{j} \) |
| Alberston index \((AT_9)\) | \( Alb(G) = \sum_{e \in E(G)} |i - j| \) |
| Atom-Bond Connectivity index \((AT_{10})\) | \( ABC(G) = \sum_{e \in E(G)} \sqrt{\frac{i+j}{2}} \) |
| Symmetric Division index \((AT_{11})\) | \( SD(G) = \sum_{e \in E(G)} \frac{i+j}{2} \) |
| Augmented Zagreb index \((AT_{12})\) | \( AZI(G) = \sum_{e \in E(G)} (\frac{i+j}{2})^3 \) |

#### Table 3. The boiling points of alkanes in K

| S.No | Compound          | \( T_{bp}(K) \) |
|------|-------------------|-----------------|
| 1    | 2-methylbutane    | 300.95          |
| 2    | 2,2-dimethylpropane | 282.65          |
| 3    | n-hexane         | 342.15          |
| 4    | 2-methylpentane   | 333.45          |
| 5    | 3-methylpentane   | 336.45          |
| 6    | 2,2-dimethylbutane | 322.85          |
| 7    | 2,3-dimethylbutane | 331.15          |
| 8    | n-heptanes        | 371.55          |
Table 4. The degree based Multiplicative connectivity indices of alkanes

| Compound          | $MT_1$  | $MT_2$  | $MT_3$  | $MT_4$  |
|-------------------|---------|---------|---------|---------|
| 2-methylbutane    | 108     | 240     | 57600   | 11664   |
| 2,2-dimethylpropane | 256    | 625     | 390625  | 65536   |
| n-hexane          | 256     | 576     | 331776  | 65536   |
| 2-methylpentane   | 432     | 960     | 921600  | 186624  |
| 3-methylpentane   | 432     | 900     | 810000  | 186624  |
| 2,2-dimethylbutane| 1024    | 2250    | 5062500 | 1048576 |
| 2,3-dimethylbutane| 729     | 1536    | 2359296 | 531441  |
| n-heptanes        | 1024    | 2304    | 5308416 | 1048576 |
| 2-methylhexane    | 1728    | 3840    | 14745600| 2985984 |
| 3-methylhexane    | 1728    | 3600    | 12960000| 2985984 |
| 2,2-dimethylpentane| 4096   | 9000    | 81000000| 16777216|
| 2,3-dimethylpentane| 2916   | 5760    | 33177600| 8503056 |
| 2,4-dimethylpentane| 2916   | 6400    | 40960000| 8503056 |
| 3,3-dimethylpentane| 4096   | 8100    | 65610000| 16777216|
| 3-ethylpentane    | 1728    | 3375    | 11390625| 2985984 |
| n-octane          | 4096    | 9216    | 84934656| 16777216|
| 2-methylheptane   | 6912    | 15360   | 23592960| 47775744|
| 3-methylheptane   | 6912    | 14400   | 207360000| 47775744|
| 4-methylheptane   | 6912    | 14400   | 207360000| 47775744|
| n-nonane          | 16384   | 36864   | 1358954496 | 268435456 |

Table 5. The degree based Multiplicative connectivity indices of alkanes

| Compound          | $MT_5$  | $MT_6$  | $MT_7$  | $MT_8$  |
|-------------------|---------|---------|---------|---------|
| 2-methylbutane    | 0.0645  | 0.0962  | 0.3330  | 0.6928  |
| 2,2-dimethylpropane | 0.0400 | 0.0625  | 0.5625  | 0.4096  |
| n-hexane          | 0.0416  | 0.0625  | 0.1768  | 0.8880  |
| 2-methylpentane   | 0.0323  | 0.0481  | 0.2357  | 0.6928  |
| 3-methylpentane   | 0.0333  | 0.0481  | 0.2041  | 0.7390  |
| 2,2-dimethylbutane| 0.0211  | 0.0313  | 0.3248  | 0.4551  |
| 2,3-dimethylbutane| 0.0255  | 0.0370  | 0.2963  | 0.5625  |
| n-heptanes        | 0.0208  | 0.0313  | 0.1250  | 0.8889  |
| 2-methylhexane    | 0.0161  | 0.0241  | 0.1667  | 0.6928  |
| 3-methylhexane    | 0.0167  | 0.0241  | 0.1443  | 0.7390  |
| 2,2-dimethylpentane| 0.0105 | 0.0156  | 0.2296  | 0.4551  |
| 2,3-dimethylpentane| 0.0183 | 0.0156  | 0.1875  | 0.2528  |
| 3-ethylpentane    | 0.0172  | 0.0241  | 0.1250  | 0.7883  |
| n-octane          | 0.0104  | 0.0156  | 0.0884  | 0.8889  |
| 2-methylheptane   | 0.0081  | 0.0120  | 0.1179  | 0.6928  |
| 3-methylheptane   | 0.0083  | 0.0120  | 0.1021  | 0.7390  |
| 4-methylheptane   | 0.0083  | 0.0120  | 0.1021  | 0.7390  |
| n-nonane          | 0.0052  | 0.0078  | 0.0625  | 0.8889  |

