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Application of New Group Contribution Method and Artificial Neural Network-Group Contribution Method in the Prediction of Critical Properties of Pure Hydrocarbons

Ouardia REBAS[1*], Samir FEKRACHE[2] and Chems Eddine CHITOUR[1]

[1] Laboratory of valorization of fossil energies, Department of Chemical Engineering. École Nationale Polytechnique, Algiers, Algeria

[2] Drilling Fluid Engineer Specialist III, MI SWACO- Schlumberger Company. Algiers, Algeria

*Corresponding author's email: ouardia.rebas@g.enp.edu.dz

ABSTRACT

The aim of this work is to determine the critical properties of pure hydrocarbons by two methods: the method of group contribution with interactions and the method of artificial neural networks. A New group contribution method was developed to predict critical temperatures, pressures and volumes of hydrocarbon compounds by using intramolecular interactions. For neural networks we have developed networks that can approximate the critical properties of pure hydrocarbons which are functions of boiling point and structure of the hydrocarbons. When we compared these methods with other group contributions methods, we have obtained better results and satisfactory accuracy. This study involved two approaches: In the first approach, we proposed new correlations based on the principle of contribution of groups with interactions (IGC) for the prediction of critical properties of six families of pure hydrocarbons: n-paraffins, isoparaffins, olefins, alkynes, naphthenes and aromatics. The deviations obtained by these correlations are relatively small compared to experimental data, and other correlations in the literature. The second approach aimed at predicting critical properties by coupling artificial neural networks to the method of non-interacting group contributions. The established method allows a better prediction of the studied properties compared to conventional methods cited in the literature. The results obtained show small deviations from experimental data including the simulation of neural networks on different isomers. These results justify the addition of the boiling temperature as an additional input next to the compound structure.

Keywords: Hydrocarbons, Critical properties, Neurals networks, Groups contribution, Intramoleculair intreractions.

1. Introduction

The knowledge of the physico-chemical properties of oil and petroleum fractions has always been a major concern for the chemical, refining and petrochemical engineer. The mastery of all the stages of separation and transformation of petroleum products, from the transportation of oil from the wells to the storage of finished products requires a perfect knowledge of the characteristics of oil and its derivatives.The determination of these characteristics begins with preliminary tests on crude oil and its various products. Analytical methods have been developed and standardized to determine the main physico-chemical properties that will condition their subsequent processing and to ensure that the controls performed by the various parties are comparable. These specifications often correspond to standards (ASTM, AFNOR, ...). Experience provides some of the properties, but in most cases it has a number of limitations due to its complexity, high cost and often significant handling time. In order to circumvent these constraints, correlations have been proposed by different authors for more than half a century. They are based in particular on the law of the corresponding states and the methods of group contributions. In the present study, we propose methods for predicting the critical properties of pure hydrocarbons based on the structure-property relationship using the group contribution method with interactions and the group contribution method coupled to artificial neural networks (GC-ANN).

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2. Results and Discussion

2.1. Group contribution method with interactions

2.1.1 Proposed correlations

The approach used to develop the new method for contributing groups with interactions is described below.

1st Step: Data Collection

2nd Step: Definition of structural groupings

3rd Step: Definition of the main terms of interactions between structural groupings and their environments

The approach to introducing interaction terms into group contribution correlation is :

1- Write the semi-developed formula for each family of hydrocarbons studied.

2- Define the main interaction terms.

4th Step: Establishment of new correlations of group contribution with interactions

5th Step: Selection of new correlations

6th Step: Comparison of correlations established with other group contribution methods in the literature

The study of the reliability of the proposed correlations was conducted by comparing the proposed correlations with other methods based on molecular structure and recommended in the literature. This comparison was based on the mean absolute deviations recorded by the different methods from the reference data and for the six hydrocarbon families studied. The comparison of the deviations recorded by the established equations and the correlations recommended in the literature. We find that the correlations of contribution of interacting groups are better than other correlations for the prediction of the critical properties of pure hydrocarbons.

2.2. Use of coupling contribution of artificial neural network groups to the determination of critical properties

The aim of this part is to propose methods (or networks) allowing the calculation of the physical properties of pure hydrocarbons belonging to the most important chemical families. These methods are essentially based on the Quantitative structure-property relationships (QSPRs), in other words, the physical properties are a function of the groupings that make up the molecule. In order to do this, we first started by collecting a database with physical properties of pure bodies of different families (DIPPR and TRC), composed of about 400 hydrocarbons, which we divided into two parts. The first part concerns non-cyclic hydrocarbons (Non Ring group) and includes kerosenes (iso and normal) and alkenes, the second part includes aromatics and naphthenes (Cyclic group, Ring group). From the comparison of the different methods, the GC-ANN method proposed and applied to pure bodies gives better results concerning critical properties, suggesting that this method better approaches the experimental values.

3. Conclusion

This study involved two approaches: In the first approach, we proposed new correlations based on the principle of contribution of groups with interactions (IGC) for the prediction of critical properties of six families of pure hydrocarbons: n-paraffins, isoparaffins, olefins, alkynes, naphthenes and aromatics. The deviations obtained by these correlations are relatively small compared to experimental data, and other correlations in the literature. The second approach aimed at predicting critical properties by coupling artificial neural networks to the method of non-interacting group contributions. The established method allows a better prediction of the studied properties compared to conventional methods cited in the literature. The results obtained show small deviations from experimental data including the simulation of neural networks on different isomers. These results justify the addition of the boiling temperature as an additional input next to the compound structure.

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