COMMUNICATION ON COUNTING POLYNOMIALS FOR ALKANES

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ABSTRACT

Henry's law constant of a sample of nonane isomers was modeled by using characteristic and counting polynomials. The characteristic polynomial and counting polynomials on the distance matrix, on the maximal fragments matrix, on the complement of maximal fragments matrix, and on the Szeged matrix were calculated for each compound and multi-varied models were identified and analyzed. Two multi-varied models, one with four and other with five variables, revealed to had estimation abilities. Both models used the characteristic and counting polynomials on Szeged matrix as criteria. The statistical characteristics of the models were analyzed and are presented. The obtained results shown that Henry's law constant of studied nonane isomers could be estimated by using characteristic polynomial and counting polynomial on Szeged matrix.

INTRODUCTION

Graph theory, defines as the study of graphs that are mathematical structures used to model pair-wise relations between objects from a certain collection, was introduced by Leonhard Euler in 1736 [1]. Sub-graphs that result through applying of the matrix criteria of fragmentation are using in investigation of chemical structures and of relationships between structures and properties. Some criteria as characteristics polynomial, Szeged and Cluj matrices are used methods. Two new criteria that proved to had abilities in characterization of compounds properties were recently introduced and analyzed [2].
The aim of the present research was to investigate the abilities in estimation of Henry's law property of nonane isomers by using characteristic and counting polynomials.

MATERIAL & METHOD

A sample of thirty-five compounds, representing the isomers of nonane ($C9H20$), where included into the study. The values of Henry's law constant (the ratio of the gaze phase concentration and the liquid phase concentration of a substance), expressed as [M/atm] unit, were taken from a previously reported research [3].
The Henry's law constant was modeled by using characteristic polynomial and counting polynomials. Five matrices were used in counting polynomials: characteristic polynomial (ChP), counting polynomial on the maximal fragments matrix (CMx), counting polynomial on the complementary of the maximal fragments matrix (CcM), and counting polynomial on the Szeged matrix (CSz). Comparisons between correlation coefficients obtained by different models were analyzed by using the Steiger's Z test [4] at a significance level of 5%.

RESULTS

One out of thirty-five compounds (4-methyl-octane) was considered an outliner and was not included into the analysis. Two models proved to had abilities in estimation of the Henry's law constant for the nonane isomers.

- Model with four variables:

$$\hat{Y}_{KHL\text{-}4v} = 1100 - 1.23\cdot10^{-4}\cdot P_{CSz}(-2.83) + 0.1269\cdot P_{ChP}(-1.72) + 2.73\cdot10^{-5}\cdot P_{ChP}(0.33) - 2.61\cdot P_{ChP}(-9.36) \quad (1)$$

where $\hat{Y}_{KHL\text{-}4v}$ is the estimated Henry's law constant by the model with four variable, $P_{CSz}(X_i)$ is counting polynomial on the Szeged matrix and $P_{ChP}(X_i)$ are characteristic polynomials.

- Model with five variables:

$$\hat{Y}_{KHL\text{-}5v} = 5669 - 3.36\cdot10^{-2}P_{CSz}(-3.07) + 1.80\cdot10^{-2}P_{CSz}(0.9) + 8.67P_{ChP}(0.11) - 1.74\cdot10^{-2}P_{ChP}(1.83) - 3.70\cdot10^{-4}P_{ChP}(7.11) \quad (2)$$

where $\hat{Y}_{KHL\text{-}5v}$ is the estimated Henry's law constant by the model with five variable, $P_{CSz}(X_i)$ are counting polynomials on the Szeged matrix and $P_{ChP}(X_i)$ are characteristic polynomials.

The statistical characteristics of the models are presented in table 1.

Table 1. Statistical characteristics of the models

Parameter	Model	
	Eq.(1)	Eq.(2)
Correlation coefficient (r)	0.9663	0.9705
95% confidence interval for (r)	[0.9329-0.9831]	[0.9411-0.9852]
Squared correlation coefficient (r^2)	0.9337	0.9418
Model significance	< 0.0001	< 0.0001

The graphical representation of the model obtained by Eq.(2) versus the measured Henry's law constant is shown in figure 1.
In order to test the null hypothesis that the correlation coefficient obtained by Eq.(1) is not different by the correlation coefficient obtained by Eq.(2), the Steiger's Z test was applied. The value of Z test was equal with 0.657 (p = 0.255) showing us that there are not statistical difference between the correlation coefficients.