Table 6. The degree based Additive connectivity indices of alkanes

| Compound          | $AT_1$  | $AT_2$  | $AT_3$  | $AT_4$  | $AT_5$  | $AT_6$  |
|-------------------|---------|---------|---------|---------|---------|---------|
| 2-methylbutane    | 2.2701  | 3.6547  | 2.0246  | 2.0667  | 16      | 14      |
| 2,2-dimethylpropane | 2      | 3.2     | 1.7889  | 1.6     | 20      | 16      |
| n-hexane          | 2.9142  | 4.8856  | 2.6548  | 2.8334  | 18      | 16      |
| 2-methylpentane   | 2.7701  | 4.6547  | 2.5246  | 2.5667  | 20      | 18      |
| 3-methylpentane   | 2.8081  | 4.7112  | 2.5491  | 2.6333  | 20      | 19      |
| 2,2-dimethylbutane| 2.5607  | 4.2856  | 2.3272  | 2.2     | 24      | 22      |
| 2,3-dimethylbutane| 2.6427  | 4.464   | 2.4082  | 2.3333  | 22      | 21      |
| n-heptanes        | 3.4142  | 5.8856  | 3.1547  | 3.3333  | 22      | 20      |
| 2-methylhexane    | 3.2701  | 5.6547  | 3.0246  | 3.0667  | 24      | 22      |
### Table 7. The degree based Additive connectivity indices of alkanes

| Compound            | $AT_1$ | $AT_3$ | $AT_5$ | $AT_{10}$ | $AT_{11}$ | $AT_{12}$ |
|---------------------|--------|--------|--------|------------|------------|------------|
| 3-methyl(hexane)    | 3.3081 | 5.7112 | 3.0491 | 3.1333     | 24         | 23         |
| 2,2-dimethylpentane | 3.0607 | 5.2856 | 2.8272 | 2.7        | 28         | 26         |
| 2,3-dimethylpentane | 3.1807 | 5.5207 | 2.9328 | 2.9        | 26         | 26         |
| 2,4-dimethylpentane | 3.1259 | 5.4237 | 2.8944 | 2.8        | 26         | 24         |
| 3,3-dimethylpentane | 3.1213 | 5.3712 | 2.8656 | 2.8        | 28         | 28         |
| 3-ethylpentane      | 3.3461 | 5.7678 | 3.0737 | 3.2        | 24         | 24         |
| n-octane            | 3.9142 | 6.8856 | 3.6547 | 3.8333     | 26         | 24         |
| 2-methylheptane     | 3.7701 | 6.5647 | 3.5246 | 3.5667     | 28         | 26         |
| 3-methylheptane     | 3.8081 | 6.7112 | 3.5491 | 3.6333     | 28         | 27         |
| 4-methylheptane     | 3.8081 | 6.7112 | 3.5491 | 3.6333     | 28         | 27         |
| n-nonane            | 4.4142 | 7.8856 | 4.1547 | 4.3333     | 30         | 28         |

### Table 8. The correlation coefficient between multiplicative indices and boiling points of alkanes

| Topological invariants | $r$  |
|------------------------|------|
| Second Multiplicative Zagreb index ($MT_1$) | 0.774717 |
| New multiplicative version of first Zagreb index ($MT_2$) | 0.766797 |
| First multiplicative hyper-Zagreb index ($MT_3$) | 0.598968 |
| Second multiplicative hyper-Zagreb index ($MT_4$) | 0.610895 |
| multiplicative sum connectivity index ($MT_5$) | -0.80006 |
| Multiplicative product connectivity index ($MT_6$) | -0.80370 |
| Multiplicative atom bond connectivity index ($MT_7$) | -0.91724 |
| Multiplicative geometric-arithmetic index ($MT_8$) | 0.503631 |

### Table 9. The correlation coefficient between additive indices and boiling points of alkanes

| Topological invariants | $r$  |
|------------------------|------|
| Randic index ($AT_1$) | 0.9958 |
| Geometric-Arithmetic index ($AT_2$) | 0.99593 |
| Sum Connectivity index ($AT_3$) | 0.99528 |
| Harmonic index ($AT_4$) | 0.98546 |
| First Zagreb index ($AT_5$) | 0.77146 |
| Second Zagreb index ($AT_6$) | 0.78002 |
| Second Modified Zagreb index ($AT_7$) | 0.97878 |
| Inverse Sum index ($AT_8$) | 0.9791 |
| Alberston index ($AT_9$) | -0.5264 |
| Atom-Bond Connectivity index ($AT_{10}$) | 0.90386 |
| Symmetric Division index ($AT_{11}$) | 0.24289 |
| Augmented Zagreb index ($AT_{12}$) | 0.95123 |

