

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 introduced and analyzed [1].

Aim: The aim of the research was to investigate the Henry's law constant, defined as the ratio of the gaseous 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 were 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

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