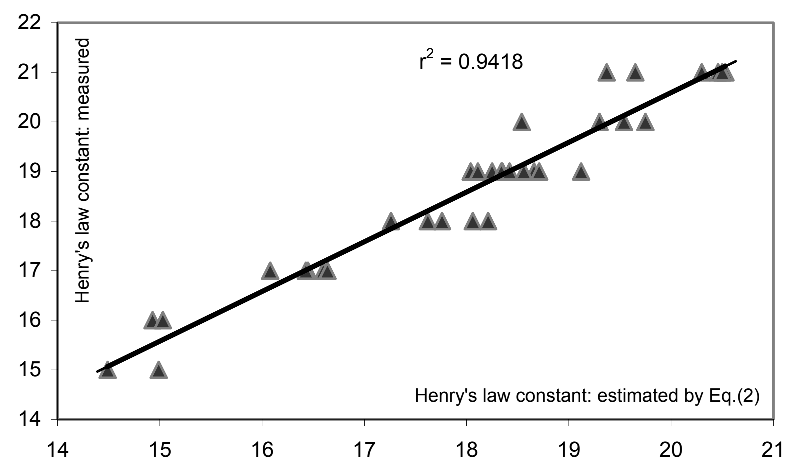

Figure 1. Estimated by Eq.(2) versus measured Henry's law constant for studied nonane isomers

CONCLUSION

The characteristic polynomial and counting polynomial on Szeged matrix criteria revealed to be useful in modeling of Henry's law constant for studied nonane isomers. Both models (Eq.(1) and Eq.(2)) revealed to had abilities in estimation of the Henry's law constant. External and internal validations of the models are intended to be done in future research in order to characterize the validity and relevance of the obtained models.

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The research was partly supported by UEFISCSU Romania through project ET108/2006.

Use of Graph Polynomials for Characterization of Alkanes Properties

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Introduction: Investigation of chemical compounds can be done by using subgraphs that result after applying of matrix criteria of fragmentation. Characteristics polynomial, Szeged and Cluj matrix criteria are used in counting polynomials. Other two criteria, maximal fragments matrix and complementary of maximal fragments matrix, were recently introduce and analyzed [1].

Aim: The aim of the research was to investigate the Henry's law constant, defined as the ratio of the gaze phase concentration and the liquid phase concentration of a substance [2], of a sample of alkanes by using counting polynomials approach.

Material and Method: A sample of thirty-four alkanes where included into the study. The values for the Henry's law constant, expressed in [M/atm] unit, were taken from a previously reported research [3].
The multivariate linear regression analysis method was used in order to find the model able to estimate the Henry's law constant of studied compounds. The models used the following criteria: characteristic polynomial (ChP), counting polynomial on Maximal Fragments Matrix (CMx), counting polynomial on complementary of Maximal Fragments Matrix (CcM) and counting polynomial on Szeged Matrix (CSz).
The characterization of obtained models was performed by analyzing the correlation coefficients, the 95% confidence interval of the correlation coefficient and the squared correlation coefficient.

Results & Discussions: Two models proved to have abilities in estimation of the Henry's law constant for the studied alkanes. One model used four variables while the other model used five variables.

Both models were statistically significant at a significance level less than 0.001. The correlation coefficients between observed and estimated by the models Henry's law constant, associated 95% confidence interval for correlation coefficients and the squared correlation coefficients are as followed:

- Model with four variables: r = 0.9663; 95% CI [0.9329-0.9831]; r^2 = 0.9337;
- Model with five variables: r = 0.9705; 95% CI [0.9411-0.9852]; r^2 = 0.9418;

The values obtained by the correlation coefficient and by the squared correlation coefficients sustained the goodness-of-fit of the obtained models and their estimation abilities. Further research on internal and external validation must be done in order to analyze the validity and relevance of the model with four and respectively five variables.

Conclusions: The characteristic polynomial, counting polynomial on maximal fragments matrix, counting polynomial on complementary of maximal fragments matrix, and counting polynomial on Szeged matrix criteria reveal to be useful criteria in modelling of the Henry's law constant of studied alkanes. More researches are necessary to be done in order to validate the obtained models.

Keywords: Counting Polynomials, Alkanes, Henry's law constant, Correlation Coefficient

Acknowledgement

The research was partly supported by UEFISCSU Romania through project ET108/2006.

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