### Table 10. Regression equation of boiling point BP based on its multiplicative topological invariants $T$

| Topological invariants | R.E of BP on $MT(G)$ | $R^2$ |
|------------------------|----------------------|-------|
| Second Multiplicative Zagreb index ($MT_1$) | $B.P = 0.006MT_1 + 334.9$ | 0.600 |
| New multiplicative version of first Zagreb index ($MT_2$) | $B.P = 0.003MT_2 + 335.7$ | 0.588 |
| First multiplicative hyper-Zagreb index ($MT_3$) | $B.P = 7E - 08MT_3 + 349.0$ | 0.358 |
Also, with MT

According to equation in the Table 10 and the square values in Table 12.

Table 12. MLR Statistics: Predictors Topological Invariants, Pearson correlation coefficient $R^2$, $R^2_{\text{Adj}}$, Standard error of estimate S, Fisher Coefficient F, Mean Square MS, Residual, Significance of models Sig.

| Topological Invariants | $MT_1$, $MT_2$, $MT_6$, $MT_7$ | $MT_3$, $MT_6$, $MT_7$ |
|------------------------|--------------------------------|------------------------|
| $R^2$                  | 0.987                         | 0.958                  |
| $R^2_{\text{Adj}}$    | 0.984                         | 0.95                   |
| S                     | 4.3569                        | 7.60121                |
| F                     | 284.165                       | 120.792                |
| MS                    | 5394.293                      | 6979.154               |
| Residual              | 18.983                        | 57.778                 |
| Sig. (p)              | 0.000$^b$                     | 0.000$^b$              |

Here the highest square correlation coefficient is 0.987 and its F value is 284.165. Standard error of estimate is 4.3569. If $p < 0.001$ then the overall regression model is significant. Also Adjusted R square is 0.984. Therefore 98.4% of variability of boiling points explained by its invariants. The corresponding MLR model is given by

$$BP = 404.407 - 8029.049MT_3 + 5017.711MT_6 - 209.805MT_7 + 0.002MT_1$$ (2.1)

This equation has four invariants Second Multiplicative Zagreb, Multiplicative sum connectivity, Multiplicative product connectivity, Multiplicative atom bond connectivity with high calibration statistics and prediction ability. According to equation in the Table 11 and the square correlation coefficients gives better correlation between $T_{BP}$ with $MT_1 > MT_2 > MT_3 > AT_4 > AT_7 > AT_5 > AT_12$ of alkanes respectively. Also, $AT_3, AT_6, AT_7, AT_10$ and $AT_11$ of alkanes are having poor correlation with $T_{BP}$. In next stage, by using SPSS software different MLR model were examined and the best MLR model was obtained by using correlation coefficient, coefficient of determination, standard error of estimate, Mean square, The Fisher statistic and Durbin-Watson significance values in Table 12.

### 2.1 Result and discussion

According to equation in the Table 10 and the square correlation coefficients gives better correlation between $T_{BP}$ with $MT_1 > MT_6 > MT_5 > MT_1$ of alkanes respectively. Also, $MT_6, MT_3, MT_2$ and $MT_4$ of alkanes are having poor correlation with $T_{BP}$. In next stage, by using SPSS software MLR model is examined by using correlation coefficient, coefficient of determination, standard error of estimate, Mean square, The Fisher statistic and Durbin-Watson significance values in Table 12.

| Topological Invariants | R.E of BP on $AT(G)$ | $R^2$ |
|------------------------|----------------------|-------|
| Randic index($AT_1$)   | $BP = 57.32AT_1 + 174.9$ | 0.991 |
| Geometric-Arithmetic index($AT_2$) | $BP = 29.35AT_1 + 196.5$ | 0.991 |
| Sum Connectivity index($AT_3$) | $BP = 58.18AT_1 + 186.7$ | 0.990 |
| Harmonic index($AT_4$) | $BP = 50.94AT_1 + 206.2$ | 0.971 |
| First Zagreb index($AT_5$) | $BP = 6.771AT_1 + 193.8$ | 0.595 |
| Second Zagreb index($AT_6$) | $BP = 6.227AT_1 + 216.5$ | 0.608 |
| Second Modified Zagreb index($AT_7$) | $BP = 93.04AT_1 + 190.0$ | 0.958 |
| Inverse Sum index($AT_8$) | $BP = 31.19AT_1 + 192.5$ | 0.958 |
| Alberston index($AT_9$) | $BP = -5.256AT_1 + 392.7$ | 0.277 |
| Atom-Bond Connectivity index($AT_{10}$) | $BP = 46.14AT_{10} + 156.0$ | 0.817 |
| Symmetric Division index($AT_{11}$) | $BP = 3.4446AT_{11} + 303.4$ | 0.059 |
| Augmented Zagreb index($AT_{12}$) | $BP = 2.454AT_{12} + 262.6$ | 0.904 |
Table 13. MLR Statistics: Predictors Topological Invariants, Pearson correlation coefficient $R^2$, $R^2_{adj}$, Standard error of estimate S, Fisher Coefficient F, Mean Square MS, Residual, Significance of models Sig.

