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Short communication

A new method based on elements and chemical bonds for organic compounds critical properties estimation

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ABSTRACT

A new method based on elements and chemical bonds was proposed to estimate the critical properties of organic compounds. Three equations were established using this method. New elements and chemical bonds groups are defined by considering the structure of organic compounds. The values of elements and chemical bonds groups of compounds containing carbon, hydrogen, oxygen, nitrogen, chlorine, and sulfur were obtained though regression calculation. The average relative deviation for prediction critical properties were compared with that were from the proposed method, the Joback-Reid, Constantinou-Gani and our group methods. The proposed method provided a new and easy approach for estimation critical properties of organic compounds through defining of the new elements and chemical bonds groups and exhibited a very satisfactory accuracy. Furthermore, the new method can also estimate the critical properties of compounds containing silicon.

1. Introduction

The critical properties of organic compounds are importance for thermodynamic calculations in chemical engineering and simulation as well as product design. However, experimental data on the critical properties of organic compounds are unavailable because of the limitation of experimental conditions and compounds. Thus, the generally reliable estimation methods development for the critical properties is very imminent.

Most methods-factor analysis-correlation equations were developed by adding the data of other measurable properties, such as normal boiling, density, and molecular weight [1]. Lee and Kesler [2] (1975) proposed a complex correlation to predict the hydrocarbons critical properties based on density and normal boiling. A new method developed by Klincewicz and Reid [3](1984) then proposed an estimation method that was dependent on three parameters: molecular weight, normal boiling, and number of atoms. In addition, a number of method for factor analysis methods have been proposed by several researchers, including Lin and Chao [4] (1984), Vetere [5] (1989, 1995), Riazi et al. [6] (1998) and Pazuki et al. [7] (2005) and Vejahati and Nikoo [8] (2007). Factor analysis can offer precise estimation and often depend on molecular weight, density, and normal boiling point, but has no tabulations of molecular descriptor properties for substances.

The molecular structure of group contribution has been developed and widely applied in number of studies. In 1955, Lydersen [9] first proposed a reliable method to estimate critical parameters, and then Ambrose [10], Joback and Reid [11]introduced another method that were the most widely used. Several experts also developed other group-contribution methods, such as Klincewicz and Reid method [3], MXXC method [12,13]. Basically, these methods are simply determined by adding different group contributions, and the interaction among groups were not be considered, which result could not distinguish isomers because of oversimplification.

Several methods were developed to overcome this limitation. Constantinou and Gani [14] proposed a complex method to estimate the critical properties of organic compounds. This method considers two levels of group contribution: the basic level is composed of simple groups, and the second level considers the effects among groups and isomers. In 1997, Pardillo-Fontdevila and Gonzalez-Rubio [15] proposed a structural approach called group-interaction contribution that considered the contributions of interactions among groups instead of the contribution of simple groups. Based on this approach, Jorge Marrero-Morejon and Eladio Pardillo-Fontdevila [16], Liang Yinghua and Ma Peisheng [17], Xu Wen and Yang Qiang [18], and Nannoolal [19–21]developed several methods for estimating the critical constants of pure organic

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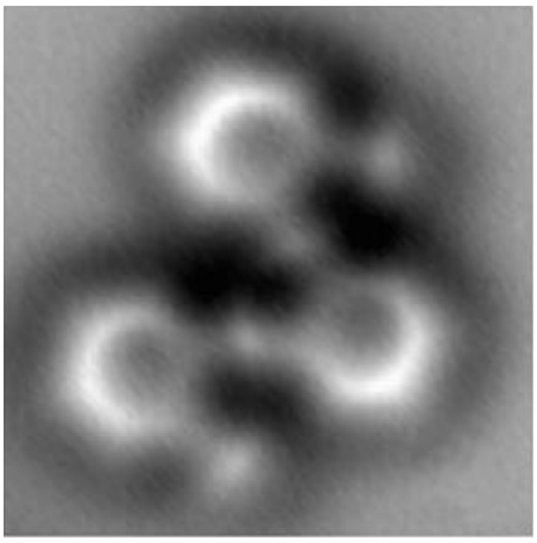

Fig. 1. The image of graphene.

compounds. Furthermore, some methods for prediction the critical properties of organic compounds have been proposed, including the position group contribution method [22–25], the neural network group contribution method [26–31], group-contribution$^+$ method [32], improving group contribution methods by distance weighting [33], fragment contribution-corresponding states method [34], as well as a benzene chain-based contribution method [35], and so on.

However, these group contribution methods use groups as the contribution group, and some compounds could not be split with existing groups because of incomplete group parameters, thereby limiting further application. In the 2004, our group [36,37] proposed a new method for estimating critical properties based on elements and chemical bonds. In previous work, our group proposed six equations for T_C, four equations for P_C, two equations for V_C, that cannot estimate compounds containing silicon. At the same time, the equations for estimation P_C and V_C must know density of compounds at a certain temperature.

In this study, the method for estimating critical properties based on elements and chemical bonds was further extended. The new equations estimate P_C and V_C which don not know density of compounds at a certain temperature when compared with our group previous method. The predicted results were compared with Joback-Reid (J-R), Constantinou-Gani(C-G), and our group methods to verify their accuracy.

2. Method and property modeling

2.1. Data

The quality of the method strongly depends on the experimental data. The sources of data were Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds [Carl L. Yaws, 2003] [38] and Thermophysical Properties of Chemicals and Hydrocarbons [Carl L. Yaws,2008] [39], which includes linear and branched alkanes and cycloalkanes, alkenes, esters, alcohols nitrogen, chlorine, and sulfur. We collected the critical properties of different compounds, including critical temperature (number of values: 485), critical pressure (number of values: 372), and critical volume (number of values: 339).

2.2. Methodology

In 2013, Felix Fisher et al. [40] found the image of individual atoms and bonds made by a noncontact atomic force microscope, as shown in Fig. 1. It proved elements and chemical bonds really exist in the material The proposed method based on elements and chemical bonds was developed according to molecular structure theory, which indicates that the properties of matter not only depends on the quantity of its constituent elements, but also on the chemical structure chemical bonds.

The methodology as illustrated in Fig. 2.

2.3. Groups

The proposed method used elements and chemical bonds as the

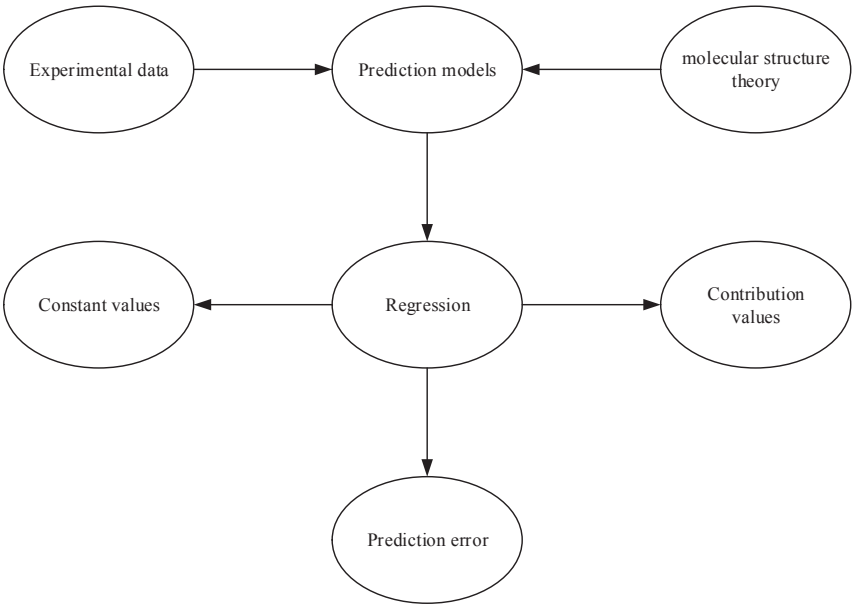

Fig. 2. Methodology for property modeling.