| Topological Invariants | $AT_1$ | $AT_2$ | $AT_3$ | $AT_4$ | $AT_5$ | $AT_6$ | $AT_7$ | $AT_8$ | $AT_9$, $AT_{10}$, $AT_{11}$ | $AT_1$, $AT_2$, $AT_3$, $AT_4$, $AT_5$, $AT_6$, $AT_7$, $AT_8$, $AT_9$, $AT_{10}$, $AT_{11}$ |
|------------------------|--------|--------|--------|--------|--------|--------|--------|--------|---------------------------------|--------------------------------------------------|
| $R^2$                  | 0.995  | 0.995  | 0.995  | 0.995  | 0.995  | 0.995  | 0.995  | 0.995  | 0.995                                          | 0.995                                            |
| $R^2_{adj}$            | 0.994  | 0.994  | 0.994  | 0.994  | 0.994  | 0.994  | 0.994  | 0.994  | 0.994                                          | 0.994                                            |
| S                      | 2.625  | 2.6084 | 2.7017 | 2.6847 | 2.5818 |        |        |        |                                               |                                                 |
| F                      | 789.19 | 1065.66| 986.365| 1005.72| 1087.85|        |        |        |                                               |                                                 |
| MS                     | 5439.63| 7251.016| 7248.11| 7248.865| 7251.753|        |        |        |                                               |                                                 |
| Residual               | 6.893  | 6.804  | 7.348  | 7.208  | 6.666  |        |        |        |                                               |                                                 |
| Sig. (p)               | 0.000b | 0.000b | 0.000b | 0.000b | 0.000b | 0.000b | 0.000b | 0.000b | 0.000b                                         | 0.000b                                           |

To predict the boiling points, the following models were obtained.

$$BP = 195.761 + 23.27TA_4 + 5.483AT_7 + 14.973AT_8$$
$$- 0.0984AT_2 - 3.651AT_1 - 10.654AT_2$$
$$- 4.327AT_3$$
$$2.1$$

$$BP = 185.307 + 19.755AT_3 + 30.879AT_7 + 11.088AT_8$$
$$- 2.161AT_1 + 1.606AT_5 + 5.452AT_4$$
$$3.2$$

$$BP = 183.665 + 33.407AT_2 - 38.848AT_4 + 58.872AT_7$$
$$- 1.599AT_1 - 2.841AT_3$$
$$4.3$$

$$BP = 247.504 + 154.592AT_2 - 278.535AT_3$$
$$+ 26.910AT_4 + 2.536AT_1$$
$$5.4$$

$$BP = 185.543 + 158.708AT_1 + 92.567AT_2$$
$$- 286.512AT_3$$
$$6.5$$

Finally, one model with highest square correlation coefficient 0.99, Fisher coefficient ($F = 1087.854$), Standard error of estimate S, Fisher Coefficient F, Mean Square MS, Residual, Significance of models Sig.

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$$- 2.161AT_1 + 1.606AT_5 + 5.452AT_4$$
$$3.2$$

$$BP = 183.665 + 33.407AT_2 - 38.848AT_4 + 58.872AT_7$$
$$- 1.599AT_1 - 2.841AT_3$$
$$4.3$$

$$BP = 247.504 + 154.592AT_2 - 278.535AT_3$$
$$+ 26.910AT_4 + 2.536AT_1$$
$$5.4$$

$$BP = 185.543 + 158.708AT_1 + 92.567AT_2$$
$$- 286.512AT_3$$

Finally, one model with highest square correlation coefficient 0.99, Fisher coefficient ($F = 1087.854$), Standard error of estimate S, Fisher Coefficient F, Mean Square MS, Residual, Significance of models Sig.
3. Conclusion

Mathematical regression models are very useful in QSPR studies. In very particular, MLR model is used to find the regression between more than two variables in QSPR studies. In this article, we have found the MLR model for prediction of boiling points of alkanes in terms of its topological invariants. Also, the result of this article indicated that the boiling points of alkanes highly correlated with Second Multiplicative Zagreb, Multiplicative sum connectivity, Multiplicative product connectivity, Multiplicative atom bond connectivity also Randić, geometric-arithmetic, sum connectivity indices.

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